Aalto University

CHEM-E6100 Fundamentals of chemical thermodynamics

General information

Fall 2022

General

- **Course personnel**
  - Prof. Daniel Lindberg (lectures) (Daniel.k.Lindberg@aalto.fi)
  - D.Sc. Jari Aromaa (tutorials and workshops) (jari.aromaa@aalto.fi)

General

- **Compulsory course for Sustainable Metals Processing and Creative Sustainability MSc programs**
- **Course is composed of lectures, workshops and exercises**
- **Lectures twice a week 24.10-29.11.2022**
  - Mondays 13:15-15:00 (Change: Exercise Wed 2.11 ↔ Lecture Mon 7.11)
  - Tuesdays 12:15-14:00
  - All lectures will be held on campus
    - *Lecture hall Platinium, C104, Critical Raw Materials Hub, Vuorimiehentie 2*
    - *Except 31.10 and 28.11, Puunjalostustekniikka 1, 241 L1*

General

- **Compulsory course for Sustainable Metals Processing and Creative Sustainability MSc programs**
- **Course is composed of lectures, workshops and exercises**
- **Lectures twice a week 24.10-29.11.2022**
  - Presentation material and videos of the weekly topics will be uploaded to MyCourses
  - Weekly quizzes will made be available in MyCourses after the lectures regarding the topic of the week
  - Quizzes will be graded max 1 point per quiz (total 6 x 1 p = 6 p) – roughly one week time to do the quizzes (Deadline on Wednesday the following week)

General

- **Exercises/tutorials starting 26.10.2022 → 30.11.2022**
  - Wednesdays 15:15-17:00 (Exercise November 2 will be moved to lecture time November 7)
  - Exercises will be held on campus
  - Exercises will deal with practical issues of theoretical key topics discussed in the lectures
  - Examples in the tutorials follow the lectures on most weeks.
  - Exercise examples often in exam.
  - Link will be provided later on MyCourses

General

- **Workshops**
  - Four interactive workshops(WS) will be organized and these will be graded (max 1 pts each):
  - Workshops will be held in computer classes and assignments will be uploaded to MyCourses after the exercise.
  - 12.11., 19.11., 26.11. and 3.12.
  - 14:15-17:00
  - Friday workshop link will be provided later.

Skills needed

- Inorganic and physical chemistry form the key disciplines and they are the necessary background of the course.
  - E.g. stoichiometry of chemical reactions, chemical equilibrium of reactions, basic understanding of concepts in thermodynamics
- Some maths are also needed –typically calculus, differential and integral equations which are high school material.

Rules for Integrals

Power Rule

$$\int x^n dx = \frac{x^{n+1}}{n+1} + C \quad n \neq -1$$

$$\int x^{-1} dx = \ln|x| + C$$

Exponential

$$\int e^x dx = e^x + C$$

$$\int a^x dx = \frac{a^x}{\ln a} + C$$

Constant Multiples

$$\int kf(x)dx = k\int f(x)dx$$

Absolute Value

$$\int |x| dx = \frac{x|x|}{2} + C$$

Sums and Differences

$$\int [f(x) + g(x)]dx = \int f(x)dx + \int g(x)dx$$

$$\int [f(x) - g(x)]dx = \int f(x)dx - \int g(x)dx$$

Differentiation Rules	
Constant Rule	$\frac{d}{dx}[c] = 0$
Power Rule	$\frac{d}{dx}x^n = nx^{n-1}$
Product Rule	$\frac{d}{dx}[f(x)g(x)] = f'(x)g(x) + f(x)g'(x)$
Quotient Rule	$\frac{d}{dx}\left[\frac{f(x)}{g(x)}\right] = \frac{g(x)f'(x) - f(x)g'(x)}{[g(x)]^2}$
Chain Rule	$\frac{d}{dx}[f(g(x))] = f'(g(x))g'(x)$

Learning outcomes of the course

- **After the course the student wil be able to**
  - ILO 1 Know the meaning of and interrelation between different thermodynamic properties
  - ILO 2 Describe the laws of thermodynamics in relation to chemical reactions
  - ILO 3 Show the relations between thermodynamic properties and phase equilibria
  - ILO 4 Calculate thermodynamic properties (Entropy, Enthalpy, Heat capacity, Gibbs energy, Volume) of materials and reactions as a function of temperature
  - ILO 5 Solve heat balances in industrial reactors based on thermodynamic data in order to develop sustainable chemical and metallurgical processes
  - ILO 6 Interpret simple phase stability diagrams

Learning outcomes of Sustainable Metals Processing

- **Core scientific and engineering knowledge to be obtained:**
  - Adequate knowledge of transport phenomena in homogeneous, heterogeneous and particulate systems, and a general knowledge of their atom-level origins; knowledge of their mutual interactions in extraction and refining operations and how their equipment and processes are designed.
  - Adequate knowledge of chemical kinetics in various fields related to metallurgical processing industries.
  - **Knowledge about chemical thermodynamic, phase equilibrium and property calculations.**
  - **Understanding on chemical equilibria, process dynamics, system engineering and their connections to process design, the best practices and flow-sheet integration.**
  - Understanding on societal, economic and environmental impacts to process designs and responsibilities related to metal making on the basis of system engineering.

Learning outcomes of Sustainable Metals Processing

- **Core scientific and engineering skills to be developed:**
  - System engineering and its connections to process design, the best practices and flow-sheet integration thus quantified sustainability linking product design and geology to metal production while also considering links to energy recovery as well as water recycling.
  - **Study experimentally metals extraction reactors and unit processes at low and high temperatures, gather data and evaluate process performance.**
  - **Model, develop and optimize production equipment, processes and plants with the help of numerical tools.**
  - **Act as metallurgical engineering expert in multidisciplinary groups developing feasible metals extraction processes, equipment and plants.**

Learning outcomes of Creative Sustainability - CHEM

- **Multidisciplinary approach:** Students learn to combine knowledge and skills from different disciplines to co-create innovative solutions for real-life challenges and to promote transformations towards ecologically, economically and socially sustainable futures.
- **Systems thinking:** Students learn to use systems thinking to create new holistic understandings of complex situations and to problem-solve.
- **Sustainable use of materials**: Students understand basic scientific principles and processes of bioeconomy and circular economy, and are able to use analytical tools and develop solutions for sustainable resource use.
- **Design thinking:** Students learn to use tools and methods to support creativity and imagination and to facilitate dialogue and collaboration in design processes**.**
- **Sustainability management:** Students learn to develop, support and manage sustainability initiatives in businesses and other organizations and to work proactively to promote sustainable development through business.

Core content analysis

	Must know	Should know	Nice to know
Knowledge	- Know the interrelation between different thermodynamic properties - Understand the laws of thermodynamics in relation to chemical reactions - Understand relations between thermodynamic properties and phase equilibria	- Know how to derive the thermodynamic functions based on the laws of thermodynamics	
Skills	- Calculate thermodynamic properties (Entropy, Enthalpy, Heat capacity, Gibbs energy, Volume) of materials and reactions as a function of temperature - Calculate heat balances in industrial reactors based on thermodynamic data - Interpret simple phase stability diagrams	- Create simple phase stability diagrams - Calculate heat balances and thermodynamic properties using thermodynamic software	
Attitudes			

Course information

- Mainly through MyCourses portal and in lectures as well as tutorials
- Group e-mails from Sisu will be used if necessary

Study materials

- The lecture hand-outs will be available as pdf files in MyCourses
- Textbook: D.R. Gaskell, Introduction to the Thermodynamics of Materials (4^{th} or 5^{th} edition); available to you as e-book in the Aalto library
  - Chapters 1-8 deal with issues in this course
- Written docs in tutorials and workshops
- Other useful material

Pelton, Phase Diagrams and Thermodynamic Modeling of Solutions
https://www.sciencedirect.com/book/9780128014943/phase-diagrams-andthermodynamic-modeling-of-solutions

- Section 2 is an overview of Thermodynamics
- Access to Aalto network via VPN is required for access

Testing and marks

- **Your skills will be tested in an exam (max. 30 points)**
  - Exam is Wednesday 7.12 9:00-13:00
  - Simple fundamental problems based directly on the lecture notes, as well as more demanding problems requiring independent skills in the art.
  - 6 questions, 0-2 essays and 4-6 computational problems.

- **Weekly quizzes will add max. 1 point/quiz (Max 6 points)**
- **Your performance in the workshops will add max. 1 points/WS to your total (Max 4 points).**
- **Thus the max. number of points will be 40 points.**
- **Minimum 20 points is needed to pass the course, e.g. 5 points from quizzes and 15 points from exam.**
- **In addition 1 point if over 50% of course participants answer the official course feedback**

Testing and marks

- Exam is planned as a normal exam on campus
- No other materials allowed except calculator and a sheet of main thermodynamic equations, that will be provided in the exam