UNIVERSITY OF ABERDEEN SCHOOL OF ENGINEERING

COURSE INFORMATION SESSION 2013/14

EG3029 Chemical Thermodynamics

CREDIT POINTS
15

COURSE CO-ORDINATOR
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CONTRIBUTORS
N/A

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PRE-REQUISITE
EG2002 Process Engineering
EG2004 Fluid Mechanics & Thermodynamics

CO-REQUISITE
None

COURSES FOR WHICH THIS COURSE IS A PRE-REQUISITE
EG3501 Chemical Reaction Engineering
EG3502 Separation Processes 1
EG3503 Chemical Engineering Design
EG3504 Process Modelling

AIMS

The course aims to give a thorough treatment of the ***real*** PVT behaviour exhibited by multicomponent, multiphase systems by giving candidates the knowledge required to determine: a) the heat and/or work required to bring about a given change of state; b) the change of state resulting from a transfer of energy in the form of heat and/or work, or as a result of a chemical reaction. To build on the knowledge of process simulation gained in Level 2 and emphasize, in examples and laboratories, the importance of selecting an appropriate *fluid package*.

DESCRIPTION

The course begins with an introduction to process modelling incorporating a revision of essential chemical engineering thermodynamics. The ideal gas law and equations for the computation of process heat/work requirements for isochoric, isobaric and isothermal processes are briefly revised. Adiabatic and polytropic processes are also treated. Advanced concepts including virial and cubic EOS are introduced.

The P-V and P-T phase diagrams, as well as the thermodymanic T-S, H-S, P-H diagrams for a pure substance are introduced together with the terms 'reduced pressure' and 'reduced temperature'. The isothermal compressibility and volume expansivity are discussed for liquids. Heat effects in terms of latent heats, standard heats of reaction and formation are introduced.

Vapour pressure and the Antoine Equation are treated allowing two-component vapour-liquid equilibrium to be discussed in terms of Raoult's law and modified Raoult's law.

PVT relations for real gas mixtures are addressed; Dalton's & Amagat's laws modified by compressibility and the pseudo-critical method employing Kay's law are covered.

Residual properties and the experimental determination of thermodynamic properties are addressed.

Solution thermodynamics concepts including fugacity and excess properties are introduced together with property changes of mixing. Activity models are discussed.

Chemical reaction equilibria are treated including an evaluation of equilibrium constants and their relation to composition. The phase rule for reacting systems is discussed. Multireaction equilibria are introduced.

LEARNING OUTCOMES

By the end of the course students should:

A: have knowledge and understanding of:

- Phase behaviour of pure substances
- Several equations of state useful for describing the PVT behaviour of single-component systems
- Non-Equation-of-State methods for describing PVT behaviour of single-component systems
- Thermodynamic computations of heat/work requirements for processes involving real gases
- Thermodynamic properties of fluids and residual properties
- Two-component vapour-liquid equilibrium: ideal & modified Raoult's law
- The equilibrium of chemically reacting systems
- Thermodynamic state changes as a result of mixing and chemical reaction.

B: have gained intellectual skills so that they are able to:

- Identify appropriate methods for the analysis of single component PVT behaviour
- Undertake thermodynamic process computations for single component systems involving non-ideal behaviour
- Undertake thermodynamic process computations for multi-component systems involving non-ideal behaviour
- Select appropriate thermodynamic concepts for analysing multi-component, multi-phase systems
- Support the results of computer simulation with appropriate hand computations
- Undertake bubble-point and dew-point computations for two-component VLE

C: have gained practical skills so that they are able to:

- Efficiently use the UNISIM Design R390 process simulator to model and analyse processes as required by a given task
- Efficiently use Matlab to implement sets of equations and carry out systematic parameter studies
- Compute mass/molar flow rates of non-ideal gas mixtures via a variety of techniques
- Confidently approach single and multi-component PVT problems and identify an appropriate model for their solution
- Undertake process heat/work computations for multi-component, non-ideal systems
- Compute the equilibrium composition of a reacting system

D: have gained or improved transferable skills so that they are able to:

- Effectively report on laboratory-based work – simulation & experimental
- Effectively use the UNISIM Design R390 process simulation engine as well as Matlab
- Identify reliable sources of PVT data for a variety of components

SYLLABUS

1. **Introduction and Principles**: Revision of general concepts; dimensions and units; first law of thermodynamics for open and closed systems; state functions; reversible ideal gas processes.
   (3 lectures - Dr Kiefer)

2. **Volumetric Properties of Pure Fluids:** PVT behaviour; PT and PV diagrams; lever rule; critical point; virial equation of state; cubic equations of state; reduced pressure and reduced temperature; volume expansivity and isothermal compressibility; latent heats.
   (4 lectures - Dr Kiefer)

3. **Second Law of Thermodynamics:** Entropy; Carnot engine; Entropy changes of ideal gas; reversibility of ideal gas processes; exergy.
   (3 lectures - Dr Kiefer)

4. **Thermodynamic Properties of Pure Fluids**: Property relations for homogeneous phases; Maxwell's equations; residual properties; two-phase systems; Clapeyron equation; Antoine equation; PH and TS diagrams; Mollier diagram; property tables.
   (4 lectures - Dr Kiefer)

5. **Vapour/Liquid Equilibrium of Mixtures**: Phase rule; Duhem's theorem; PTxy diagram of binary mixtures; Pxy and Txy diagrams; PT diagram; Raoult's law; Henry's law; modified Raoult's law; K-value correlations.
   (5 lectures - Dr Kiefer)

6. **Solution Thermodynamics**: Property relations; chemical potential; partial properties; ideal gas mixture model; fugacity; treatment of solutions; ideal solution model; excess properties; liquid-phase properties from VLE; activity models; property changes of mixing; heat effects of mixing.
   (6 lectures - Dr Kiefer)

7. **Chemical reaction equilibrium**: reaction coordinate; equilibrium criteria; equilibrium constant; temperature effects; composition effects; single-reaction systems; multireaction equilibrium; phase rule in reacting system; heat of formation; heat of reaction.
   (5 lectures - Dr Kiefer)

This is a guide to the taught content of EG3029 and it should be noted that this is subject to change at the discretion of the course instructor.

TIMETABLE

30 one-hour lectures, 10 one-hour tutorials and 3 three-hour laboratories in total. Detailed times are provided separately.

ASSESSMENT

1st attempt: 1 three-hour written examination paper (80%), and continuous assessment (20%).

Resit: A three-hour resit paper may be provided for candidates who fail the course at the first attempt. Where a resit paper is offered, the mark reported for the resit will be the better of:

a) 100% of the resit examination mark
b) 80% of the resit examination mark + 20% of the continuous assessment mark.

Notes on Assessment

- *Candidates who pass the examination at the first attempt but fail to pass the course will be required to pass the resit examination.*

The continuous assessment will be based on the submission of engineering reports detailing the laboratory work. Detailed information relating to the format of reports will be given during course contact time.

FORMAT OF EXAMINATION

Candidates must attempt ALL FIVE questions. All questions carry 20 marks.

Notes:

(i) Candidates are permitted to use approved calculators only.

(ii) Candidates are permitted to use the Engineering Mathematics Handbook, which will be made available to them

(iii) Data sheets will be provided where necessary.

PLEASE NOTE THE FOLLOWING

(i) You must not have in your possession at the examination any material other than that expressly permitted by the examiner. Where this is permitted, such material must not be amended, annotated or modified in any way.

(ii) During the course of the examination, you must not have in your possession or attempt to access any material that could be determined as giving you an advantage in the examination.

(iii) You must not attempt to communicate with any candidate during the examination, either orally or by passing written material, or by showing material to another candidate, nor must you attempt to view another candidate's work.

Failure to comply with the above will be regarded as cheating and may lead to disciplinary action as indicated in the Academic Quality Handbook (http://www.abdn.ac.uk/registry/quality/)**.**

Your attention is drawn to key University policies which can be accessed via https://abdn.blackboard.com/bbcswebdav/institution/Policies It is important that make yourself familiar with the University's policies and procedures on the subjects covered.

FEEDBACK

a) Students can receive feedback on their progress with the Course on request at the weekly tutorial/feedback sessions.

b) Students are given feedback through formal marking and return of laboratory reports.

c) There will be a test exam at the end of the teaching session. The test exam will be marked (but is not part of the continuous assessment) and the test exam paper questions will be discussed in the Revision week.

d) Students requesting feedback on their exam performance should make an appointment within 4 weeks of the publication of the exam results.

STUDENT MONITORING

Attention is drawn to Registry's guidance on student attendance and monitoring at: http://www.abdn.ac.uk/registry/monitoring

1.1 of this guidance says that students will be reported as "at risk" if the following criteria are met:

Either (i) Absence for a continuous period of 10 working days or 25% of a course (whichever is less) without good cause being reported;

or (ii) Absence from two small group teaching sessions for a course without good cause (eg tutorial, laboratory class, any other activity where attendance is expected and can be monitored);

or (iii) Failure to submit a piece of summative or a substantial piece of formative in-course assessment for a course, by the stated deadline (eg class test, formative essay).

For the purposes of this, course attendance will be monitored at the tutorial and lab sessions and the formative in-course assessment are the lab reports.

RECOMMENDED BOOKS

The course is largely based on the treatment of undergraduate chemical engineering thermodynamics presented in

1. “Introduction to Chemical Engineering Thermodynamics”, J.M. Smith, H.C. van Ness, M.M. Abbott, McGraw-Hill; current edition – 7th Edition, ISBN 9780071247085.

The course also makes reference to, and uses a limited volume of material from;

2. “Elementary Principles of Chemical Processes”, R.M. Felder, R.W. Rousseau, John Wiley & Sons, Inc.; current edition – 3rd Edition, ISBN 9780471375876

3. “The Properties of Gases and Liquids”, B.E. Poling, J.M. Prausnitz, J. O’Connell, McGraw-Hill; current edition – 5th Edition, ISBN 9780071189712

4. “Fundamentals of Thermodynamics”, C. Borgnakke, R.E. Sonntag, Wiley; current edition, ISBN 9781118321775

INSTITUTIONAL INFORMATION

Students are asked to make themselves familiar with the information on key institutional policies which have been made available within MyAberdeen (https://abdn.blackboard.com/bbcswebdav/institution/Policies). These policies are relevant to all students and will be useful to you throughout your studies. They contain important information and address issues such as what to do if you are absent, how to raise an appeal or a complaint and how seriously the University takes your feedback.

These institutional policies should be read in conjunction with this programme and/or course handbook, in which School and College specific policies are detailed. Further information can be found on the University’s Infohub webpage or by visiting the Infohub.