Unit 206 Chemical thermodynamics, kinetics and reactor design

Unit summary

This unit is about the chemistry and chemical engineering concerned with the thermodynamics and kinetics of chemical reactions, the thermodynamics of phase behaviour, and the design of chemical reactors.

Aims

The unit aims to explore chemical thermodynamics, kinetics, phase behaviour, and chemical reactors

Prerequisites

It is expected that candidates will have a working knowledge of the materials in the four compulsory papers of the Certificate examination.

Learning outcomes

There are **four** outcomes to this unit. The candidate will be able to:

- Appreciate and analyse chemical thermodynamics and phase equilibria.
- Appreciate and analyse the kinetics of chemical reactions.
- Understand heterogeneous catalysed reactions.
- Appreciate and design chemical reactors

Guided learning hours

It is recommended that 300 hours should be allocated for this unit. 120 of those hours are actual taught hours. This may be on a full time or part time basis.

Key Skills

This unit contributes towards the Key Skills in the following areas:

N4.1

Develop a strategy for using application of number skills over an extended period of time.

N4.2

Monitor progress and adapt your strategy, as necessary, to achieve the quality of outcomes required in work involving:

- deductive and inferential reasoning;
- algebraic manipulation.

N4.3

Evaluate your overall strategy and present the outcomes from your work, including use of charts, diagrams and graphs to illustrate complex data.

PS4.1

Develop a strategy for using skills in problem solving over an extended period of time.

PS4.2
Monitor progress and adapt your strategy, as necessary, to achieve the quality of outcomes required when tackling **one** complex problem with at least three options.

PS4.3
Evaluate your overall strategy and present the outcomes from your work using a variety of methods

Occupational Standards
This unit has been mapped to the following National Occupational Standards:

1.1.1 Identify the requirements of clients for engineering products or processes
1.1.2 Produce specifications for engineering products or processes
1.2.3 Propose and specify research into engineering products or processes
1.3.1 Undertake research into engineering products or processes
1.3.2 Evaluate the results of research
3.1.1 Determine the installation requirements for engineering products or processes
3.1.2 Specify installation methods and procedures to achieve installation requirements
3.1.4 Schedule installation activities to implement the installation methods and procedures
4.1.1 Determine the operational requirements of engineering products or processes
4.2.2 Solve operational problems with engineering solutions
6.1.1 Analyse the risks arising from engineering products and processes
6.1.2 Specify methods and procedures to reduce risks
7.2.3 Evaluate projects
8.1.1 Maintain and develop own engineering expertise

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Outcome 1 Appreciate and analyse chemical thermodynamics and phase equilibria.

Knowledge requirements
The candidate knows how to:

1 appreciate the concept of reversible work and free energy
2 calculate the temperature and pressure dependence of free energies
3 determine free energy functions
4 describe and calculate fugacity and activity
5 appreciate the standard-state concept
6 assess quantitatively free energy and equilibrium
7 describe phase equilibria
8 determine T and P dependence of free energies
9 apply the Gibbs-Helmholtz equation
10 determine solubilities of solids, liquids and gases
11 apply Raoult's and Henry's laws
12 determine activity coefficients
13 use the Gibbs-Duhem Equation and perform thermodynamic consistency tests
14 ascertain chemical equilibrium and determine T and P dependence
15 recognize and be able to calculate, using tables of data
   a standard free energies
   b enthalpies
   c entropies
16 assess equilibrium constants
17 describe gas and liquid phase reactions with T and P dependence
18 investigate reversible electrochemical cells and standard electrode potentials
19 appraise concentration cells
20 analyse experimental determination of thermodynamic data

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Outcome 2 Appreciate and analyse the kinetics of chemical reactions.

Knowledge requirements
The candidate knows how to:

1 use simple homogeneous rate equations

2 assess overall rates

3 analyse temperature dependence of reaction rates

4 apply the Arrhenius equation and understand the role of an activated complex

5 determine
- a equilibrium constants
- b rate constants
- c free energy of reaction
- d free energy of activation
- e activation energy and frequency factor

6 analyse collision theory and frequency factors

7 interpret experimental results, determine reaction order and calculate activation energies

8 understand parallel and consecutive reactions

9 apply the concept of rate limiting steps

10 determine the effect of temperature on relative rates of competing processes
- a reaction
- b diffusion

11 assess reactions which are
- a chain
- b isothermal
- c adiabatic

12 appreciate free radicals

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Outcome 3 Understand heterogeneous catalysed reactions.

Knowledge requirements
The candidate knows how to:

1 analyse physical adsorption and chemisorption

2 determine the enthalpy of adsorption and dependence of surface coverage on temperature and pressure

3 determine surface areas by Langmuir and BET isotherms

4 determine adsorption coefficients

5 apply rate equations of simple reactions

- a first and second order
- b adsorption – desorption controlled
- c surface reaction controlled

6 assess the significance of the specific rate constants in reactions

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Outcome 4 Appreciate and design chemical reactors

Knowledge requirements
The candidate knows how to:

1 assess tubular reactors

2 investigate the solution of the elementary design equation based on plug flow for isothermal and adiabatic cases

3 assess continuous stirred-tank reactors (CSTR)

4 assess design equations based on the perfect mixing assumption in CSTRs

5 compare stirred tank and tubular reactors

6 apply residence time studies to reactors

7 compare batch and continuous processes with regard to

- a reactor volume
- b reaction yield

8 assess the logic of a choice of process

9 investigate optimisation problems and optimum temperature sequences

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Recommended reading list

Core texts	Author(s)	Publisher	ISBN
Physical Chemistry includes CD Rom	Atkins, PW	Oxford University Press	0198501013
Chemical Reaction Engineering	Levenspiel	John Wiley	047125424X
Introduction to Chemical Engineering Thermodynamics	Smith, Van Ness	McGraw Hill	0071147373
The Principles of Chemical Equilibrium	Denbigh, KG	Cambridge University Press	0521281504
Chemical Metallurgy	Moore	Butterworth-Heinemann	0408053690 o/p
Chemical Reactor Theory: an Introduction	Denbigh, Turner	Cambridge University Press	0521276306 o/p