Title:	Fluid Properties Analysis APPROVED
Long Title:	Properties of Liquids and Gase

Module Code:	CHEP8011	**Duration:**	1 Semester

Credits:	5
NFQ Level:	Advanced
Field of Study:	Chemical & Process Eng
Valid From:	Semester 1 - 2016/17 (September 2016)
Module Delivered in	1 programme(s)
Module Coordinator:	NIALL MORRIS
Module Author:	NOEL DUFFY
Module Description:	This module introduces students to more advanced aspects of thermodynamic analysis including the estimation of thermodynamic & transport properties of fluid mixtures and the application of solution thermodynamics to the solution of practical Chemical Engineering problem.

Learning Outcomes	
On successful completion of this module the learner will be able to:	
LO1	Estimate the molar volume, molar enthalpy and molar entropy of real fluid mixtures, using modern equations of state, applied to practical engineering problems.
LO2	Estimate transport and thermodynamic properties of pure fluids and then apply these correlations to solve practical engineering problems.
LO3	Estimate the thermodynamic and transport properties of real fluid mixtures, and then apply these methods to solve practical engineering problems.
LO4	Estimate the heat of reaction and equilibrium concentration for chemical reactions in non-ideal systems.

Pre-requisite learning
Module Recommendations *This is prior learning (or a practical skill) that is strongly recommended before enrolment in this module. You may enrol in this module if you have not acquired the recommended learning but you will have considerable difficulty in passing (i.e. achieving the learning outcomes of) the module. While the prior learning is expressed as named CIT module(s) it also allows for learning (in another module or modules) which is equivalent to the learning specified in the named module(s).*
None
Incompatible Modules *These are modules which have learning outcomes that are too similar to the learning outcomes of this module. You may not earn additional credit for the same learning and therefore you may not enrol in this module if you have successfully completed any modules in the incompatible list.*
None
Co-requisite Modules
No Co-requisite modules listed
Requirements *This is prior learning (or a practical skill) that is mandatory before enrolment in this module is allowed. You may not enrol on this module if you have not acquired the learning specified in this section.*
No requirements listed

Module Content & Assessment

Indicative Content
Review of PvT behaviour of pure substances Pv, PT diagrams; triple point, critical point. Equations of state: ideal, virial; Pitzer acentric factor. Compressibility factor. Reduced temperature and pressure, corresponding states principle. Generalised compressibility charts. Vapour pressure: Clapeyron equation, Clausius-Clapeyron equation; Antoine equation. Gibbs Phase Rule.
Cubic Equations of State Cubic EOS (van der Waals, Redlich-Kwong and variants, Peng Robinson and variants); high-precision equations of state. Use of cubic EOS to determine molar volume given P, T. Inter-relationships between thermodynamic properties: P, v, T, u, s, h, g, a. Heat capacity; evaluation paths; reference states. Residual properties / departure functions for real fluids.
Correlation and estimation of pure component properties Scalar properties e.g. critical data, acentric factor, normal boiling point. Temperature dependent thermodynamic properties e.g. vapour pressure, enthalpy of vapourisation, heat capacity. Transport properties e.g. viscosity, conductivity. Estimation of property values using published and software-mediated methods. Group contribution methods: Joback, Gani et al.
Properties of Mixtures Property changes on mixing; partial molar properties (volume, enthalpy, Gibbs energy); chemical potential. Significance of Gibbs energy and chemical potential. Gibbs-Duhem equation. Ideal mixtures of ideal gases and real fluids. Excess properties. Fugacities and fugacity coefficients, activities and activity coefficients. Lewis-Randall rule. Liquids. Ideal solutions. Application of equations of state using mixing rules. Introduction to activity coefficient models, local composition models.
Chemical reaction equilibrium Review of determination of heat of reaction from heats of formation: Hess' Law. Determination of heat of reaction at non-standard conditions of temperature (Kirchoff's Law) and pressure for ideal and non-ideal systems. Determination of equilibrium composition from Gibbs energy of formation at non-standard conditions of temperature for ideal and non-ideal systems.

Assessment Breakdown	%
Course Work	40.00%
End of Module Formal Examination	60.00%

Course Work

Assessment Type	*Assessment Description*	*Outcome addressed*	*% of total*	*Assessment Date*
Short Answer Questions	Examination of material covered to date: use of cubic equations of state, etc.	1,2	40.0	Week 6

End of Module Formal Examination

Assessment Type	*Assessment Description*	*Outcome addressed*	*% of total*	*Assessment Date*
Formal Exam	End-of-Semester Final Examination	1,2,3,4	60.0	End-of-Semester

Reassessment Requirement

Repeat examination
Reassessment of this module will consist of a repeat examination. It is possible that there will also be a requirement to be reassessed in a coursework element.

The institute reserves the right to alter the nature and timings of assessment

Module Workload

Workload: Full Time				
Workload Type	*Workload Description*	*Hours*	*Frequency*	*Average Weekly Learner Workload*
Lecture	Lectures/Discussions/Class Tutorials.	3.0	Every Week	3.00
Independent & Directed Learning (Non-contact)	Study/Past Papers/Self-Study Tutorials.	3.0	Every Week	3.00
Lab	Use of thermodynamics related software	1.0	Every Week	1.00
			Total Hours	7.00
			Total Weekly Learner Workload	7.00
			Total Weekly Contact Hours	4.00

Workload: Part Time				
Workload Type	*Workload Description*	*Hours*	*Frequency*	*Average Weekly Learner Workload*
Lecture	Lectures / Discussions / Class tutorials	3.0	Every Week	3.00
Independent & Directed Learning (Non-contact)	Study/Past papers/Self-study tutorials	3.0	Every Week	3.00
Lab	Use of thermodynamics related software	1.0	Every Week	1.00
			Total Hours	7.00
			Total Weekly Learner Workload	7.00
			Total Weekly Contact Hours	4.00

Module Resources

Recommended Book Resources

- **Elliott, J.R, & Lira, C.T. 2012, *Introductory Chemical Engineering Thermodynamics*, 2nd Edn. Ed., Pearson [ISBN: 978-0-13-275624-2]**

Supplementary Book Resources

- **Jurgen Gmehling, Barbel Kolbe, Michael Kleiber, Jurgen Rarey, 2012, *Chemical Thermodynamics for process simulation*, Wiley-VCH Weinheim, Germany [ISBN: 9783527312771]**
- **Koretsky, M. D. 2013, *Engineering and chemical thermodynamics*, 2nd Ed., Wiley [ISBN: 0470259612]**
- **Sandler, S.I. 2015, *Using Aspen PLus in Thermodynamics Instruction: a step by step guide*, Wiley [ISBN: 9781118996]**
- **Smith, J.M., van Ness, H.C., Abbott, M.M. 2000, *Introduction to Chemical Engineering Thermodynamics*, 6th Edn Ed., McGraw-Hill**
- **Noel de Nevers, 2012, *Physical and Chemical Equilibrium for Chemical Engineers*, 2nd Ed., Wiley [ISBN: 9780470927106]**
- **Poling, B.E., Prausnitz, J.M., O'Connell, J.P. 2000, *Properties of Liquids and Gases*, 5th Edn Ed., McGraw-Hill**
- **Abbott, M.M., van Ness, H.C. 1989, *Thermodynamics with Chemical Applications (Schaum's Outline Series)*, 2nd Edn Ed., McGraw-Hill**
- **Stanley I. Sandler 2006, *Chemical, biochemical, and engineering thermodynamics*, 4th Edn Ed., John Wiley & Sons Hoboken, N.J. [ISBN: 9780471661740]**
- **Prausnitz, J.M., Lichtenthaler, R.N., de Azevedo, E.G. 1998, *Molecular Thermodynamics of Fluid Phase Equilibria*, 3rd Edn Ed., Prentice-Hall**
- **Obrey, H., Sandler, S.I., Varma, A. 1998, *Modeling Vapor-Liquid Equilibria: Cubic Equations of State and their Mixing Rules*, Book & Disk Edn Ed., Cambridge University Press**

This module does not have any article/paper resources

Other Resources

- **Process Simulation Software: Aspen Technology Inc. 2014, *Aspen ONE*, AspenTech, 10 Canal Park, Cambridge, MA, USA**

Module Delivered in

Programme Code	Programme	Semester	Delivery
CR_ECPEN_8	Bachelor of Engineering (Honours) in Chemical and Biopharmaceutical Engineering	5	Mandatory