Title:	Process & Properties Analysis APPROVED
Long Title:	Process & Properties Analysis

Module Code:	CHEP8014	**Duration:**	1 Semester

Credits:	5
NFQ Level:	Advanced
Field of Study:	Chemical & Process Eng
Valid From:	Semester 1 - 2017/18 (September 2017)
Module Delivered in	1 programme(s)
Module Coordinator:	NIALL MORRIS
Module Author:	NOEL DUFFY
Module Description:	This module develops students' capability to solve real phase equilibrium separation problems, applying fundamental theory with industry-grade software. Advanced functions of the steady-state process simulation package, Aspen Plus, will be covered and the students will be introduced to the capabilities of a batch process simulator.

Learning Outcomes	
On successful completion of this module the learner will be able to:	
LO1	Assess the applicability of correlative and predictive phase equilibrium models to specific ideal and non-ideal system separations.
LO2	Assess the separability of a non-ideal mixture using Aspen software.
LO3	Construct sensitivity analyses, design specifications, calculator blocks and optimization blocks in Aspen Plus
LO4	Prepare a simulation of a batch process using batch simulation software.

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 vapour liquid equilibrium (VLE) for ideal systems. Vapour pressure of pure components: Antoine equation. Pxy, Txy, yx diagrams for ideal mixtures; K-values; relative volatility; bubble and dew point calculations; isothermal and adiabatic flash calculations.
Non-ideal phase equilibrium VLE in non-ideal systems: using equations of state; using activity coefficient models with equations of state. Variation of activity coefficients with temperature; local composition (excess Gibbs energy) models: Wilson, UNIQUAC, NRTL. Azeotropes. High pressure systems: retrograde condensation.
Highly non-ideal systems (VLE, GLE, SLE) Liquid-liquid equilibrium; variation with temperature and pressure. Supercritical components; solubility of gases in liquids, gas-liquid equilibrium. Introduction to electrolyte solutions: Debye-Huckel Law, modifications: Bromley, Pitzer; Chen NRTL electrolyte model. Introduction to solid-liquid equilibria: salt solubility, influence of salts on vapour-liquid equilibria.
Predictive methods for phase equilibrium Local composition models - group contribution methods: UNIFAC and modified UNIFAC. Predictive equations of state: PSRK and VTPR-GC methods. Strengths and weaknesses of such methods. Introduction to COSMO and PC-SAFT models. Semi-predictive NRTL-SAC for drug solubility prediction.
Data quality assessment Checking phase equilibrium data for thermodynamic consistency. Regression of published experimental data to models. Examination using alternative databases e.g. Aspen, NIST, Dortmund DataBank. Combination of data sources and predictive methods.
Application of phase equilibrium to separation processes Azeotrope variation with pressure. Non-ideal ternary systems: nodes, saddles, residue curves, distillation curves, distillation boundaries. Determination of feasible product compositions. Determination of operating pressure.
Advanced Capabilities of Aspen Plus Sensitivity analysis, design specifications, calculator blocks and optimization blocks
Batch Simulation Using Batch Process Developer Determine cycle time and identify bottlenecks, create a multiple batch Gantt chart, generate equipment content and capacity reports to determine equipment size.

Assessment Breakdown	%
Course Work	100.00%

Course Work

Assessment Type	*Assessment Description*	*Outcome addressed*	*% of total*	*Assessment Date*
Practical/Skills Evaluation	Software Project - high end tools in AspenPlus	3	10.0	Week 6
Practical/Skills Evaluation	Phase Equilibrium prediction	1,2	25.0	Week 7
Practical/Skills Evaluation	Aspen Batch Process Developer	4	15.0	Week 12
Open-book Examination	Thermodynamics Exam, using software, texts and notes, to predict and assess reaction and phase equilibrium and feasible separation.	1,2	50.0	Sem End

No End of Module Formal Examination

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/Worked examples/Tutorials	1.0	Every Week	1.00
Lab	Process Simulation for Batch and Continuous Processes	1.0	Every Week	1.00
Lab	Phase equilibrium assessment	2.0	Every Week	2.00
Independent & Directed Learning (Non-contact)	Study, Solving Problems	3.0	Every Week	3.00
			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 / Worked examples / Tutorials	1.0	Every Week	1.00
Lab	Process simulation for Batch and Continuous processes	1.0	Every Week	1.00
Lab	Phase equilibrium assesment	2.0	Every Week	2.00
Independent & Directed Learning (Non-contact)	Study / problem solving	3.0	Every Week	3.00
			Total Hours	7.00
			Total Weekly Learner Workload	7.00
			Total Weekly Contact Hours	4.00

Module Resources

Recommended Book Resources

- **Warren D. Seider, J.D. Seader, Daniel R. Lewin, Soemantri Widagdo, 2010, *Product and Process Design Principles: Synthesis, Analysis and Design, 3rd Edition*, 3rd Ed., Wiley [ISBN: 9780470414415]**

Supplementary Book Resources

- **Elliott, J.R., Lira, C.T. 2012, *Introductory chemical engineering thermodynamics*, 2nd Ed., Pearson [ISBN: 9780132756242]**
- **Jurgen Gmehling, Barbel Kolbe, Michael Kleiber, Jurgen Rarey, 2012, *Chemical Thermodynamics for process simulation*, Wiley-VCH Weinheim, Germany [ISBN: 9783527312771]**
- **Stanley I. Sandler 2006, *Chemical, biochemical, and engineering thermodynamics*, 4th Ed. Ed., John Wiley & Sons Hoboken, N.J. [ISBN: 9780471661740]**
- **Sandler, S.I. 2015, *Using Aspen Plus in Thermodynamics Instruction: A Step-by-Step Guide*, Wiley [ISBN: 978-1-118-996]**
- **Smith, J.M., van Ness, H.C., Abbott, M.M. 2004, *Introduction to Chemical Engineering Thermodynamics*, 7th Ed. Ed., McGraw-Hill**
- **Abbott, M.M. & van Ness, H.C. 1989, *Thermodynamics with Chemical Applications (Schaums Outline Series)*, 2nd Ed. Ed., McGraw-Hill**
- **Prausnitz, J.M., Lichtenthaler, R.N., de Azevedo, E.G. 1998, *Molecular Thermodynamics of Fluid Phase Equilibria*, 3rd Ed. Ed., Prentice-Hall**
- **M. F. Doherty and M. F. Malone 2001, *Conceptual design of distillation systems*, McGraw-Hill Boston [ISBN: 0072488638]**
- **Poling, B.E., Prausnitz, J.M., O'Connell, J.P. 2000, *The Properties of Gases and Liquids*, 5th Ed. Ed., McGraw-Hill**
- **Obrey, H., Sandler, S.I., Varma, A. 1998, *Modeling Vapor-Liquid Equilibria: Cubic Equations of State and their Mixing Rules*, Disk Ed. Ed., Cambridge University Press**

This module does not have any article/paper resources

Other Resources

- **Software: Aspen Technology Inc 2015, *Aspen Suite*, AspenTech, 10 Canal Park, Cambridge, MA, USA**
- **Software: DDBST *Dortmund Databank (Teaching Edition)*, Oldenburg**

Module Delivered in

Programme Code	Programme	Semester	Delivery
CR_ECPEN_8	Bachelor of Engineering (Honours) in Chemical and Biopharmaceutical Engineering	8	Mandatory