

**COMMONWEALTH GRADUATE ENGINEERING PROGRAM
DISTANCE LEARNING COURSE PLANNING SHEET
UNIVERSITY OF VIRGINIA**

Course CHE 615 - Advanced Chemical Engineering Thermodynamics Semester Fall 2006

Instructor John P. O'Connell Phone No. 434-924-3428

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Textbook(s): (Student to purchase)

J.P. O'Connell & J.M. Haile, "Thermodynamics: Fundamentals for Applications", Cambridge Press, 2005, ISBN 0521582067

Reference(s):

"Chemical & Engineering Thermodynamics" by S.I. Sandler, 3rd Ed., John Wiley, 2001

"Phase Equilibria in Chemical Engineering" by S.M. Walas, Butterworths, 1985

"Thermodynamics", 2nd Edition, by H.C. Van Ness & M.M. Abbott, Schaum's Outlines, McGraw-Hill, 1989

"Molecular Thermodynamics of Fluid Phase Equilibria, 3rd Ed.", by J. M. Prausnitz, R.N. Lichtenthaler & E.G. de Azevedo, Prentice-Hall, 1999

Computer Needs:

Computer Capability None necessary, though among choices for required project are computer coded programs

Software required? Spreadsheet, MathCad/MatLab might be useful Provided? No

Other _____

University of Virginia - Fall, 2006
Beginning of Course Memorandum
CHE 615 - Advanced Chemical Engineering Thermodynamics

Instructor: John O'Connell

Office: (434) 924-3428 Chemical Engineering 310

URL: <http://www.che.virginia.edu/faculty.html>

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Class Home Page URL: http://toolkit.itc.virginia.edu/cgi-local/tk/UVa_SEAS_2006_Fall_CH_E615-1

Classes: TR 1530-1645; Office Hours: TBA

GTA: TBA

Text: "Multicomponent Thermodynamics: Fundamentals for Applications" by J. P. O'Connell and J.M. Haile (O'CH); Cambridge University Press, 2005; ISBN 0-521-58206-7. All chapters 0-13 covered, except little in Chapter 11.

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"Chemical & Engineering Thermodynamics" by S.I. Sandler, 3rd Ed., John Wiley, 2001

"Phase Equilibria in Chemical Engineering" by S.M. Walas, Butterworths, 1985

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Course Objectives

1. Review Fundamental Thermodynamic Principles for Improved Knowledge and Understanding.
2. Gain Experience with Professional Level Use of Physical Property Models & Chemical Reaction Equilibrium Calculations
3. Implement Thermodynamics in Some Complex Systems

Grading Basis (650 points)

Quizzes (2)	200
Final Examination	300
Term Project	100
Homework	<u>50</u>
	650

Homework

Problems assigned will be found in "Assignments - Homework Submission" from the Class Home Page. Due in class on Tuesdays. 1/4 of problems chosen will be randomly graded; papers are not returned. Brief outlines of all solutions given on the Toolkit Web Site by noon the day after; questions to be asked in class after solutions appear.

Term Project

Students will pick one option from the options A - D described briefly below with details in the "Projects" directory of the "Materials" section of the Class Home Page. The project option selected is to be communicated to Mr. O'Connell during the 2nd week of November & the project must be submitted by 1700 on the day of the final exam.

A. Term Paper & Article Analysis For article from the instructor's list describing method for correlating physical property or computing equilibria of multiple chemical reactions, write a paper of up to 7 pages (plus figures, tables & appendices) to discuss nature of model, its basis, breadth & limitations of application, accuracy & expected usefulness. Also, submit both (1-page) "Scope" & "Conclusions & Significance" sections & "Reviewer's Comments".

B. Computer Problem I. Write, or obtain, a computer program for using a student-selected activity coefficient, vapor pressure and vapor equation of state models to obtain vapor-liquid equilibria (x,y,T,P) for a binary of complex substances (specified by the instructor) from the heavy component triple point to light component critical point.

C. Computer Problem II. Write, or obtain, computer program for using a student-selected multiphase equation of state to obtain vapor-liquid equilibria (x,y,T,P) and phase volumes for binary of normal substances (specified by instructor) from triple point to critical point of the heavier component.

D. Computer Problem III. Submit programs and solutions for O'CH problems 11.16, 11.19, 11.20, 11.23.

Copies of Lecture slides are placed on the Toolkit Web Site by noon of the lecture day.