ChE 548 Syllabus

A. Course Details

ChE 548 Advanced Transport Phenomena II

Meeting Place: Room 108, Perkins Hall
Meeting Time: MWF at 8:00-8:50

Instructor: Dr. David Keffer, room 617 Dougherty Hall, dkeffer@utk.edu
Teaching Assistant: None

Required Text: "Transport Phenomena", Bird, Stewart, & Lightfoot, Wiley, second edition is preferred but first edition is acceptable.

Course Website: http://clausius.engr.utk.edu/che548/index.html

B. Course Objective:

The objective of this course is to continue a mathematically rigorous study of transport phenomena. In this course, particular emphasis will be given to mass and energy transport, as momentum transport was featured in the first semester of the course, ChE 547.

C. Grading Policy

C.1. Grade Breakdown

• Exams (1 mid-term and 1 final exam @ 25% each):	50%
• Homeworks (6 assignments):	25%
• Computer Project and Report (1 project @ 25% each):	25%
• Total:	100%

C.2. Homework

- Homework assignments are made each Wednesday and due in two weeks unless a change is announced in class.
- Homework assignments are due at the beginning of class.
- Late homework assignments are not accepted.
- Students can work together to solve homework assignments. However, each student must turn in his/her own work in his/her own handwriting. For homework assignments where computer-generated code or graphs are required, each student must generate their own codes and graphs.
- Instances of plagiarism will be dealt with as stipulated by University guidelines, outlined in *Hill Topics*. A copy of *Hill Topics* is available in the main office of the Chemical Engineering Department. Please do not force me to have to deal with

plagiarism. Remember, you are here to learn. If you are in doubt about whether a particular action constitutes plagiarism, feel free to discuss it with the instructor.

C.3. Exams

- There are 2 exams, as indicated on the schedule.
- Each exam counts 25% of the course grade.
- Do not miss exams. Make-up Exams are not given. In the event of a serious problem, e.g. extreme illness, death in the family, etc., a substitute will be assigned on a case-by-case basis, totally at the instructor's discretion. A cold is not a satisfactory excuse for missing an exam. The University Student Health Clinic does not write medical excuses for prescribing common cold prescription medicine. Therefore, do not expect a prescription slip to get you anything but a zero on a missed exam.

C.4. Computer Projects

- There is a computer project worth 25% of the course grade.
- The computer projects will be done individually and will be assigned approximately one month before it is to be collected.
- The projects will be performed using the programming platform of your choice. Recommended platforms are FORTRAN, C, and MATLAB. Other platforms and languages are discouraged and will not be supported by the instructor .

D. Getting Help

Although lectures and text are the primary means of instruction in this course, the instructor is here to help you successfully complete this course. When you do not understand something in class or have difficulty with an exam or homework, you are encouraged to seek out the instructor. Efforts will only be made to meet with students who regularly attend lecture.

D.1. Email

The best way to contact the TA or the instructor is via email.

- Questions regarding course content should be sent via email to the Instructor
- To guarantee that the email is read promptly, make the subject of the email “ChE 548”

D.2. Office Hours

- The Instructor holds office hours on Friday afternoon 3:30-5:00. Frequently these office hours are held in Dougherty 314. Otherwise, check the instructor's office, 617 Dougherty.

E. Outline

I. Generating Transport Properties

I.A. Traditional Methods of Estimating Diffusivities
- read Chapter 17 of Bird, Stewart, & Lightfoot, 2nd edition
- work homework set 1 (on web)

I.B. Using Molecular Dynamics Simulations to Estimate Diffusivities
- read *molecular dynamics* hand-out (on web)
- read *self diffusion coefficients from molecular dynamics* hand-out (on web)
- read the *Lennard-Jones equation of state* hand-out (on web)
- work homework set 2 (on web)

- read *how to make an MD movie with freeware* hand-out (on web)
- read *multicomponent molecular dynamics* hand-out (on web)
- read *transport diffusion coefficients from self diffusion coefficients* hand-out (on web)
- read *transport diffusion coefficients from self diffusion coefficients Appendix: The practical evaluation of the thermodynamic partial derivatives* hand-out (on web)
- work homework set 3

II. Solving Transport Equations

II.A. PDE Review from ChE 505
- review numerical solution of parabolic partial differential equations

II.B. Solving systems of material balances
- read Chapter 18 of Bird, Stewart, & Lightfoot, 2nd edition
- rework BSL problems with numerical solution
- cover: accounting for adsorption phenomena (pore and surface) (notes)
- cover: accounting for reaction phenomena (homogeneous and heterogeneous) (notes)
- work homework set 4

II.C. Solving systems of material and energy balances
- read Chapter 9 of Bird, Stewart, & Lightfoot, 2nd edition
- cover: including the energy balance (basics)
- cover: incorporating reaction and adsorption
- cover: parametric sensitivity analysis
- work homework set 5

III. Other Topics of Interest (time permitting)

- Chapter 24. Other Mechanisms for Mass Transport
- The practical and quantitative consequences of approximating chemical potential gradients with concentration gradients
- The basis of transport properties and transport equations in irreversible thermodynamics
- work homework set 6