

**CHEM789**  
**Experimental Design and Statistics in Chemistry**  
Spring Term 2014

Instructor: Dr. Kevin Owens

Class Time: Mon 6:00-7:20 pm  
Wed 7:30-8:50 pm

Office: Stratton Hall 415

Class Room: Curtis 452

Phone: 215-895-2621

Office Hours: Wed 4:00-6:00 pm

Fax: 215-895-1265

e-mail: kevin.owens@drexel.edu

**Required Textbook:**

Douglas C. Montgomery, Design and Analysis of Experiments, 8<sup>th</sup> ed., New York: John Wiley & Sons, Inc., 2013, ISBN-13: 978-1-1181-4692-7.

Note there is a student companion website for the textbook at <http://bcs.wiley.com/he-bcs/Books?action=index&itemId=0470128666&bcsId=4460>

Note: If you have access to the 7<sup>th</sup> edition (while it is no longer available directly from Wiley, it is still available from 3<sup>rd</sup>-party sellers such as Amazon) you may use it, but you will have to carefully check any problems assigned from the text.

**Course Objectives:**

- To develop basic statistical analysis skills, including the calculation of summary statistics, propagation of error and confidence intervals
- To develop an understanding of methods for comparing means (t-test) and variances (F-test)
- To gain an understanding of the calibration process, including selection of a model, calculation of experimental parameters from measured values, evaluation of the fitness of the model using an analysis of variance (ANOVA) approach, and application of the model to the analysis of unknowns, including the calculation of the appropriate confidence intervals of predicted values
- To gain an understanding of basic experimental design, specifically factorial and fractional factorial approaches
- To gain an understanding of experimental optimization methodology, particularly steepest ascent and simplex methods
- To gain a proficiency with Microsoft Excel and other freeware packages to solve basic statistical problems

**Topic Outline:**

Basic Statistics  
measures of central tendency  
measures of dispersion  
confidence intervals  
pooling of standard deviations  
treatment of outliers  
means testing

Chapter 2

variance testing	
Error Analysis	
propagation of error	
Regression Analysis	Chapter 10
derivation of normal equations	
regression analysis tables (analysis of variance of regression)	
treatment of outliers	
use of regression lines	
prediction	
discrimination	
confidence intervals	
sensitivity	
detection limits	
Analysis of Variance	Chapter 3
one-way designs	
two-way designs	
Experimental Design Methods	Chapter 5
factorial designs	Chapter 6-7
fractional factorial designs	Chapter 8
central composite designs	
Three-level and mixed-level designs	Chapter 9
Optimization Methods	Chapter 11
steepest ascent methods	
simplex optimization	
genetic algorithms	

**Proposed Schedule:**

May 5	<b>EXAM I</b> (possibly including take-home section)
May 26	No class, Memorial Day Holiday
Finals week	<b>EXAM II</b> (possibly including take-home section)

**Course Grading:**

Mid-term exam	35%
Final exam	40%
Problem sets (several of which will total)	25%

**Additional Texts of Interest:**

John R. Taylor, An Introduction to Error Analysis: The Studies of Uncertainties in Physical Measurements, 2<sup>nd</sup> edition, Mill Valley, CA: University Science Books, 1997, paperback ISBN-13: 978-0-935702-75-0.

Norman Draper, Harry Smith, Applied Regression Analysis, 3<sup>rd</sup> ed., New York: John Wiley & Sons, Inc., 1998, ISBN-10: 0-471-17082-8.

- David G. Kleinbaum, Lawrence L. Kupper, Applied Regression Analysis and Other Multivariable Methods, 3<sup>rd</sup> edition, North Scituate, MA: Duxbury Press, 1997, ISBN-10: 0534209106.
- George E.P. Box, J. Stuart Hunter, William G. Hunter, Statistics for Experimenters: Design, Innovation and Discovery, 2<sup>nd</sup> ed., New York: John Wiley & Sons, 2005, ISBN-10: 0-471-71813-0.
- Charles K. Bayne, Ira B. Rubin, Practical Experimental Designs and Optimization Methods for Chemists, Deerfield Beach, FL: VCH Publishers, Inc., 1986, ISBN-10: 0895731363, (currently out of print).
- William J. Diamond, Practical Experimental Designs for Engineers and Scientists, 3<sup>rd</sup> edition, New York: John Wiley & Sons, 2001, paperback ISBN-10: 0471390542.
- Joseph Adler, R In a Nutshell: A Desktop Quick Reference, Sebastopol, CA: O'Reilly Media, Inc., 2010, ISBN-13: 978-0-596-80170-0.
- Paul Teetor, R Cookbook, Sebastopol, CA: O'Reilly Media, Inc., 2011, ISBN-13: 978-0-596-80915-7.

## Recorded Lectures

The lectures for this class will be recorded; the screencasts will be made available on the *Lecture Archive* page available on the course homepage on Bb Learn. Every effort will be made to have the screencasts posted within 48 hours of the class. They will be available in both Shockwave (Flash) and zipped Ipad (\*.m4v) format. In some cases additional material will be assigned as recorded lectures only. You are responsible for the material presented in those lectures as well.

## Microsoft Office Availability

Unfortunately, the university decided approximately a year and a half ago to discontinue the student license for Microsoft Office products as a cost-saving measure. This affects you if you downloaded and installed your copy of MS Office from the Drexel software server; if you purchased your own copy of Office when you purchased your computer you are *not* affected by this situation. This creates a problem in that we have extensively used Excel for problem solving and data analysis in CHEM789; in particular we use many of the tools in Excel's Data Analysis Toolpack Add-on that do not have good replacements in either Calc (as part of Open Office) or Spreadsheets (as part of Google Docs). After a good deal of hunting I have found an alternative freeware spreadsheet program named Gnumeric that in my opinion has better statistical analysis tools than those in Excel's Data Analysis Toolpack. You should download the software (the current version is 1.12.9) from <http://projects.gnome.org/gnumeric/>. The on-line User's Manual for the program can be found at <http://projects.gnome.org/gnumeric/doc/gnumeric.shtml>. Another package that is highly recommended is R (see <http://www.r-project.org/>), an amazingly complete (and free) statistical analysis environment. An overview can be found at <http://www.r-project.org/about.html> (the current version is 3.0.2). It is a "statistical analysis environment" much like Maple is a "mathematical computing environment" as opposed to a spreadsheet like Excel, Google Spreadsheet or Gnumeric. There are extensive on-line manuals at <http://cran.r-project.org/manuals.html>. I will provide further information about R in class.

*Note to Macintosh Users:* For some reason, Microsoft has decided *not* to include the Data Analysis Toolpack Add-on in the latest versions of Microsoft Office for the Macintosh. There is

a free alternative for the missing Add-on: StatPlus:mac LE offered by a company named AnalystSoft, Inc (see <http://www.analystsoft.com/en/products/statplumacle/> for details). The free LE version includes ANOVA and linear regression. The free edition can be upgraded to the regular version (student price of \$90 for a single license and \$199 for a 4-pack) which includes polynomial regression, amongst other tools. IF anyone finds other possible solutions for this Mac issue, please let me know.

## Bb Learn

We will be using Bb Learn 9, Drexel's on-line Course Management System, extensively to enhance communication in CHEM789. The instructions below tell you how to log on and begin using Bb Learn:

- 1) Login through DrexelOne at <http://one.drexel.edu>.
- 2) Enter your Drexel domain ID and password, click on **Login**.
- 3) Click on the **Students** Tab.
- 4) Click on the **My Courses** link.

or

- 1) Enter the Drexel Bb Learn website directly at <https://learn.dcollege.net/>.
- 2) Enter your Drexel domain ID and password, click on **OK**.

If you enter these correctly you will now be on your Bb Learn dashboard. Select **CHEM789 Statistics & Experimental Design** from the list of courses in the center pane of the screen under the heading **My Courses**. You will now be on the course homepage. Please note that **ALL** of your homework assignments will be posted as assignments on the homepage. The *Announcements* page will be used for assignment and exam reminders, etc.

## Communication

It is assumed that all students have a Drexel computer account for email and easy access to the Internet and to the Drexel University network.

## Academic Integrity

As you are working towards becoming a chemical professional, you are expected to maintain the highest degree of integrity in your work, as reflected by the Ethical & Professional Guidelines as published by the American Chemical Society (available at the ACS website under Careers, Professional Development, Ethics and Professional Guidelines). Your efforts as a student here at Drexel are covered by the academic dishonesty policy found at [http://www.drexel.edu/provost/policies/academic\\_dishonesty.asp](http://www.drexel.edu/provost/policies/academic_dishonesty.asp).

## Course Drop/Withdrawal

Courses may only be dropped during the "drop period" lasting from the beginning of the enrollment period through the end of the second week of the quarter. Dropping a course results in the course being removed from the student's academic record without a "W" appearing on the transcript; i.e., neither the course nor the grade of "W" appears on the student's transcript. Students may withdraw from a course during the "withdrawal period" lasting from the beginning of the third week through the end of the seventh week of the quarter. Withdrawing from a course

causes both the name of the course and the grade of “W” to appear on the student’s transcript. Before withdrawing from a course, students should consult with the instructor. You should consult the information found on the Provost’s office website [http://www.drexel.edu/provost/policies/academic\\_transactions.asp](http://www.drexel.edu/provost/policies/academic_transactions.asp) for complete details.

### **Disability Services**

Students with disabilities who wish to request accommodations and services at Drexel University need to present a current accommodation verification letter (“AVL”) to the instructor before accommodations can be made. AVL's are issued by the Office of Disability Resources, which is based in the Office of Equality & Diversity (see <http://www.drexel.edu/oed/disabilityResources/> ).

### **Syllabus Modification**

I reserve the right to modify the syllabus, including the course schedule and list of topics, at anytime during the course. I will announce any changes both in lecture and by posting on Bb Learn.

Rev 3/29/14 kgo