CHEM 454L – Chemometrics
Class Syllabus
Dr. Grady Hanrahan

Instructor: Dr. Grady Hanrahan, Phone (323) 343-2365
Email: ghanrah@calstatela.edu

Office Hours: P.S. 807 M, W, F 10:30am-12:00pm or by appointment

Lecture: M, W, F 09:00-10:10 am, BIOS 246

Course Description & Objectives:

CHEM 454L - *Chemometrics* will offer a more practical training experience for students compared to traditional statistical method courses. An array of powerful chemometric techniques for experimental design and data analysis will be covered, ultimately providing students with modern analytical training.

The purpose of this course is to train students in chemometric methods for optimizing experimental design, data processing, calibration and quality control.

Upon completion of this course, students will be able to:

1. Apply basic statistical methods to their independent research efforts;
2. Perform advanced chemometric analysis on large data sets;
3. Apply the knowledge learned to all scientific data analyses during their studies and future career-related activities.

Prerequisites:

CHEM 201, MATH 206 and PHYS 103.

Required Textbook:

Chemometrics: Statistics and Computer Applications in Analytical Chemistry, Matthias Otto, Wiley-VCH Publisher.

Lecture Style: PowerPoint slides, overheads, scientific papers and take home exercises. Both independent research (computer-based) and group learning will be offered to compliment the classroom lectures.

Lecture Schedule: CHEM 454L - Spring 2005

Dates	Subject	Chapter(s)
Week 1	Class Introduction, Descriptive Statistics, Excel Exercises	Chapters 1 & 2
Week 2	Signal Processing and Time-Series Analysis Excel Exercises	Chapter 3
Weeks 3-4	Principles of Experimental Design & Optimization Excel Exercises	Chapter 4, Handouts
Week 5	Factorial Designs and Analysis	Chapter 4, Handouts
Week 6	Fractional Factorial Designs and Analysis, Sequential Analysis, Excel Exercises	Chapter 4, Handouts
	MIDTERM EXAM April 29	
Week 7	Univariate Calibration & Least Squares Excel Exercises	Chapter 6, Handouts
Week 8	Linear –vs- Multivariate Regression	Chapter 6
Week 9	Principal Component Regression Partial Least Squares Regression	Chapter 6, Handouts
Week 10	Quality Assurance and Good Lab Practice	Chapter 9
Week 11	**FINAL PROJECT DUE – June 6th, 8:00 am**	

***** Note: Dates subject to change (except for the Midterm and Final Project)**

Point Distributions for Grades

Lecture: 1 x 100 point Midterm Exam
10 x 20 point quizzes (lowest dropped) = 180 points
5 x 10 point Excel Exercises
20 points - Class participation
Final Project - 200 points

Total = 550 points

Grades will be assigned as traditional (A, B, C, D, & F) and based on points accumulated. However, class attendance, distribution of points and individual participation will be taken into consideration on final grades (+ and – considered). To pass this course, students must complete all assigned work. Students will receive an (F) if all work is not completed (unless a documented excuse, e.g., medical).

Final Project

There will be two separate research projects available: 1) Experimental Design or 2) Multivariate Data Analysis. Students who are performing research in individual laboratories are encouraged to use multivariate analysis on their data. You will use the various multivariate techniques learned to analyze your data. Those students who do not have research data will design and optimize an experiment using the techniques learned in the classroom and Excel exercises. Students with research data may also do the Experimental Design in collaboration with the Multivariate Analysis to better optimize their experimental conditions. Project guidelines and expectations will be covered extensively during the 6-7th week by your instructor.

For the project, a formal, typed-written report must be handed in during finals week. This report must follow the format below. Reports must be a concise description of the experiment/data analysis with all appropriate data and graphs. The format includes (in order):

1. Cover page with title of experiment, name and date.
2. Abstract
3. Introduction
4. Experimental procedures
5. Results, including data and relevant graphs
6. Conclusion
7. References
8. Acknowledgments

Dropping the course/Incompletes

Hopefully, a student will not be dropping this course. However, in the event that this is necessary the student must meet all university rules and deadlines. In the case of an incomplete, the student must be making a (C) in the course and the reason for the incomplete an illness or an accident. An INCOMPLETE GRADE REPORT form must be completed and given to the instructor by the end of the examination week.

Formal Report Sections – Detailed Description

Abstract

A concise summary of the work performed and contains the key results. No introduction or background material should be placed here.

Introduction

Here one states the aim, the historical and theoretical context of the work. Include any relevant chemical equations or reactions. Should be concise, but have enough information for a complete introduction.

Experimental Procedures

This section is used for describing experimental procedures, conditions, apparatus and reagents used in the experiment.

Results

The data obtained in the experimental section is either tabulated and/or graphically displayed. Results from these data are calculated in this section. Show all data and calculations used.

Conclusion

This section contains a critical evaluation of the data gathered and the errors inherent in them. Be specific and thorough in your narrative.

References

Throughout the body of the manuscript, statements used which derive from external sources require defense based on previous work. These statements must be denoted

numerically either with a superscript or in parenthesis in the text, and then the source listed in the Reference section by that number.

For example:

1. J. Peabody and H. Originales, "The Behavior of Copper Ions in Aqueous Solution." Journal of Analytical Results, **21**, 345-350.

-where **21** is the journal volume and 345-350 are the page numbers.

Acknowledgments

All assistance, funds and gifts should be acknowledged as a matter of courtesy. For example, financial support and scholarships, laboratory assistance, etc…should be stated.