CHEMICAL ENGINEERING 621
(CHE 621)
Model Building and Response Surface Methodology

Term F22

Instructor
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For 'live' meetings: **Please set up via e-mail message**

Please prefer to e-mail me directly and via regular e-mail (see above). I am very responsive to e-mails (9:00 am to 9:00 pm), unless I am lecturing or tied up in long meetings. I will certainly respond within 24 hours or earlier.

Grading

Assignments	45%
Mid-term	10% 'take-home' style
Final	45% 'take-home' style

See below for more details on course delivery.

Textbook

(a) D.C. Montgomery (2009). Design and Analysis of Experiments (8^{th}, 9^{th} or 10^{th} edition), Wiley: to complement lecture notes; the three editions are very similar

(b) Course Notes (to be posted on UW-LEARN a few days before each chapter is initiated, Ch 1 to 12; Ch 13-16 as special topics, in parallel, or as reading material); additional handouts (exercises, homework problems, other examples, etc.) may be distributed during lectures or posted via UW- LEARN; please check UW-LEARN (LEARN from now on) regularly for course-related announcements.

Teaching Assistant
Ms Bhoomi Mavani
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Email is preferred for immediate communication + appointments, etc.

For 'live' meetings: **Please set up via e-mail message**

More about the role of TA during the first week of lectures.

Lecture Schedule/Room **[first lecture on Thurs, Sept 8, 2022]**

Tuesday 12:30-2:00 pm E6-4022
Thursday 12:30-2:00 pm E6-4022
Last lecture on Tues, Dec 6, 2022

Note: Fall Reading week: Oct 8-16, 2022; no lectures.

Course Objectives

This is a ***quantitative course*** on Applied Stats, and more specifically on the design of experiments (DOE) and the related analysis of data sets. The course will discuss the role of statistical design of experiments (and subsequent data analysis) for process/recipe improvement and product development (modeling, process troubleshooting and steps towards optimization). Topics: Linear and non-linear regression situations. Given the need for an experimental investigation, determine an optimal experimental design (and alternative scenarios). Screening designs. Single and multifactor factorial designs (combined with regression and analysis of variance principles) in aid of process understanding and further process/product design. Empirical modelling and non-linear mechanistic models. Model-based designs. Data transformations. Response surface methodology for investigating process/product performance. Determining optimal conditions and designs.

Very few graduate curricula cover this (internationally)!

Assignment and homework problems, along with examples in notes/book (and other practice exercises/questions given in class during lectures) are important to understand principles and techniques. Numerical results are as important as the methodology/algorithms! Most of the chapters in the course notes are indeed **glorified (long) examples!**

Interactions between instructor/students and TA/students via e-mail are strongly encouraged (for addressing quick/simple questions and clarifications). If a question is longer, then individual/group meetings (over Teams or in-person) will be schedules via e-mail. If you have questions, the time to ask and clarify them is **during the course** and before the assignments (or other homework problems) are due!

Course Outline [Ch 1-12 will be covered in detail. Ch 13-16 are special complementary topics or simply reading material, depending on time and class appetite.]

General themes follow:

1. Ch 1, review, Statistical Background
   Quick review of a typical 2nd year Engineering/Science introductory Statistics course

2. Ch 2, review (70%; new 30%) Regression Analysis
   Linear regression with matrix calculus; analysis of variance and residuals; emphasis on regression diagnostics

3. Ch 3, review (reading material) Statistical Design of Experiments
   Overview of DOE

4. Ch 4, review, Design/Analysis of Single Factor Experiments
   Randomization; replication; multiple comparisons

5. Ch 5, review, Design/Analysis of Single Factor Experiments with Blocking
   Emphasis on blocking (variance reduction techniques); paired comparisons; multiple comparisons; special metrics

6. Ch 6, Multifactor Experiments (basis and main building blocks of DOE)
   Two-level full factorial experiments and related models

7. Ch 7, Multifactor Experiments (DOE)
   Two-level fractional factorials and screening designs

8. Ch 8, Non-Linear Regression and Model-Based Designs
   Non-linear regression; mechanistic models; model-based designs (alphabetical optimal designs, for both linear and non-linear model situations)

9. Ch 9, Response Surface Methods
   Response surface methodology; uses and basic background; central composite designs (CCD) and other designs; expansion of 2^k to 3^k designs; locating optimal operating points and conditions; occurrence and elucidation of ridge systems; exploration of maxima

10. Ch 10, Data Transformations
    Adequacy of estimation; Y-data transformations; Box-Cox family of transformations

11. Ch 11, Analysis of Undesigned (Happenstance) Data
    What to do and not to do, pitfalls, variance inflation factor and other diagnostics

12. Ch 12, Concluding Remarks
    What is next? More tips

13. Ch 13, Design/Analysis of Mixture Experiments (if time and appetite)
    Designing formulations and appropriate models

14. Ch 14, Evolutionary Operation (EVOP) (reading material)
    Towards (continuous) plant experimentation

15. Ch 15, Hierarchical (Nested) Designs (reading material)
    Designs and the related variance components

16. Ch 16, Multivariate Techniques (if time and appetite)
    Quick overview

Ch 9 is the culmination of the course. The first seven chapters (certainly Ch 1-5) represent review/overview material, or material that some people may be more familiar with, so they will be covered more quickly.

About a week per chapter above (some are reading material, some are shorter than others); references to book chapters and specific sections/subsections will be given during lectures; course material covered will be summarized/posted before mid-term and final exams.

Course Delivery Specifics

Lectures in the F22 term are expected to be in-person.

A CHE 621 'Team' has been generated, in case.

I will do my best to update you with concrete information either via e-mail or via LEARN.

Important points to remember: Do not panic; we will try to resolve issues, if any. Anything can be resolved, provided there is good/open/honest/ communication and good will. Even if you miss a lecture, you can resort to notes (chapters, etc.) posted on LEARN. Communicate with me well, and we will find a solution, for all reasonable requests.

All students will have access to course notes (posted chapters on LEARN). The notes read more or less like a book and slides have recently been annotated with extra explanatory comments. As you go through the notes/slides, check the 'bubbles' that appear. They contain extra explanations for the specific slide. Often, they also pose questions related to food-for-thought; this will help you to understand better the specific concepts or algorithmic steps described. All these will be complemented with additional postings (addenda per chapter) and/or other announcements on LEARN. If a slide is more or less blank/empty (and just poses a question or contains a brief statement), again it is related to either food-for-thought or something I will explain during a lecture.

If a slide is not clear, or if what I write on the white-board is not clear, you can always indicate it to me, and I can always post more explanations, especially when long equations are involved.

I am always willing to spend considerably more time on a course (than the usually allotted lecture time) in order to offer a better learning experience for all.

During the term, **feel free to discuss** with me possible experimental plans for your own research projects. That is the best way to apply course concepts to what you do. The best way is to do that before you embark on experiments without planning!

All students can arrange for meetings, online or in-person, if there are questions. We will see how things develop after the first week of the course.

Learning will be more inductive in the first part of the course (CH 1-5) and more deductive later. As I alluded to above, questions posed in the notes/slides help you to understand the material better (and, hence, check your knowledge). The same with simple exercises/examples/problems within a chapter. In all cases, I will be giving you a few days to a week (depending on the specific question/exercise/problem), for you to work on a question and try to arrive at an answer. We will always discuss the most important answers in class and/or I will also post an extra file, if needed.

Policy for Assignments and/or other Homework Problems (CHE 621 had 9 assignments, with problems designated towards assignments or mid-term exam (before the mid-point of the course), or final exam (after the mid-point of the course).

Assignment and other homework problems are the heart of the course, so you understand and clarify the different algorithmic steps. Problems are for general practice but also count towards assignment and exam contributions (i.e., towards the course grade components).

Consider the assignment and other homework problems to be sets of problems to be counted as assignments, **and also** towards the mid-term (ME) and final exam (FE) contributions. This will happen seamlessly during the course between the first and last lecture.

Let me give a representative example. Let's say that you are given Assignment 2 (A2) after course chapter 2 (CH 2) is completed. Let's say (hypothetically) that A2 consists of 4 problems. I may indicate that 3 problems will count towards grading, two towards A2 and one towards the mid-term exam (ME2). The 4th problem may only be for you as a 'practice' problem. Which problems count and for what contribution will be designated very clearly when A2 is posted on LEARN. That way you will be working in parallel to the course lectures **and 'building up' your final course mark. In essence, all homework problems (for assignments and exams) will be of the 'take home' type. Hence, you will be able to wrap up the course grading requirements by Dec 19, 2022, or earlier. In previous terms, grading requirements were complete by the date exams were supposed to begin (Dec 9, 2022, for F22).**

I (and/or the course TA) will explain very clearly (via LEARN announcements/messages to all in the class) how assignments are to be submitted, and related deadlines and/or other comments per assignment (Dropbox via LEARN, etc.).

You will have the option (your choice) to submit assignment and ME problems in groups of 3 (groups will be formed via LEARN), but FE problems will be submitted individually.

Assignments (and other homework problems) will be due at instructor-designated deadlines (almost every 10 days), usually after we complete a course chapter. Answers to practice exercises/questions/problems might be submitted via e-mail directly to me, via regular e-mail, and I would be getting back to you with comments. This will create a useful 'e-dialogue' between students and instructor/TA. All these options will be clarified accordingly, as we move along.

The submitted problems will be graded (by the TA or myself) and the mark will become available to you within 7-10 days (usually). This is for assignment and ME-designated problems. Submitted problem solutions should be legible, well organized and easy to follow (to be taken into account during grading). Late assignments *will not be accepted*, unless you have *notified me (NOT the TA!) in advance* before the due date (with a justification).

If a submission is late, a grade of zero will be assigned.

Note: Any homework related files (and/or mid-term and final exams or any other written documents for the course from students to instructor/TA) **will be deleted/destroyed towards the end of 2023.**

Mid-term Exam (ME)

Mid-term exam-designated problems will give you (and me) a chance to review the material and see where you are, i.e., whether you understand the basic concepts.

Date: N/A in F22 course offering; see section above; **Open book(s)/notes**. More details in class or via LEARN.

Re-examination requests for a missed mid-term exam (**with a legitimate** reason) will not be considered; rather, the mid-term weight will be transferred to the final exam weight. If the reason is not legitimate, a zero will be assigned.

Final Exam (FE)

Final exam-designated problems will give you (and me) a chance not only to review the covered material but also to practise typical data analysis and design of experiments situations. All data sets and scenarios will be coming from actual process examples.

Date: N/A in F22 course offering; see section above; **Open book(s)/notes**. More details in class or via LEARN.

Continuity of education plan and course contingency planning

- Every course outline for an in-person class has been designed with a plan that considers alternate arrangements for:
    - a short-term (e.g., one-week) cancellation of in-person classes, whether for the particular course or University-wide;
    - a longer-term cancellation of in-person meetings, whether for the particular course or University-wide;

- The basic guideline here is that, in case of unforeseen circumstances (course cancellations for different reasons, illness, self-isolation, etc.), we will try to be consistent with department/faculty/university-wide plans/decisions.
- We will also try to provide reasonable accommodation(s), as per department/faculty/ university guidelines.
- Hopefully, we will not have to make use of such alternate arrangements!

Fair Contingencies for Emergency Remote Teaching

The course outline presents the instructor's intentions for course assessments, their weights, and due dates in Fall 2022. As best as possible, we will keep to the specified assessments, weights, and dates. To provide contingency for unforeseen circumstances, the instructor reserves the right to modify course topics and/or assessments and/or weight and/or deadlines with due and fair notice to students. In the event of such challenges, the instructor will work with the Department/Faculty to find reasonable and fair solutions that respect rights and workloads of students, staff, and faculty.

Course Learning Outcomes (related to CEAB Graduate Attributes and course accreditation; see also Graduate Attributes Table below; numbers in brackets correspond to the numbered outcomes of the Table on Graduate Attributes below)

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

Estimate confidence and prediction intervals and construct ANOVA tables (variance decomposition) in both regression and design of experiments situations (1, 2)

Be fluent with advanced linear and non-linear regression situations (correlation, prediction, analysis of residuals, model comparisons, model diagnostic checks); metrics to describe parameter uncertainty (3, 4, 5)

Differentiate between design scenarios vs data analysis (randomization, replication, blocking) (6, 7, 8)

Basic tools of DOE: Design single factor experiments: data analysis, multiple comparisons, comparison-wise vs experiment-wise error, with and without blocking of (lurking) stochastic variables (3, 4, 5, 9)

Basic tools of DOE: Design multifactor experiments: emphasis on 2-level full and fractional factorial designs, assessing significance of factor and factor interaction effects, confounding of effects, benefits of orthogonal and rotatable designs, estimation of process error, selection of best design fraction, screening designs to generate process information (3, 4, 5, 9)

Address questions like: why apply experimental designs, what if experiments are not designed, what if experiments do not go as planned, what if results are unexpected, do data need transformations, empirical observations vs meaningful physico-chemical interpretations (6, 7, 8, 12)

Construct response surface methodology maps and implement central composite designs for locating optimal operating points and experimental conditions, understand and explore the 'geography' of maxima, understand prediction variance. Link empirical and mechanistic models, apply model-based designs, and implement data transformations. Question undesigned data, understand variance component parts, understand special extensions into plant experimentation, and tackle different design scenarios (3, 4, 5, 9)

Graduate Attributes

As defined by the Canadian Engineering Accreditation Board (CEAB), listed below as a reference:

Outcome	Definition
1. A knowledge base for engineering	Demonstrated competence in university level mathematics, natural sciences, engineering fundamentals, and specialized engineering knowledge appropriate to the program.
2. Problem analysis	An ability to use appropriate knowledge and skills to identify, formulate, analyze, and solve complex engineering problems in order to reach substantiated conclusions.

3. Investigation	An ability to conduct investigations of complex problems by methods that include appropriate experiments, analysis and interpretation of data, and synthesis of information in order to reach valid conclusions.
4. Design	An ability to design solutions for complex, open-ended engineering problems and to design systems, components or processes that meet specified needs with appropriate attention to health and safety risks, applicable standards, economic, environmental, cultural and societal considerations.
5. Use of engineering tools	An ability to create, select, apply, adapt, and extend appropriate techniques, resources, and modern engineering tools to a range of engineering activities, from simple to complex, with an understanding of the associated limitations.
6. Individual and team work	An ability to work effectively as a member and as a leader in teams, preferably in a multi-disciplinary setting.
7. Communication skills	An ability to communicate complex engineering concepts within the profession and with society at large. Such abilities include reading, writing, speaking and listening, and the ability to comprehend and write effective reports and design documentation, and to give and effectively respond to clear instructions.
8. Professionalism	An understanding of the roles and responsibilities of the professional engineer in society, especially the primary role of protection of the public and the public interest.
9. Impact of engineering on society and the environment	An ability to analyze social and environmental aspects of engineering activities. Such abilities include an understanding of the interactions that engineering has with the economic, social, health, safety, legal, and cultural aspects of society; the uncertainties in the prediction of such interactions; and the concepts of sustainable design and development and environmental stewardship.
10. Ethics and equity	An ability to apply professional ethics, accountability, and equity.
11. Economics and project management	An ability to appropriately incorporate economics and business practices including project, risk and change management into the practice of engineering, and to understand their limitations.
12. Life-long learning	An ability to identify and to address their own educational needs in a changing world to sufficiently maintain their competence and contribute to the advancement of knowledge.

Academic Offences and Plagiarism

The Senate of the University of Waterloo requires that all course descriptions contain material related to plagiarism and academic offences. The web link below describes relevant material, and you are asked to read this information carefully. If you have any questions, please ask your instructor.

http://uwaterloo.ca/secretariat/policies-procedures-guidelines/policy-71

Academic Integrity: In order to maintain a culture of academic integrity, members of the University of Waterloo community are expected to promote honesty, trust, fairness, respect and responsibility. [Check www.uwaterloo.ca/academicintegrity/

for more information.]

Grievance: A student who believes that a decision affecting some aspect of university life has been unfair or unreasonable may have grounds for initiating a grievance. Read Policy 70, Student Petitions and Grievances, Section 4,

https://uwaterloo.ca/secretariat/policies-procedures-guidelines/policy-70

When in doubt please be certain to contact the department's graduate administrative assistant who will provide further assistance.

Discipline: A student is expected to know what constitutes academic integrity [check www.uwaterloo.ca/academicintegrity/] to avoid committing an academic offence, and to assume responsibility for certain actions. A student who is unsure whether an action constitutes an offence, or who needs help in learning how to avoid offences (e.g., plagiarism, cheating, etc.), or about "rules" for group work/collaboration, should seek guidance from the course instructor, academic advisor, or the graduate/undergraduate Associate Chair or Associate Dean. For information on categories of offences and types of penalties, students should refer to Policy 71 (see link above).

Appeals: A decision made or penalty imposed under Policy 70 (Student Petitions and Grievances) (other than a petition) or Policy 71 (Student Discipline) may be appealed if there is ground for appeal. A student who believes that there is ground for appeal should refer to Policy 72 (Student Appeals)
https://uwaterloo.ca/secretariat/policies-procedures-guidelines/policy-72

AccessAbility Services: AccessAbility Services, https://uwaterloo.ca/accessability-services/ collaborate with all academic departments to arrange appropriate accommodations for students who need such services. If you require academic accommodations, please register with the office at the beginning of each academic term.

Anything else? We are here to help you! Talk to and clarify with the instructor as soon as possible! Ask questions before the due dates, not 5 minutes before the due date (or at mid-night)! Do not leave questions for the period after classes have ended! Now is the time!