# CHEM E 599 B: Current Topics In Chemical Engineering: Design of Experiments

## Course description

The main goal of this course is to provide students with sound and intelligible experimental design, and to supply the machinery for "unambiguous interpretation". This course focuses on developing a set of statistical tools to perform the design of experiments (DOE) with applications to chemical engineering and materials science. It provides sufficient background to design a suitable set of experiments (either computer simulations or laboratory experiments) to obtain evidence and validate a scientific hypothesis. We outline and discuss four aspects of DOE : a) Comparative – understanding whether changes to a variable (e.g.: composition) result in a change in a property (e.g.: structure). b) Screening – understanding an unknown process by sampling and ranking different factors of influence on a property/process. c) Modeling – representing a functional relationship using a mathematical model that can then later be used for predictions (e.g.: linear regression, response surfaces, etc). d) Optimizing – determine values of each design variable that optimize the property/process response

This course aims to provide a modern approach using machine learning to DOE tailored towards scientific discovery and understanding in general. This course covers both classical DOE (i.e. regression and sampling, random designs, factorial design, response surfaces, etc) and an introduction to the machine learning-based approach to DOE using techniques such as active learning. This course covers the computational and data analysis aspects of the DOE with an emphasis on writing computer programs for various data sampling methods, learning, and optimization. We use multiple case studies from open-sourced datasets to demonstrate the application of the four aspects of DOE mentioned above.

## Course location and schedule

Primary instructor contact: kiranvad@uw.edu, Benson Hall B14 (basement)
Schedule: Mon, Wed, Fri $01:30-02:20$ PM
Location: THO 334
Office hours: On request via Zoom or in the office (please send an email)

## Prerequisites

The course makes use of data science methods such as regression and classification. Students need to be familiar with programming in Python for assignments and course projects. We will cover the basics of multi-variate analysis and probabilistic modeling required to understand the course materials and successfully finish the projects. Courses in data science such as "MSE 477/542 and CHEM 441/541: Data Science and Materials Informatics" is a plus but not required.

## Books

There is no required textbook for this course. Detailed course notes will be provided as a PDF for each lecture along with references for further reading.

## Course objectives

To acquaint students with the basic principles of design of experiments and computational methods for accelerated material discovery and development.

## Topics covered in Lecture

- Module 1: Introduction to DOE and analysis
  - What is DOE: Objective, Variables, and Experiments
  - Review of basic statistics and probability
  - Measures of information and probability
- Module 2: Randomized block designs and classical DOE
  - Introduction to the grid and random sampling methods
  - Latin hypercube and sobol indices
  - Factorial design
  - Criteria-based and Space-filling design
- Module 3: Adaptive design, discovery, and optimization
  - Probabilistic modeling and Gaussian processes
  - Modern approaches to DOE: Introduction to active learning and Bayesian optimization

## Course evaluation (Percentage of total grade)

- Home works and assignments (two assignments $25\%$ each): This would require you to apply the methods discussed so far on simple design problems related to chemical engineering or material science. Total : $50\%$
- Final project: Implement a material discovery campaign on the computer, compare it with baselines and evaluate the results and write them in a report $45\%$
- In-class participation $5\%$