Choose Your Own Kinetics Adventure: Student-Designed Case Studies for Chemical Reaction Engineering Course Projects

Ashlee N. Ford Versypt
School of Chemical Engineering, Oklahoma State University

Abstract

This paper presents an innovative approach for a chemical reaction engineering course project. The project tasks students to conduct the preliminary design of a reactor or series of reactors to produce a chemical product of their choice. The constraints on this open-ended “choose your own project” are that the chosen process must involve a catalyst, multiple reactions, and heat transfer. The students must use published kinetics and physical property data from the literature, heat and mass balances, and software to complete their design. Students work in groups and write a report summarizing their findings. The activity connects course concepts to real world applications and requires students to design their own case studies through exploring the research and patent literature. These aspects engage students in topics they are interested in while simultaneously relieving the burden off of faculty for constructing new projects each course offering.

Introduction

Problem-based learning and laboratory experiments are common teaching methods for the undergraduate kinetics and reaction engineering courses in chemical engineering (Silverstein 2011). However, these approaches typically are concentrated on one course topic at a time. Most problems that can be found in the common reaction engineering textbooks, such as Folger’s text that is widely used in the field (Silverstein 2011), tend to focus on topics related only to isolated segments of the text. For example, a problem involving a catalytic rate law can only be found in the few chapters dealing explicitly with catalysis. Likewise, heat transfer problems are only found in the unit on heat transfer. Formulas are provided for how to calculate heat transfer for single or multiple reactions, yet very few examples or problems have simultaneous heat transfer and multiple reactions (Fogler 2011). This same limitation also often applies to laboratory experiments that need to be conducted within a few laboratory sessions safely, inexpensively, and without many variables changing simultaneously. In the real world, catalysis, multiple reactions, and heat transfer are likely to occur in concurrently. According to Falconer and Huvard (Falconer 1999),

1. Real processes involve multiple reactions with multiple heat effects.
2. Most industrial chemical reactions are exothermic and heat transfer is often the most important design criteria.
3. Most bioreactions can only be carried out within a narrow temperature range….
4. The largest number of different chemical reactions (but not the largest quantify of material) are run in batch reactors, which are common in the pharmaceutical, biotech, polymer, and cosmetics industries….
6. Continuous catalytic reactors are common in the petrochemical industries and, by far, the largest quantities of materials are produced in these types of reactors.

Project-based approaches have been utilized in chemical engineering to emphasize emerging technologies and to engage students in in-depth realistic projects such as multi-semester project sequences (Ragusa 2012) and industrially relevant case studies throughout the curriculum (Glassey 2013). These approaches are excellent but require significant coordination amongst several faculty and a lot of planning. Project reuse could become a major issue due to many students working on the same multi-year project. There is a need to reduce the workload for faculty while still providing complex, interesting problems for students to learn to deal with real-life challenges.

This paper details a course project assignment used for the past three years in the Oklahoma State University junior level course CHE 3123 Chemical Reaction Engineering that aims to fill the gap in realistic case studies while not being overly burdensome to faculty to create new detailed problem statements each year for course projects. The goals of the assignment are (1) to give the students more experience with real world problems beyond the scope of those typically included in undergraduate textbooks, (2) to connect major concepts from the course, and (3) to provide students with opportunities to explore industrial applications in areas of interest to them: e.g., traditional chemicals, fuels, food and beverages, pharmaceuticals, or biotechnology.

Methods

Choose your own kinetics adventure

The project assignment is modeled after “choose your own adventure” novels where different choices within a structured context lead to different experiences. In this context, the instructor provides the students with a project prompt and a set of constraints (the system must involve multiple reactions, catalysis, and heat transfer effects). The students must meet the project objectives while staying within the constraints, but they have freedom to make reasonable choices in topic selection and process design. A one-page preliminary report and a project update meeting with the professor before the final project is completed are used to assess that students are identifying their case study of interest, obeying the constraints, finding appropriate references, and not designing a process that is beyond the scope of the project (mass transfer effects are neglected for this project). These checkpoints can redirect projects with only minor deductions at the preliminary report stage. After the case study is selected and approved, the final report focuses on open-ended design of that case using the methodologies and software tools (Polymath) used in the course homework.

Six weeks are allocated for the course project. The preliminary report is due after three weeks. The update meeting between each group and the instructor must occur in weeks four or five. The meeting typically takes 15 minutes and is scheduled through a Google spreadsheet shared with the class online. The project is weighted as 6.5% of the course grade (65 points out of 1000 total). 10 points are allocated for the preliminary report, 5 points for the update meeting (each student earns this credit independently for attendance), and 50 points for the project report. The next subsections provide the prompt for the project and the requirements for the preliminary report and the final report. Supplemental information about citation style and final report formatting and general structure guidelines are provided to the students but are not shown here.

Prompt given to students at the start of the project

Your company wants to investigate the potential for developing a new product generated by a chemical reaction. They are trusting your team to choose the product and to conduct a preliminary study on the chemical kinetics and reaction engineering design. If promising, the company will later pursue economics and full process design involving all the other components of their existing chemical plant.

The purpose of the project is to give you experience putting together the various components in chemical reaction engineering. You will work in teams to study an industrial reaction system of your choice with reference to the scientific research literature. The system **MUST** involve multiple reactions, catalysis, and heat transfer effects. You will use Polymath to model the reaction system. You will summarize your findings in a written report.

Each group must the published literature for an industrial reaction system of interest to the group. This could be motivated by interest in specific industries or products. Example areas include biofuel production from enzymatic degradation of cellulosic feedstocks, catalytic membrane reactor for generation of hydrogen from carbon dioxide syngas, biopharmaceutical manufacturing of monoclonal antibodies, catalytic cracking of petrochemicals, or food chemistry involved in yeast fermentation of beer. The system must involve multiple reactions, catalysis, and non-isothermal effects. At least one reference must be included for the kinetics of the system chosen. For general literature searches, Web of Science is the recommended database, which can be accessed through the university library.

You will need to determine the best reactor conditions for your reaction system. You will use the chemical reaction engineering algorithm (Fogler 2011) and the design principles covered in the course to do so. You will use Polymath to solve the differential equations or system of algebraic equations for the amounts of each species, pressure drop, and temperature or heat duty within the reactor for the reaction system you are studying. All of the equations should be defined and shown in the final report. Output plots for important quantities such as concentrations, moles, or molar flow rates as functions of time or reactor volume or catalyst weight and others like pressure drop and temperature or heat duty should be generated and included in the results. You may also want to calculate and plot selectivity and yield. You should provide enough evidence with your Polymath simulations to support your decision to use a particular reactor and what conditions are best for operating your reaction system. You should describe the metrics you have used for “optimal” design in your final report and justify why these were chosen. You should also explore a variety of values for key input parameters and show the consequences of those parameters on your output metrics. You must submit your .pol Polymath codes and include your Polymath report and relevant plots in your final report.

All groups must have 3 or 4 team members. You are allowed to work in groups of your choosing. You are responsible for forming your own teams.

Preliminary report

The preliminary report is a one page (maximum) document submitted via the online class management system by one member of each group. The preliminary report is worth 15 points. The preliminary information is considered as a preplan for this project. It should be updated and included in the introduction of the final report. The preliminary report must include the following (point values listed in parenthesis):

- list of group members (1)
- very brief description of the reaction system (1) – this description can be similar to the phrases used in the examples listed above.
- motivation for studying this reaction system (1) – describe personal motivation for studying this system and at least one potential benefit for the company.
- at least two reactions to be considered in the reaction system (2) –list all of the chemical species involved in the reactions and show the reactions in A, B, C, D, etc. notation. These need not be all of the reactions that occur in the real system. Note that a multi-step catalytic reaction mechanism with one overall rate law (e.g., Michaelis-Mention, Monod, or Langmuir-Hinshelwood) counts as one reaction.
- information about the rate laws (2) – is a rate law known for a particular catalyst? Or will an expression from Ch. 9 or 10 of (Fogler 2011) be used for the rate law? Identify sources of data relevant to the rate laws for the system.
- information about the thermal properties of the reaction system (1) – are the reactions exothermic, endothermic, or both? Will the reactor be insulated or cooled/heated? The process may be isothermal, but in that case how will energy be added or removed to hold it constant?
- information about the type of reactor (1) – will a batch reactor, CSTR, PFR, PBR, membrane reactor, semibatch reactor, or some other reactor configuration be used and why?
- references (1) – include your reference(s). A required citation style is included in the assignment statement.

Final report

The final report for the project should follow the same formatting and general structure of the written final reports in CHE 4002 Unit Operations Laboratory with some modifications as listed below. Point breakdowns for the 50 points allocated to the final report are indicated in parenthesis. Grammar and formatting errors may be deducted from any relevant sections. The report must be submitted electronically via the class management system. No handwritten notes are allowed, and all equations must be typed. Label all of the following sections and subsections in the order listed.

1. Title Page (1) – course number, project title, project group number, group members, date
2. Executive Summary (3) – A 1/3-page, or less, statement that should contain the objective (1), results (2), and conclusions (3). The purpose is to succinctly convey why the project was done, what the objective was, what the result of the work was (values, evidence that it works, cautions related to assumptions), and what action the enterprise needs to take.

3. Introduction (4)
    a. Objective (1) – simple, clear, explicit, specific, statement of objective or deliverable (substantial redundancy with Item 2)
    b. Rationale (1) – statement of why the enterprise needs the deliverable and what issues about the situation might impact the work process or measures of quality of the deliverable (perhaps an elaboration on statements in Item 2)
    c. Overview (1) – summary of the reaction system, methods for modeling the reaction system, and the recommended reactor design. This should be updated from the preliminary report. List your chemical reactions and reaction rate laws here. Do not plug in numbers. Leave those as variables to be specified in the Data section below.
    d. Update Meeting Summary (1) – record when your group met with the instructor and any modifications you made to your plan as a result of that meeting.
4. Methods (15) – Organize your methods section into two subsections labeled as follows:
    a. Reaction System Design (7) – describe the procedures for sizing the reactor system, why the reactor conditions are appropriate for this application, and what metrics (such as selectivity, yield, safety, etc.) were considered and their definitions. If the reaction system involves determining a rate law from published kinetic data or determining the kinetics parameters in the Arrhenius equation, determine the data-dependent quantities and describe the methods for regression analysis. If the rate law and kinetic parameters were given in the literature, then make sure to acknowledge the sources.
    b. Chemical Reaction Engineering (CRE) Algorithm Modeling Using Polymath (8) – include typed version of all the equations following the CRE Algorithm applied to the reaction system and any additional equations needed to model the reactor in Polymath. Explain why these are appropriate for tje system. Number all equations as (1), (2), etc. on the right column. Polymath reports should be included in Appendix, and Polymath .pol file should be submitted on the class management system. All the variables must be are defined once with units.
5. Results (20)
    a. Data (5) – include any data and physical property values obtained or estimated from the literature with references. Rate law and kinetic parameters must be either estimated from data or obtained directly from a reference. Either way, citations are required. Other values such as initial or inlet concentrations and components, pressures, temperatures, flow rates, and other operating conditions should be given explicitly. Summarize these data in tables.
    b. Results (15) – description of reaction system design and Polymath results including figures and screenshots. Include results that correspond to all of the methods described in the methods section. Be clear on how the “optimal” design was selected, which means that comparisons between different cases must be shown and the best must be selected from among them.
6. Discussion (3) – describe quality issues and simulation results. Discuss results from Polymath, procedures, errors, idealizations. Compare results to expectations.
7. Conclusions (1) – describe the “bottom-line” finding – what should be done, how confident is the finding or recommendation, if the project were to be repeated what should be done differently.

8. References (3) – list of citations that acknowledge sources. You must follow the reference style for full credit. You must include all of the references mentioned in the text in the References section, and all references listed in the References section must be cited in the text. You must use the following format to refer to a reference in the text. "We obtained rate constant data from [1]." or "The rate law is [1]" followed by an equation.

Results

Course learning objectives covered in the project

The course project explicitly satisfies CHE 3123 course learning objective #9. Additionally, the project is designed to assess all of the CHE 3123 course learning objectives listed in Table 1, except #7.

Table 1: CHE 3123 course learning objectives

Engineering Technical and Science Skills
1. Identify, understand, and characterize the fundamentals of chemical reaction rate laws.
2. Size and model continuous and batch reactors (isothermal and non-isothermal).
3. Obtain a knowledge of reactor principles that will provide guidelines for the design of chemical reactors.
4. Model reactors involving multiple reactions, pressure drops, and changing stoichiometry (for gas reactions).
5. Understand the basic principles of catalysis and characterize simple catalytic reactions.
6. Analyze and interpret data from reactors for obtaining rate laws or design criteria.
7. Understand the basic principles of modeling non-ideal reactors.
8. Use computer packages (Polymath, Microsoft Excel, and Aspen) to solve reactor models.
9. Complete group project(s) involving the concepts of chemical kinetics and chemical reactor design.
Engineering Effectiveness and Professional Skills
10. Enhance team skills, particularly by working with other students.
11. Present written work that is logical, neat, well documented, guides the reader, fully qualified, and uses standard and good practice for graphical, equation, and data presentation.

Workload for the faculty instructor for the course project

With this project approach, there is very little set up involved in the course project. The dates are updated year to year in the project prompt, and the project is assigned at the appropriate time. Preliminary reports are fast to grade with deductions primarily for missing information or references for the rate laws or statements about the heat transfer modes that do not make sense. Students are penalized for exceeding the one page limit. A new Google spreadsheet is provided to the students for update meetings. There are typically about 20 groups in the CHE 3123 course. Within a two week period, those groups all have 10 – 20 minute meetings with the professor, requiring approximately 4 – 7 hours. Typically some groups will have questions about references from the literature or will be missing references. An introduction to using Web of Science with their topic combined with the keyword "kinetics" often yields good results. Final report grading is still a time-intensive process, but less so than for a project that has one set of reasonable answers. With each group potentially selecting different topics for their case studies, there is no feasible way for the instructor to generate "right" answers. Instead, the report is evaluated from a project manager's perspective. Each case study must be presented and referenced in an acceptable way. The data should be complete. The constraints of multiple reactions, catalysis, and heat transfer must be satisfied. The methods of the chemical reaction engineering algorithm must be followed (mole balances, rate laws, stoichiometry, energy balances, combine the equations, and numerically evaluate using the Polymath software). For insulated reactors, a calculation of the temperature change in the reactor is required. For isothermal reactors, the heat duty to be removed or added to the reactor by a heat exchanger is necessary. For other heat exchange modes, the reactor temperature, heat duty, and ambient temperature changes must be determined. Design decisions must be justified. Each mistake in the algorithm or in mathematics, physics, chemistry, or engineering principles receives a 1 point deduction.

Representative topics from student-designed case studies

To date, there have been exactly 60 student-designed case study projects over the three offerings of CHE 3123 taught by the author. The perennial most prevalent topic is fermentation of various alcohol beverages (beer, wine, sake, tequila, scotch, champagne have all been topics). Many college students have strong personal interests in alcohol, plus they find it amusing and engaging to study it for their course project. Making fermentation even more appealing, the CHE 3123 class tours a local craft beer brewery annually, and there is a great example of Monod fermentation kinetics in (Fogler 2011). The challenge in this case study is identifying multiple rate laws. To satisfy this constraint, students often refer to a kinetics study for the fermentation of apple wine from different sugars (Wang 2004) and treat the fermentation with at least two types of sugars simultaneously in the same batch reactor. The Haber process for synthesis of ammonia has also been studied by at least one group each year.

From experience, the topics of explosives, polymers, and chemical vapor deposition are strongly advised against. Explosives manufacturing has very limited legally accessible data before raising security concerns with the government. Polymeric density changes are not covered in (Fogler 2011), so the methods studied in the class are not sufficient for dealing with polymer production. Chemical vapor deposition has very complex kinetics and strong mass transfer contributions that are beyond the undergraduate course coverage of these aspects.

Student feedback and issues

Student feedback has been positive or neutral on using this type of project. Many students have given positive verbal comments about the fun of investigating a topic of their choice or about getting to learn more about a topic that they are interesting in that is not explicitly covered in the curriculum. Compared to other classes, fewer complaints were received since students recognized that they were responsible for choice of bad project topics or teammates.

A detailed grading rubric is given to students in advance. Those that follow the rubric carefully typically earn between 80 and 100% on the project with 85% being the approximate mean over the three project offerings. All projects have received at least a passing grade. The two weakest projects involved students who waited until the last minute with only one person working on the project while the other teammates completed a project for a concurrent course. One of these teams also completely ignored the instructor’s advice to simplify their problem involving chemical vapor deposition, which was certainly beyond the scope required for the project.

Having the in-person update meetings with the instructor and office hours have helped to keep the projects stay on track. Additionally, in the third offering, examples of old reports were provided in class for a mini-critique by student groups. The students were able to gain exposure to the application of the rubric and to practice evaluation and judgement of other student work. These examples were only available for a limited time as read only electronic files. The students were not informed in advance that the access would be temporary, so none tried to save the files. Identifying information and numerical values were redacted before distribution. No difference in project grade distribution was observed before and after showing these examples in class.

Conclusions

The course project assignment described here for the CHE 3123 Chemical Reaction Engineering course can easily be implemented in other chemical engineering programs in a similar course. The approach for student-designed case studies as real-world relevant course projects can be adapted into other engineering disciplines provided that there are clear constraints that can be established for the project that define the project scope and offer industrially relevant challenges. It is highly recommended to have a preliminary report and an update meeting with the instructor to provide low stakes early feedback to students in this type of project.

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Biographical Information

Dr. Ashlee N. Ford Versypt is an assistant professor in the School of Chemical Engineering at Oklahoma State University. She earned her Ph.D. and M.S. degrees in chemical engineering from the University of Illinois at Urbana-Champaign and her B.S. at the University of Oklahoma. She conducted postdoctoral research at the Massachusetts Institute of Technology. Her research focuses on developing computational models for systems biomedicine and pharmaceutics and using computing and reflection in the classroom. She teaches chemical reaction engineering, process controls, and an elective course on applied numerical computing for scientists and engineers.