

CE 561, Fall 2009 – Expectations and Ideas for Final Project

The project proposal is due in class on Wednesday, October 14, 2009.

A progress report on the project is due in class on Friday, November 20, 2009.

The final project is due by 5:00 p.m. on the last day of finals, Monday, December 21, 2009.

You may work individually or in teams of two or three. If you work in a team, you will submit a single proposal, progress report, and final report and each team member will receive the same grade. A project done by a team of two or three is expected to be proportionally more substantial than a project done by an individual.

Your final project should:

- (1) demonstrate your ability to research a topic and solve problems independently;
- (2) be written clearly for a target audience that has a background in chemical kinetics and reaction engineering;
- (3) be a substantial undertaking – I expect a final report of order ten pages (text) plus figures, calculations, computer programs used, etc. The report should include *your original work and ideas*, not just a literature review or compilation (though a literature review should be included);
- (4) be relevant to the subject matter of this course;
- (5) if possible, relate to your interests for thesis research or other research projects that you may undertake.

Example project ideas include:

- (1) Development or modification of a reactor design or reactor configuration for a real industrial process. For a topic like this, consider getting into the nuts and bolts of reactor design, like what material to make it out of, how to start it up, a control scheme, interactions with upstream and downstream processes, etc. You would probably want to include a patent search for related reactor designs and processes (both to get ideas and to avoid patent infringement).
- (2) Application of reaction engineering tools learned in this class to a novel problem – the Niagara river or your large intestine modeled as a plug flow reactor with axial mixing, for example. You could develop an analytical or a computer model of the system with a degree of detail appropriate to the complexity of the problem and the time you have to solve it. This would probably require a fairly broad literature survey, since important information might lie outside the chemistry and chemical engineering literature.
- (3) Development of a model of a real industrial reactor. Rather than designing a reactor, as in (1), get a detailed description of a real reactor (from the literature, patent applications, friends in industry, or whatever) and try to model it with sufficient detail (both in the chemical kinetics and transport) to make quantitative predictions of reactor performance over a range of conditions. This would presumably involve developing a computer code as well as researching the reactor design and reaction kinetics.
- (4) Find a paper in the literature in which overall kinetics are reported but either no mechanism is given or you do not believe the mechanism that is given. Propose a reaction mechanism and try to fit the data in the paper using known values for rate parameters, or chemically reasonable values where no known rate parameters are available. Analyze the sensitivity of

the predictions to various rate constants and see if the overall kinetic results can be used to fit any of the rate constants in your mechanism.

- (5) Study an individual reaction or a reaction mechanism in depth. Use appropriate reaction rate theories to interpret experimental data from the literature. See if there are theoretical estimates of the rate constant in the literature. Critically evaluate both theory and experiment to make recommendations for the rate parameters. Try to estimate error limits for your recommendations. Make your own theoretical estimates of rate parameters.

These are just a few suggestions to give you a flavor of the type of project that I am hoping to get from you. Many other kinds of project are acceptable, and you are encouraged to discuss any and all project ideas with me.

The project proposal and progress report

To reduce procrastination and to give me the opportunity to provide some feedback on your project ideas, I would like you to submit a 1-page project proposal early in the semester, and a 5 to 10 page progress report later in the semester.

The proposal is due in class on Oct. 14, as noted in the course schedule. It should include

- (1) a brief outline of what you propose to do
- (2) why you think it is an important and/or interesting problem
- (3) how it relates to the content of this course
- (4) results of any preliminary calculations and/or a preliminary literature survey indicating that what you propose is feasible

I will return a copy of these proposals to you with my comments. I will also keep a copy. The quality of this proposal and the degree to which you follow through with your plans will contribute to your final grade for the project.

The progress report is due in class on Nov. 20, as noted in the course schedule. It should include

- (1) a summary of what you have accomplished so far – including a literature survey
- (2) a summary of what remains to be done
- (3) a description of any changes in the scope of the project that will be required, relative to your original proposal
- (4) a timeline for completion of the project.

Again, I will return these to you with my comments, and the quality of this project report will contribute to the overall grade. This progress report, as the name implies, should show substantial **progress** toward completion of the project. By the time you submit this report, the bulk of the work should be done (i.e. literature surveys should be complete, any computer codes should be written and working, any designs should be drawn up, etc.).

Grading

Grading of a project like this is highly subjective. Please remember that the main goal of the project is that you learn about something that you find interesting and that is not covered in detail in this course. Getting a good grade is a secondary goal. Projects that meet the five expectations listed at the top of the previous page will get A's. Projects that narrowly fail to meet all of those expectations will get B's. Projects that fall far short of meeting those expectations will get appropriately lower grades.

Academic Integrity and Attribution of Credit

The contents of your project report must be in your own, original words. All sources must be properly cited. You should look at current journals in chemistry or chemical engineering to see common citation formats. Select a format and use it consistently. You may not copy complete sentences, phrases, or paragraphs from a book, journal article, web page, or elsewhere, unless you clearly indicate that it is a direct quotation (e.g. by putting it in quotation marks) and give proper credit to the source. In general, you should write the literature survey in your own words with references to all of the original sources upon which it is based. Because of problems that I have encountered in the past, I want to make this absolutely clear: ***If you submit a project report in which significant portions have been copied from another source, you will fail this course. Doing so constitutes plagiarism and will not be tolerated.***