Guidelines for the main 5.68J/10.652J Project, Spring 2008

1) By April 4, you must:
    a) Write a one-page outline proposing the project
    b) (Optionally) Find a partner to work with
    c) Meet with Prof. Green to discuss your proposed project, and get my advice and consent about the project.
2) By May 15, you must turn in your written report, containing:
    a) Motivation – why someone should care about the system you are studying and about your results
    b) Background Information on the system you are studying and the methodology you are using/proposing to use, including a brief summary of some relevant scientific literature with citations.
    c) Your results, probably including some tables and figures.
    d) Bibliography

    The report must total 20 pages or less, in legible 12 point type.
3) The week of May 13-15, you and your partner will make a 15-20 minute oral presentation on your project to the class, and answer questions.

Types of Projects:

1) Feasibility (including S/N) Analysis for a Proposed Kinetics Experiment.
2) Analysis of real experimental data (you'll have to arrange access to the data).
3) Computation of a Rate Constant, or Thermochemical or Transport Parameters for an individual molecule.
4) Estimation of how a rate constant will change with changes in its environment, e.g. solvent effects, pressure effects.
5) Construction / Analysis / Reduction of a many-step Kinetic Model.
6) Error/uncertainty analysis on an individual parameter, or on the predictions of a kinetic model.

Ideally, the project will connect to your research, and might ultimately lead to a journal publication. If you are not involved in research yet, you should try to partner with someone who has a real research problem.

Some example projects:

1) Develop a kinetic model for a gas phase process for producing CH_2O from CH_4 and O_2, using NO_2 as a catalyst, using literature rates and rate estimates.
2) Compute the thermochemistry of some radicals formed by abstracting H's from amines.
3) Design an experiment for detecting allyloxyl radical CH_2CHCH_2O and measuring its reaction rates, and compute the expected S/N.
4) Adapt literature models for ignition or polycyclic aromatic formation to predict what happens initially in a rapid compression machine or a diesel engine.