A First Course on Kinetics and Reaction Engineering

Unit 16. Lesson Plan

Before Class

- Provide the redacted slides and the handouts to the students and tell them to bring them to class
- The activity will involve calculations and least squares fitting that are most easily performed using a computer; either make arrangements so the students have access to whatever software they need/use for these activities or adapt the lesson plan so that they only set up the calculations but don't actually perform them

During Class

- Introduce today's topic and where it fits in the course (Slides 1 and 2)
- Review of Unit 16 (5 to 10 minutes)
  - Slides 3 and 4: go over the key concepts on the slides
- Ask whether the students have any questions from their pre-class preparation and answer them
  - Slide 5
- Learning Activity 16.1 (~20 minutes)
  - Slides 6 and 7: Show the students the problem statement and remind them how it was solved using the integral method of analysis. Note that sometimes you can't analytically integrate the differential equations, and sometimes when you can integrate them, you can't linearize them. In such cases numerical least squares can be used. As this example will show, numerical least squares also can be used when you can integrate and linearize.
  - Slide 8: Show them the steps they are going to take to solve the problem numerically; encourage them to try to compare and contrast with the previous solution. Have them work in teams or individually and tell them to write mole balances for every reactant and product with the rate expression substituted into the mole balances. Give them a few minutes to complete the task.
  - Slide 9: Make sure everyone got the mole balances correct, noting the sign. Tell them that if these equations are going to be solved numerically, they'll need to provide some information/data to the software. Tell them to list the things they will need to provide and give values for variables they'll provide and show the equations that will be provided in the form of code. Give them ~5 minutes to come up with an answer. (circulate as they work, answering questions, etc.)
  - Slide 10: Go over each of the things they need to provide: initial values, final t value, code to evaluate ODEs. Make sure that they understand what quantities will be available to their code (values of independent and dependent variables, set variable values and parameter values). Hold a brief discussion contrasting the amount of work they did to solve the ODEs compared to the integral method.

- Slide 11: Tell them that now they have code to solve the ODEs, they need to use the answer provided by that code to fit the model to the data using numerical least squares. Tell them to list the things they will need to provide and give values for variables they'll provide and show the equations that will be provided in the form of code. Give them ~5 minutes to come up with an answer. (circulate as they work, answering questions, etc.)
- Slide 12: Have them tell you what they listed and use this slide to summarize. As before, make sure that they understand what quantities will be available to their code. If possible, provide them with the MATLAB solution for this activity, or if you use different software, provide them with code that is set up for this problem and have them run the code and get the results. Discuss any numerical issues they encounter.
- Slide 13: Summarize the results and answer any questions

• Activity 16.2 (~20 minutes) This activity is structured just like the first, the difference is that the model involves a set of algebraic equations instead of differential equations. As you work through it, highlight differences associated with algebraic equations vs. ODEs
  - Slides 14 and 15: Show the problem, review previous solution via linearization, show the tasks they'll undertake in the numerical solution
  - Slide 16: Give them a few minutes to write three mole balance design equations.
  - Slide 17: Make sure everyone got the mole balances correct, noting the sign. Tell them that if these equations are going to be solved numerically, they'll need to provide some information/data to the software. Tell them to list the things they will need to provide and give values for variables they'll provide and show the equations that will be provided in the form of code. Give them ~5 minutes to come up with an answer. (circulate as they work, answering questions, etc.)
  - Slide 18: Go over the things they need to provide; highlight the need to provide a guess for the solution of the set of algebraic equations and how the experimental responses can be used to generate a guess.
  - Slide 19: Tell them that now they have code to solve the mole balances, they need to use the answer provided by that code to fit the model to the data using numerical least squares. Tell them to list the things they will need to provide and give values for variables they'll provide and show the equations that will be provided in the form of code. Give them ~5 minutes to come up with an answer. (circulate as they work, answering questions, etc.)
  - Slide 20: Have them tell you what they listed and use this slide to summarize. As before, make sure that they understand what quantities will be available to their code. If possible, provide them with the MATLAB solution for this activity, or if you use different software, provide them with code that is set up for this problem and have them run the code and get the results. Discuss any numerical issues they encounter.
  - Slide 21: Summarize the results and answer any questions

• Slide 22: Put the material covered in this class into the overall context of the course.

After Class

- Provide the complete slides to the students.
- Provide the MATLAB code to the students if they use MATLAB.

Variations and Options

- When they are given the code (Slides 12 and 20) assign part of the class to identify where each of the input items they listed are located in the code while others execute the code, then the second time around, have them switch roles. Briefly go over the code.