A First Course on Kinetics and Reaction Engineering

Unit 14. Lesson Plan

Before Class

- Provide the redacted slides and the handouts for Activity 14.1 to the students and tell them to bring them to class
- The activity will involve problem solving (particularly polynomial fitting and linear least squares); it would be best to make arrangements so the students have access to whatever software they need/use for these activities

During Class

- Introduce today's topic and where it fits in the course (Slides 1 and 2)
- Review of Unit 14 (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 14.1a (~15 minutes)
  - Slide 6: Read through the problem statement; point out that they will need to first calculate nA for each data point, ask if they have questions, then get them started. If you suspect that they won't be able to fit a polynomial, use the 2nd order fit as a demo and tell them to do the others. Circulate, observe, correct and answer questions as they work.
  - Slide 7: After ~10 minutes, discuss the results. Start by asking what the expected behavior for nA vs. t is (monotonically decreasing) and explain why (a single, isothermal reaction is not going to proceed for a while and then suddenly start going in reverse). Point out that the 5th order plot is very "curvy" because the polynomial order is too high, allowing overemphasis of the individual data points. Note the the 3rd order has a pronounced minimum, and since that is not expected, it should be rejected. Let them argue whether 2nd or 4th order is better and then use whichever they choose to calculate dnA/dt for each data point. Give them a few minutes to do so. (If many don't know how, show them the polynomial found by fitting the quadratic (see solution) and how to take its derivative)
- Learning Activity 14.1b (~15 minutes)
  - Slide 8: Read through the problem statement and point out that they already have nA vs. t. Tell them to get started and circulate as they work. The fact that there isn't an estimate for the first point (backward differences) or last point (forward differences) should become apparent to them; they may ask about it. In either case, make sure they see why
  - Slide 9: Ask what they are finding and whether it appears acceptable in light of the expectation already discussed (nA monotonically decreasing). Show how the central differences average out some of the noise (red highlighting), but not all

- Slide 10: Use the circled data points to show how the individual data points are being given too much weight, leading to the oscillations shown in the highlighted cells on the previous slide.

- Learning Activity 14.1c (~15 minutes)
  - Slide 11: Read through the slide and then let them get started. Tell them that the first thing they'll need to do is write the mole balance design equation. This should be straightforward, but at this point it may finally become clear to some what is meant by treating the derivative like an experimentally measured variable. Circulate as they work, answering questions, observing, correcting wrong impressions, resolving arguments, etc.
  - Slide 12: When most are done, go through the design equation development and make sure all see how it is a linear equation, then discuss the results. Point out that while the central differences did average out some of the noise, it wasn't enough. Point out that even the polynomial fit is not very good (r^2 is 0.85). In addition, there are systematic deviations in the model plot for the polynomial data. Allow them to draw conclusions that polynomial is better than finite differences when data are noisy, but beyond a certain point, noisy data lead to uncertain results no matter how the derivative is estimated. Best action here would to find a more accurate way to measure concentration and repeat the experiment.
- Slide 13: 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 solution to activity 14.1 and the MATLAB code to the students.