CE 329

Class 1 on Unit 1

Agenda

- Why are we here?
- About the course
  - About Dr. Lund
  - Primary learning resources
  - Topics that will be explored
  - Student learning outcomes
  - Course requirements
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  - Academic integrity
  - Accessibility resources
  - Professionalism
- Teaching and learning methods for the course
- Unit 1 review
- Questions
- Activity 1.1
  - MATLAB script for identifying independent reactions or equations
- What's up next

Why Are We Here?

- We are here so that I can help you learn about kinetics and reaction engineering
  - Learning is something done *by* students, not something done *to* them; teaching is helping students learn
  - You must *want to learn* and you must *make the effort* necessary to learn
  - I cannot learn for you and I cannot cause you to learn, but I can create an environment that is conducive to learning
- My roles
  - To help you to learn, i. e. I am your “coach” for learning kinetics and reaction engineering
    - Provide readings and videos to read/watch before class; these are the “lectures” for the course
      - online quiz due before the start of class as a prod
    - Provide in-class learning environment
      - review readings/videos, answer questions, conduct learning activities
    - Provide opportunities for practice and self-assessment
      - homework and practice exams
  - To assess how much you have learned and how well you have learned it
    - Selected homework assignments
    - MATLAB assignments
    - Exams
- Your grade will be based upon the effort you put forth as well as what you have learned

About the Course

- About Dr. Lund
  - B. S. Purdue (1976), Ph. D. Wisconsin (1981) both in chemical engineering
  - Exxon Research and Engineering 1981-1986
  - U. B 1986 - present
  - Expertise in heterogeneous catalysis, reaction pathways and kinetics, reaction engineering
  - Has taught CE 429/329 every time it has been offered since 1986 except 1998 - 2000
  - Die-hard Wisconsin Badger fan
- Primary learning resources for CE 329
  - UBLearns (https://ublearns.buffalo.edu)
    - Course Syllabus and Schedule are posted under Course Information
  - “A First Course on Kinetics and Reaction Engineering,” AFCoKaRE (http://wwwresearch.sens.buffalo.edu/karetext/title/title.shtml)
- Oh the things you will learn
  - About kinetics: the origin of rate expressions for chemical reactions, the generation of kinetics data and the analysis of those data for the purpose of assessing the adequacy of rate expressions. Rate expressions for systems involving combined transport and kinetics effects will be introduced
  - About reaction engineering: the design and modeling of ideal reactors involving multiple reactions and thermal effects will be studied for both steady state and transient operation. Augmented operation the ideal reactors will also be examined. Modeling of reactors that are not ideal will be introduced.

- Student learning outcomes
  - Design experiments to generate kinetics data using any of the three ideal reactor types, perform tests to ensure the ideal reactor model assumptions are obeyed and utilize the resulting experimental data to generate an acceptable rate expression for a chemical reaction (CBE Student Outcomes a, b, e and k)
  - Postulate a mathematical form for a rate expression empirically or on the basis of the theory of chemical reactions (CBE Student Outcomes a and e)
  - Qualitatively analyze the effect of operating parameters upon the final or outlet properties of a fluid that is reacting in one of the three ideal types of reactor (CBE Student Outcomes e and k)
  - Construct accurate analytical models of systems of one or more ideal or augmented reactors and use those models for the design, simulation or optimization of a reactor process (CBE Student Outcomes a, c, e and k)
  - Describe and formulate alternatives to the ideal reactor models (CBE Student Outcome e)
  - Analyze simple systems where chemical and physical kinetics are coupled (CBE Student Outcomes a, e and k)
- Course requirements
  - 38 online quizzes
  - 39 in-class worksheets
  - 5 MATLAB files for solution of in-class problems
  - 32 homework problems
  - 32 corrections to homework problems
  - 3 mid-term exams
  - 1 comprehensive final exam

- Grading (see syllabus for more details)
  - Course score
    - Online pre-class quizzes (5%)
    - In-class worksheets (5%)
    - Homework effort (5%)
    - Homework corrections (5%)
    - Homework accuracy; five assignments selected at random (10%)
    - MATLAB assignments (10%)
    - Three mid-term and one final exam (15% each)
  - Course grades
    - Students earning 90% or more of the maximum possible total score will earn an A
    - Students earning 80% or more of the maximum possible total score will earn a B
    - Students earning 70% or more of the maximum possible total score will earn a C
    - Students earning 60% or more of the maximum possible total score will earn a D
    - In no case will the grade cutoffs be higher than those listed above; they may need to be decreased to account for unexpected difficulty of exams or other factors
  - First violation of the policy on academic integrity will result in lowering of the student's final grade by one full letter
  - Two violations of the policy on academic integrity will result in a grade of F
  - A grade of I (incomplete) will only be given if
    - student's work to date is satisfactory
    - student has a legitimate inability to complete the course requirements within the semester
- U. B. policy on academic integrity - http://academicintegrity.buffalo.edu/

- Accessibility resources
  - office 25 Capen
  - phone: (716) 645-2608
  - email: stu-accessibility@buffalo.edu
  - Please inform Dr. Lund as soon as possible about your needs to allow coordination of your accommodations.
- Act like professionals
  - In all correspondence
  - In the classroom
  - In posts on the discussion forums on UBLearns

Teaching and Learning Methods for the Course

- This course is taught as a “flipped classroom”
  - Presentation of information (lectures and reading) occurs outside of class
  - Class time is used for active learning
  - Felder, R., Chem. Eng. Education 25(3), 132-133 (1991)
    - The fact is that what routinely goes on in most college classes is not teaching and learning, but stenography: professor transcribes notes from notebook to chalkboard, students transcribe from chalkboard back to notebook. Even if the notes are supplemented with all sorts of insightful commentary, research shows that students in lectures generally retain a reasonable percentage only of what they hear in the first ten minutes and relatively little of anything that happens thereafter. They really only learn by thinking and doing, not watching and listening.
- Your expected workflows as CE 329 students
  - Before Class Meets
    - Complete assigned readings and videos, write down any questions you have
    - Complete the online quiz for that class meeting
  - During Class
    - Ask any questions that you have from your pre-class completion of the assigned units
    - Participate in learning activities
      - Ask questions whenever something is not clear
      - Help fellow students who are having difficulty with a particular point
      - Volunteer when called upon to participate

- Your expected workflows as CE 329 students (continued)
  - After Class Ends
    - Make sure you can fulfill the learning objectives listed in the AFCoKaRE Unit
    - Work on homework assignments
      - Complete and submit the next solution that is due
      - Correct the most recently submitted solution and submit your corrections
  - Homework
    - Start work on the assignment the same day that the unit was considered in class
      - Set up solution to each problem
      - If you get stuck or something is unclear, seek help
        - office hours
        - UBLearns discussion forum
    - Complete and submit the assignment by the assigned day and time
      - Immediately after it is due, the solution will be posted
    - As soon as possible after the solution is posted, go through your solution and identify all mistakes
      - show how to correct them, making sure you understand why your solution was in error and why the posted solution is correct
    - Complete and submit your corrected solution by the assigned day and time
- Treat CE 329 homework as a learning and self-assessment tool, not as a course assessment tool
  - Download the AFCoKaRE Exam Info handout
  - When you solve problems in class and on assignments try to do so referring ***only*** to that handout; it is the same information you will be provided on exams

Reasons for Using the Flipped Classroom Method

- To make learning ***easier*** and more ***efficient*** and to foster ***deeper understanding***
- When do you learn?
  - Not much during a lecture
  - *You learn when* you attempt to solve a problem, without following the solution to a similar problem, and *you get stuck*
    - You already have learned the things before the point where you got stuck
    - "Getting stuck" reveals concepts and subtleties that you do not fully understand
- With the approach used in this class, you encounter the things you don't fully understand in the classroom where there is an expert ready to help you fill in the missing understanding
  - Not late at night, right before an exam or assignment due date
  - Not alone or with equally uncertain peers as your only source of help
- ***But it only works***, or at least it works much better, ***if you follow the workflow I've laid out***
  - If you come to class without having done the readings and watched the videos, the effectiveness of the approach becomes more like the traditional way of teaching and learning
  - If you don't participate in the classroom activities, you again end up trying to figure things out by yourself or with the help of equally confused classmates

Where We've Been

- Part I - Chemical Reactions
    - 1. Stoichiometry and Reaction Progress
    - 2. Reaction Thermochemistry
    - 3. Reaction Equilibrium
- Part II - Chemical Reaction Kinetics
- Part III - Chemical Reaction Engineering
- Part IV - Non-Ideal Reactions and Reactors

Unit 1 Summary/Review

- Fields that Involve Chemical Reactions
  - Kinetics – field of science concerned with understanding and modeling the rates of chemical reactions
    - The resulting model is called the rate equation or rate expression
  - Reaction Engineering – branch of chemical engineering concerned with understanding and modeling chemical reactors
    - Reaction engineering models are called design equations and are comprised of mole balances, an energy balance and a momentum balance
    - Rate expressions (kinetics models) appear within the design equations (reaction engineering models)
  - Reaction Thermodynamics includes equilibrium analysis and energy changes associated with reactions
- Chemical Reactions
  - Involve bond breaking and forming among reactants and products
    - No atoms gained or lost so reaction must be "balanced"
  - Written similar to mathematical equations except arrows instead of equals sign
    - Use the symbol $\nu_{i,j}$ to denote the stoichiometric coefficient of species i in reaction j
      - If i is a reactant, $\nu_{i,j} < 0$
      - If i is a product, $\nu_{i,j} > 0$
  - Some biological phenomena, including cell growth and enzyme-catalyzed reactions, can be treated in a manner analogous to chemical reactions
    - Nomenclature can be different
    - Cell growth doesn't have a fixed stoichiometry; use an effective stoichiometry

Characterizing How Far a Reaction has Gone (Reaction Progress)

- Extensive and Intensive Variables
- Reaction Progress Variables
  - Single reaction: extent, conversion, etc.

$$\xi_j = \frac{\left(n_i - n_i^0\right)}{\nu_{i,j}} \qquad f_i = \frac{n_i^0 - n_i}{n_i^0}$$

  - Multiple reactions: extent, yield, selectivity, etc.

$$n_i = n_i^0 + \sum_{j=1}^{N_{ind}} \nu_{i,j}\xi_j$$

    - Complete mathematically independent sub-set of the reactions that are taking place
  - Reversible reactions: fraction of equilibrium conversion
- Limiting Reagent: the one that will run out first
- Mole Tables

Species	Initial Moles	Final Moles
i	n_i^0	$n_i^0 + \sum_{j=1}^{N_{ind}} \nu_{i,j}\xi_j$
⋮	⋮	⋮
Total	$\sum_{\text{all } i} n_i^0$	$\sum_{\text{all } i}\left(n_i^0 + \sum_{j=1}^{N_{ind}} \nu_{i,j}\xi_j\right)$

Questions?

Reaction Progress Learning Activity

Consider the reaction 4 NH_3 + 5 O_2 → 4 NO + 6 H_2O taking place in a closed, constant volume reactor (V = 1 L). At the start of the process, the reactor held one mole of NH_3 and 0.15 mole of O_2.

- To solve some problems in this course, you will need to write an expression for the concentration of O_2 in terms of the concentration of NH_3 and the initial composition of the system.
- To solve other problems (in Part I of the course) you will need to write expressions for the mole fractions of each of the four species (NH_3, O_2, NO and H_2O) in terms of the extent of the reaction and the initial composition of the system.
- To solve still other problems in this course, you will need to calculate the concentration of O_2, given the fractional conversion of NH_3 and the initial composition of the system.

Identifying Stoichiometry Problems

- To succeed, you need to be able to
  - Read a problem statement and analyze it to determine what type of problem it is
  - Know how to approach each particular problem (without reference to solved examples, etc.)
- Chemical reactions will be central to almost every type of problem in this course
  - As we progress through the course new problem types will be encountered
  - Each time this happens, the associated learning activities will provide some guidance on how to identify the new problem type and how to approach the solution of the problem
- Stoichiometry problems are introduced in Unit 1
  - Key features of typical reaction stoichiometry problems
    - The reactions taking place are known
    - The initial composition of the system is known
    - One or more quantities related to the final composition or the progress of the reactions taking place are known
    - The problem entails finding values or expressions for other, unknown quantities related to the final composition or the progress of reactions
  - Solving stoichiometry problems is sometimes a step within larger problems
    - Calculation of equilibrium compositions (Unit 3 of AFCoKaRE)
    - Analysis of kinetics data (Section C of Part II of AFCoKaRE)

General Approach to Stoichiometry Problems

- Identify a complete, mathematically independent sub-set of the reactions that are taking place (see Supplemental Unit S1)
- Construct a mole table (optional)
- Write the defining equations for each of the quantities given in the problem statement in terms of the extent(s) of the independent reactions
  - Most are defined in terms of moles, so write definition in terms of moles and then substitute expressions for final moles in terms of extents
- Solve for the extents of the independent reactions (as values or as expressions in terms of the given quantities)
- Write the defining equations for each quantity you are asked to find in terms of the extent(s) of the independent reactions
  - Again, most are defined in terms of moles, so write definition in terms of moles and then substitute expressions for final moles in terms of extents
  - Substitute the extents found above to obtain the requested quantities
- See the How-To files provided with Unit 1

Practice Applying the General Approach to Stoichiometry Problems

- Your group has been assigned one of the three problems for this activity
- Work through the general approach given on the previous slide, applying it to your problem
  - Do NOT refer to any solved examples from the readings or other sources
  - Don't bother to solve any of the equations that result
  - Just set the problem up
- If you get stuck, feel free to talk to other groups or to call me over to help you
- In a few minutes you will combine with other groups and explain your solution procedure to them

Mole Table

Consider the reaction 4 NH_3 + 5 O_2 → 4 NO + 6 H_2O taking place in a closed, constant volume reactor (V = 1 L). At the start of the process, the reactor held one mole of NH_3 and 0.15 mole of O_2.

Species	*Initial Moles*	*Final Moles*
NH_3	1	$1 - 4\xi$
O_2	0.15	$0.15 - 5\xi$
NO	0	4ξ
H_2O	0	6ξ
Total	1.15	$1.15 + \xi$

Solution to the First Problem

Consider the reaction 4 NH_3 + 5 O_2 → 4 NO + 6 H_2O taking place in a closed, constant volume reactor (V = 1 L). At the start of the process, the reactor held one mole of NH_3 and 0.15 mole of O_2. Write an expression for the concentration of O_2 in terms of the concentration of NH_3 and the initial composition of the system.

$$C_{NH_3} = \frac{n_{NH_3}}{V} = \frac{1-4\xi}{1} = 1-4\xi \quad \Rightarrow \quad \xi = \frac{1-C_{NH_3}}{4}$$

$$C_{O_2} = \frac{n_{O_2}}{V} = \frac{0.15-5\xi}{1} = 0.15-5\xi$$

$$C_{O_2} = 0.15 - 5\left(\frac{1-C_{NH_3}}{4}\right) = 0.15 - 1.25 + 1.25C_{NH_3} = 1.25C_{NH_3} - 1.1$$

Solution to the Second Problem

Consider the reaction 4 NH_3 + 5 O_2 → 4 NO + 6 H_2O taking place in a closed, constant volume reactor (V = 1 L). At the start of the process, the reactor held one mole of NH_3 and 0.15 mole of O_2. Write expressions for the mole fractions of each of the four species (NH_3, O_2, NO and H_2O) in terms of the extent of the reaction and the initial composition of the system.

$$y_{NH_3} = \frac{n_{NH_3}}{n_{total}} = \frac{1-4\xi}{1.15+\xi}$$

$$y_{O_2} = \frac{n_{O_2}}{n_{total}} = \frac{0.15-5\xi}{1.15+\xi}$$

$$y_{NO} = \frac{n_{NO}}{n_{total}} = \frac{4\xi}{1.15+\xi}$$

$$y_{H_2O} = \frac{n_{H_2O}}{n_{total}} = \frac{6\xi}{1.15+\xi}$$

Solution to the Third Problem

Consider the reaction 4 NH_3 + 5 O_2 → 4 NO + 6 H_2O taking place in a closed, constant volume reactor (V = 1 L). At the start of the process, the reactor held one mole of NH_3 and 0.15 mole of O_2. Calculate the concentration of O_2, given the fractional conversion of NH_3 and the initial composition of the system.

$$f_{NH_3} = \frac{n_{NH_3}^0 - n_{NH_3}}{n_{NH_3}^0} = \frac{1-(1-4\xi)}{1} = 4\xi \quad \Rightarrow \quad \xi = \frac{f_{NH_3}}{4}$$

$$C_{O_2} = \frac{n_{O_2}}{V} = \frac{0.15 - 5\xi}{1} = 0.15 - 5\xi$$

$$C_{O_2} = 0.15 - 5\left(\frac{f_{NH_3}}{4}\right) = 0.15 - 1.25 f_{NH_3}$$

What's Up Next

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