Course Outline and Outcomes

What is Chemical Engineering ?

You are majoring in Chemical Engineering and have been chosen to return to your high school and recruit the *best and the brightest* to follow in your footsteps. How would you explain your newfound profession and convey an idea regarding the types of tasks others may encounter in the ChE job market ?

- Explain the role of a ChE in "traditional" contexts
  - # Define and give examples of a process (or ChE process)
  - # Identify tasks a ChE would perform in a given industry / situation
- Explain the role of a ChE in emerging markets
  - # Distinguish between product and process design / analysis
  - # List the steps involved in product design
- Identify the tools used in process design / analysis
  - # Define the term balance equation and give examples of things that might be balanced
  - # Describe the characteristics and purpose of a flowchart
  - # Identify a valid flowchart for a given process description

Engineering Calculations

In order to properly communicate with other engineers / scientists you must use the correct *language* .How can you use concise language to convey not only what you measured, but how precise the measurement was ?

- Explain the utility of the proper use of units
  - # Define and give examples of value, units, and dimensions in a given expression
  - # Convert from one set of units to another
  - # Identify an invalid equation, based on dimensional arguments
  - # Compare two quantities using a dimensionless group
- Correctly use scientific notation
  - # Write a value in scientific notation(using the correct number of significant digits)
  - # Determine the number of significant digits both in a given value as well as in the result of arithmetic

While measuring data is enormously useful you cannot possibly measure every possible bit of information under every possible condition(it would take too long and would be far too expensive).How can you use limited data to obtain *enough* information to get by ?

- Utilize curve - fitting or linear interpolation to estimate unmeasured data from measured data
- "Check" your results by order - of - magnitude estimation, back substitution, etc.

Process and State Variables

Describing and analyzing processes requires that you can understand, calculate, and manipulate both process data as well as state variables.

How would you calculate process variable *values* from *measurements* ?

- Manipulate process flow data
  - # Interconvert mass, volume, and moles(and their flows)
  - # Calculate mass(mole) fractions from mole(mass) fractions for a mixture
- Calculate pressures using a manometer(and explain the concept of gauge pressure)
- Interconvert between different temperature scales
- Explain the difference between intensive and extensive variables

Certain calculations require you to know quite a bit about the "state" of a material(i.e., its state of aggregation(phase), temperature, pressure, chemical composition, etc.).How can we quantify properties about a material 's state?

- Calculate State Variables U and H
  - # Define "state variable"
  - # Explain why one must choose a reference point when calculating state variables
  - # Generate "fictitious paths" from your reference state to your desired state
  - # Use heat capacities and phase data to calculate H and U from fictitious paths
- Use tabular data to determine U and H

Balance and Process Fundamentals

Balances are simple accounting procedures used to aid in the overall analysis of a process 's viability.

Exactly *how* ; a process is run, often determines much regarding what the balance equations will look like.What are some of the characteristics that a running process may have ?

- Characterize system operation
  - # Give original examples of(and identify) batch, semi - batch, continuous, steady, and transient processes
  - # Define open system, closed system, adiabatic, isothermal

What are quantities for which we can write balances ? Just like a checkbook, we can have inputs / deposits / credits and we can have outputs / withdrawals / debits.What are some of the *ways* in which these ins and outs can occur ? What happens if we put more in than we take out ?

- Explain the origin and physical meaning of each of the terms in the General Mass Balance Equation
- Write a General Energy Balance Equation
  - # Explain the origin and physical meaning of each of the terms in the General Energy Balance Equation
  - # Explain the difference between shaft work and flow work
  - # Simplify the appropriate form of the Energy Balance Equation

Now that we have written our balance equations, how can we concisely depict the information that we require to actually *do* the balance (or show our results after we have completed the balance) ?

- Draw and label a flowchart from a process description

Performing Non - Reactive Mass and Energy Balances

Now that we know *how* to write the equations that will get us started for balances, we need to worry about *when* they are useful.How do we know when to write these equations, or how many we need ?

- Perform single - unit mass balances
  # Perform a degree - of - freedom analysis for a single - unit mass balance process
  # Do the calculations suggested in the degree - of - freedom analysis

Real processes often include more than one process unit.How do we handle arbitrary numbers of units ? arbitrarily complex arrangements of those units ?

- Identify relevant sub - systems within a multi - unit process on which to perform a degree - of - freedom analysis(and subsequently do the required calculations)
- Perform mass balances(degree - of - freedom plus calculations) for systems with recycle, bypass, and purge streams

Energy balances can be used as an additional equation in mass balances.

- Simplify and solve the General Energy Balance for non - reactive systems

Performing Reactive Mass and Energy Balances

When reactions occur, material balances become more difficult, and energy balances are often more important.How do we handle generation and consumption of molecular species ? What if we don 't even *know* the stoichiometry ?

- Calculate quantities necessary for reaction / chemistry benchmarking
  # Calculate the limiting reactant, excess reactants, percent excess, and fractional conversion in a given reaction
  # Define and calculate the yield and selectivity for reaction networks
  # Define and calculate the "atom economy" of a process proposal
- Perform reactive mass balances(degree - of - freedom plus calculations)
  # Write extent - of - reaction expressions from stoichiometry
  # Utilize equilibrium expressions to determine equilibrium compositions and extents of reaction
  # Perform atomic species balances

What effect do reactions have on energy balances ? How do we handle fictitious paths of material that is generated or consumed ?

- Perform reactive energy balances
  # Explain how chemical reactions are handled in the General Energy Balance
  # Use Hess 's Law to determine the heat of reaction of given reactions

Thermodynamics

Thermodynamics can be used to make the number of necessary measurements smaller, or to make the *type* of measurement easier.

It turns out that *volumetric* flowrates are far easier to measure than mass or molar flows.How can we make use of this information ?

- Use single - phase thermodynamics to convert from volumetric flows to mass / molar flows
  - Determine the density of a mixture of liquids
  - Use the ideal gas law to determine P, V, or T of a single component
  - Determine the composition of a mixture of ideal gases from their partial pressures or volume fractions
  - Use one(or all) of the covered non - ideal equations(SRK, compressibility factor, van der Waals, virial equation) to determine P, V, or T
  - Use equations of state for mixtures of gases
- Use equations of state in material balances

When *multiple* phases are in equilibrium with each other, the problem becomes *constrained* .Can we use this information, along with Thermodynamics, to further reduce the number of necessary measurements ?

- Sketch a phase diagram and label relevant regions / points(solid, liquid, gas, critical point, etc.)
- Use Gibbs phase rule to determine how much information is necessary to specify the thermodynamic state of a system
- Explain the difference between the Gibbs phase rule and a Degrees - of - freedom analysis
- Perform vapor - liquid equilibrium(VLE) calculations
  - Estimate the vapor pressure of liquid components
  - Use ideal solution expressions to determine the composition of liquids and their corresponding vapors
  - Define and use K values, Raoult 's law, and relative volatility
  - Distinguish between when Henry 's Law and Raoult' s Law would be applicable
  - Use Txy or Pxy diagrams for non - ideal(and ideal) solutions
  - Explain the relationship between y - x, Txy, and Hxy diagrams
- Estimate the composition of liquids in equilibrium with solids
- Estimate the composition of immiscible liquids in equilibrium with each other(using either partition ratios or ternary phase diagrams)

Performing Multi - Phase Mass and Energy Balances

Using thermodynamics in mass / energy balance problems means that additional equations are available for solving the required unknowns.

How can VLE calculations be used in mass balance applications?

- Solve multi - component flash distillation problems
  - Derive and use the lever - arm rule
  - Explain and sketch the basic flash distillation process
  - Derive and plot the operating equation for a binary flash distillation on a y - x diagram
  - Solve both sequential and simultaneous binary flash distillation problems.Explain the difference between these types of problems
- Write and solve mass and energy balances for multi - stage distillation
  - Write the mass and energy balances and equilibrium expressions for any stage in a column

    - # Explain what constant molal overflow(CMO) is, and determine if it is valid in a given situation
    - # Determine the operating equations for CMO systems
    - # Calculate the feed quality and determine its effect on flowrates.Plot the feed line on a y - x diagram
    - # Determine the number of stages required to achieve a separation, using the Lewis method
    - # Determine the number of stages required to achieve a separation, using the McCabe - Thiele method
    - # Solve total and minimum reflux problems when CMO is valid
    - # Explain why multicomponent distillation is trial - and - error
    - # Make appropriate assumptions and make external mass balances for multicomponent distillation problems
- Perform gas - liquid(solubility) and liquid - liquid equilibrium mass balances
    - # Explain what absorption and stripping do and describe a complete gas treatment plant
    - # Use the McCabe - Thiele method to analyze absorption and stripping systems for both concentrated and dilute systems
    - # Solve both immiscible and partially miscible extraction problems

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