Final Exam: Friday, December 20, 9:00 - 11:30 p.m. 245 Olin Hall
Comprehensive - covers chapters 2 through 5, with emphasis on chapter 5: dimensional analysis and dynamic scaling.
Open book, open notes, open exercise solutions.
Bring a calculator and a ruler/straightedge.
Graphing calculators are okay. No laptops.

Office Hours before Final Exam …
# December 2019

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<td><strong>Phys 2213 9 a.m.</strong></td>
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End-of-Semester Self-Assessment of Design & Analysis Skills

Assignment: Complete the End-of-Semester Assessment posted at
https://stanforduniversity.qualtrics.com/jfe/form/SV_3KQO95VVf6or62p

To be completed individually, not as teams.

Will require about an hour to complete.

This is excellent review of your design and analysis strategies you developed this semester.

Must be completed by Friday, December 20 at 9 a.m.
EngrD 2190 – Chemical Process Design & Analysis

Course Summary and Review – Part 1

Mathematical Modeling
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<th>week</th>
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<td>8/30</td>
<td>course content, course objectives, and course organization. reading: chapter 1, pp. 1-7, chapter 2, pp. 8-19.</td>
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<td>Concept: process design - unit operations and process flowsheets. Context: green chemistry for hydrazine synthesis. reading: chapter 2, pp. 20-25.</td>
<td>CS 1 9/4, 9/6</td>
<td>problem redefinition, process analysis &amp; design by incremental evolution. exercises 2.45, 2.38, 2.40, 2.9, and 2.22.</td>
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<td>3</td>
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<td>Concept: process design - problem solving. Context: strategies for separation - purification of Br₂. reading: chapter 2, pp. 25-42. homework: exercises 2.5, 2.21, 2.28, 2.43, 2.50, and 2.52.</td>
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<td>3</td>
<td>9/11</td>
<td>Concept: process design - reactors for solid reactants and products; reactants in excess to simplify separations. Context: CH₄ from CO₂ and thermal energy, cont’d.</td>
<td>CS 2 9/11, 9/12</td>
<td>process analysis and process design by incremental evolution. exercises 2.34, 2.32, and 2.35.</td>
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Chemical engineers create processes and products based on chemical and biochemical change. Processes are divided into unit operations, represented by process flowsheets. How to create processes?
Course Objectives

*Overall*
To introduce basic principles of engineering design and analysis in the context of chemical and biomolecular engineering.

*Engineering Skills*
To design a chemical and biomolecular process by the following steps:
- define the *real* problem
- generate ideas.
- create a design.
- analyze the design.

Real Problem: Produce $P$.

Problem: Deliver Pure $A$ and Pure $B$ to a reactor.

To analyze a chemical and biomolecular process with three methods:
- mathematical modeling.
- graphical modeling.
- dimensional analysis & dynamic scaling
Reactant $A$ decomposes to $P$ (product) and $B$ (by-product).

$$A \rightarrow P + B$$

The molecular weight ratio of $P$ to $B$ is 7:3, so 10 kg of $A$ reacts to form 7 kg of $P$ and 3 kg of $B$. The reactor converts 40% of $A$. 

Mathematical Modeling
Which to build?
How to compare?
Mass flow rates
Energy flow rates
Asset flow rates
Hydrogen Fuel from Thermal Energy

Overall Reaction: \( \text{H}_2\text{O} \rightarrow \text{H}_2 + \frac{1}{2}\text{O}_2 \)
Manufacturing Human Tissue Plasminogen Activator (tPA)

Overall Reaction:  532 amino acids → tPA
Mass Balance at the Cellular Level

- CHO cell: $\text{CH}_{1.8}\text{N}_{0.2}\text{O}_{0.5}$
- tPA: $\text{CH}_{1.7}\text{N}_{0.26}\text{O}_{0.26}\text{S}_{0.05}$

Chemicals:
- Glucose
- Oxygen ($O_2$)
- Ammonia ($NH_3$)
- Water ($H_2O$)
- Carbon dioxide ($CO_2$)
Mass & Energy Balances for Space Travel
The Earth’s Carbon Cycle
The Earth’s Carbon Cycle

atmosphere

\[ M_1 = 612 \text{ Pg C} \]

- terrestrial biota
  \[ M_5 = 580 \text{ Pg C} \]
  \[ F_{15} = 100 \text{ Pg/yr} \]
  \[ F_{51} = 50 \text{ Pg/yr} \]

- soils & detritus
  \[ M_6 = 1500 \text{ Pg C} \]
  \[ F_{61} = 50 \text{ Pg/yr} \]
  \[ F_{56} = 50 \text{ Pg/yr} \]

- fossil fuels
  \[ M_7 = 5300 \text{ Pg C} \]
  \[ F_{df} \]

- hydrosphere

- deep waters
  \[ M_4 = 37,000 \text{ Pg C} \]
  \[ F_{71} \]

- cool surface waters
  \[ M_3 = 140 \text{ Pg C} \]
  \[ F_{23} = 57 \text{ Pg/yr} \]

- warm surface waters
  \[ M_2 = 730 \text{ Pg C} \]
  \[ F_{12} = 57 \text{ Pg/yr} \]
  \[ F_{21} = 58 \text{ Pg/yr} \]

- fossil fuels
  \[ M_7 = 5300 \text{ Pg C} \]

- terrestrial biota
  \[ M_5 = 580 \text{ Pg C} \]
  \[ F_{15} = 100 \text{ Pg/yr} \]
  \[ F_{51} = 50 \text{ Pg/yr} \]

- soils & detritus
  \[ M_6 = 1500 \text{ Pg C} \]
  \[ F_{61} = 50 \text{ Pg/yr} \]
  \[ F_{56} = 50 \text{ Pg/yr} \]

- fossil fuels
  \[ M_7 = 5300 \text{ Pg C} \]
  \[ F_{df} \]
The Earth’s Carbon Cycle - Coupled Differential Equations

\[ \frac{dM_1}{dt} = -\left( k_{12} + k_{13} \right) M_1 - k_{15} \alpha_{tb} \frac{M_1 - M_{1, \text{threshold}}}{M_1 + M_{1, \text{saturation}}} + k_{21} \left( \frac{M_2}{730} \right)^\beta + k_{31} \left( \frac{M_3}{140} \right)^\gamma 
\]

\[ + k_{51} M_5 + k_{61} M_6 + F_{71} + F_{df} \]

\[ \frac{dM_2}{dt} = k_{12} M_1 - (k_{23} + k_{24}) M_2 - k_{21} \left( \frac{M_2}{730} \right)^\beta + k_{42} M_4 \]

\[ \frac{dM_3}{dt} = k_{13} M_1 + k_{23} M_2 - k_{34} M_3 - k_{31} \left( \frac{M_3}{140} \right)^\gamma + k_{43} M_4 \]

\[ \frac{dM_4}{dt} = k_{24} M_2 + k_{34} M_3 - (k_{42} + k_{43}) M_4 \]

\[ \frac{dM_5}{dt} = k_{15} \alpha_{tb} \frac{M_1 - M_{\text{threshold}}}{M_1 + M_{\text{saturation}}} - \left( k_{51} + k_{56} \right) M_5 - F_{df} \]

\[ \frac{dM_6}{dt} = k_{56} M_5 - k_{61} M_6 \]

\[ \frac{dM_7}{dt} = -F_{71} \]

\[ \frac{d\alpha_{tb}}{dt} = \frac{-\epsilon_{df} F_{df}}{M_5, \text{reference}} \]
The Earth’s Carbon Cycle - Numerical Integration

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The Earth’s Carbon Cycle - Numerical Integration

linear extrapolation of fossil fuel burning and deforestation

reservoir mass (Pg C)

1000
900
800
700
600
500
400
300
200
100
0
-100

1950 1975 2000 2025 2050 2075 2100

year

[CO2] = 750 ppm

[CO2] = 380 ppm

2003
The Earth’s Carbon Cycle - Numerical Integration
The Earth’s Carbon Cycle - Numerical Integration

linear extrapolation of deforestation - fossil fuel burning set at 1990 levels in 2010

reservoir mass (Pg C)

year
The Earth’s Carbon Cycle - Numerical Integration

deforestation stopped 2005 - fossil fuel burning set at 1990 level in 2010

---

reservoir mass (Pg C)

year

1950 1975 2000 2025 2050 2075 2100

cool surface ocean

warm surface ocean

air

soil

plants

deep ocean
Mass & Energy Balances

- Define nomenclature.
- Show system borders and state assumptions.
- State source of equation -
  “apply conservation of mass” or
  “reaction specification” or
  “stream composition.”
- Describe derivation.
  “Substitute eqns (1) and (2) into eqn (3).”
- Box answer:
  number with no insignificant figures
  and units, such as kJ/min.
Energy Balances

1. Cannot calculate energy of a mass stream;
   cannot state \( q_1 = 100 \text{ kJ/min} \)
   Must calculate the change in energy of a mass stream;
   must calculate \( \Delta q_{1 \rightarrow 2} = q_2 - q_1 \)

2. Cannot measure \( \Delta q \); must measure \( \Delta T \) or \( \Delta \text{phase} \)
   and use thermodynamics to convert to energy.

3. Simple mass units can be complex energy units.
   Create an equivalent unit of elementary energy units.

   An elementary energy unit has -
   one mass stream in, one mass stream out,
   one energy change; \( \Delta T \) or \( \Delta \text{phase} \), and
   all mass passing through the unit is heated or changes phase.
Mathematical Modeling - Are Flow Rates Consistent with Steady State?

- **Not Steady State**
  - Men: 25/hour
    - Women: 25/hour
  - Party: 500 men, 500 women

- **Steady State**
  - Men: 20/hour
    - Women: 10/hour
  - Party: 500 men, 500 women

- **Steady State**
  - Men: 20/hour
    - Women: 10/hour
  - Liquid-solids separator:
    - 100 kg liquids
    - 10 kg solids
    - 2 kg/min liquids
    - 2 kg/min solids
    - Wet with 1 kg/min liquids
3.48 $A$ and $P$ cannot be separated. The process below increases the ratio of $P$ to $A$ by the reaction $A \rightarrow P$. The reactor converts 10% of the $A$ that enters.

1. Reactor creates $90 - 10 = 80$ mol $P$/min.

2. $80 = (800) \times (720)$

3. All streams into and out of a splitter have the same composition.

4. $A(710) \rightarrow P(6390)$

5. $A(800) \rightarrow P(6400)$

Calculate the flow rates of $A$ and $P$ in all streams.

$\frac{80}{0.1} = 800$ mol $P$/min.
The process below produces $X$ by the reaction $E \rightarrow X$. The reactor converts 50% of the $E$ that enters.

Product $X$ is in equilibrium with useless by-product $Z$. The ratio of $X$ to $Z$ is 1:1.

Calculate the flow rates of $E$, $X$, and $Z$ in all streams.

$E$: \[
\frac{100}{0.5} = 200
\]
Mathematical Modeling - Informal Mass Balances

3.51 The process below produces $X$ from the reaction $A + B \rightarrow H + X$. The reactor conversion is 50% if 10 mol $A$ and 10 mol $B$ enter the reactor, 5 mol $A$ and 5 mol $B$ leave the reactor.

4. $H$ and $X$ have same stoichiometry in reaction; $H$ and $X$ both created at 90 mol/min.

5. $A$ and $B$ have same stoichiometry in reaction; $A$ and $B$ both consumed at 90 mol/min.

6. All streams into and out of a splitter have the same composition.

Calculate the flow rates of $A$, $B$, $H$, and $X$ in all streams.
3. The reactor below converts 50% of A and B for equal molar flow rates of A and B. The ratio of A to I in the feed is 10 to 1. The ratio of A to I in the purge output is 1 to 1.

4. Overall mass balance:
   \[ B_{\text{in}} = B_{\text{out}} + P_{\text{out}} \]

5. Guess \( A_{\text{in}} = 100 \) \( \Rightarrow I_{\text{in}} = 10 \)
   \( (110), B(100), (11), I(10) \)

6. Guess \( A_{\text{in}} = 110 \) \( \Rightarrow I_{\text{in}} = 11 \)

7. All streams into and out of a splitter have the same composition.

8a. No guess
   \[
   \begin{align*}
   A_{\text{out}} &= I_{\text{out}} \\
   I_{\text{out}} &= I_{\text{in}} \\
   A_{\text{in}} &= 10I_{\text{in}}
   \end{align*}
   \]

9. \( A + B \rightarrow P \)
   \[ P_{\text{out}} = 99 \]
   \[ A_{\text{in}} = A_{\text{out}} + 99 \]
   \[ 10A_{\text{out}} = A_{\text{out}} + 99 \]
   \[ A_{\text{out}} = 11, A_{\text{in}} = 110 \]
Mathematical Modeling - Informal Mass Balances

3. The reactor below converts 10% of A and B for equal molar flow rates of A and B. Product P also reacts with B to form by-product X. Separating A from X is impractical because A and X have the same melting point and boiling point; X is removed from the process by a purge which also removes some A.

3. \( P_{\text{created}} = P_{\text{out}} + X_{\text{out}} = 90 + 10 = 100 \)  
   \[ A \text{ into reactor} = B \text{ into reactor} = \frac{100}{0.1} = 1000 \]

1. Overall mass balances
   \[ A_{\text{in}} = A_{\text{out}} + P_{\text{out}} + X_{\text{out}} \]
   \[ = 10 + 90 + 10 = 110 \]
   \[ B_{\text{in}} = B_{\text{out}} + P_{\text{out}} + 2X_{\text{out}} \]
   \[ = 0 + 90 + 2 \times 10 = 110 \]