Lecture 4-5
Finish Conservation of Mass
✓ Review few
Review packet for midterm
Glucose Metabolism in Cells

We know that glucose is needed in our system to fuel our bodies. Oxygen is needed to metabolize glucose according to the following chemical reaction:

\[ \text{C}_6\text{H}_{12}\text{O}_6 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} \]

Let’s say that we flow glucose and oxygen in by eating candy and breathing. Let’s assume a basis of 400 g/day with a mass fraction of \( \text{O}_2 \) at 0.4.

What is the limiting reactant? What is the rate of \( \text{O}_2 \) consumption? What is the rate of \( \text{CO}_2 \) production? What is the exit rate of the components at steady state?
Avengers – Assemble!

• Assemble what you know
• Draw your diagram
• Set your basis
• Write your assumptions
Calculate the limiting reactant

\[ \dot{M}_{O_2} = \omega_{O_2} \dot{M}_{in} = 0.4 \times 400 = 160 \text{ g/day} \]

\[ \dot{M}_a = \omega_a \dot{M}_{in} = 1.6 \times 400 = 240 \text{ g/day} \]

Calculate what we can produce based on this input (in a day!)

160 g/day \( \frac{\text{mole}}{32 \text{ g O}_2} \) \( \frac{6 \text{ moles CO}_2}{10 \text{ moles O}_2} \) = 6 moles CO\(_2\) formed/day

240 g/day \( \frac{\text{mol}}{180 \text{ g CO}_2} \) \( \frac{1 \text{ mol G}}{1 \text{ mol CO}_2} \) = 8 moles CO\(_2\) formed/day

O\(_2\) is limiting b/c produces less CO\(_2\)

Now, let's assume our system fully depletes our limiting reactant.
Calculate the rate of O2 consumption and CO2 production

Rate of consumption is calculated based on the limiting reactant.

\[ \frac{160 \text{ g}}{\text{day}} (\frac{1 \text{ mole O}_2}{32 \text{ g O}_2}) (\frac{1 \text{ mol glucose}}{6 \text{ moles O}_2}) = 0.83 \frac{\text{ moles glucose}}{\text{ day}} \]

\[ \text{nglucose} = 0.83 \frac{\text{ mol}}{\text{ day}} \]

\[ \text{nco}_2 = 5 \frac{\text{ mol}}{\text{ day}} \]
Calculate the exit rate of products

\[ \dot{N}_{\text{o}_2} = 0 \]

\[ \dot{N}_{\text{glucose}} = \text{?} \]

Mass out, mass balances

Total - \( O_2 \) = glucose

Molar \( r \cdot \text{mw} \)

\[ \dot{m}_{\text{glucose}} = 89.92 \text{ g day} \]

\[ \text{5 moles day} \]
Calculate the fractional conversion of O2 and glucose

\[ f = \frac{\text{rate of consumption}}{\text{rate of input}} = \frac{0.03}{1.33} = 0.03 \%
\]

O2 100% glucose
Now, we live in a land where candy is sparse and we don’t have as much. We don’t want to change the flowrate b/c the pump requires a technician to change the values and that costs $$. How could we change our mass fractions to conserve glucose but keep CO2 yield the same.

Set glucose as limiting reagent
Set yield CO2 same as before

\[
f_{\text{glucose}} = 1 = \frac{\text{rate consumed}}{\text{rate input}} = \frac{0.83}{\text{6.83 mol}} \text{ day}^{-1}
\]

0.83 mol \text{ day} \times \left( \frac{180 \text{ g}}{\text{mol}} \right) \times \left( \frac{\text{day}}{400 \text{ g}} \right) = \omega_{\text{glucose}} = 0.37 \text{ fraction input glucose}
1. List extensive and intensive properties

2. Define: mass fraction, mole fraction, molar flow rate, mass flow rate. Give symbol for each.

3. Write the relationship between mass and volume in a flowing system


5. Describe the difference between steady state and dynamic

6. Write the algebraic, differential and integral form of the accounting equation. When is each valid? Given an example.

7. Find $\dot{n}_A$, $\dot{n}_B$, and $\dot{n}_C$.

8. In order to make the titanium alloy needed for a hip implant, metal reduction must be performed. The reduction of a metal by another is called metallothermic reduction. Metallic titanium is produced by reduction of titanium tetrachloride ($\text{TiCl}_4$) with magnesium. In one plant, a steel reactor vessel is charged with 320 lb of Mg bars, and heated in an inert atmosphere to about 850°C to form a pool of molten Mg on the bottom of the furnace. Then 1070 lb of liquid TiCl$_4$ is run in through a pipe at the top, while a small amount of inert gas is added to maintain a positive pressure in the reactor. The figure below shows a sketch of the reactor vessel. Determine the limiting reactant.

The reaction occurs according the following:

$$\text{Mg} + \text{TiCl}_4 \rightarrow \text{MgCl}_2 + \text{Ti}$$
9. Acetyl Co-A is produced by the following reaction:

\[
C_{21}H_{36}N_7O_{16}P_3S + C_{3}H_{4}O_3 + C_{21}H_{27}N_7O_{14}P_2 \rightarrow C_{21}H_{28}N_7O_{14}P_2 + C_{23}H_{38}N_7O_{17}P_3S + CO_2 + H^+
\]

Pyruvate \( C_3H_4O_3 \)
NAD\(^+ \) \( C_{21}H_{27}N_7O_{14}P_2 \)
NADH \( C_{23}H_{38}N_7O_{17}P_3 \)

This reaction is aided by the pyruvate dehydrogenase complex, which is comprised of three enzymes, pyruvate dehydrogenase (E1), dihydrolipoly transacetylase (E2), and dihydrolipoly dehydrogenase (E3).

You have decided to design a reactor system to produce citrate. The first step is the Acetyl Co-A reaction, the second step is a mixer to introduce water, and the last step is the bioreactor described in problem #3. Design a low-cost Acetyl Co-A reactor and Mixer needed to produce citrate at the same rate determined in problem #3, with the same component mass flow rates as described in problem #3. Assume that the pyruvate dehydrogenase complex is present in the first reactor. What are the mass percentages and mass flow rates of the materials exiting the citrate reactor?

What are the mass flow rates of the components entering the Acetyl Co-A reactor and the Mixer? (Assume 100% reaction efficiency, assume that nothing is lost, and assume that all components are liquid).

<table>
<thead>
<tr>
<th>Component</th>
<th>Price/pound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pyruvate</td>
<td>$111.75/100 g</td>
</tr>
<tr>
<td>NAD(^+)</td>
<td>$25.05/1 mg</td>
</tr>
<tr>
<td>Coenzyme-A</td>
<td>$128.34/25 mg</td>
</tr>
<tr>
<td>Oxaloacetate</td>
<td>$56/2 mg</td>
</tr>
<tr>
<td>Water</td>
<td>$27.24/100 mL</td>
</tr>
</tbody>
</table>

10. Your project supervisor has asked you to reduce the costs associated with the process. After analyzing the process, you notice that Coenzyme A is both a product of the citrate reaction and a reactant in the Acetyl-Co-A reaction, so you design a separator that is 90% efficient, and recycle the Coenzyme-A to the Acetyl-Co-A reactor as a separate input stream. At steady state, how will you change your Acetyl-Co-A reactor input stream to make best use of this new recycle stream? If the plant runs for 24 hours/day for 3 weeks, how much will you save with the recycle stream?

Thought exercises:

(a) How would change your Acetyl-Co-A reactor flow rates if the pyruvate dehydrogenase complex conversion efficiency is only 40%?

(b) If your project supervisor asked you to reduce costs by optimizing the process, what are some cost-cutting options? How much would they save you?