ABE 201
Biological Thermodynamics 1

Module 6:

Mass Balances with

Chemical Reactions

Outline

- <u>Conservation of Mass</u> and Chemical Reactions

- <u>Useful Concepts</u> for Solving Mass Balances with Chemicals Reactions

- <u>Approaches</u> to Solving Mass Balances with Chemical Reaction

Conservation of Mass

Accumulation = In – Out + Generation - Consumption

- **Steady-state: Accumulation = 0**

- **No chemical Reactions: Gen = Con = 0**

- **Chemical Reactions?**
  - **Two Approaches**
  - **Atomic Species Balance**
  - **Chemical Compound Balance**

Concepts

- Stoichiometry: balanced chemical reaction that is mathematical representation of the relationship between atoms in reactants and atoms in products
- Yield: amount of <u>actual</u> product produced divided by <u>theoretical</u> product that could be produced

$$Yield = \frac{Actual\ Product}{Theoretical\ Product}$$

Stoichiometry

To start, lets consider the burning of ethanol in the presence of oxygen which produces carbon dioxide and water.

$$C_2H_5OH + O_2 \longrightarrow CO_2 + H_2O$$

As the equation is given, this is ***not*** a balanced stoichiometric equation.

Stoichiometry

To balance this equation, you must have equal amounts of each component on each side of the equation.

$$C_2H_5OH + 3O_2 \longrightarrow 2CO_2 + 3H_2O$$

Carbon - 2	Carbon - 2
Hydrogen - 6	Hydrogen -6
Oxygen - 7	Oxygen - 7

Balancing a chemical reaction is really an ***atomic*** mass balance! (In -> Out)

Stoichiometry

- Describes the relationship between reactants and products <u>if and when</u> a chemical reaction occurs
- Does **<u>not</u>** tell us
  - that the reaction <u>in fact</u> occurred in this system;
  - how <u>fast</u> it occurred;
  - how <u>completely</u> the reaction occurred

Stoichiometry vs Yield

2 mole C_2H_5OH

6 moles O_2

1 moles C_2H_5OH

3 moles O_2

3 moles H_2O

2 moles CO_2

$$1C_2H_5OH + 3O_2 \rightarrow 2CO_2 + 3H_2O$$

$$Yield_{H_2O} = \frac{3}{6} = 0.50$$

Limiting and Excess Reagents

Ethanol is <u>excess</u>

2 mole C_2H_5OH

1 moles C_2H_5OH

2 moles O_2

3 moles H_2O

2 moles CO_2

5 moles O_2

Oxygen is <u>limiting</u>

$$1C_2H_5OH + 3O_2 \rightarrow 2CO_2 + 3H_2O$$

$$Yield_{H_2O} = \frac{3}{\frac{5}{3} * 3} = 0.60$$

Extent of Reaction

To describe the extent to which a reaction proceeds, there are two parameters, the fractional conversion (f) and the extent of reaction (ξ).

fractional conversion = f = $(n_{i,in}-n_{i,out})/n_{i,in}$

extent of reaction = $\xi = (n_{i,out} - n_{i,in})/v_i$

$n_{i,in}$ - moles of compound i going in

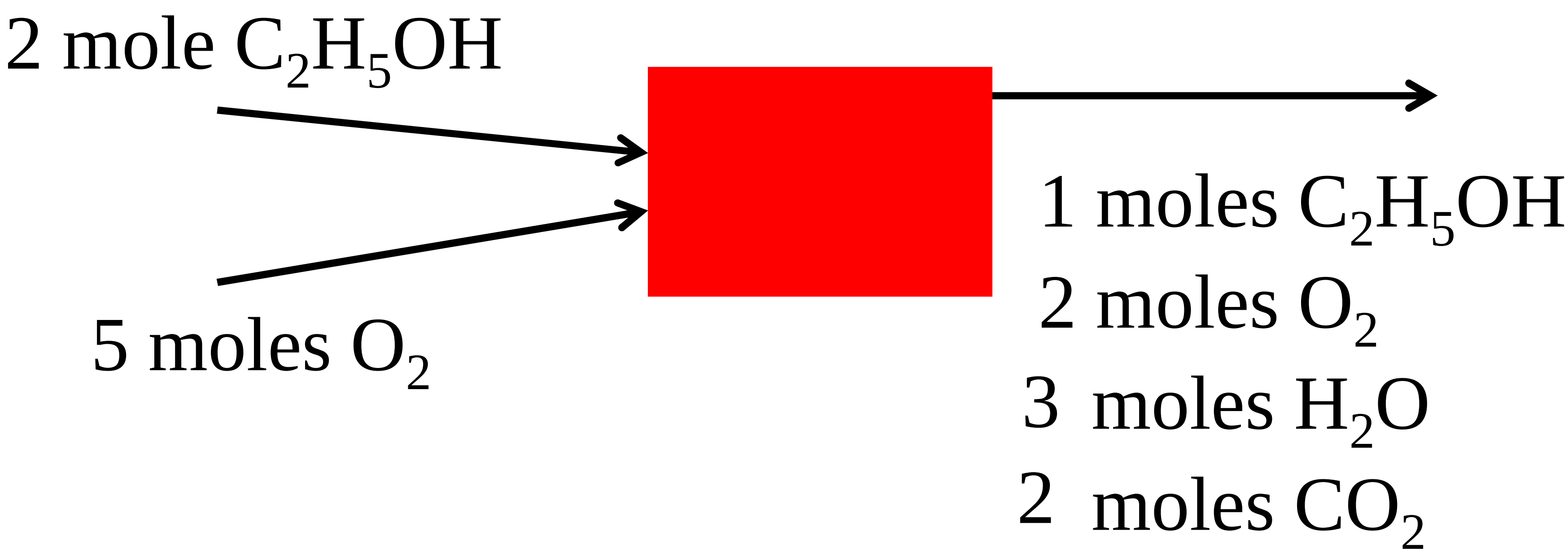
$n_{i,out}$ - moles of compound i going out

v_i - stoichiometric coefficient for compound i

Note: v_i is <u>negative</u> for <u>reactants</u>
v_i is <u>positive</u> for <u>products</u>

These factors are vital because they must be used to account for generation or consumption.

Fractional Conversion and Extent of Reaction



$$1C_2H_5OH + 3O_2 \rightarrow 2CO_2 + 3H_2O$$

$$f_{etOH} = \frac{2-1}{2} = 0.50$$

$$\xi_{etOH} = \frac{1-2}{-1} = 1$$

$$f_{O2} = \frac{5-2}{5} = 0.60$$

$$\xi_{O2} = \frac{2-5}{-3} = 1$$

Using Extent of Reaction

- Tells you how many “turns of the crank” occurred in your process.
- Is a <u>single</u> variable that is common to all <u>reactants and products</u>
- <u>Simplifies</u> the number of variables for solving mass balances
- <u>Each separate reaction</u> will have a <u>unique</u> extent of reaction

Mass Balance Using Extent of Reaction

100 g/min C_2H_5OH

165 g/min O_2

48.0 g/min C_2H_5OH

? g/min O_2

? g/min H_2O

? g/min CO_2

$$1C_2H_5OH + 3O_2 \rightarrow 2CO_2 + 3H_2O$$

etOH = 46 g/mol water = 18 g/mol

Oxygen = 32 g/mol CO_2 = 44 g/mol

Accumulation = In – Out + Generation - Consumption

Assume steady-state operation

0 = In – Out + Generation - Consumption

$$0 = In - Out + v_i * \xi * MW_i$$

Ethanol Balance

$$0 = In - Out + v_{etOH} * \xi * MW_{etOH}$$

$$0 = 100\ g/min - 48\ g/min + (-1) * \xi * (46\ g/mol)$$

$$\xi = 1.13\ mol/min$$

Oxygen Balance

$$0 = 165\ g/min - m_{O2,out}\ g/min + (-3) * 1.13 * (32\ g/mol)$$

$$m_{O2,out} = 56.5\ g/min$$

Water Balance

$0 = In - Out + v_{water} * \xi * MW_{water}$

$0 = 0 \text{ g/min} - m_{water,out} \text{ g/min} + (+3) * 1.13 * (18 \text{ g/mol})$

$m_{water,out} = 61.0 \text{ g/min}$

CO2 Balance

$0 = In - Out + v_{CO2} * \xi * MW_{CO2}$

$0 = 0 \text{ g/min} - m_{O2,out} \text{ g/min} + (+2) * 1.13 * (44 \text{ g/mol})$

$m_{CO2,out} = 99.4 \text{ g/min}$

Check – Total Mass Balance

$0 = In - Out$

$0 = (100 + 165) - (48 + 56.5 + 62.0 + 99.4)$

$0 = (265) - (48.0 + 56.5 + 61.0 + 99.4) = 265 - 264.9$

Atomic Species Balance

- Generation = Consumption = 0
- Similar to balancing stoichiometry (make each element balance)
- Does not depend upon <u>knowing</u> the stoichiometry of the reaction
- Often used when <u>multiple</u> reactions occur simultaneously in one reactor

Mass Balance Using Extent of Reaction

100 g/min C_2H_5OH

165 g/min O_2

48.0 g/min C_2H_5OH

? g/min O_2

? g/min H_2O

? g/min CO_2

$$1C_2H_5OH + 3O_2 \rightarrow 2CO_2 + 3H_2O$$

etOH = 46 g/mol   water = 18 g/mol

Oxygen = 32 g/mol CO_2 = 44 g/mol

Accumulation = In – Out + Generation - Consumption

Assume steady-state operation

0 = In – Out

Carbon Balance

0 = 100 g/min / 46 g/mol * 2 mol C/mol etOH –
(48 g/min / 46 g/mol * 2 mol C/mol etOH
+ m_{CO2}/ 44 g/mol * 1 mol C/mol CO2)

m_{CO2} = 99.5 g/min

Oxygen Balance

*0 = (100 g/min / 46 g/mol * 1 mol O/mol etOH*

*+ 165 g/min / 32 g/mol * 2 mol O/mol O2)*

*- (48 g/min / 46 g/mol * 1 mol O/mol etOH*

*+ $m_{O2,out}$ / 32 g/mol * 2 mol O/mol O2*

*+ $m_{water,out}$ / 18 g/mol * 1 mol O/mol water*

*+99.5 g/min + / 44 g/mol * 2 mol O/mol CO2)*

Summary

- Mass balances with chemical reactions can be solved in two ways:
  - Extent of reaction
  - Atomic species (elemental) balance