Computers

- I encourage you to use Excel or Python for as many homework problems as possible for the rest of class
- Turn in a copy of the Excel sheet or Python code along with any handwritten notes

- The Case Study is coming…..

Dean's Lecture Credit

- Dean's lecture credit
  - Dean's lectures
    - (Oct 13 & Nov 17, JSB Aud, 11 am)
  - Leadership lectures
  - ChE graduate seminars that have outside speakers (Thursdays at 4 pm in 325 EB)
    - https://apm.byu.edu/che791/index.php/Main/Fall2022
  - Other seminars if approved by Dr. F.

You will mark the # of seminars on a box on the final exam

Practice Exam

- Last year's (F'21) practice exam now posted on learning suite
  – Final answers given
- This is the only exam you are allowed to study
- Take-home exam details
  – Available Wednesday (Sept 28)
  – Due Monday morning, 9 am (Oct. 3)
  – Closed book but one 8.5 x 11 sheet of paper with notes (one side) is allowed
  – TA's will have help sessions next Wednesday and Thursday
  – 3-hour time limit on exam
    - 1 point per minute deduction for every minute more than 180 minutes
  – Plan your time (this will be General Conference weekend)

3

Balances with Reactions

Class 10

4

Class Review:

(a) What is the equation for the %excess of a reactant?

$$\%excess = \frac{n_{i,0} - n_{i,stoich}}{n_{i,stoich}}$$

(b) What is equation for the fractional conversion?

$$f_i = X_i = \frac{n_{i,0} - n_{i,f}}{n_{i,0}} \quad \text{or} \quad n_{i,f} = n_{i,0}(1 - X_i)$$

(c) What is the equation for the extent of reaction (if there is only one reaction)?

$$\xi = \frac{n_i - n_{i,0}}{\nu_i} \quad \text{or} \quad n_i = n_{i,0} + \nu_i \xi$$

(d) What is the equation for the moles of species i if there are multiple reactions?

$$n_i = n_{i,0} + \nu_{i,1}\xi_1 + \nu_{i,2}\xi_2 + \ \ldots$$

5

ADVICE

- Work through the examples in sections 4.7, 4.8
  - Ex 4.7-1 thru 3 (today)
  - Ex 4.8-1 thru 4 (for next time)

- Don't just browse through!

(Otherwise you will not learn this material)

6

3 Different Methods of Balances for Reacting Systems

1. Molecular Species Balances
2. Atomic Element Balances
3. Extent of Reaction

7

1. Molecular Species Balances
(reacting systems – used least)

- Use generation and consumption terms

$$accum = in - out + gen - cons$$

8

1. Molecular Species Balances
(reacting systems – used least)

- Use generation and consumption terms
- Use ratios of species based on stoichiometry
  - Moles species j generated/moles species i consumed
- Add # of independent chemical rxns to DOF analysis

Page 144 (128 in 3rd Ed.)

+ # of unknowns
+ # of independent chemical reactions
- # of independent molecular species balances
- # of other equations
= DOF

9

2. Atomic Element Balances
(reacting systems – useful)

- No generation and consumption terms
  In = Out
- Count moles of atoms
  - Split up species into atoms
- Include # of independent atomic element balances to DOF analysis

Page 143 129 in 3rd Ed.

+ # of unknowns
- # of independent atomic element balances
- # of independent non-reacting molecular species balances
- # of other equations
= DOF

10

3. Balances Using Extent of Reaction
(useful)

- Use definition of ξ

  $n_i = n_{i,o} + \nu_i \xi$, or using flow rates
- One ξ_j for each reaction
  - Use problem info to get ξ_i's, then calculate unknown variables
- Add extent of reaction variables to DOF analysis

Page 145
130 in 3rd Ed

+ # of unknowns
+ # of independent ξ_i's
- # of independent reacting molecular species balances
- # of independent non-reacting species
- <u># of other equations</u>
= DOF

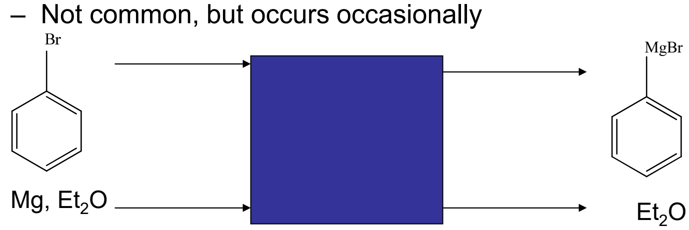
11

Recommendations

- Book recommends <u>element balances</u>
  - I say only for complex reactions or solids
  - Extent of reaction approach is easiest if simple reactions

Caution:

- Element balances are not always independent!!!
  - If ratio of two elements is constant everywhere, the element balances are not independent!
  - Not common, but occurs occasionally



C/H ratio is same in two streams (twice)

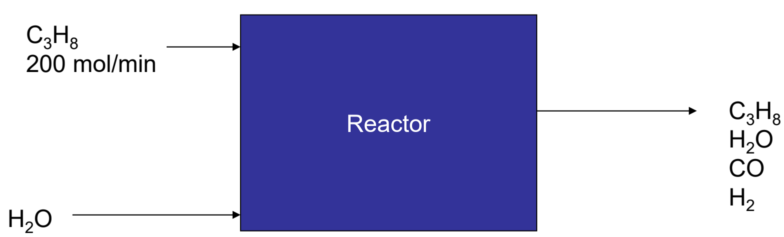
12

Cautions

- If no reactions occur in the subunit, use the DOF for non-reacting systems
- If reactions occur in the overall system, you must use the DOF for reacting systems for the overall system

13

Example Problem



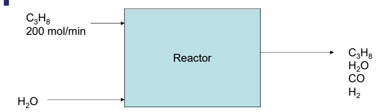
I will work this problem in each of three ways:

1. Molecular Balances
2. Element Balances
3. Extent of Reaction

Start with DOF! See Worksheet…

14

Molecular Species Balances with DOF Analysis



$C_3H_8 + 3\ H_2O \rightarrow 3\ CO + 7\ H_2$

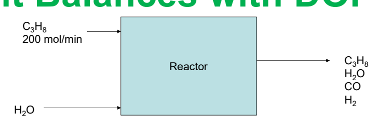
DOF Analysis

Unknowns: $n_{H2O,in}$, n_{C3H8}, n_{H2O}, n_{CO}, n_{H2}	= +5
# of Rxns	= +1
# of Species Balances	= -4
# of Other Equations	= 0
Degrees of Freedom	= 2!!!

(need to specify two things in order to solve problem)

15

Element Balances with DOF Analysis



$C_3H_8 + 3\ H_2O \rightarrow 3\ CO + 7\ H_2$

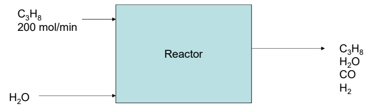
DOF Analysis

Unknowns: $n_{H2O,in}$, n_{C3H8}, n_{H2O}, n_{CO}, n_{H2}	= +5
# of Reacting Elements	= -3
# of Non-reacting Species Balances	= -0
# of Other Equations	= -0
Degrees of Freedom	= 2!!!

(need to specify two things in order to solve problem)

16

Extent of Reaction with DOF Analysis



$$C_3H_8 + 3\,H_2O \rightarrow 3\,CO + 7\,H_2$$

DOF Analysis

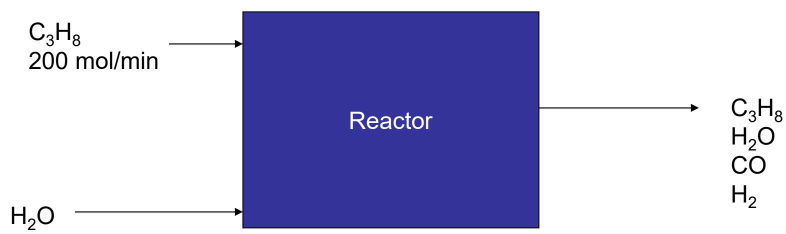
Unknowns: $n_{H2O,in}$, n_{C3H8}, n_{H2O}, n_{CO}, n_{H2}	= +5
# of ξ's (# or reactions)	= +1
# of Independent Species Balances	= -4
# of Other Equations	= -0
Degrees of Freedom	= 2!!!

(need to specify two things in order to solve problem)

17

Example Problem

with zero DOF



Additional Relationships:

1. 65% conversion of C_3H_8
2. 25% excess H_2O

18