Chapter 2
Lecture # 2-3

- **The Input-Output Structure of the Process (Part 2).**

Input – Output Structure

Other Consideration for the Input – Output Structure of the Process Flowsheet

- Feed Purity and Trace Components
  - Small Quantities and "Inerts" – Do Not Separate

E.g. H_2 in feed to THDA process contains CH_4

CH_4 does not react

so, do not remove

Input – Output Structure

Other Consideration for the Input – Output Structure of the Process Flowsheet

- If Separation of Impurities is Difficult – Do Not Separate
  - Azeotrope – (water and ethanol)
  - Gases – (requires high P and low T)
- If impurities foul or poison catalyst then ***separate***
  - Sulfur – Group VIII Metals such as iron, nickel, and platinum
  - A guard bed of activated carbon (or Zinc Oxide) is placed upstream of the reactor for protection

Input – Output Structure

Other Consideration for the Input – Output Structure of the Process Flowsheet

If impurity reacts to form difficult-to-separate material or hazardous product then ***separate***

If impurity is in large quantities then ***purify*** the feed.

Input – Output Structure

ADD MATERIAL TO FEED

- Stabilize Products
- Enable Separation/Minimize Side Reactions
  - Anti-Oxidants and Scavengers
  - Solvents and Catalysts

Input – Output Structure

ADD MATERIAL TO FEED

- Control Exothermic Reactions
  - Steam for oxidation reactions
- Control Equilibrium
  - Adding inerts shifts equilibrium to the right

Example: styrene reaction

$$C_6H_5CH_2CH_3 \longleftrightarrow C_6H_5CHCH_2 + H_2$$

Input – Output Structure

Information Obtained From Input-Output Diagram

- Basic economic analysis on profit margin.
- What chemical components must enter with the feed and leave as products.
- All the reactions, both desired and undesired, that take place.

Profit Margin (PM)

PM = Value of products – Cost of raw materials

- If PM < 0, then don't bother to pursue this process but start looking for an alternate route

<u>Toluene HDA vs. Toluene Disproportionation</u>

$C_6H_5CH_3 + H_2 \rightarrow C_6H_6 + CH_4$

Toluene benzene

$2C_6H_5CH_3 \rightarrow C_6H_6 + C_6H_4(CH_3)_2$

Toluene benzene xylene

Toluene used more efficiently

Profit Margin (PM)

- Some processes are more sensitive to product and feed prices than others.
- Average cost data over a period of several years should be used in evaluating PM.
- Cost of raw materials play a role in deciding which chemical path to choose to produce a given product.

Example 2.1

Evaluate the profit margin for the HDA process.

From Tables 6.3 and 6.4 (Year 2001)

Benzene = $ 0.349/kg

Toluene = $ 0.322/kg

Natural gas (methane and ethane, MW =18) = $ 6.00/GJ
= $ 6.7/1000 std. ft' = $ 0.293/kg

Hydrogen = $ 0.721 /kg

Using 1 kmol of toluene feed as a basis

Example 2.1 (cont.)

Consider 1993 prices

Cost of *Raw Materials*

92 kg of Toluene = (92 kg)($ 0.24kg) = $ 22.08

2 kg of Hydrogen = (2 kg)($ 0.312/kg) = $ 0.624

Value of Products

78 kg of Benzene = (78 kg)($ 0.27 /kg) = $ 21.06

16 kg of Methane = (16 kg)($ 0.126/kg) = $ 2.016

Profit Margin

Profit Margin = (21.06 + 2.016) - (22.08 + 0.644) = $ 0.372 or
$ 0.0040/kg of toluene

Conclusion

This is significantly lower than the 2001 margin. Production of benzene via the HDA of toluene would probably not be economical

Example 2.2

Evaluate the profit margin for the toluene disproportionation process.

From Tables 6.4 (Year 2001)

Mixed Xylenes = 0.323 $/kg

Using 2 kmols of toluene feed as a basis

Cost of *Raw Materials*

184 kg of Toluene = (184 kg)($0.322/kg) = $ 59.25

Value of Products

78 kg of Benzene = (78 kg)($0.349/kg)= $ 27.22

106 kg of xylene = (106 kg)($0.323/kg) = $ 34.24

Example 2.2

Margin

Profit Margin = 34.24 + 27.22 - 59.25 = $ 2.21

or $ 0.012/kg toluene feed

Currently this process is significantly better than the hydrodealkylation process.

Year 1993

Mixed Xylenes = 0.323 $/kg

Margin = (78)(0.27) + (106)(0.25) - (184)(0.24) = $ 3.4

or $ 0.0185/kg of toluene

We conclude that the margin for the disproportionation process is significantly less sensitive to product and feed prices than is the hydrodealkylation process.