CHE 425

Engineering Economics and Design Principles

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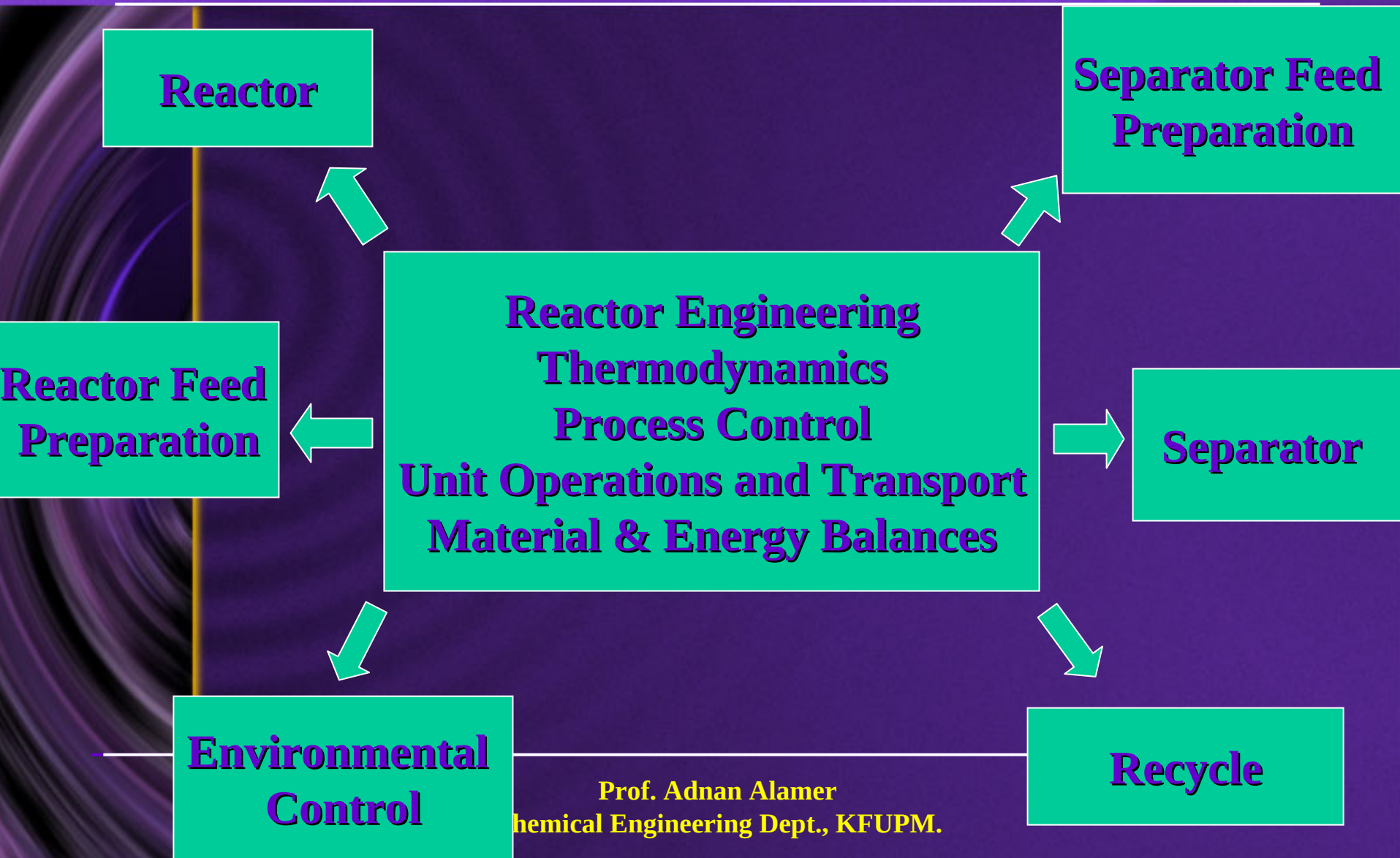
CHAPTER 10

Synthesis of the PFD from the Generic BFD

Introduction

- The full PFD truly defines the process in a chemical engineering sense.
- It is the starting point for engineers to design components needed to translate the chemical engineers vision to reality.

Introduction (cont.)



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Introduction (cont.)

Broader context of project

- **Environmental concerns**
- **Customer expectations**
- **Return on investment, etc.**

Important details

- **Type of heat transfer medium**
- **Number of stages in a column**
- **Volume of a reactor, etc.**

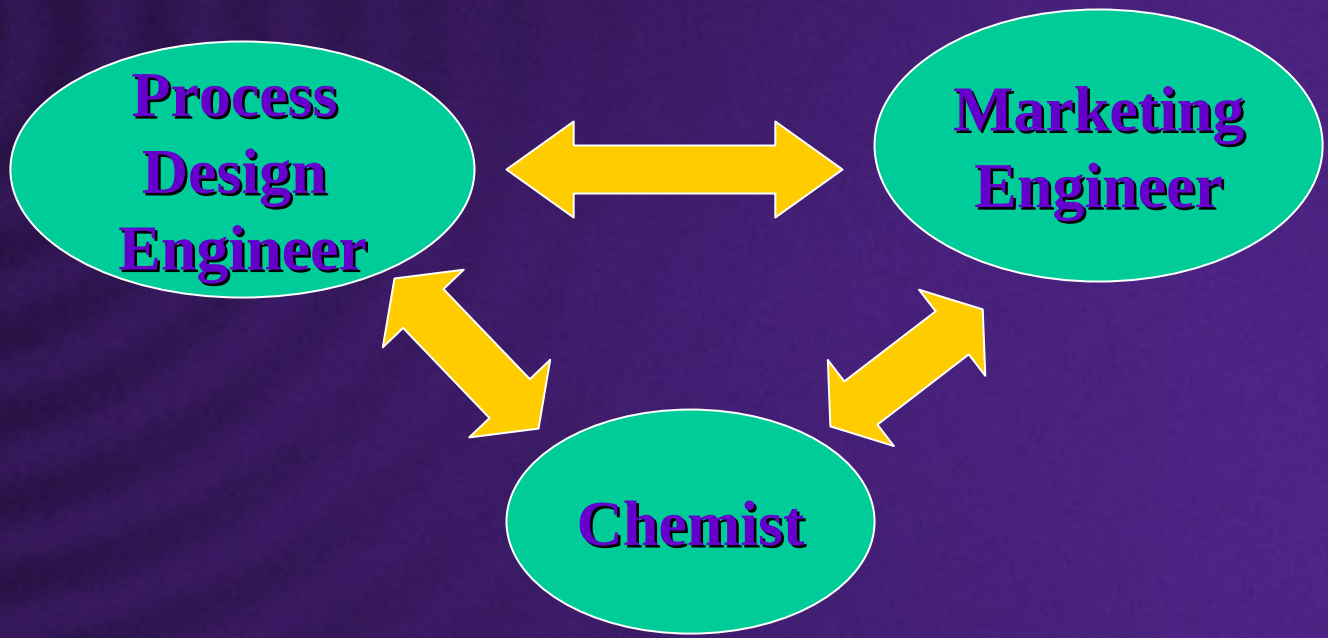
Introduction (cont.)

- Consider as many alternatives as possible in the early stages of PFD synthesis.

It is a common human trait to resist change more strongly as more effort is expended on a task, design, or product. We describe this as not wanting to abandon our "investment" in the activity.

10.1 INFORMATION NEEDS & SOURCES

- **Interactions with other engineers and scientists**
  - Team of engineers work on development of the process



10.1 INFORMATION NEEDS & SOURCES (cont.)

- **Reaction kinetic data**
  - Kinetics of the main reaction must be known

    Rate of Rxn = function(T, P, composition)
  - Knowledge of the kinetics of unwanted side reactions is also crucial to the development of PFD structure or topology
  - Knowledge of detailed rxn pathways, elementary rxns, and unstable rxn intermediates is NOT required

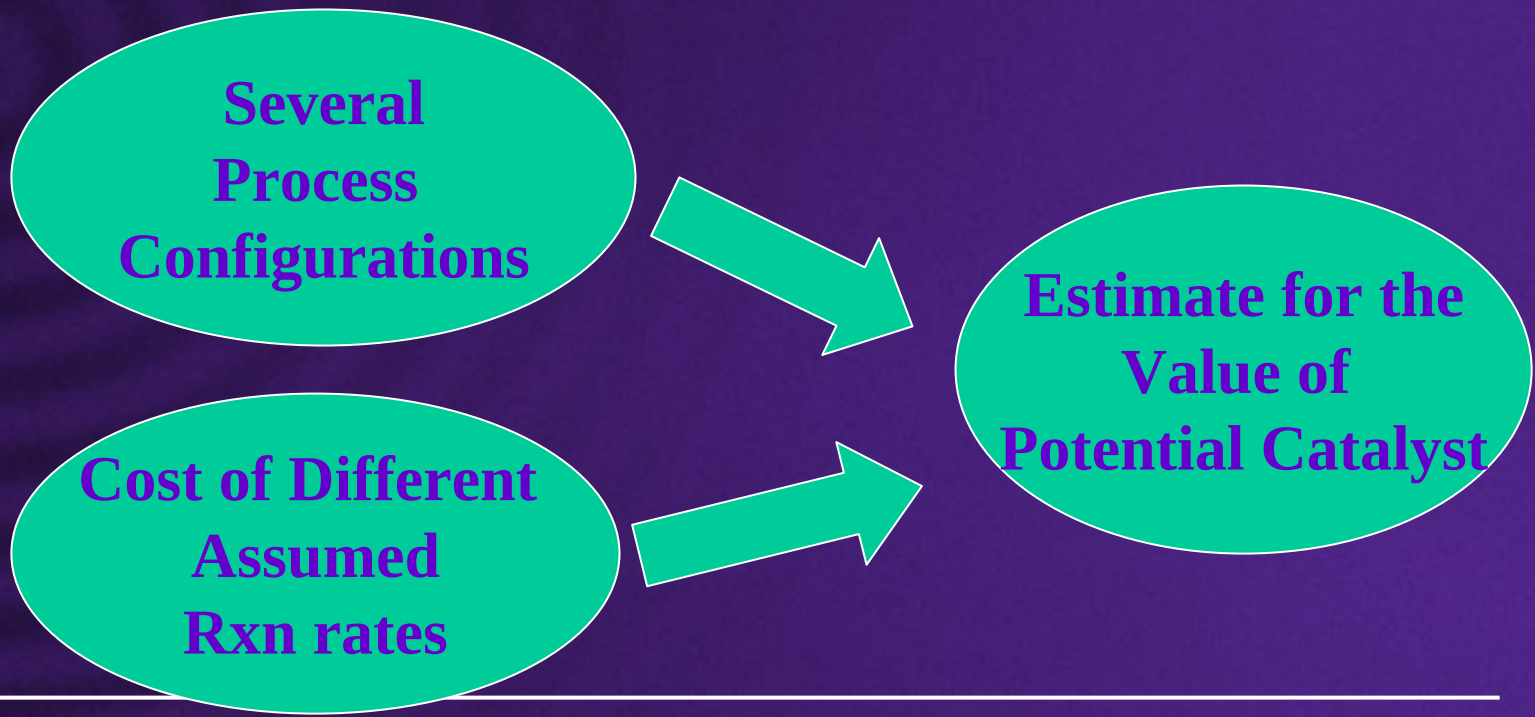
10.1 INFORMATION NEEDS & SOURCES (cont.)

- For common homogeneous rxns, kinetics are available.
- Kinetics for catalyzed rxns are not readily available in the open literature. *The competitive advantage of a company is often the result of a unique catalyst*
  - Available in company files
  - Patent literature
- Key data to obtain from patent literature are:
  - Inlet and outlet compositions
  - Temperature
  - Pressure
  - Space time

10.1 INFORMATION NEEDS & SOURCES (cont.)

Q: Can preliminary PFD and cost analysis be done without kinetic data?

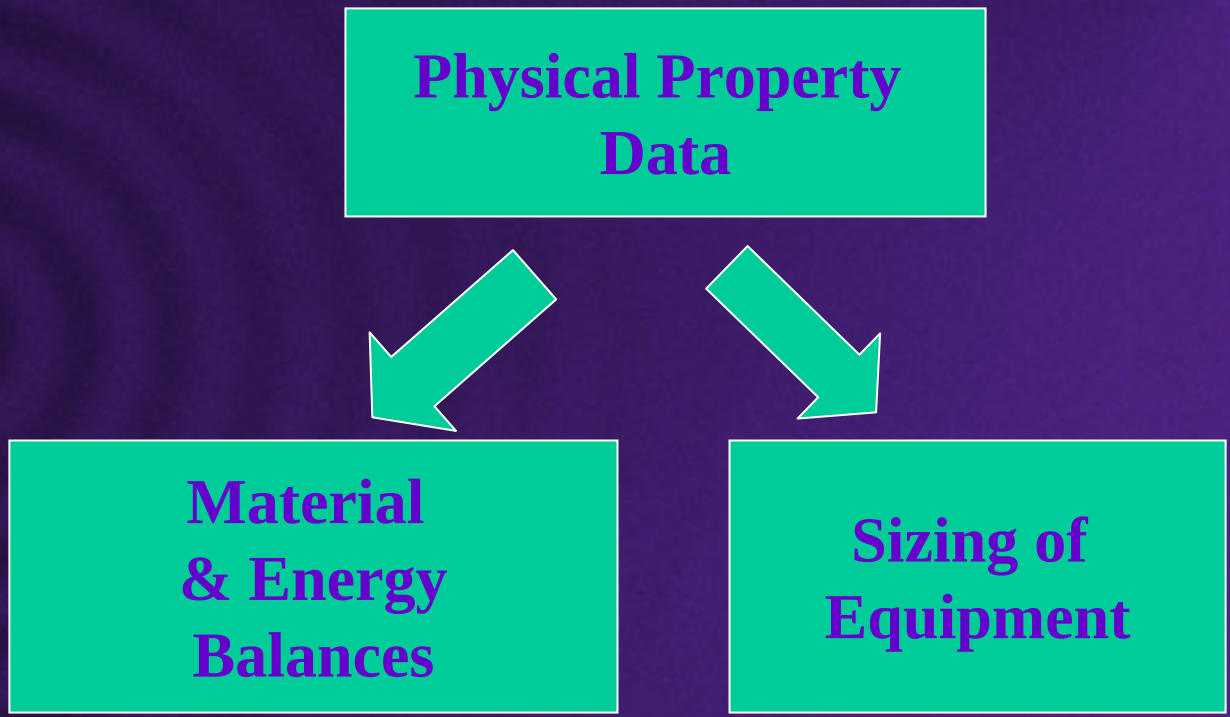
Ans: Yes



10.1 INFORMATION NEEDS & SOURCES (cont.)

- If doubling rxn rate reduces cost of manufacture by $1 million dollar per year then catalysis research is warranted.
- The economic breakpoint is often a catalyst productivity of desired product of ~0.10 kg product per kg catalyst per hour.
- Another guide is that activation energies are usually between 40 and 200 kJ/mol.

10.1 INFORMATION NEEDS & SOURCES (cont.)



- Physical property data are easier to obtain or estimate than kinetic data

10.1 INFORMATION NEEDS & SOURCES (cont.)

- Material and energy balances
  - Heat capacity data
  - Density data

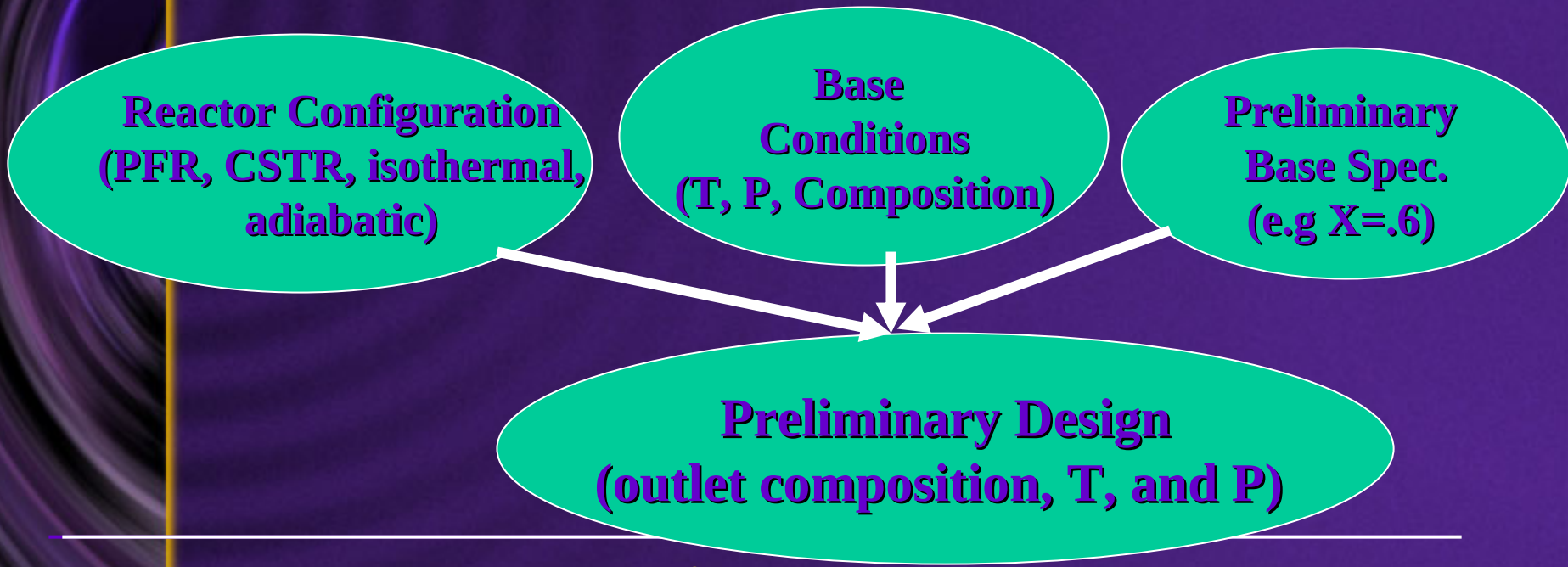
Measured data are available in database of process simulators. If unavailable, can be estimated by group contribution techniques.

10.1 INFORMATION NEEDS & SOURCES (cont.)

- Design of Heat Exchangers:
  - Thermal conductivity data
  - Viscosity data
- Design of Separators:
  - Phase equilibrium data

10.2 REACTOR SECTION

- For a process with a reactor, synthesis of PFD often begins with the reactor section.
- Develop a feasible PFD (base-case design)



10.2 REACTOR SECTION (cont.)

Important Questions

1. In what phase does the reaction take place?
2. What are the required temperature and pressure ranges for the reactor?
3. Is the reaction kinetically or equilibrium controlled?
4. Does the reaction require a solid catalyst or is it homogeneous?

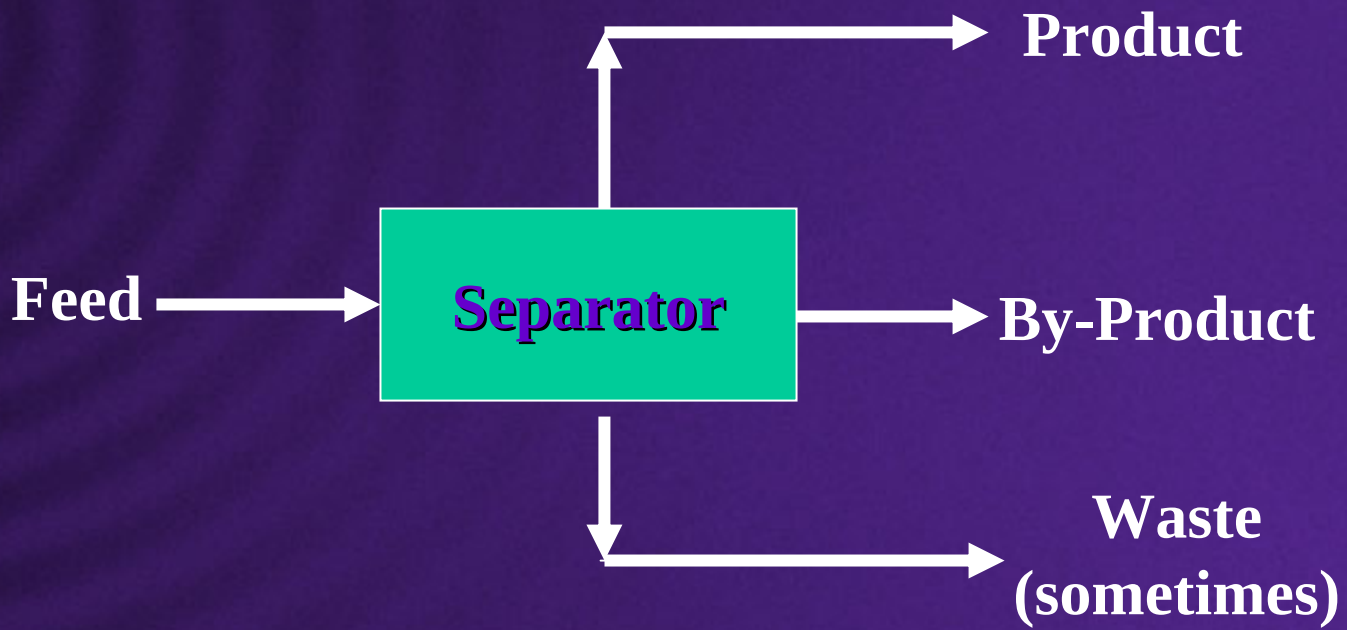
10.2 REACTOR SECTION (cont.)

Important Questions (cont.)

5. Is the main reaction exothermic or endothermic?
6. What side reactions occur, and what is the selectivity of the desired reaction?
7. What is the approximate single-pass conversion?
8. For gas-phase oxidations, should the reactor feed be outside the explosive limits?

10.3 SEPARATOR SECTION

- After the reactor section, the separator section should be studied.



10.3 SEPARATOR SECTION (cont.)

Important Questions

1. What type of units should be used?
2. How should the units be sequenced?
3. What are the product specifications for all the products?
4. Are any of the products heat sensitive?

10.3 SEPARATOR SECTION (cont.)

Table 10.1 Guidelines for Choosing Separation Units

- Use distillation as a first choice for separation of fluids when purity of both products is required.
- Use gas absorption to remove one trace component from a gas stream.
- Consider adsorption to remove trace impurities from gas or liquid streams.
- Consider pressure-swing adsorption to purify gas streams, especially when one of the components has a cryogenic boiling point.
- Consider membranes to separate gases of cryogenic boiling point and relatively small flowrates.
- Choose an alternative to distillation if the boiling points are very close or if the heats of vaporization are very high.

10.3 SEPARATOR SECTION (cont.)

- Consider extraction as a choice to purify a liquid from another liquid.
- Use crystallization to separate two solids or to purify a solid from a liquid solution.
- Use evaporation to concentrate a solution of a solid in a liquid.
- Use centrifugation to concentrate a solid from a slurry.
- Use filtration to remove a solid in almost dry form from a slurry.
- Use screening to separate solids of different particle size.
- Use float/sink to separate solids of different density from a mixture of pure particles.
- Consider reverse osmosis to purify a liquid from a solution of dissolved solids.
- Use leaching to remove a solid from a solid mixture.

10.3 SEPARATOR SECTION (cont.)

Table 10.2 Guidelines for Sequencing Separation Units

- Remove the largest product stream first. This makes all of the subsequent separation units smaller.
- For distillation, remove the product with the highest heat of vaporization first, if possible. This reduces the heating/cooling duties of subsequent units.
- Do not recombine separated streams. (This may seem obvious, but it is often disobeyed.)
- Do the easy separations first.
- Do not waste raw materials, and do not overpurify streams based on their uses.
- Remove hazardous or corrosive materials first.

10.3 SEPARATOR SECTION (cont.)

For the separation section, other important questions to be considered include:

1. *What are the product specifications for all the products?* Product specifications are developed to satisfy customers who will use these products in their own processes. The most common specification is a minimum concentration of the main constituent, such as 99.5 wt%. Maximum impurity levels for specific contaminants may also be specified, as well as requirements for specific physical properties such as color, odor, and specific gravity. A single separation technique may not be sufficient to meet all the required product specifications.

10.3 SEPARATOR SECTION (cont.)

Example 10.1

In the production of benzene via the HDA of toluene, it is necessary to produce a benzene product stream that contains >99.5 wt% benzene that is water white in color (i.e, absolutely clear). If the feed toluene to the process contains a small amount of color, determine a preliminary separation scheme to produce the desired benzene product

10.3 SEPARATOR SECTION (cont.)

- As a guide, look at Fig 1.5 (HDA of toluene).
- Separation can be accomplished using distillation due to wide difference in volatility between toluene and benzene.
- Compound causing coloration is soluble in both benzene and toluene
- Laboratory test shows that benzene can be decolorized by passing it through a bed of activated carbon
- Thus, add an activated carbon adsorber as a second separation step to decolorize the benzene product.

10.3 SEPARATOR SECTION (cont.)

2. *Are any of the products heat sensitive?* If any of the products or by-products are heat sensitive (i.e., they decompose or polymerize at elevated temperatures), the conditions used in the separations section may have to be adjusted.

10.3 SEPARATOR SECTION (cont.)

Example 10.2

It is known that acrylic acid starts to polymerize at 90 °C. Acrylic acid must be separated from acetic acid to produce the required purity product, and the volatilities of both acids are significantly different. This points to distillation as the separation method. The normal boiling points of acrylic acid and acetic acid are 140 °C and 118 °C, respectively. How should the separation be accomplished to avoid degradation of the Acrylic acid product?

10.3 SEPARATOR SECTION (cont.)

- The distillation column must be run under vacuum to avoid the problem of acrylic acid degradation.

- The pressure should be set so that the bottom temperature of the column is below 90 ^{o}C.

- From Figure B.2 and Table B.4, we see that a column pressure of 0.16 bar at the bottom can accomplish the desired separation without exceeding 90 ^{o}C