Chapter 10
Lecture # 1-2

- Overview
- Introduction
- Information needed before Synthesizing a PFD
- Reactor Section

Chapter 10 Overview

Title: Synthesis of the PFD from the Generic BFD

Topics:

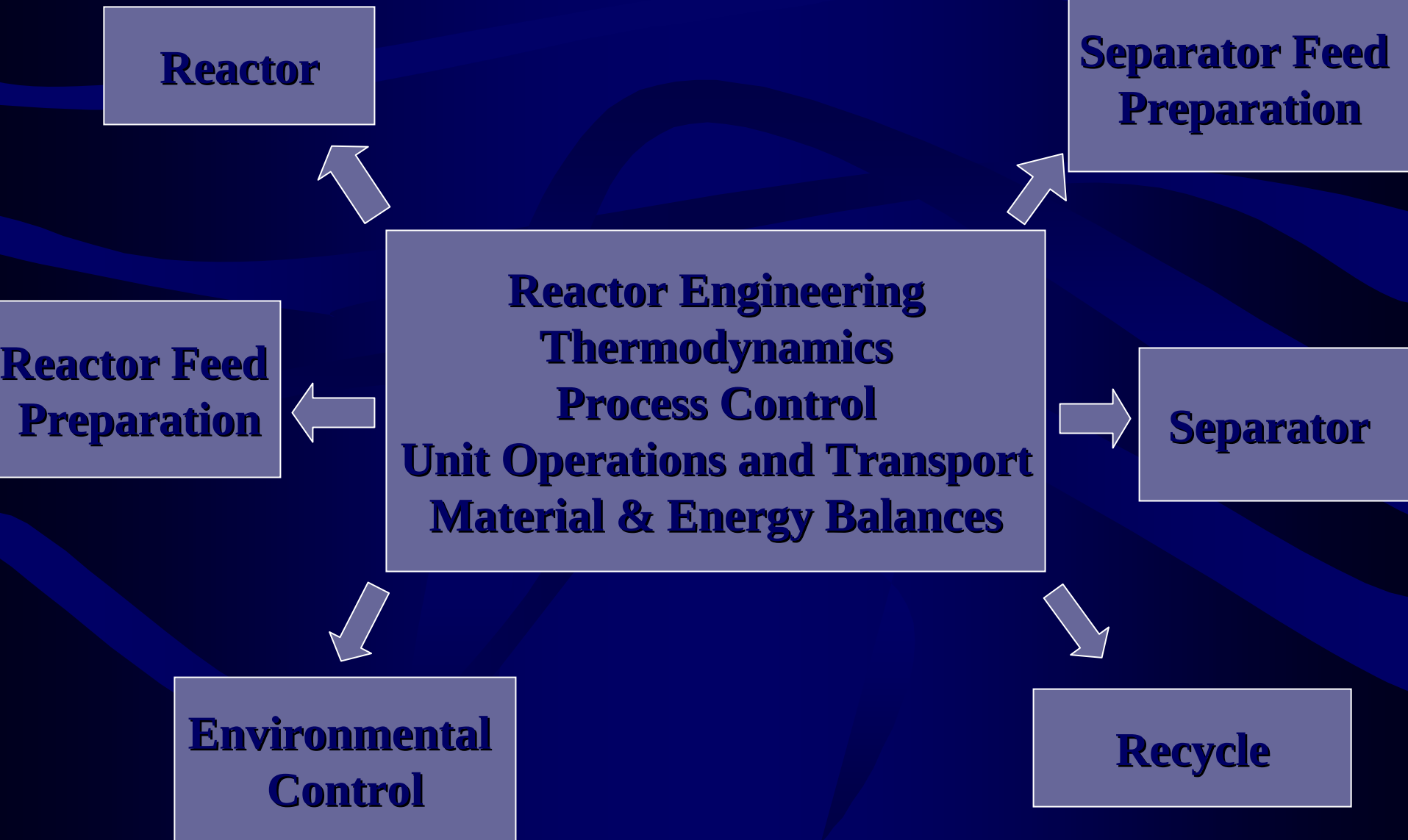
1) Introduction

2) Information needed prior to Synthesis of a PFD.

3) Reactor Section.

4) Separator Section.

Introduction



Introduction

Broader context of project

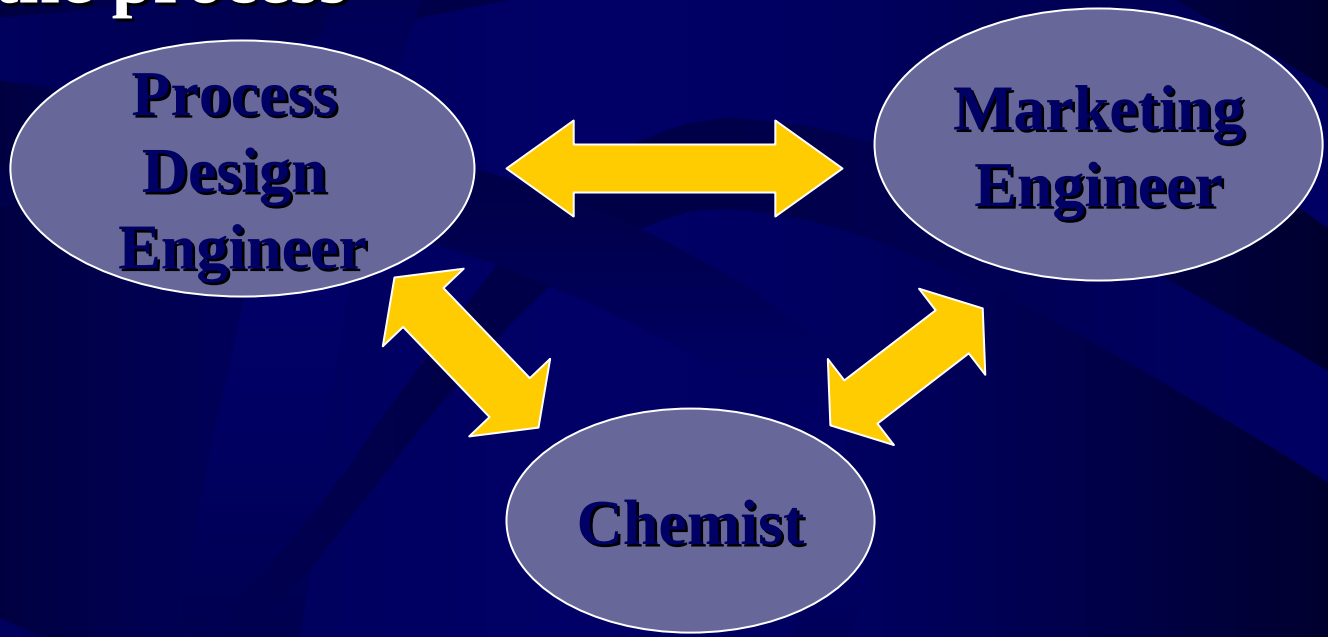
- **Environmental concerns**
- **Customer expectations**
- **Return on investment, etc.**

Important details

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

Introduction

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



Information

- **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.**

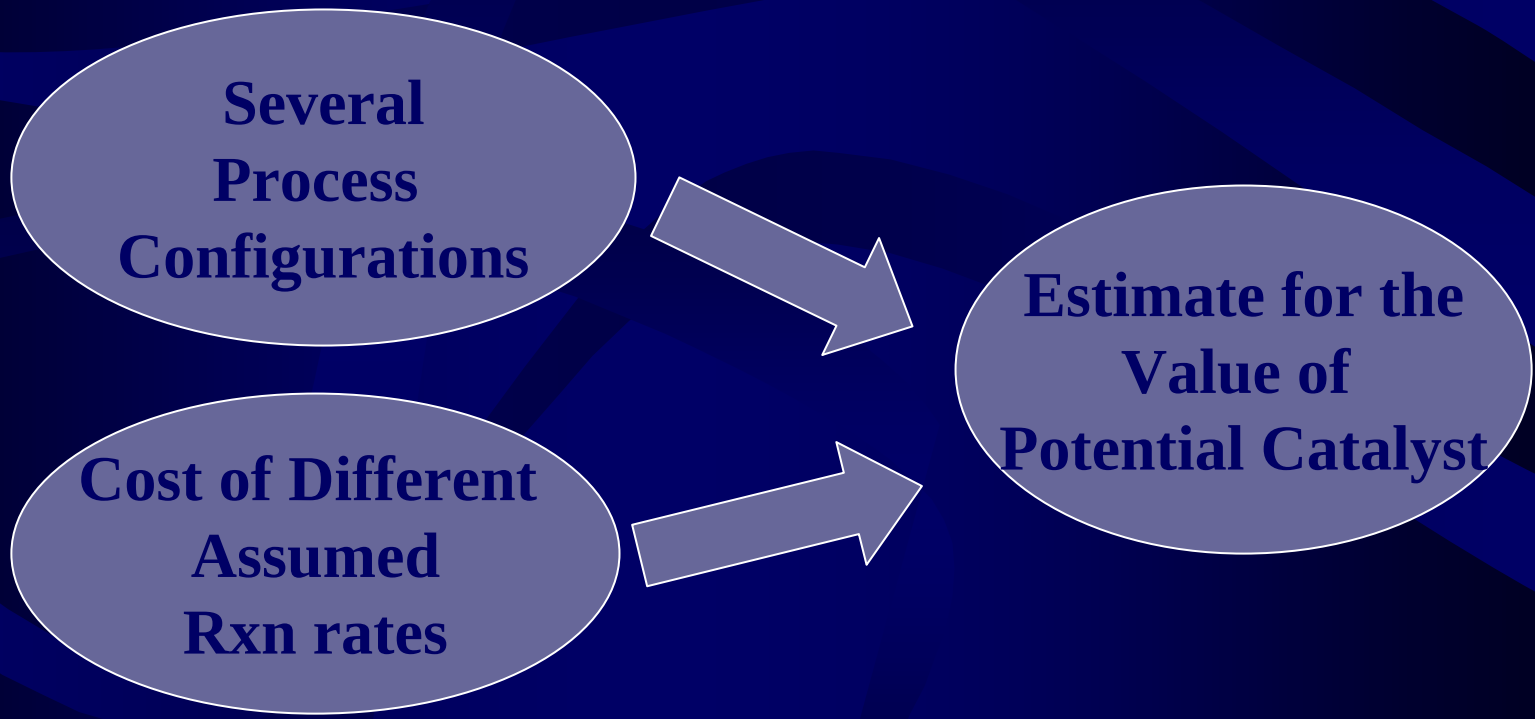
Information

- 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

Information

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

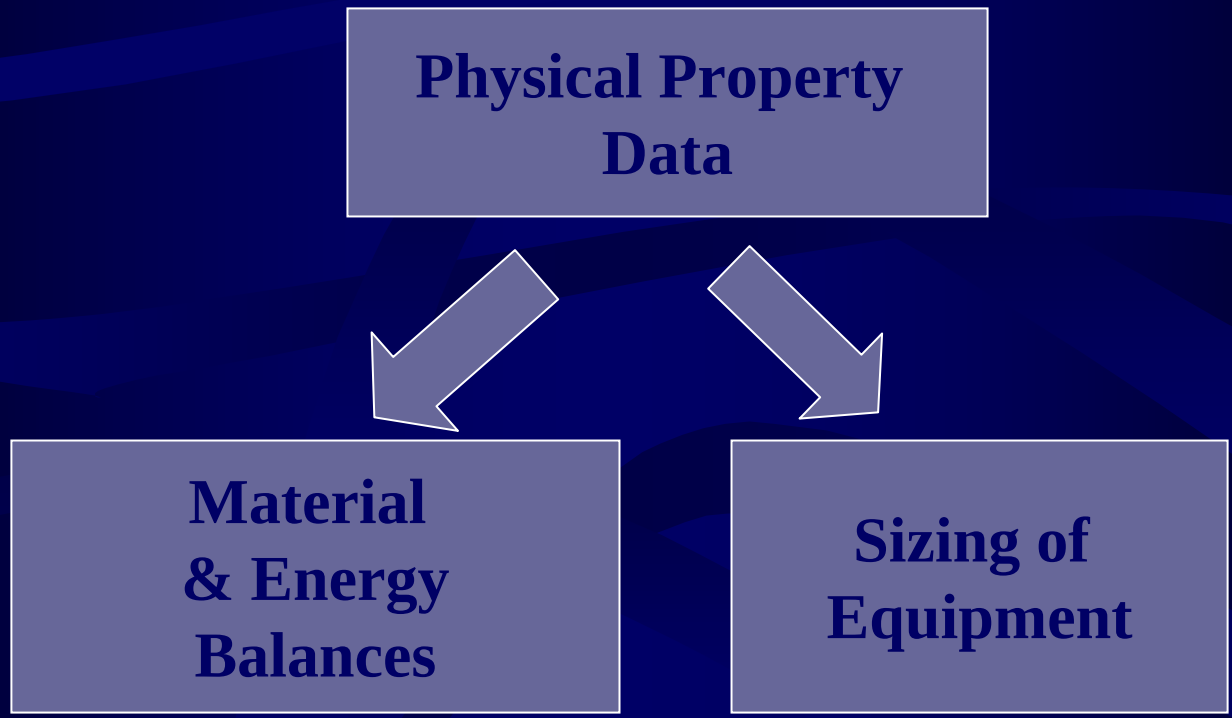
Answer: Yes



Information

- 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.

Information



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

Information

- 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.

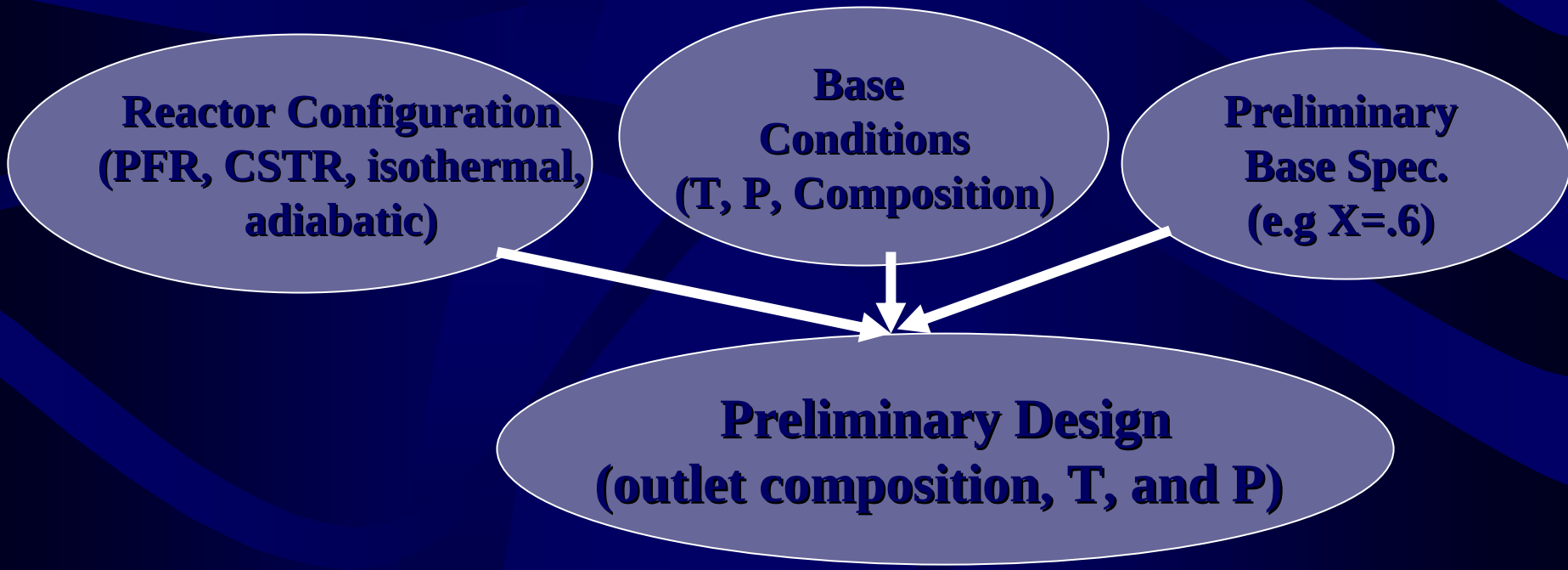
Information

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

Reactor Section

- For a process with a reactor, synthesis of PFD often begins with the reactor section.

- Develop a feasible PFD (base-case design)



Reactor Section

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?

Reactor Section

Important Questions

❺ Is the main reaction exothermic or endothermic?

❻ What side reactions occur, and what is the selectivity of the desired reaction?

❼ What is the approximate single-pass conversion?

❽ For gas-phase oxidations, should the reactor feed be outside the explosive limits?