Lecture 2 Fundamentals of Conversion, Product Yield, and Calculation of Key Reactor Parameters

Goal of the lecture: To study the fundamental principles of chemical conversion, product yield, and the main parameters used to evaluate and design chemical reactors.

Brief lecture notes: In this lecture, we explore the essential macrokinetic parameters that characterize the performance of chemical reactors. Students will learn how to define and calculate conversion, selectivity, and yield, and how these parameters are connected with reactor design and process efficiency. The lecture also introduces the main types of reactors (batch, plug flow, and continuous stirred-tank reactors) and their mathematical descriptions. Special attention is given to the derivation of basic rate expressions, material balance equations, and methods to evaluate reaction performance under isothermal and non-isothermal conditions. The lecture concludes with a discussion on the optimization of reactor parameters for maximum product yield and economic efficiency.

Main part

Chemical reactions rarely reach complete conversion of reactants; thus, understanding conversion (X), selectivity (S), and yield (Y) is crucial for reactor design and process optimization. These parameters quantitatively describe how effectively raw materials are transformed into desired products.

Conversion (X) represents the fraction of a reactant that reacts:

$$X_A = \frac{F_{A0} - F_A}{F_{A0}}$$

where F_{A0} and F_A are the molar flow rates of reactant A at the inlet and outlet of the reactor, respectively.

Selectivity (S) measures how efficiently the reactant is converted into the desired product compared to undesired by-products:

$$S = \frac{\text{moles of desired product formed}}{\text{moles of reactant consumed}}$$

Yield (Y) combines both conversion and selectivity, providing an overall measure of the efficiency of producing the target compound:

$$Y = X \times S$$

Key Reactor Parameters

The design and analysis of reactors rely on material and energy balances, kinetic data, and flow characteristics. The most common types of reactors include:

1. Batch Reactor (BR):
   Suitable for small-scale production or laboratory studies, where reactants are charged, reacted for a set time, and then discharged.
   The material balance is expressed as:

$$\frac{dN_A}{dt} = -r_A V$$

where r_A is the reaction rate and V is the reactor volume.

2. Continuous Stirred-Tank Reactor (CSTR):
   Operates at steady state with perfect mixing. The outlet composition equals the reactor composition.
   The design equation is:
$$F_{A0} - F_A = -r_A V$$
3. Plug Flow Reactor (PFR):
   Assumes no back-mixing; concentration changes along the reactor length. The design equation is:
$$\frac{dF_A}{dV} = r_A$$

Factors Affecting Conversion and Yield

- Temperature: Higher temperature increases reaction rate but may promote side reactions.
- Pressure: Especially important in gas-phase reactions; affects equilibrium and rate.
- Catalyst: Enhances desired reaction rate and selectivity.
- Residence Time: Determines how long reactants stay in the reactor; too short leads to incomplete conversion, too long may increase by-products.
- Reactor Design: Flow regime (mixing, turbulence, laminarity) significantly affects conversion and selectivity.

Optimization of Reactor Performance

In industrial practice, optimization involves balancing conversion, yield, and reactor cost. High conversion may not always mean high yield due to competing reactions.Process engineers use computational modeling and experimental data to select the most suitable reactor type and operating conditions.

Figure 1 – Schematic representation of different reactor types

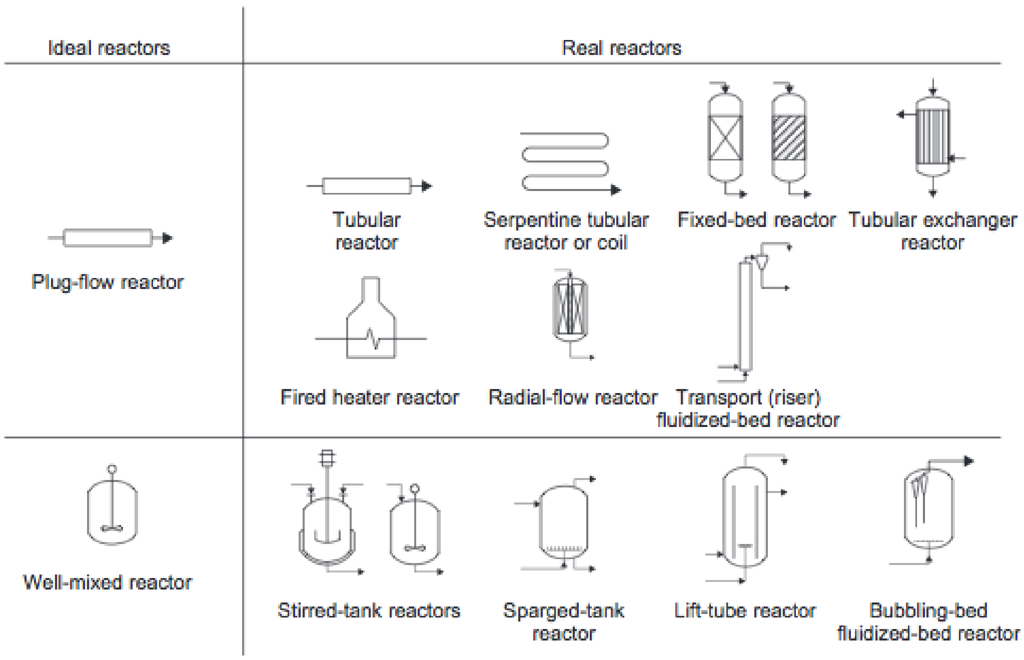

Table 1 – Comparison of Key Reactor Characteristics

Reactor Type	Operation Mode	Mixing Behavior	Typical Use	Advantages	Limitations
Batch Reactor	Unsteady-state	Perfect mixing	Small-scale, lab	Flexible operation	Poor control at scale
CSTR	Steady-state	Perfect mixing	Liquid-phase reactions	Uniform composition	Lower conversion per pass
PFR	Steady-state	No mixing along flow	Gas-phase, continuous	High conversion	Complex design and control

Questions for self-control

1. What is the difference between conversion, selectivity, and yield?
2. How does temperature influence selectivity in parallel reactions?
3. What are the main differences between batch and continuous reactors?
4. How is residence time related to conversion in plug flow reactors?
5. What factors determine the optimal reactor type for a specific reaction?

Literature

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