

Lecture 6 Molar Flows and Volumes in Continuous Reactors

Goal of the lecture: To study the relationships between molar flow rates, concentration, and volumetric flow in continuous reactors and how these parameters affect reactor performance and conversion.

Brief lecture notes: This lecture explores the fundamental relationships between molar flow, volumetric flow, and reactor volume in continuous chemical reactors. It covers steady-state mass balances, the influence of density changes due to chemical reactions, and the connection between flow properties and reactor design equations. The discussion includes both liquid-phase and gas-phase systems, emphasizing the impact of compressibility and conversion on molar flow and volumetric rate. The lecture also compares how these parameters vary in Continuous Stirred-Tank Reactors (CSTRs) and Plug Flow Reactors (PFRs), forming the basis for kinetic analysis and process optimization.

Main Part

In continuous reactors, reactants and products continuously flow in and out, maintaining steady-state operation. The molar flow rate F_i of component i is defined as the number of moles passing through a given cross-section per unit time. It is linked to the concentration C_i and volumetric flow rate v through the relation:

$$F_i = C_i v$$

This equation is central to reactor design, as it allows expressing balances and rate equations in terms of measurable quantities.

1. Molar Flow Balance

At steady state, the molar balance for a reacting species A in a continuous reactor can be expressed as:

$$\frac{dF_A}{dV} = r_A$$

where r_A is the rate of reaction per unit volume and V is the reactor volume. This equation applies directly to plug flow reactors (PFRs). For a CSTR, the balance simplifies to:

$$F_{A0} - F_A = -r_A V$$

These relations form the basis for calculating conversion, reactor volume, and performance under continuous operation.

Volumetric Flow and Density Changes

In liquid-phase systems, density changes with conversion are usually negligible, and the volumetric flow rate v can be assumed constant. However, in gas-phase systems, the total number of moles and thus the volumetric flow rate may change due to reaction stoichiometry.

For a gas-phase reaction at constant temperature and pressure:

$$\frac{v}{v_0} = \frac{1 + \varepsilon X_A}{1}$$

where ε is the fractional change in moles per mole of A reacted, and X_A is the conversion of A .

The term ε is defined as:

$$\varepsilon = \frac{\sum_i v_i}{v_A}$$

where v_i are stoichiometric coefficients. This correction is crucial when dealing with gaseous reactions, as molar flow and volumetric flow are not constant along the reactor.

Relationship Between Conversion and Flow

The molar flow of A at any point in the reactor is related to its inlet flow and conversion as:

$$F_A = F_{A0}(1 - X_A)$$

Thus, combining with the rate expression:

$$\frac{dX_A}{dV} = \frac{-r_A}{F_{A0}}$$

These equations are fundamental in reactor sizing and design. The volumetric flow rate v may also vary with conversion for gas-phase reactions, affecting the residence time and reaction rate distribution along the reactor length.

Applications in CSTR and PFR Design

In a CSTR, all variables are uniform throughout the reactor, and the design equation is:

$$V = \frac{F_{A0}X_A}{-r_A}$$

For a PFR, the design must account for varying flow and concentration:

$$\int_0^{X_A} \frac{dX_A}{-r_A} = \frac{V}{F_{A0}}$$

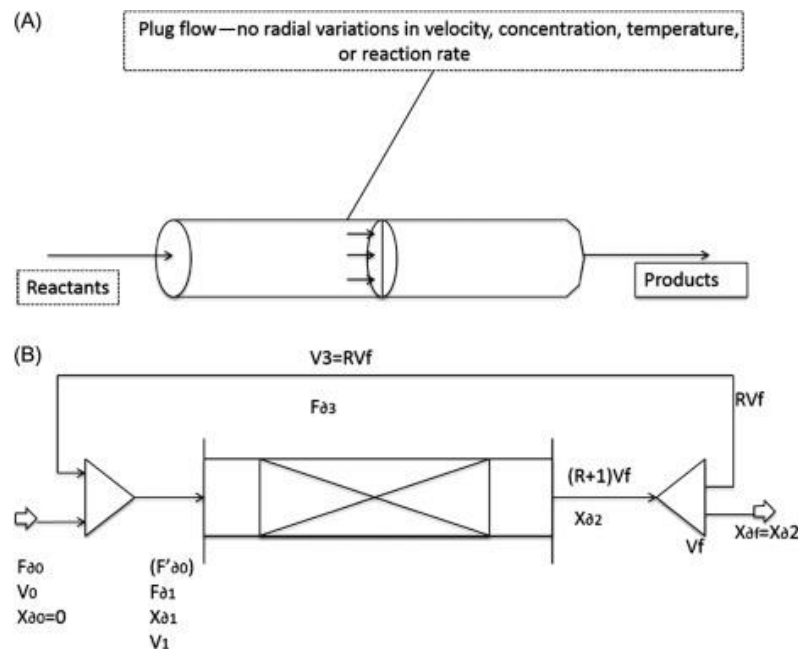
When volumetric flow is not constant, the integral becomes more complex and must include $v(X_A)$, particularly for gaseous systems.

Understanding molar and volumetric flow behavior is essential for accurately predicting reactor performance, scaling up processes, and optimizing reaction conditions. It directly influences conversion, residence time, and reactor size.

Table 1. Comparison of Flow Characteristics in Continuous Reactors

Parameter	CSTR	PFR
Flow pattern	Complete mixing	Plug flow (no mixing in axial direction)
Molar flow change	Uniform throughout reactor	Varies along length
Volumetric flow	Constant (liquid), variable (gas)	May vary with conversion
Residence time	Single value	Distributed along length
Typical application	Homogeneous liquid reactions	Gas-phase, high conversion processes

Figure 1. Plug flow



Questions for Self-Control

1. What is the relationship between molar flow rate, concentration, and volumetric flow?
2. How does the molar flow of reactant A change with conversion in a continuous reactor?
3. Why can volumetric flow rate be assumed constant in liquid-phase but not gas-phase systems?
4. How do molar flows differ between CSTR and PFR reactors?
5. What is the significance of the parameter ϵ in gas-phase reactions?

Literature

1. Fogler, H. S. Elements of Chemical Reaction Engineering, 5th Ed., Prentice Hall, 2016.
2. Levenspiel, O. Chemical Reaction Engineering, 3rd Ed., Wiley, 1999.
3. Froment, G. F., Bischoff, K. B. Chemical Reactor Analysis and Design, Wiley, 2011.
4. Hill, C. G. An Introduction to Chemical Engineering Kinetics & Reactor Design, Wiley, 1977.
5. Smith, J. M. Chemical Engineering Kinetics, 3rd Ed., McGraw-Hill, 1981.