# Reactor

## 1 Batch Reactor

### 1.1 Overview

Batch reactor is a system where a certain amount of reactants are loaded into the reactor, and then the reaction is allowed to proceed for a certain amount of time without any additional inputs or outputs. This is in contrast to a continuous reactor, where reactants continuously flow into the reactor and products continuously flow out.

### 1.2 Constant Pressure

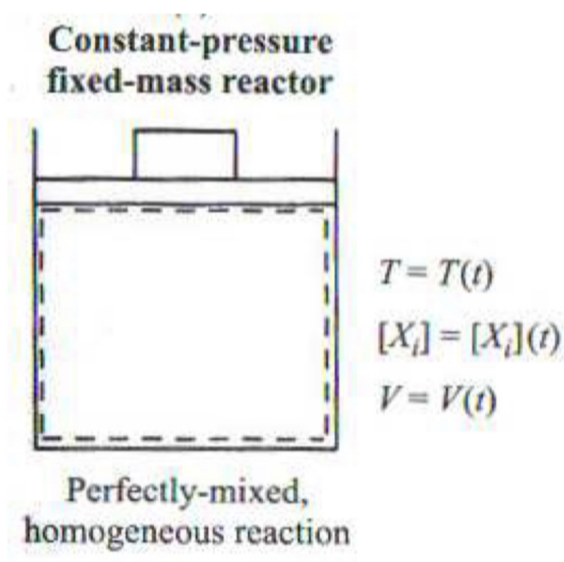


Figure 1: Constant Pressure Batch Reactor.

Features:

1. Massless piston that can rapidly allow gas to expand
2. Unconfined mixture that can't mix with ambient
3. Assume uniform
4. $Da_{mix} >> 1$

### 1.3 Constant Volume

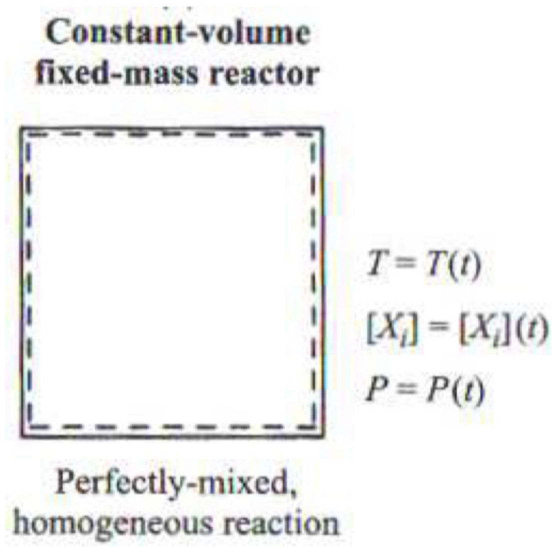


Figure 2: Constant Volume Batch Reactor.

Features:

1. Fast reactions
2. $Da_{mix} >> 1$, no mixing between fluid elements
3. Can be uniform or stratified, pressure coupling between layers

## 2 Well-Stirred Reactor

### 2.1 Overview

The well-stirred reactor model is an idealization and simplification that assumes perfect mixing within the reactor. In other words, it is assumed that the reactants (e.g., fuel and oxidizer) are immediately and perfectly mixed upon entering the reactor, and that the composition, temperature, and pressure are uniform throughout the reactor at any given moment in time.

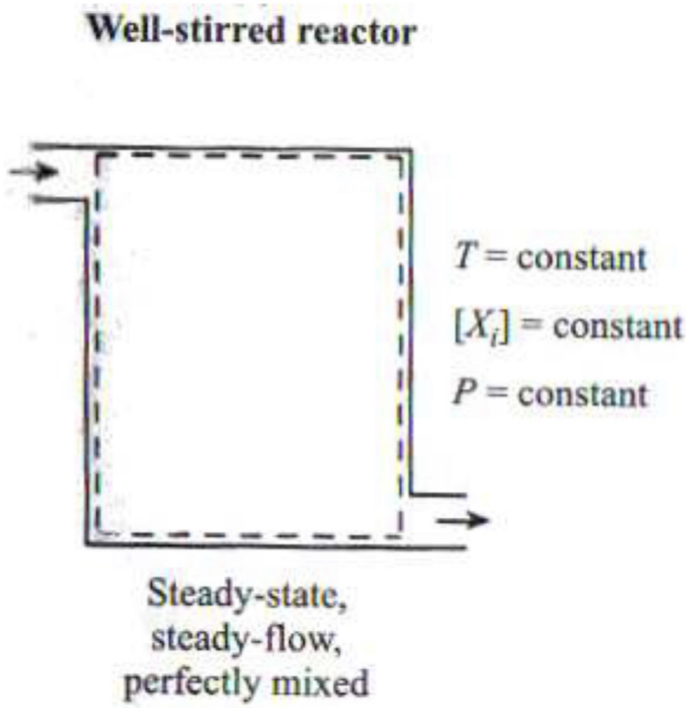


Figure 3: Well-Stirred Reactor.

## 2.2 Features

1. $Da_{mix} = \dfrac{\tau_{mix}}{\tau_{chem}} << 1$
2. Low pressure, low speed reactors
3. Internal properties are the same as the outlet due to fast mixing
4. Results depend on residence time

## 2.3 Governing Equations

**Mass conservation**

$$\frac{dm_{cv}}{dt} = \dot{m}_{in} - \dot{m}_{out}$$

**Species conservation**

$$\frac{dY_i}{dt} = \frac{\dot{m}_{in}}{\rho V}\left(Y_{i,in} - Y_i\right) + \frac{\dot{\omega}_i MW_i}{\rho}$$

**Energy**

$$c_{p_{mix}}\frac{dT}{dt} = \frac{\dot{m}_{in}}{\rho V}\sum_i Y_{i,in}\left(h_{i,in} - h_i\right) - \frac{\sum_i h_i \dot{\omega}_i MW_i}{\rho} + \frac{\dot{q}'''}{\rho} - \frac{1}{\rho}\frac{dp}{dt}$$

**Residence time**

$$\tau_{res} \equiv \frac{\rho V}{\dot{m}_{in}} = \frac{m}{\dot{m}_{in}}$$

**Variables**

- inputs: $\dot{m}_{in}$, $Y_{i,in}$, $T_{in}$, $\dot{q}'''_{in}$
- unknowns: $\rho$, $V$, $\dot{m}_{out}$, $N \times Y_i$, $T$, $p$
- $2 + N$ ODEs, 1 algebraic equation $\Rightarrow$ need 2 more constraints, e.g., $V(t)$ and $p(t)$
- steady state assumption simplifies equations to a set of $2 + N$ coupled non-linear algebraic equations, making the system solvable without additional constraints

# 3 Plug-Flow Reactor

## 3.1 Overview

In the context of combustion, PFR represents a scenario where the flow of reactants (fuel and oxidizer) moves in one direction, without any backmixing. As the mixture progresses along the length of the reactor, the chemical reactions occur, converting reactants into products.

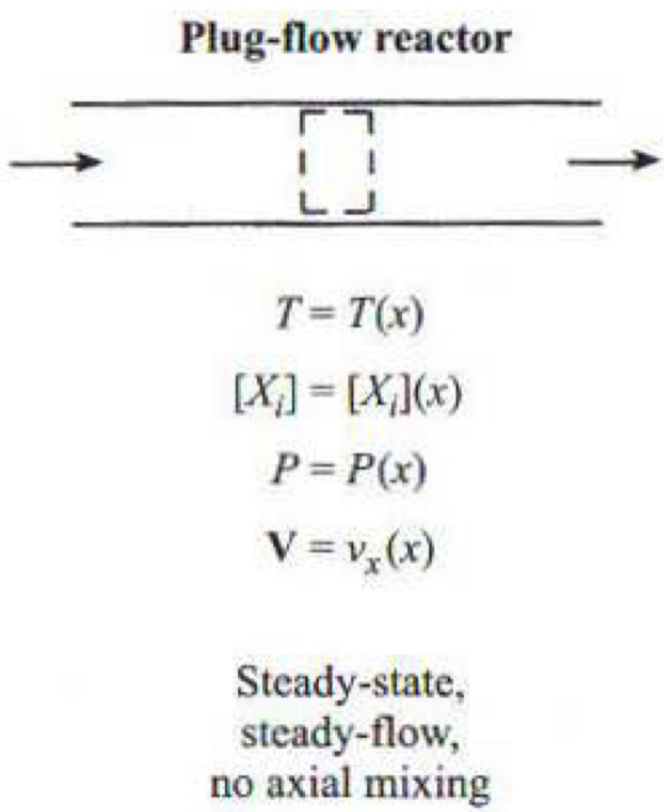


Figure 4: Plug-Flow Reactor.

## 3.2 Features

1. Steady-state, steady flow
2. Negligible kinetic energy
3. No mixing in the axial direction and no axial diffusive transport - 1D, $Da_x = \infty$
4. No cross-stream variation - 1D
5. Residence times varies inversely with velocity

## 3.3 Governing Equations

**Mass conservation**

$$\frac{d\left(\rho u_x A\right)}{dx} = 0$$

**Momentum**

$$\rho u_x A \frac{du_x}{dx} = -A\frac{dP}{dx} - P\frac{dA}{dx} - \tau_w P$$

where the friction coefficient is defined as,

$$\tau_w = f(\mathrm{Re})\frac{1}{2}\rho u^2$$

**Energy conservation**

$$\rho u_x \frac{dj}{dx} = \dot{q}'''_{in}$$

using the perfect gas assumption, i.e., $h = f(T, Y_i)$,

$$\rho u_x c_{p_{mix}} \frac{dT}{dx} = \dot{q}'''_{in} - \sum_i h_i \dot{\omega}_i MW_i$$

**Species conservation**

$$\rho u_x \frac{dY_i}{dx} = \dot{\omega}_i MW_i$$