

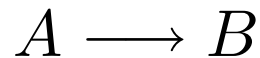
Process Model

A process model is a set of equations, including the necessary input data to solve the equations, that allow us to **predict** the behavior of a chemical process system.

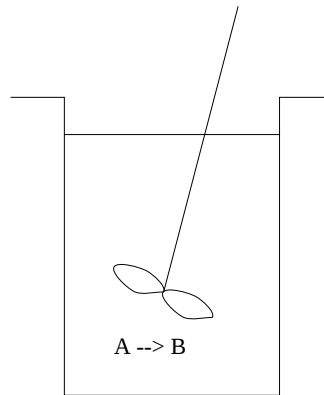
1. **Fundamental Model:** Derived from
 - Material and energy balances
 - Physical and Chemical Properties
2. **Empirical Model:** Obtained by “fitting” data
 - Numerical Methods
 - Statistical Analysis

Example 1

The following liquid-phase, isothermal first order reaction, with rate constant k , is occurring in a batch reactor.



How does the concentration of species A change with time if the initial concentration is C_{A0} ?



Batch Reactor with First Order Reaction

Fundamental Model

$$\begin{aligned}\frac{dC_A}{dt} &= -kC_A \\ C_A(0) &= C_{A0}\end{aligned}$$

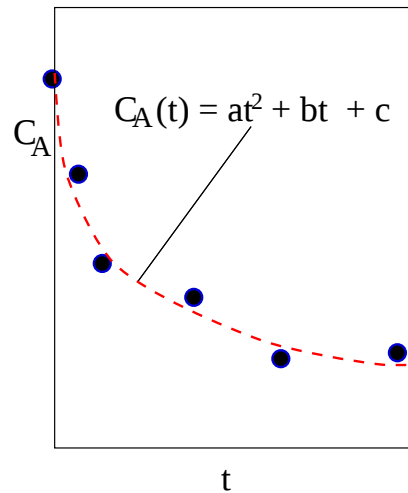
Integrating:

$$C_A = C_{A0}e^{-kt}$$

If k is known *a priori*, the above expression tells us how C_A changes with time.

Empirical Model

- **Measure** C_A with t and plot the data.
- **Find** an equation that “best fits” the data.



Types of Process Models

1. **Steady state** models.
2. **Dynamic** models.

In this course, we will develop:

- **dynamic** models from **first principles**.
- **approximate** models of chemical processes.

Reasons for Developing Process Models

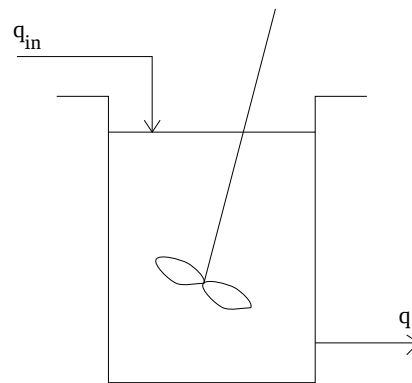
1. Operator training
2. Process design
3. Safety
4. Control system design

Developing Dynamic Process Models

- **Step 1:** Problem statement
- **Step 2:** Assembly of information
 - Sketch
 - System and Notation
 - Axiomatic laws
 - Rate laws and Constitutive relations
 - Assumptions
- **Step 3:** Combine information
- **Step 4:** Boundary conditions/Constraints
- **Step 5:** Simplify equations

Example 2

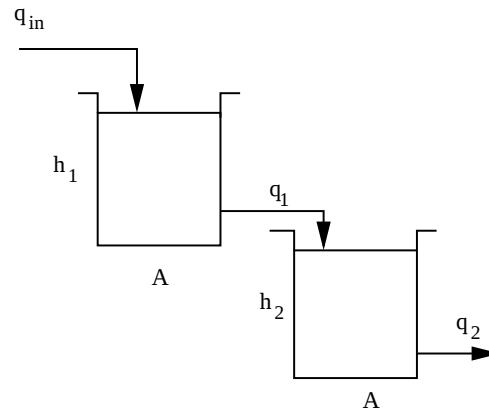
A typical liquid storage process is shown in the figure below. How does the height change with time ?



Filling Process

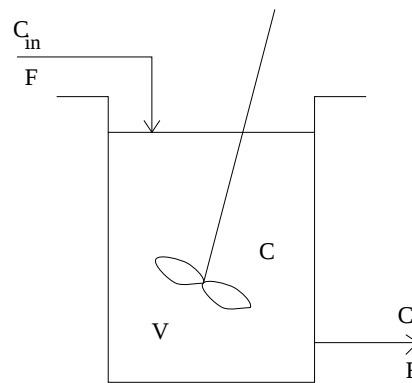
Example 3

Two tanks-in-series are shown in the figure below. How do the heights of the liquid in the two tanks change with time ?



Example 4

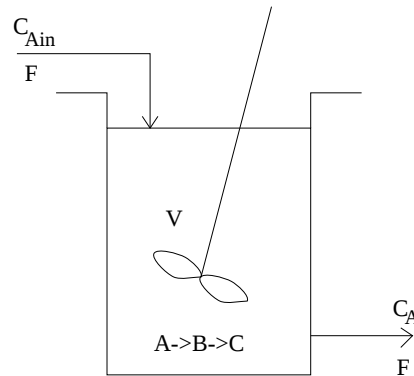
A mixing process is shown in the figure below.
How does the outlet concentration change with time ?



Mixing Process

Example 5

A series reaction is taking place in a CSTR. The first reaction is second order w.r.t. A and the second reaction is first order w.r.t. B . How do the outlet concentrations of species A , B , and C change with time ?



Series Reaction in CSTR