Overview of lecture topics

- Topic 1: Course introduction
- Topic 2: Introduction to frequency domain and Laplace transformation
- Topic 3: Dynamic Behavior of Linear systems
- Topic 4: Frequency Response Analysis and Bode plots
- Topic 5: Mathematical Description of Chemical Systems
- Topic 6: Nonlinear ODE’s, Linearity, Linearization Feedback, Stability, Root Locus
- Topic 7: Feedback Controller Design and Bode stability
- Topic 8: Advanced (Enhanced) Process Control

Dynamics and Control of Processes

Lecture 5: Mathematical Description of Chemical Systems

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Course 6E8X0

Outline

- Model definition
- Why do we need models?
- What type of models are applied?
- Models that you know
- What modelling principles may be applied?
- Model design procedure
- Some modelling examples

Model definition

Mathematical Model

- **Eykhoff (1974)**

  " A representation of the essential aspects of an existing system (or a system to be constructed) which represents knowledge of that system in a usable form"

- ***Denn (1986)***

  "A mathematical model of a process is a system of equations that for given specific input data is representative of the response of the process to a corresponding set of inputs"

Why do we need models?

- Understand processes
- Process design
- Estimate non-measured variables
- Detection of failures and limits
- Evaluate control strategies
- Process optimization

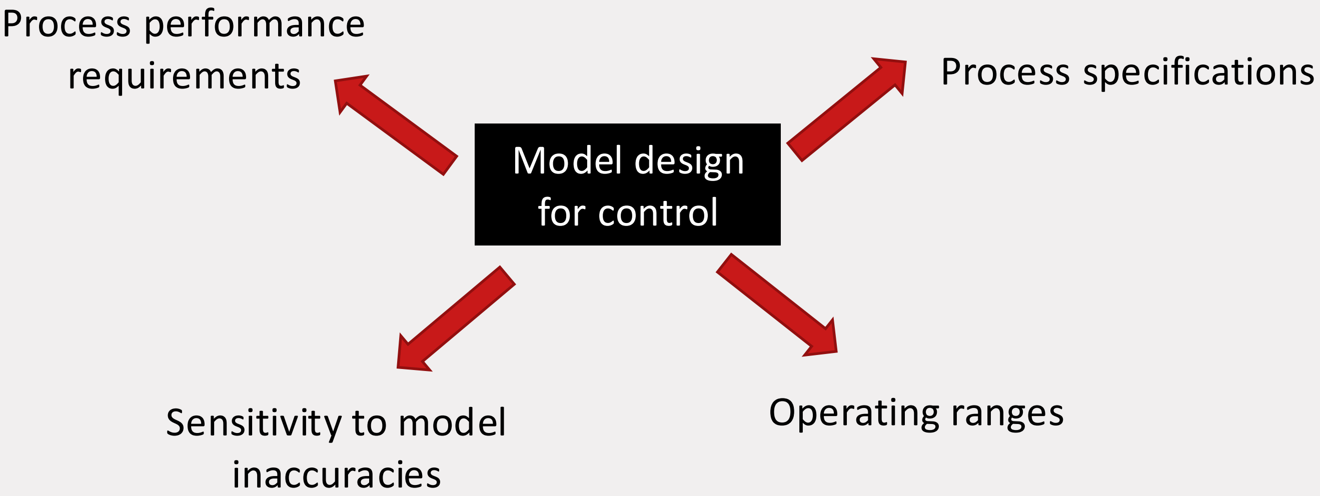
Why do we need models?

5 questions that have to be answered in **process control** through modelling:

1. Which are the variables of the process?
   - Inputs, outputs, manipulated variables, disturbances
2. Which variables can be influenced?
   - Number of degrees of freedom
   - Cause-effect relationships
   - Process controllability
3. Over what range can variables be altered?
   - Operating window
4. How effectively can feedback maintain the process at desired conditions?
   - Sign, magnitude, speed and shape of response
5. How sensitive are results obtained to small changes in process behavior?

Why do we need models?

Models represent the relevant process behavior needed for control system design



What types of models are applied?

Models applied for the design of process control and optimization systems can be categorized by the following types of mathematical models:

Fundamental models

- First principle models
- Mass, energy, momentum balances

Empirical models

- Data-driven models
- Based on experience or a priori knowledge of the system

Steady-state models

- Describe an operation point and small variations around it

Dynamic models

- Describes the transient behaviour

Other classifications

Deterministic or stochastic Variations

Lumped or distributed models Parameters

Models that you know

Conservation laws

- Conservation of mass
- Conservation of Energy
- Conservation of Momentum

Procedure

Take a control volume (system)
Define the conserved quantity
Analyze according to:

$$\left\{\begin{array}{l}\text{Rate of \textbf{accumulation}}\\ \text{of conserved quantity}\\ \text{in the system}\end{array}\right\} = \left\{\begin{array}{l}\text{Rate of \textbf{input} of}\\ \text{conserved quantity}\\ \text{in the system}\end{array}\right\} - \left\{\begin{array}{l}\text{Rate of \textbf{output} of}\\ \text{conserved quantity}\\ \text{in the system}\end{array}\right\} + \left\{\begin{array}{l}\text{Rate of \textbf{production}}\\ \text{of conserved quantity}\\ \text{in the system}\end{array}\right\} - \left\{\begin{array}{l}\text{Rate of \textbf{consumption}}\\ \text{of conserved quantity}\\ \text{in the system}\end{array}\right\}$$

Accumulation = Input - Output + Production - Consumption

Models that you know

Constitutive equations

- Properties of matter
  - Calorific capacity
  - Density
- Transport equations
  - Newton Law (momentum)
  - Fourier Law (heat transfer)
  - Fick's diffusion Law (mass)
- Reaction kinetics
  - Mass action kinetics
  - Arrhenius
- Thermodynamic equations
  - State equations (Ideal gas equation)
  - Phase equilibrium

- Heat transfer $Q = UA\Delta T$
- Chemical Reaction Rate $r_A = k_0 e^{-E/RT} C_A$
- Equation of state $pV = nRT$
- Fluid flow $F = C_v \cdot \left(\Delta P / \rho \right)^{1/2}$
- Phase equilibrium $y_i = K_i \cdot x_i$

Model Design Procedure

It is extremely important to closely follow a well structured design procedure to develop models that comply with the ultimate requirements that meet the design specifications of the process control system

Design Procedure basic steps:

- Define goals for the model
- Prepare basic process information
- Formulate the model
- Determine a solution with respect to model behaviour
- Analyse the solution results for correctness and for performance
- Validate the model

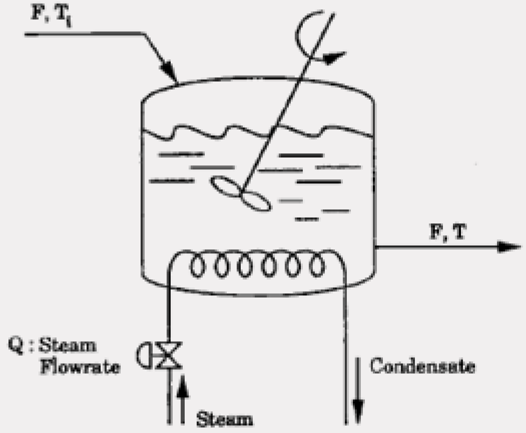
Model design procedure

Definition of goals for the model

- Why and what do I want to model?
  - Control
  - Getting new information
  - Simulations /prediction
- How simple or complex should the model be?
- Which are the important aspects to be considered in the model?
  - Requirements with respect to model accuracies
  - Design specifications
- How deep are the fundamental principles for this process?

Model Design Procedure

Example: A Continuous Stirred Tank Heating System



Goal:

Determination of the dynamic response of the tank temperature to changes in steam flow

Model Design Procedure

Prepare basic process information

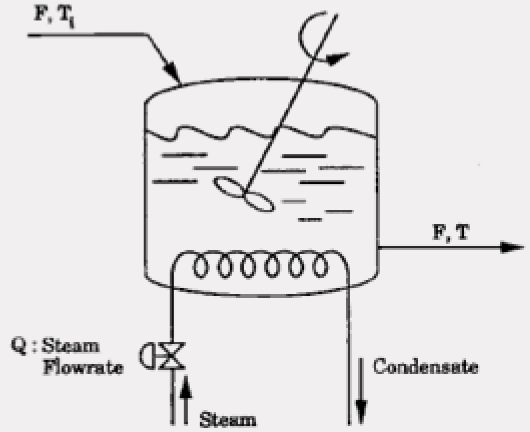
- Make a sketch of the process and identify the system that needs to be modelled
- Identify the variables of interest of the process in relation to the application of the model
- Explicitly state the assumptions made for modelling
- List the available data

Model design procedure

Example:

Information

- The system is the stirred tank
  - Important variables:
    - Temperature in the tank (output variable)
    - Heat supplied by the steam (manipulated input variable)



Assumptions

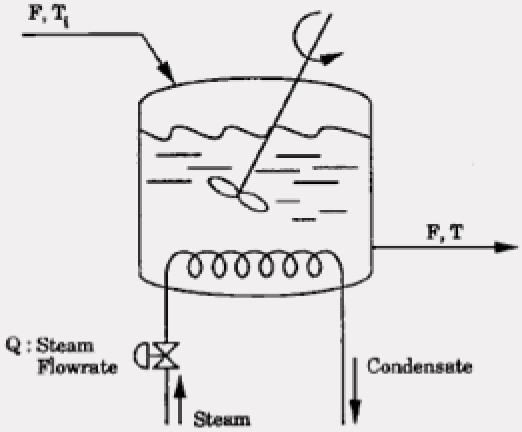
- The content of the tank is ideally mixed
- Physical properties are constant (density, heat capacity of liquid, latent heat of steam)
- All the heat supplied by the steam (including condensation heat) is transferred to the liquid content in the tank
- Heat losses to the atmosphere are considered to be negligible

Model design procedure

Example:

Process data available

- Specific heat capacity of the liquid : C_p [J/kg·K]
- Density of the liquid: ρ [kg/m^3]
- Latent heat of vaporization of steam: λ [J/kg]
- Tank volume: V [m^3]
- Initial temperature of liquid in the tank: T_0 [K]

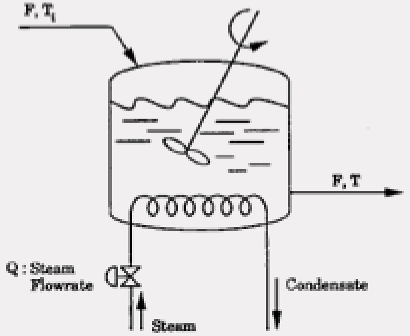


Model design procedure

Formulate the model

- Apply the relevant laws of conservation
- Apply in addition constitutive equations to get a unique solution
- Rationalize the model by combining given equations and by collecting terms
- Check the degrees of freedom
- Make the equations dimensionless by scaling of the variables

Model design procedure



The overall mass balance is not relevant (flow in = flow out) :

$$\frac{d\rho V}{dt} = \rho F - \rho F, \frac{dV}{dt} = 0$$

Mass balance

Application of the energy balance is relevant since temperature of the liquid content in the tank is of interest:

$$\underbrace{\rho C_p \frac{d\left[V\left(T - T^*\right)\right]}{dt}}_{\text{Rate of accumulation of energy}} = \underbrace{\rho F C_p \left(T_i - T^*\right)}_{\text{Rate of heat Input (Inlet steam)}} + \overbrace{\lambda Q}^{\text{Rate of heat input (steam condensation)}} - \underbrace{\rho F C_p \left(T - T^*\right)}_{\text{Rate of heat output (Outlet condensed steam)}}$$

$$\rho V C_p \frac{dT}{dt} = \rho F C_p \left(T_i - T\right) + \lambda Q$$

After simplification

Remark: T^* - reference temperature at which specific enthalpy of liquid is taken to be zero

Model design procedure

The number of degrees of freedom analysis of this model:

- Number of dependent variables: 2 (T and Q)
- Number of independent equations: 1
- Number of parameters: 4 (λ, C_p, V, ρ)
- Number of external or disturbance variables: 1 (T_{in})

Model design procedure

Determine a solution with regard to model behaviour

Two possible routes may be followed in calculating solutions of the obtained set of equations from the detailed modelling of the process:

- Try to solve the set of Differential (Algebraic) Equations analytically
  - Only feasible for relatively simple equations
  - Preferred way as it provides very much insight into the system behaviour

- Solve the equations numerically
  - Use simulation packages like Matlab/Simulink, gPROMS, Aspen Custom Modeller, Mathematica, Process Studio, Mobatec, …
  - Be aware of potential inaccuracies due to the applied solvers and the applied resolution

Model design procedure

To find a solution the equations are further simplified and re-arranged

$$\rho V C_p \frac{dT}{dt} = \rho F C_p \left(T_i - T\right) + \lambda Q \quad \Rightarrow \quad \frac{dT}{dt} + \frac{1}{\tau}T = \frac{\lambda Q}{\rho V C_p} + \frac{1}{\tau}T_i$$

with $\tau = \dfrac{V}{F}$ residence time

The model in terms of deviation variables:

$$x = T - T_s,\ u = Q - Q_s,\ d = T_i - T_{i,s}$$

@ Steady state: $\dfrac{dT}{dt} = 0$

$$\frac{1}{\tau}T_s = \frac{\lambda Q_s}{\rho V C_p} + \frac{1}{\tau}T_{i,s}$$

Model design procedure

Subtract the steady state equation from the original ODE

$$\frac{dT}{dt} - \frac{dT_s}{dt} + \frac{1}{\tau}(T - T_s) = \frac{\lambda Q}{\rho V C_p} - \frac{\lambda Q_s}{\rho V C_p} + \frac{1}{\tau}(T_i - T_s)$$

$$\frac{dx}{dt} + \frac{1}{\tau}x = \frac{\lambda}{\rho V C_p}u + \frac{1}{\tau}d \quad x(0) = 0 \text{ if } T(0) = T_s$$

Take the Laplace transform

$$sX(s) + \frac{1}{\tau}X(s) = \frac{\lambda}{\rho V C_p}U(s) + \frac{1}{\tau}D(s)$$

$$X(s) = \left(\frac{\beta\tau}{\tau s + 1}\right)U(s) + \left(\frac{1}{\tau s + 1}\right)D(s) \quad \text{with:} \beta = \frac{\lambda}{\rho V C_p}$$

Model design procedure

$$X(s) = \left(\frac{\beta\tau}{\tau s + 1}\right) U(s) + \left(\frac{1}{\tau s + 1}\right) D(s)$$

Solution:

$$x(t) = e^{-\frac{1}{\tau}} x(0) + \int_0^t e^{-\frac{t-\sigma}{\tau}} \beta u(\sigma) d\sigma + \int_0^t e^{-\frac{t-\sigma}{\tau}} \frac{1}{\tau} d(\sigma) d\sigma$$

Inverse Laplace Transformation of the terms on the right hand side

$$\frac{\beta\tau}{\tau s + 1} \Leftrightarrow \beta e^{-\frac{t}{\tau}}$$

$$\frac{1}{\tau s + 1} \Leftrightarrow \frac{1}{\tau} e^{-\frac{t}{\tau}}$$

Model design procedure

Analyse the solution results for correctness and for performance

- Check the results for correctness
  - Does the solution satisfy limiting conditions like initial and final conditions?
  - Does the solution obey implied bounds?
  - Are numerical solutions within range of expectations?

- Interpret the results obtained
  - Plot the solution
  - Check the obtained characteristic behaviour and does it meet expectations
  - Relate the results obtained to available process data and assumptions made
  - Evaluate the sensitivity of the solution
  - Answer some relevant “what if” questions

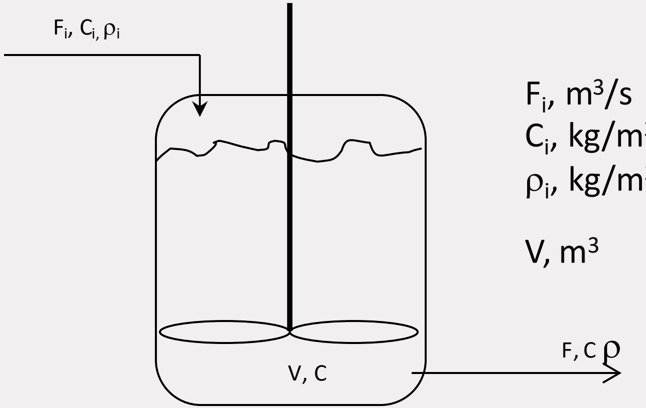
Model design procedure

Validate the model

- Select a number of key variables for validation of the model behaviour
- Compare the results obtained from validation with experimental results available
- Compare the results of a simplified model with results possibly available from a more detailed model

Some modelling examples

Continuous stirred tank reactor with no chemical reaction



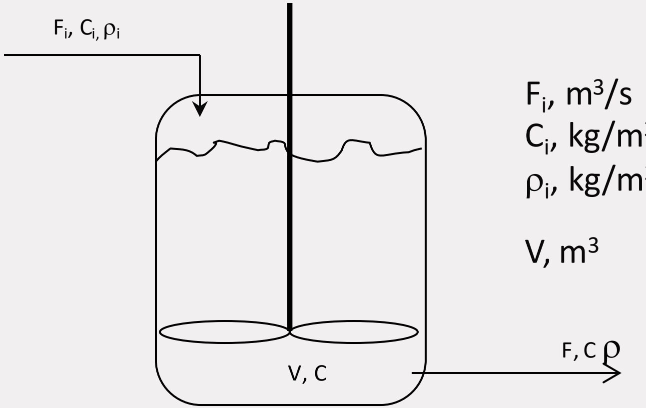
F_i, m^3/s
C_i, kg/m^3
ρ_i, kg/m^3

V, m^3

1. Define goals for the model
2. Prepare basic process information
3. Formulate the model
4. Determine a solution with regard to model behaviour
5. Analyse the solution results for correctness and for performance
6. Validate the model

Some modelling examples

Continuous stirred tank reactor with no chemical reaction



F_i, m^3/s
C_i, kg/m^3
ρ_i, kg/m^3

V, m^3

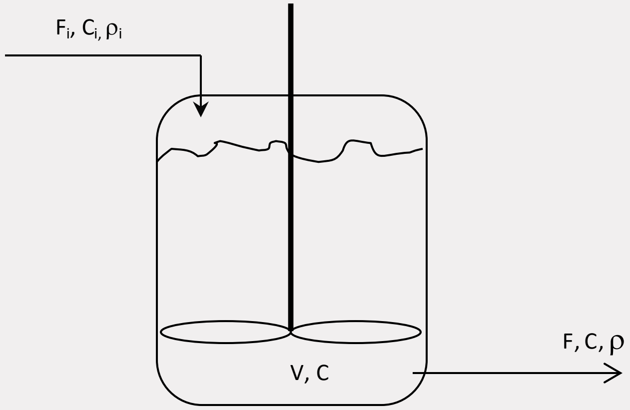
1. **Goal**: To know the changes of concentration C in the reactor
2. **Information:** density is constant
3. **Formulate the model**

Principle of conservation of mass

- Total mass
- Component balance for solute C

If you have N components, then write N-1 component balances + total mass balance

Some modeling examples



Total mass balance:

$$\frac{d(\rho V)}{dt} = \rho_i F_i - \rho F = 0$$

constant density

$$\rho_i = \rho$$

$$\frac{dV}{dt} = F_i - F$$

Component balance:

$$\frac{d(CV)}{dt} = F_i C_i - FC$$

V and C are dependent variables

$$\frac{dC}{dt} = \frac{F_i}{V} C_i - \frac{F}{V} C - \frac{C}{V}\frac{dV}{dt}$$

If we assume continuous operation F_i=F (V is constant)

$$\frac{dC}{dt} = \frac{F}{V} C_i - \frac{F}{V} C \quad \Rightarrow \quad \frac{dC}{dt} = \frac{1}{\tau}(C_i - C)$$

Some modelling examples

Rearrange

$$\frac{dC}{dt} + \frac{1}{\tau}C = \frac{1}{\tau}C_i$$

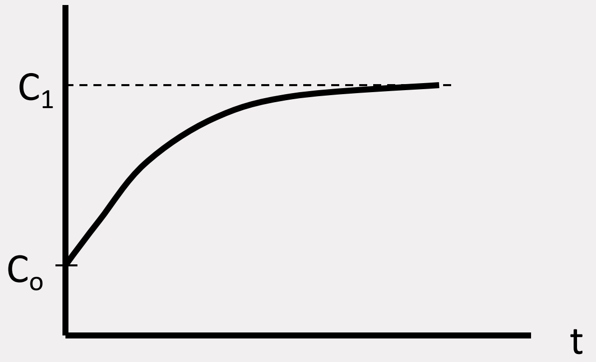
Time constant τ

Manipulated input or forcing function

$$C_i = \begin{cases} C_0 & t \leq 0 \\ C_1 & t > 0 \end{cases}$$

Solution

$$C(t) = C_1 + (C_0 - C_1)e^{-\frac{t}{\tau}}$$



Other modelling examples

Bioreactor for biomass production in continuous operation

Mass balance

$$\frac{d(\rho V)}{dt} = \rho F - \rho F = 0$$

Mass balance per component

$$\frac{d(SV)}{dt} = FS_{in} - FS - r_S V$$

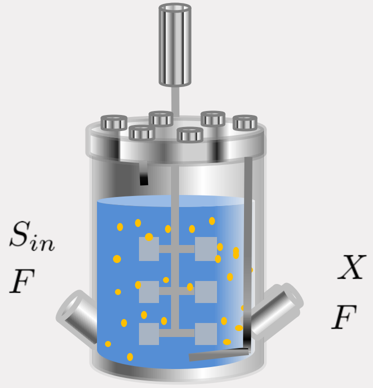
$$\frac{dS}{dt} = \frac{F}{V}(S_{in} - S) - r_S$$

$$\frac{d(XV)}{dt} = -FX + r_X V$$

$$\frac{dX}{dt} = r_X - \frac{F}{V}X$$

Define dilution rate as:

$$D = \frac{F}{V}$$



$$S \rightarrow X$$

$$r_X = \mu X$$

$$Y_{X/S} = \frac{r_X}{r_S}$$

Other modelling examples

Bioreactor for biomass production in continuous operation

Mass balance

$$\frac{dV}{dt} = F - F = 0$$

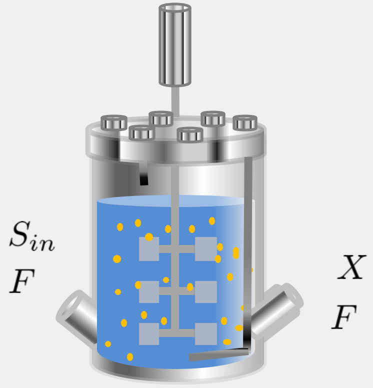
Mass balance per component

$$\frac{dS}{dt} = D(S_{in} - S) - r_S \quad \Rightarrow \quad \frac{dS}{dt} = D(S_{in} - S) - \frac{\mu X}{Y_{X,S}}$$

$$\frac{dX}{dt} = r_X - DX \quad \Rightarrow \quad \frac{dX}{dt} = (\mu - D)X$$

$$\boxed{\begin{aligned} \frac{dS}{dt} &= D(S_{in} - S) - \frac{\mu^{max}}{Y_{X,S}}\frac{S}{K_S + S}X \\ \frac{dX}{dt} &= \left(\mu^{max}\frac{S}{K_S + S} - D\right)X \end{aligned}}$$

Non linear



$$S \rightarrow X$$

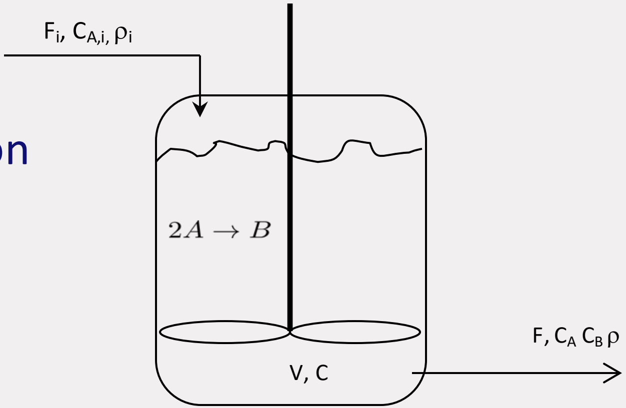
$$r_X = \mu X$$

$$Y_{X/S} = \frac{r_X}{r_S}$$

$$\mu = \mu^{max}\frac{S}{K_S + S}$$

Some modeling examples

Continuous stirred tank reactor with chemical reaction



Total balance

$$\frac{d(\rho V)}{dt} = \rho_i F_i - \rho F = 0$$

$$\frac{dV}{dt} = F_i - F$$ constant density $\rho_i = \rho$

$$\frac{dV}{dt} = 0$$ constant Volume $F_i = F$

Component balance:

$$\frac{dC_A}{dt} = \frac{F}{V} C_{A,i} - \frac{F}{V} C_A - kC_A^2$$

$$\frac{dC_B}{dt} = -\frac{F}{V} C_B - kC_A^2$$

Nonlinear