Computational Techniques
Module 8: Ordinary Differential Equations (Boundary Value Problems)

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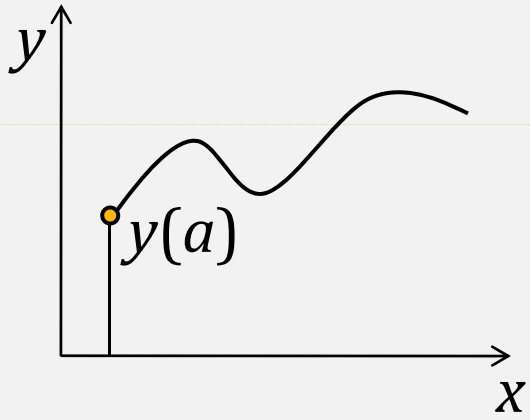
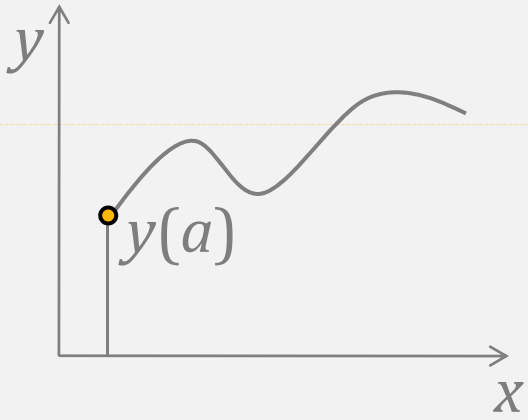
What is "Initial Value Problem"?

- Differential Equations
  - Governing equation + auxiliary conditions
- Initial value problems
  - Auxiliary conditions are specified at *one point only*



What is "Boundary Value Problem"?

- Differential Equations
  - Governing equation + auxiliary conditions
- Initial value problems
  - Auxiliary conditions are specified at *one point only*
- Boundary value problems
  - Auxiliary conditions are specified at *two points*



Reactor without Axial Dispersion

- Model for a Plug Flow Reactor
  - Model: $\left(\frac{F}{A}\right)\frac{dC_A}{dx} = -r(C_A)$
  - Initial Condition: $C_A\big|_{x=0} = C_0$

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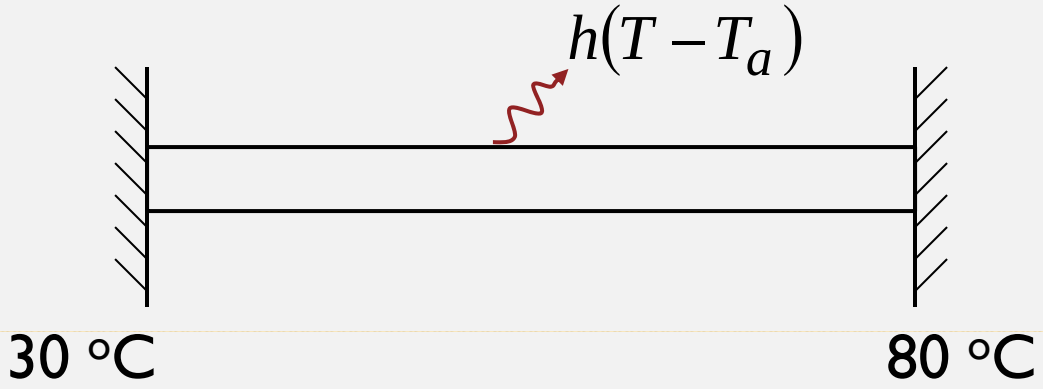
- With Axial dispersion
  - Model: $\left(\frac{F}{A}\right)\frac{dC_A}{dx} = \mathcal{D}\frac{d^2C_A}{dx^2} - r(C_A)$
  - Boundary Conditions: $C_A\big|_{x=0} = C_0;\ C'_A\big|_{x=L} = 0$

Example-2: Heat Conduction



$$0 = k\frac{\mathrm{d}^2T}{\mathrm{d}x^2} - \frac{h}{d_h}(T - T_a)$$

$$T(0) = 30;\ T(L) = 80$$

If first end is insulated, then $T'(0) = 0$

General Boundary Value Problems

- General case
  - Model $f(y'', y', y; x) = 0$
  - BCs $\varsigma_1(y', y; x)\big|_{x_1} = 0$

    $\varsigma_2(y', y; x)\big|_{x_2} = 0$

Common ChE BVP

- Second order ODE
  - Model

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + p(x,y)\frac{dy}{dx} + q(x,y) = 0$$

Linear if: $p(x)$ and $q(x,y) = r(x)\,y + s(x)$

  - Boundary conditions
    - Dirichlet: $y|_{x=a} = \alpha;\quad y|_{x=b} = \beta$
    - Neumann: $y'|_{x=a} = \alpha;\quad y'|_{x=b} = \beta$
    - Mixed: $\left(y + c_1 y'\right)\big|_{x=a} = \alpha$

In general, we have $\alpha(x,y)$ and $\beta(x,y)$

Overview

- Shooting Method
  - Solve Initial Value Problem + Algebraic Equation
- Finite Difference
  - Convert to (non-)linear equations
- Other methods (not covered in this course)
  - Function space methods
  - Finite element
  - Finite volume