PROCESS DYNAMICS AND CONTROL

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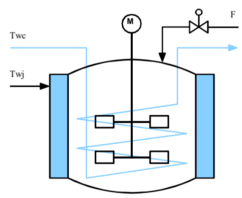
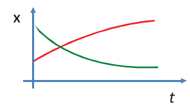
RECAP

- Importance of dynamic modeling
- Importance of process control
- Examples of control systems
- Basic definitions
  - Controlled variable, manipulated variable, disturbance variable, set point.

APPLICATIONS OF DYNAMIC MODELING

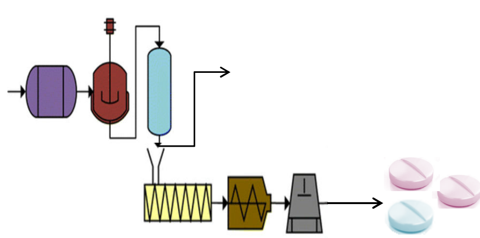
- Improve process understanding
- Train operating personnel
- Develop control strategies
- Optimize operating conditions



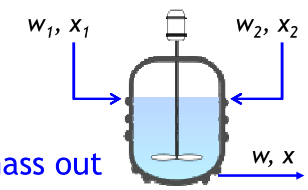


OPTIMIZING OPERATING CONDITIONS

- Examples:
  - Minimize startup time
  - Minimize startup waste
  - Maximize yield in a batch process
- We need a dynamic model for optimization



BLENDING TANK MODEL



- Steady-state model
  - Assumptions?

  0 = Rate of mass in - Rate of mass out

  $$w_1 + w_2 - w = 0$$

  $$w_1 x_1 + w_2 x_2 - wx = 0$$

- Dynamic model
  - Assumptions?

  Rate of accumulation =
  Rate of mass in - Rate of mass out

  $$\frac{d(\rho V)}{dt} = w_1 + w_2 - w$$

  $$\frac{d(\rho V x)}{dt} = w_1 x_1 + w_2 x_2 - wx$$

ORDINARY-DIFFERENTIAL EQUATIONS

- Dynamic models yield differential equations
  - Time as an independent variable

- This course is limited to ordinary differential equations (ODEs)
  - *p*: constant parameters
  - *x*: state variables

  $$\frac{d\mathrm{x}}{dt}(t) = \mathrm{f}(\mathrm{x}(t), p, t)$$

- Find state variables and parameters in the blending example.

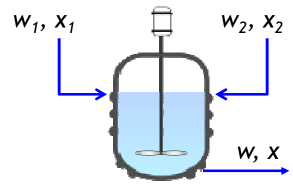
CAN WE SIMPLIFY THE MODEL?

- More assumptions?
  - Constant density

$$\rho\frac{d(V)}{dt} = w_1 + w_2 - w$$

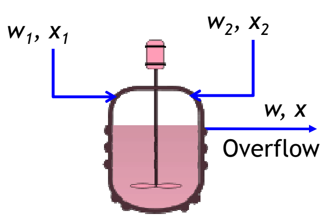
$$\rho\frac{d(Vx)}{dt} = w_1x_1 + w_2x_2 - wx$$

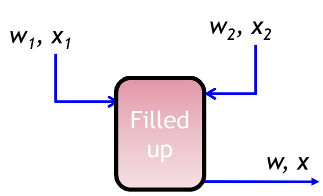
$$\rho\left(V\frac{d(x)}{dt} + x\frac{d(V)}{dt}\right) = w_1x_1 + w_2x_2 - wx$$



SIMPLIFY THE MODEL EVEN FURTHER

- Assume constant volume
- How?
  - Overflow line
  - Closed tank that is filled to capacity
  - Nearly perfect control of level





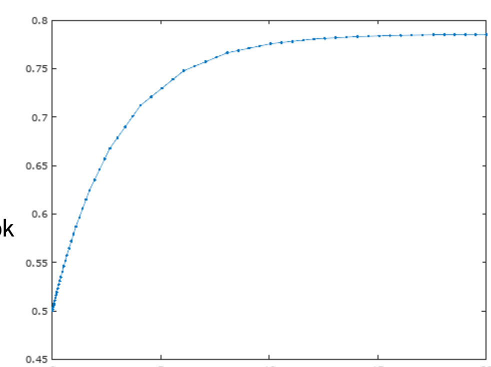
HOW TO SOLVE THE DYNAMIC MODEL

- Analytically
  - If model is simple enough
- Numerically
  - Used in most practical cases

DYNAMIC RESPONSE OF SYSTEM

- Sudden change in inlet composition x from 0.4 to 0.8.
- Initial condition
- Dynamic solution
  - Transient behavior
  - Final steady state

See Example 2.1 of Seborg's book



DEGREES OF FREEDOM (DOF) ANALYSIS

- How to know if the model can be solved?

Linear system of equations $y = Ax$

For General systems of equations $N_F = N_V - N_E$

- ➢Exactly Specified
- ➢Underspecified
- ➢Overspecified

DYNAMIC ENERGY BALANCE

Rate of accumulation of energy in system = Rate of work done on the system + Rate of heat added to the system + Rate of energy added to system by incoming material − Rate of energy removed from system by outgoing material

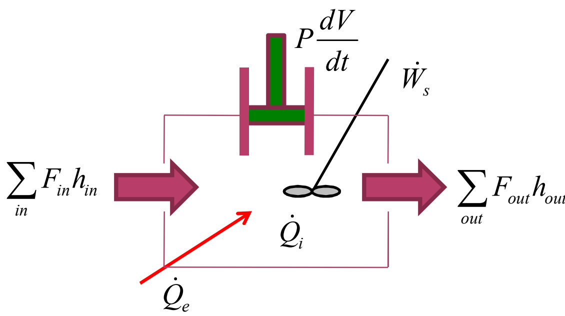
Total energy in the system

$$E_{tot} = U + E_K + E_P$$

✓Changes in kinetic and potential energies can usually be ignored in process modeling

Exceptions?

ENERGY BALANCE DERIVATION



$$\frac{dU}{dt} = \dot{Q} + \dot{W} + \sum_{in} F_{in}h_{in} - \sum_{out} F_{out}h_{out}$$

$$\dot{W} = \dot{W}_{shaft} - P\frac{dV}{dt}$$

$$\dot{Q} = \dot{Q}_e + \dot{Q}_i$$

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ENERGY BALANCE DERIVATION

$$\frac{dU}{dt} = \dot{Q} + \dot{W}_s - P\frac{dV}{dt} + \sum_{in} F_{in}h_{in} - \sum_{out} F_{out}h_{out}$$

- Constant-volume (rigid vessel)

$$\boxed{\frac{dU}{dt} = \dot{Q} + \dot{W}_s + \sum_{in} F_{in}h_{in} - \sum_{out} F_{out}h_{out}}$$

$$\frac{dU}{dt} = \frac{dH}{dt} - \frac{d(PV)}{dt} = \dot{Q} + \dot{W}_s - P\frac{dV}{dt} + \sum_{in} F_{in}h_{in} - \sum_{out} F_{out}h_{out}$$

- Constant-pressure

$$\frac{dH}{dt} - P\frac{dV}{dt} - \cancel{V\frac{dP}{dt}} = \dot{Q} + \dot{W}_s - P\frac{dV}{dt} + \sum_{in} F_{in}h_{in} - \sum_{out} F_{out}h_{out}$$

$$\boxed{\frac{dH}{dt} = \dot{Q} + \dot{W}_s + \sum_{in} F_{in}h_{in} - \sum_{out} F_{out}h_{out}}$$

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EXAMPLE: DYNAMIC NON-ISOTHERMAL CSTR

$$A \xrightarrow{k} B$$

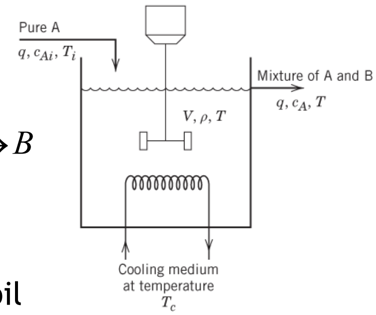

Figure 2.6 A nonisothermal continuous stirred-tank reactor.

Some assumptions
- Constant volume
- Constant density
- T_c constant through the coil

$$V\rho C\frac{dT}{dt} = wC(T_i - T) + (-\Delta H_R)Vkc_A + UA(T_c - T)$$

$$k = k_0 e^{(\frac{-E}{RT})}$$

Nonlinear ODE? Why?

EXAMPLE: DYNAMIC NON-ISOTHERMAL CSTR

Change in cooling water temperature

I. -10 K
II. +5 K

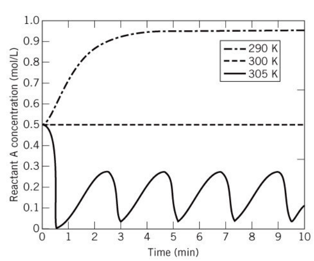

Figure 2.8 Reactant A concentration variation with step changes in cooling water temperature to 305 and 290 K.

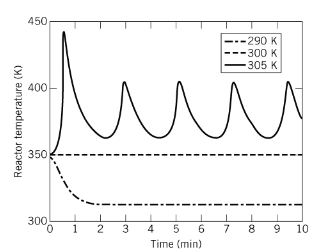

Figure 2.7 Reactor temperature variation with step changes in cooling water temperature from 300 to 305 K and from 300 to 290 K.

Response changes dramatically with **direction** & **magnitude** of change (typical for nonlinear dynamics)

ODE SIMULATION USING OCTAVE (MATLAB!)