

# Modeling Approaches

- Physical/chemical (fundamental, global)
  - Model structure by theoretical analysis
    - Material/energy balances
    - Heat, mass, and momentum transfer
    - Thermodynamics, chemical kinetics
    - Physical property relationships
  - Model complexity must be determined (assumptions)
  - Can be computationally expensive (not real-time)
  - May be expensive/time-consuming to obtain
  - Good for extrapolation, scale-up
  - Does not require experimental data to obtain (data required for validation and fitting)

- Black box (empirical)
  - Large number of unknown parameters
  - Can be obtained quickly (e.g., linear regression)
  - Model structure is subjective
  - Dangerous to extrapolate
- Semi-empirical
  - Compromise of first two approaches
  - Model structure may be simpler
  - Typically 2 to 10 physical parameters estimated (nonlinear regression)
  - Good versatility, can be extrapolated
  - Can be run in real-time

- Conservation Laws

Theoretical models of chemical processes are based on conservation laws.

## Conservation of Mass

$$\left\{ \begin{array}{l} \text{rate of mass} \\ \text{accumulation} \end{array} \right\} = \left\{ \begin{array}{l} \text{rate of mass} \\ \text{in} \end{array} \right\} - \left\{ \begin{array}{l} \text{rate of mass} \\ \text{out} \end{array} \right\} \quad (2-6)$$

## Conservation of Component i

$$\left\{ \begin{array}{l} \text{rate of component i} \\ \text{accumulation} \end{array} \right\} = \left\{ \begin{array}{l} \text{rate of component i} \\ \text{in} \end{array} \right\} - \left\{ \begin{array}{l} \text{rate of component i} \\ \text{out} \end{array} \right\} + \left\{ \begin{array}{l} \text{rate of component i} \\ \text{produced} \end{array} \right\} \quad (2-7)$$

# Conservation of Energy

The general law of energy conservation is also called the First Law of Thermodynamics. It can be expressed as:

$$\begin{aligned}
 \left\{ \begin{array}{l} \text{rate of energy} \\ \text{accumulation} \end{array} \right\} &= \left\{ \begin{array}{l} \text{rate of energy in} \\ \text{by convection} \end{array} \right\} - \left\{ \begin{array}{l} \text{rate of energy out} \\ \text{by convection} \end{array} \right\} \\
 + \left\{ \begin{array}{l} \text{net rate of heat addition} \\ \text{to the system from} \\ \text{the surroundings} \end{array} \right\} &+ \left\{ \begin{array}{l} \text{net rate of work} \\ \text{performed on the system} \\ \text{by the surroundings} \end{array} \right\} \quad (2-8)
 \end{aligned}$$

The total energy of a thermodynamic system,  $U_{tot}$ , is the sum of its internal energy, kinetic energy, and potential energy:

$$U_{tot} = U_{int} + U_{KE} + U_{PE} \quad (2-9)$$

- *Development of Dynamic Models*
- *Illustrative Example: A Blending Process*

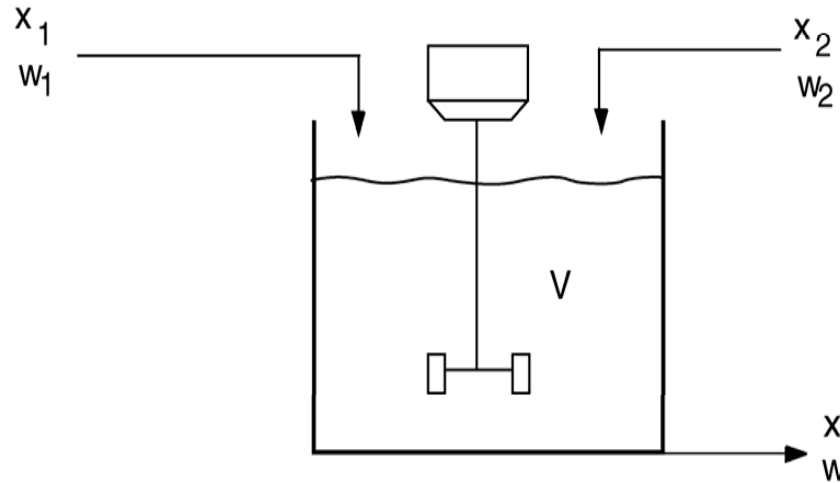


Figure 2.1. Stirred-tank blending process.

**An unsteady-state mass balance for the blending system:**

$$\left\{ \begin{array}{l} \text{rate of accumulation} \\ \text{of mass in the tank} \end{array} \right\} = \left\{ \begin{array}{l} \text{rate of} \\ \text{mass in} \end{array} \right\} - \left\{ \begin{array}{l} \text{rate of} \\ \text{mass out} \end{array} \right\} \quad (2-1)$$

or

$$\frac{d(V\rho)}{dt} = w_1 + w_2 - w \quad (2-2)$$

where  $w_1$ ,  $w_2$ , and  $w$  are mass flow rates.

- **The unsteady-state component balance is:**

$$\frac{d(V\rho x)}{dt} = w_1 x_1 + w_2 x_2 - w x \quad (2-3)$$

The corresponding steady-state model was derived in Ch. 1 (cf. Eqs. 1-1 and 1-2).

$$0 = \bar{w}_1 + \bar{w}_2 - \bar{w} \quad (2-4)$$

$$0 = \bar{w}_1 \bar{x}_1 + \bar{w}_2 \bar{x}_2 - \bar{w} \bar{x} \quad (2-5)$$

# The Blending Process Revisited

For constant  $\rho$ , Eqs. 2-2 and 2-3 become:

$$\rho \frac{dV}{dt} = w_1 + w_2 - w \quad (2-12)$$

$$\frac{\rho d(Vx)}{dt} = w_1 x_1 + w_2 x_2 - wx \quad (2-13)$$

Equation 2-13 can be simplified by expanding the accumulation term using the “chain rule” for differentiation of a product:

$$\rho \frac{d(Vx)}{dt} = \rho V \frac{dx}{dt} + \rho x \frac{dV}{dt} \quad (2-14)$$

Substitution of (2-14) into (2-13) gives:

$$\rho V \frac{dx}{dt} + \rho x \frac{dV}{dt} = w_1 x_1 + w_2 x_2 - wx \quad (2-15)$$

Substitution of the mass balance in (2-12) for  $\rho dV/dt$  in (2-15) gives:

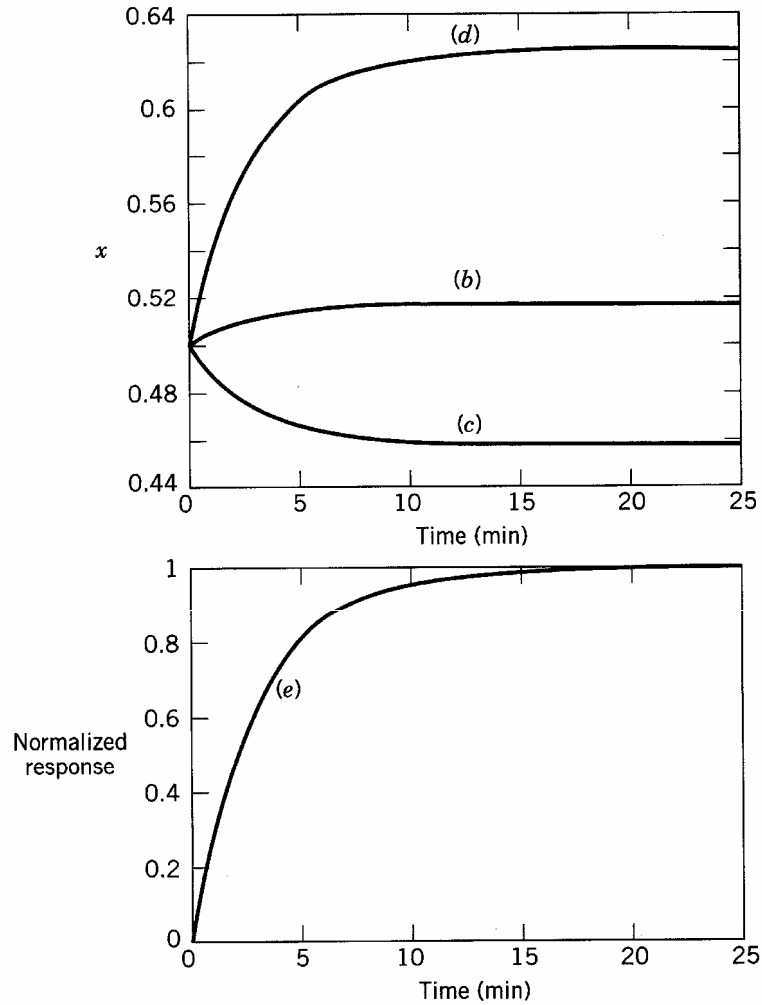
$$\rho V \frac{dx}{dt} + x(w_1 + w_2 - w) = w_1 x_1 + w_2 x_2 - wx \quad (2-16)$$

After canceling common terms and rearranging (2-12) and (2-16), a more convenient model form is obtained:

$$\frac{dV}{dt} = \frac{1}{\rho} (w_1 + w_2 - w) \quad (2-17)$$

$$\frac{dx}{dt} = \frac{w_1}{V\rho} (x_1 - x) + \frac{w_2}{V\rho} (x_2 - x) \quad (2-18)$$





**Figure 2.2** Exit composition responses of a stirred-tank blending process to step changes in:  
(b) flow rate  $w_1$   
(c) flow rate  $w_2$   
(d) flow rate  $w_2$  and inlet composition  $x_1$   
(e) Normalized response for parts (b)–(d).

# Stirred-Tank Heating Process

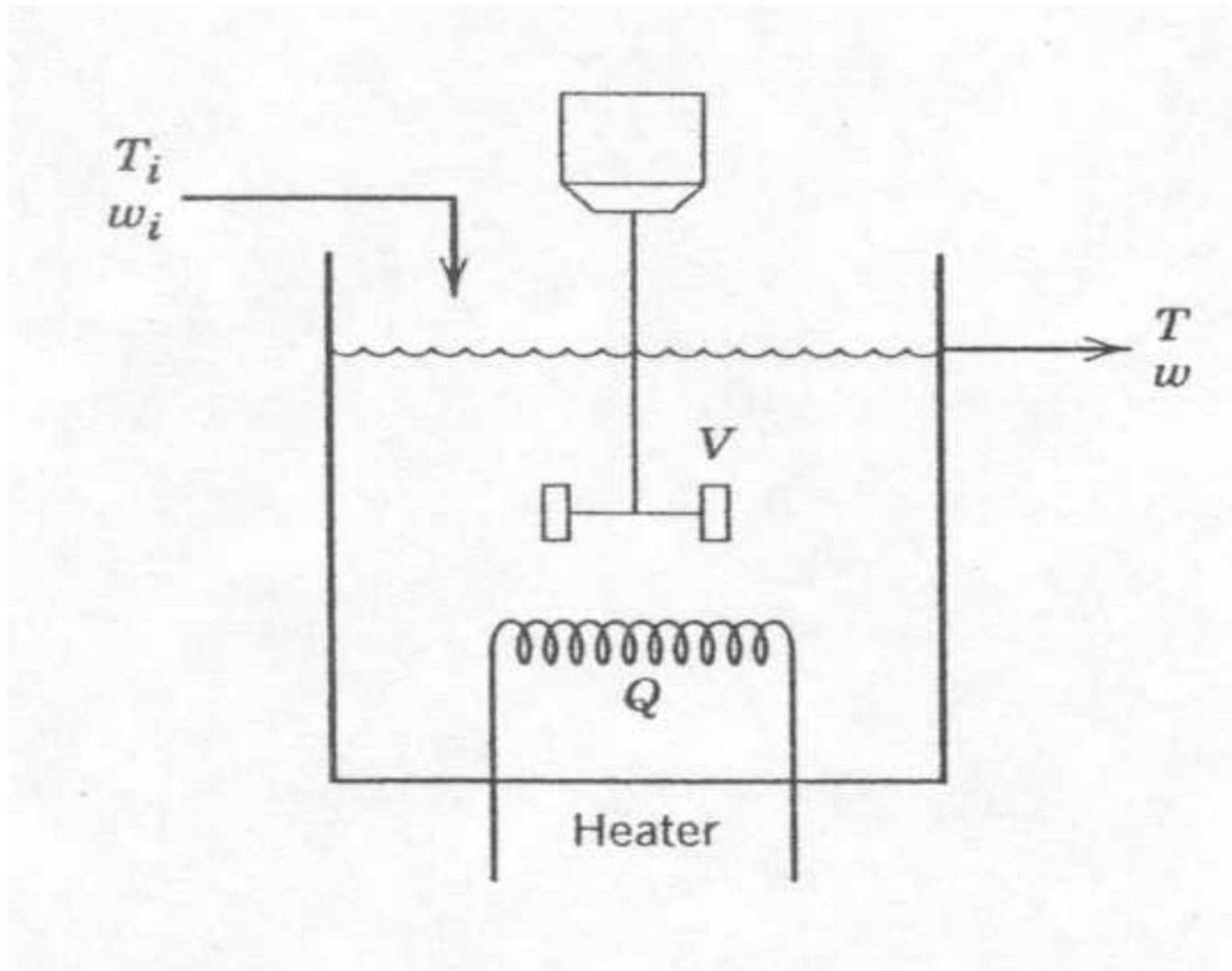


Figure 2.3 Stirred-tank heating process with constant holdup,  $V$ .

# Stirred-Tank Heating Process (cont'd.)

Assumptions:

1. Perfect mixing; thus, the exit temperature  $T$  is also the temperature of the tank contents.
2. The liquid holdup  $V$  is constant because the inlet and outlet flow rates are equal.
3. The density  $\rho$  and heat capacity  $C$  of the liquid are assumed to be constant. Thus, their temperature dependence is neglected.
4. Heat losses are negligible.

For the processes and examples considered in this book, it is appropriate to make two assumptions:

1. Changes in potential energy and kinetic energy can be neglected because they are small in comparison with changes in internal energy.
2. The net rate of work can be neglected because it is small compared to the rates of heat transfer and convection.

For these reasonable assumptions, the energy balance in Eq. 2-8 can be written as

$$\frac{dU_{\text{int}}}{dt} = -\Delta(w\hat{H}) + Q \quad (2-10)$$

$U_{\text{int}}$  = the internal energy of  
the system

$\hat{H}$  = enthalpy per unit mass

$w$  = mass flow rate

$Q$  = rate of heat transfer to the system

$\Delta$  = denotes the difference  
between outlet and inlet  
conditions of the flowing  
streams; therefore

$-\Delta(w\hat{H})$  = rate of enthalpy of the inlet  
stream(s) - the enthalpy  
of the outlet stream(s)

# Model Development - I

For a pure liquid at low or moderate pressures, the internal energy is approximately equal to the enthalpy,  $U_{int} \approx H$ , and  $H$  depends only on temperature. Consequently, in the subsequent development, we assume that  $U_{int} = H$  and  $\hat{U}_{int} = \hat{H}$  where the caret (^) means per unit mass. As shown in Appendix B, a differential change in temperature,  $dT$ , produces a corresponding change in the internal energy per unit mass,  $d\hat{U}_{int}$ ,

$$d\hat{U}_{int} = d\hat{H} = CdT \quad (2-29)$$

where  $C$  is the constant pressure heat capacity (assumed to be constant). The total internal energy of the liquid in the tank is:

$$U_{int} = \rho V \hat{U}_{int} \quad (2-30)$$

# Model Development - II

An expression for the rate of internal energy accumulation can be derived from Eqs. (2-29) and (2-30):

$$\frac{dU_{\text{int}}}{dt} = \rho V C \frac{dT}{dt} \quad (2-31)$$

Note that this term appears in the general energy balance of Eq. 2-10.

Suppose that the liquid in the tank is at a temperature  $T$  and has an enthalpy,  $\hat{H}$ . Integrating Eq. 2-29 from a reference temperature  $T_{\text{ref}}$  to  $T$  gives,

$$\hat{H} - \hat{H}_{\text{ref}} = C(T - T_{\text{ref}}) \quad (2-32)$$

where  $\hat{H}_{\text{ref}}$  is the value of  $\hat{H}$  at  $T_{\text{ref}}$ . Without loss of generality, we assume that  $\hat{H}_{\text{ref}} = 0$  (see Appendix B). Thus, (2-32) can be written as:

$$\hat{H} = C(T - T_{\text{ref}}) \quad (2-33)$$

# Model Development - III

For the inlet stream

$$\hat{H}_i = C(T_i - T_{ref}) \quad (2-34)$$

Substituting (2-33) and (2-34) into the convection term of (2-10) gives:

$$-\Delta(w\hat{H}) = w[C(T_i - T_{ref})] - w[C(T - T_{ref})] \quad (2-35)$$

Finally, substitution of (2-31) and (2-35) into (2-10)

$$V\rho C \frac{dT}{dt} = wC(T_i - T) + Q \quad (2-36)$$

## Define deviation variables (from set point)

$$y = T - \bar{T} \quad \bar{T} \text{ is desired operating point}$$

$$u = w_s - \bar{w}_s \quad \bar{w}_s(\bar{T}) \text{ from steady state}$$

$$\frac{\rho V}{w} \frac{dy}{dt} = -y + \frac{\Delta H_v}{wC} u \quad \text{note that } \frac{\Delta H_v}{wC} = K_p \text{ and } \frac{\rho V}{w} = \tau_1$$

$$\text{note when } \frac{dy}{dt} = 0 \quad y = K_p u$$

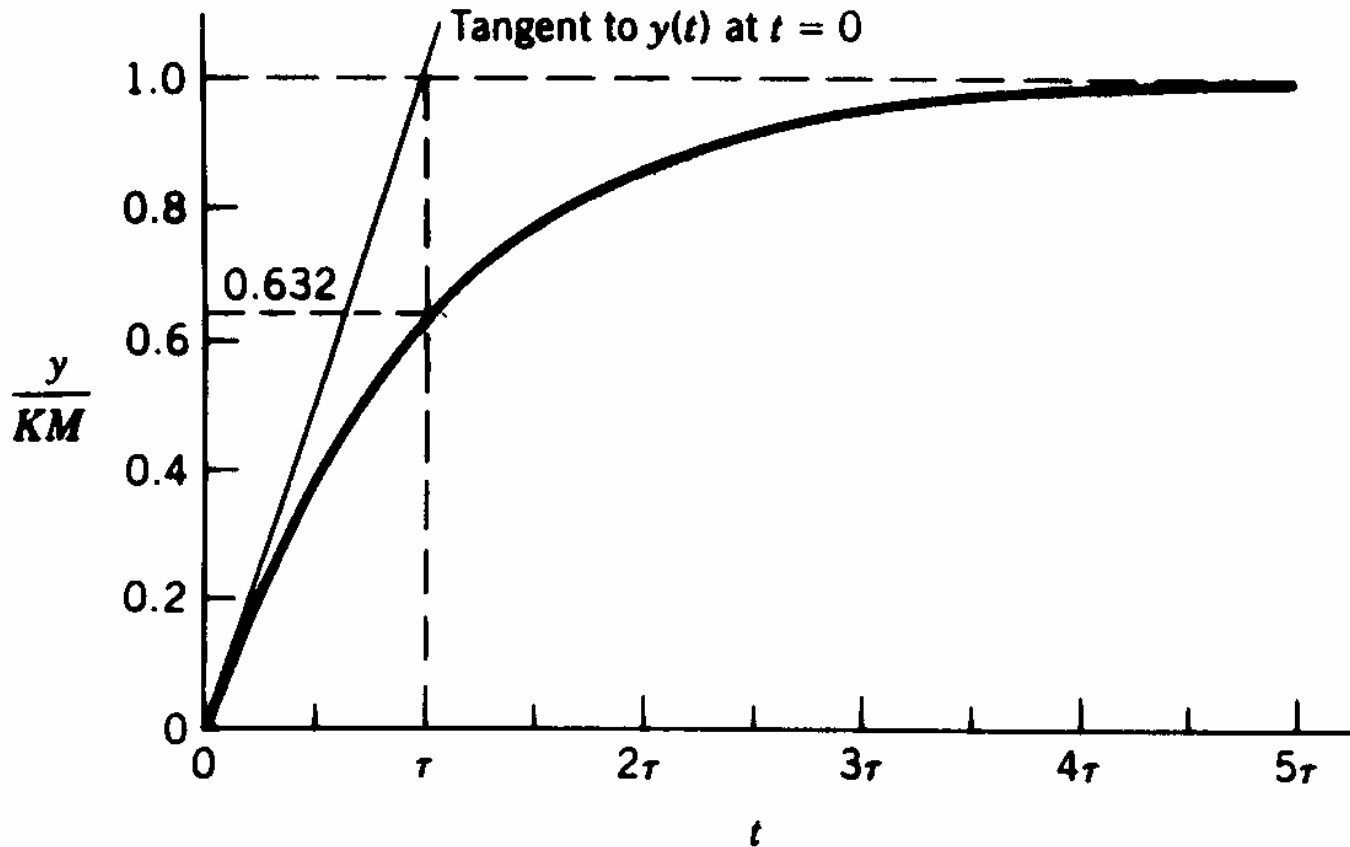
$$\tau_1 \frac{dy}{dt} = -y + K_p u$$

General linear ordinary differential equation solution: sum of exponential(s)

Suppose  $u = 1$  (unit step response)

$$y(t) = K_p \left( 1 - e^{-\frac{t}{\tau_1}} \right)$$





**Figure 7.2.** Step response of a first-order system and graphical constructions used to estimate the time constant,  $\tau$ .

## Table 2.2. Degrees of Freedom Analysis

1. List all quantities in the model that are *known* constants (or parameters that can be specified) on the basis of equipment dimensions, known physical properties, etc.
2. Determine the number of equations  $N_E$  and the number of process variables,  $N_V$ . Note that time  $t$  is *not* considered to be a process variable because it is neither a process input nor a process output.
3. Calculate the number of degrees of freedom,  $N_F = N_V - N_E$ .
4. Identify the  $N_E$  output variables that will be obtained by solving the process model.
5. Identify the  $N_F$  input variables that must be specified as either disturbance variables or manipulated variables, in order to utilize the  $N_F$  degrees of freedom.

# Degrees of Freedom Analysis for the Stirred-Tank Model:

3 parameters:  $V, \rho, C$

4 variables:  $T, T_i, w, Q$

1 equation: Eq. 2-36

Thus the degrees of freedom are  $N_F = 4 - 1 = 3$ . The process variables are classified as:

1 output variable:  $T$

3 input variables:  $T_i, w, Q$

For temperature control purposes, it is reasonable to classify the three inputs as:

2 disturbance variables:  $T_i, w$

1 manipulated variable:  $Q$

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