

## CM3310 Spring 2008

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### Lecture 2. Process Modeling, part 1

**Applications:** ( see page 32 )

1. Operator training
2. Process Design
3. Safety
4. Process Control

**Remark:** the models will be built using mathematics to describe the behavior of the process before they can be coded into a computer to become a simulator.

#### Example questions of some processes:

1. Does the water level in a reboiler increase or decrease when the liquid feed flow is stepped up by 10% ?
    - a. ... after a very long time → is process gain positive or negative ?
    - b. ... after 5 mins → will the process exhibit “inverse response” ?
  2. How long does it take for the tank pressure to reach 63.2% of the new steady state when the inlet gas flow is stepped up ?
  3. How does the temperature of the polymer in the reactor behave based on the controller used?
    - a. ... does it oscillate?
    - b. ... is the process stable?
  4. Is the heating schedule of a composite press manufacture adequate ?
- The mathematical models needed to characterize the process dynamics will be differential equations consisting of time derivatives.

### General Form of the Model:

$$\frac{dx}{dt} = f(t, x, u, d; p)$$

where

$x$	Process variable (aka states)
$t$	Time
$u$	Manipulated variable
$d$	Disturbance variable
$p$	Parameters

### Types of Models:

1. Physical ( aka phenomenological ) Models
2. Empirical Models
3. Mixed

### Physical Models:

- uses balance (conservation) equations and constitutive equations
- often results in nonlinear equations
- generally difficult to find analytical solution, thus numerical solution are used to investigate the models

### Empirical Models:

- obtained using models with fixed structure
- also known as curve-fitting methods
- quick and often effective for designing control systems
- not as insightful for design retrofits

### Some Guidelines:

1. First determine the form of the model needed: figure out which are process (state) variables, i.e. what are the time derivatives in the model ?
2. Use mass, energy or component balance equations as starting points.
3. Incorporate constitutive equations, such as heat transfer equations, kinetic equations, thermodynamic equations, that could allow only the desired variables to remain in the differential equations.

### Example 2.1: Gas Surge Drum ( page 37 )

Desired form:  $\frac{dP}{dt} = f(t, P, q_{in}, P_{out})$  where  $q_{in}$  is the molar feed flow rate

Mass balance:

$$\frac{d}{dt}(\text{mass in tank}) = (\text{mass flow})_{in} - (\text{mass flow})_{out}$$

Then using the following assumptions:

- Ideal gas law
- Constant molecular weight
- Molar flow rate out is proportional to the difference between  $P$  and  $P_{out}$ .

we get

$$\frac{dP}{dt} = \frac{RT}{V} q_{in} - \frac{RT}{V} \beta (P - P_{out})$$

Remarks:

- $V$  and  $\beta$  are design parameters.
- $T$ ,  $P_{out}$  and  $q_{in}$  are disturbance variables.
- $R$  is the gas constant – not a parameter.

### Example 2.2: Isothermal Chemical Reactor ( page 39-44 )

Desired form:

$$\begin{aligned}\frac{dV}{dt} &= f_1(F, F_{in}) \\ \frac{dC_A}{dt} &= f_2(F, F_{in}, C_{Ain}, C_A, C_P, V) \\ \frac{dC_P}{dt} &= f_3(F, F_{in}, C_{Ain}, C_A, C_P, V)\end{aligned}$$

where  $F$  and  $F_{in}$  are volumetric flow rates.

Using mass balance and component balances, plus the following assumptions:

- Density is constant
- Reaction is first order :  $r_A = -kC_A$

we get:

$$\begin{aligned}\frac{dV}{dt} &= F_{in} - F \\ \frac{dC_A}{dt} &= \frac{F_{in}}{V} (C_{Ain} - C_A) - kC_A \\ \frac{dC_P}{dt} &= -\frac{F_{in}}{V} C_P + kC_A\end{aligned}$$

**Remarks:**

1.  $F_{in}$  is the manipulated variable.
2.  $F$  is a disturbance variable.
3.  $V$ ,  $C_A$  and  $C_P$  are the state variables.
4.  $k$  is a process parameter which could be changed by choosing a different operating temperature.

**Constitutive Relationships:** (see pages 44-50)

1. Thermodynamics: state equations (ideal gas, etc.), equilibria, reversibility
2. Kinetics: rate equations, energetic and equilibria
3. Transport: heat transfer, mass transfer and momentum transfer
4. Equipment: valves, sensors, transducers, etc.

**Suggested Exercise:**

1. Problem 2-3: blanket system on page 69.