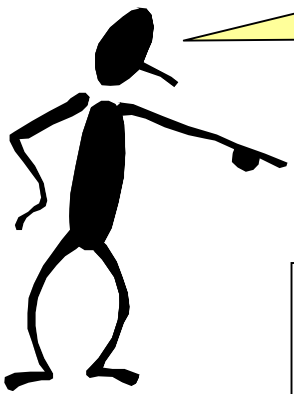
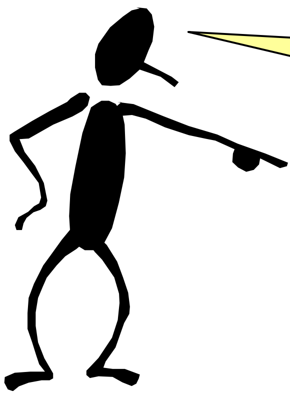
CHAPTER 3 : MATHEMATICAL MODELLING PRINCIPLES



When I complete this chapter, I want to be able to do the following.

- Formulate dynamic models based on fundamental balances
- Solve simple first-order linear dynamic models
- Determine how key aspects of dynamics depend on process design and operation

CHAPTER 3 : MATHEMATICAL MODELLING PRINCIPLES



Outline of the lesson.

- **Reasons why we need dynamic models**
- **Six (6) - step modelling procedure**
- **Many examples**
  - mixing tank
  - CSTR
  - draining tank
- **General conclusions about models**
- **Workshop**

WHY WE NEED DYNAMIC MODELS

Do the Bus and bicycle have different dynamics?

- **Which can make a U-turn in 1.5 meter?**
- **Which responds better when it hits s bump?**

Dynamic performance depends more on the vehicle than the driver!

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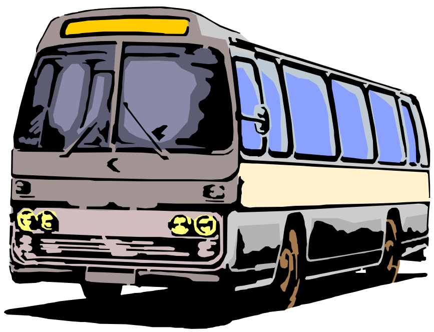
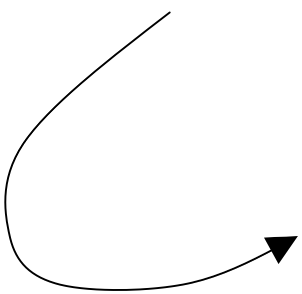


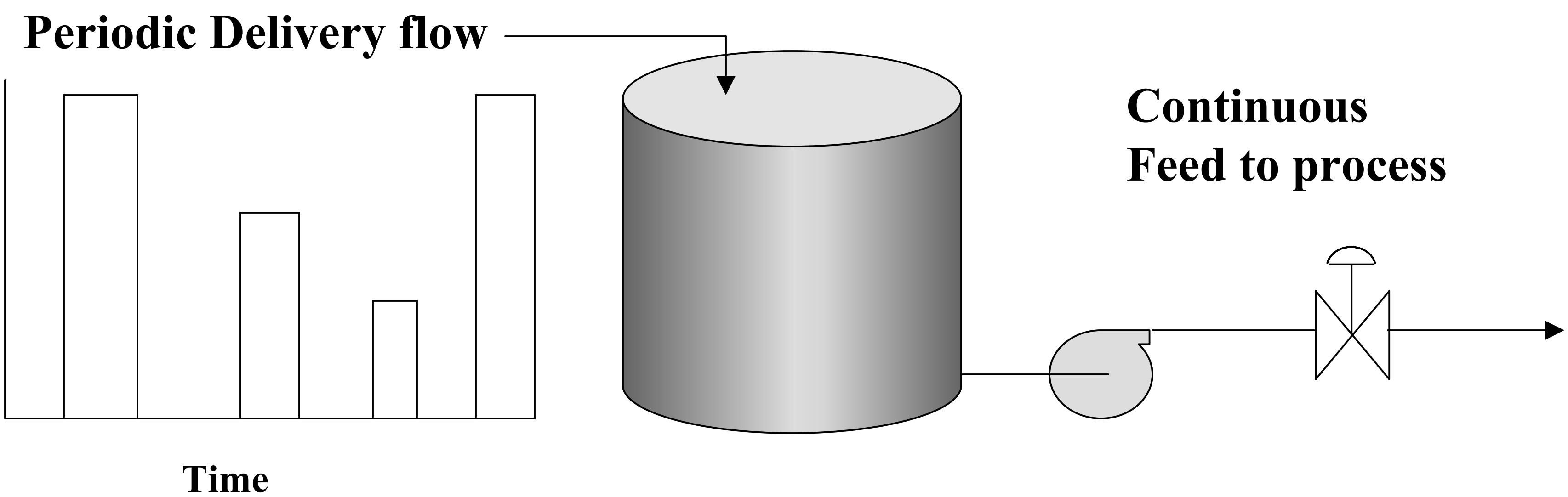
Dynamic performance depends more on the vehicle than the driver!



The process dynamics are more important than the computer control!

WHY WE NEED DYNAMIC MODELS

Feed material is delivered periodically, but the process requires a continuous feed flow. How large should should the tank volume be?



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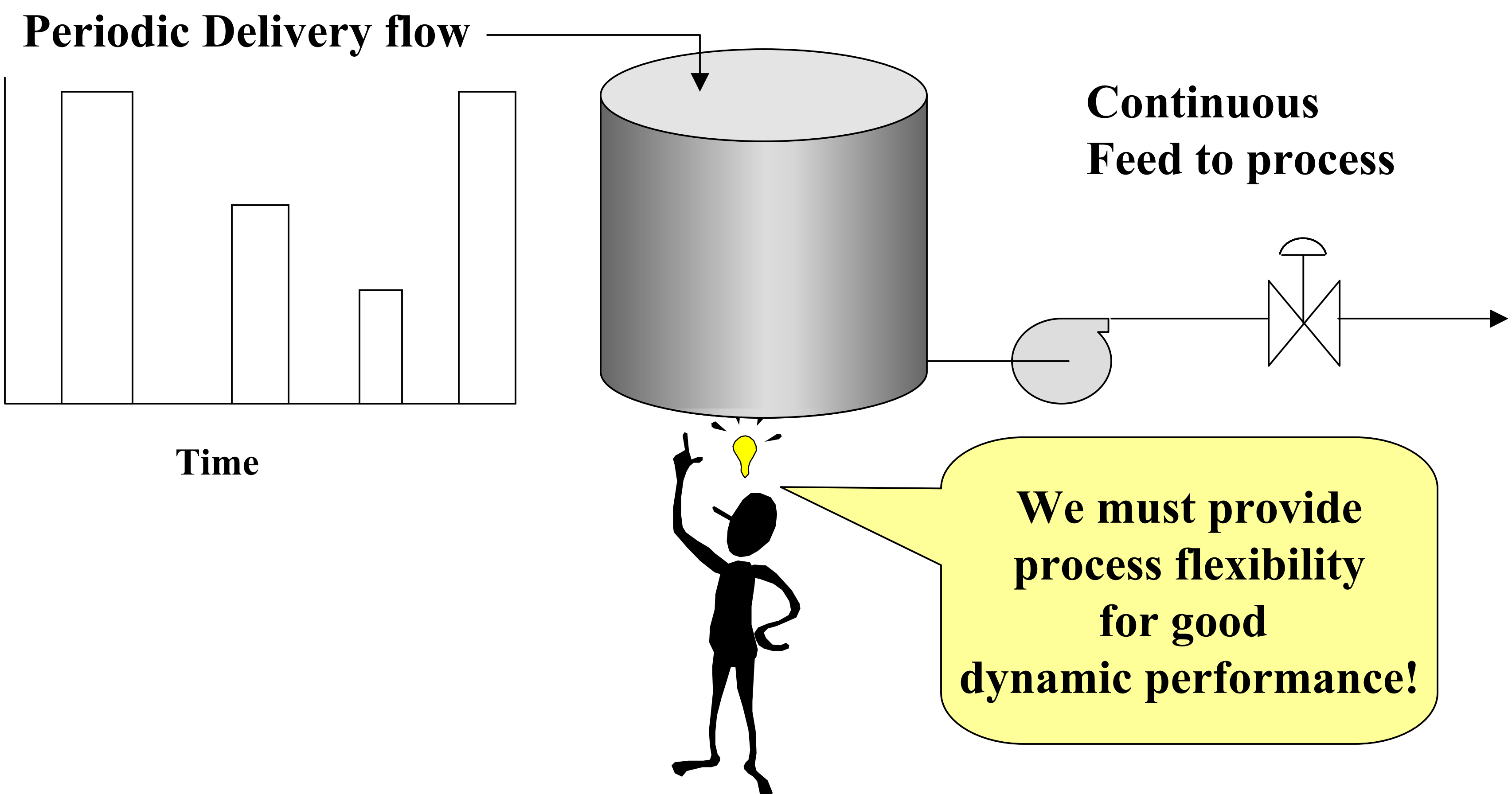
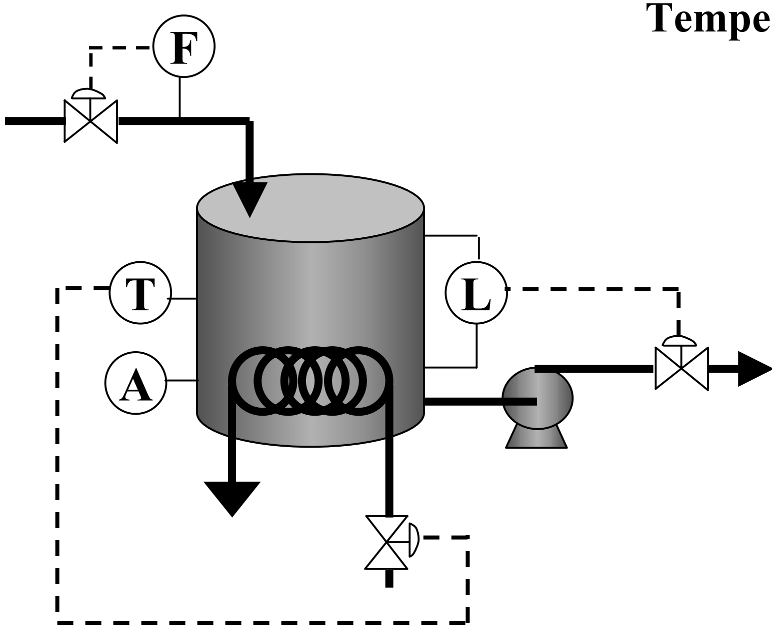
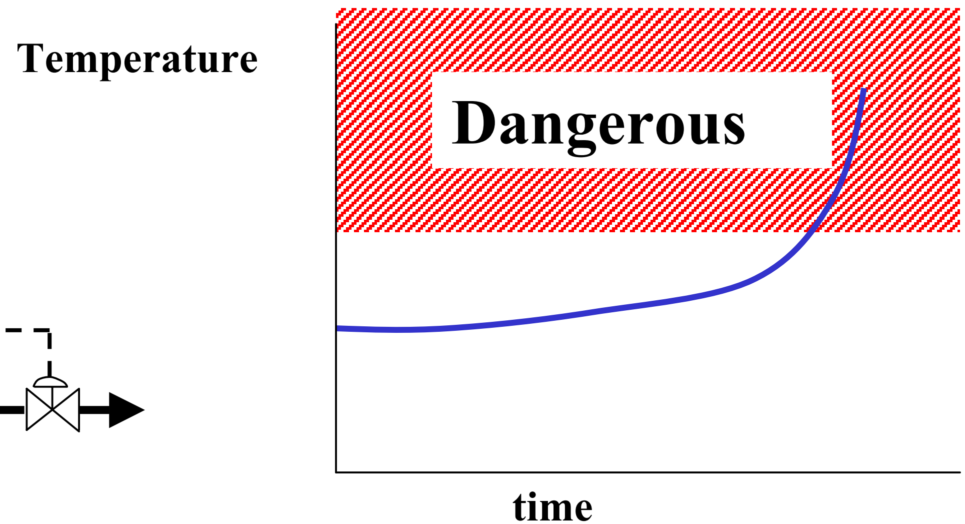


WHY WE NEED DYNAMIC MODELS

The cooling water pumps have failed. How long do we have until the exothermic reactor runs away?





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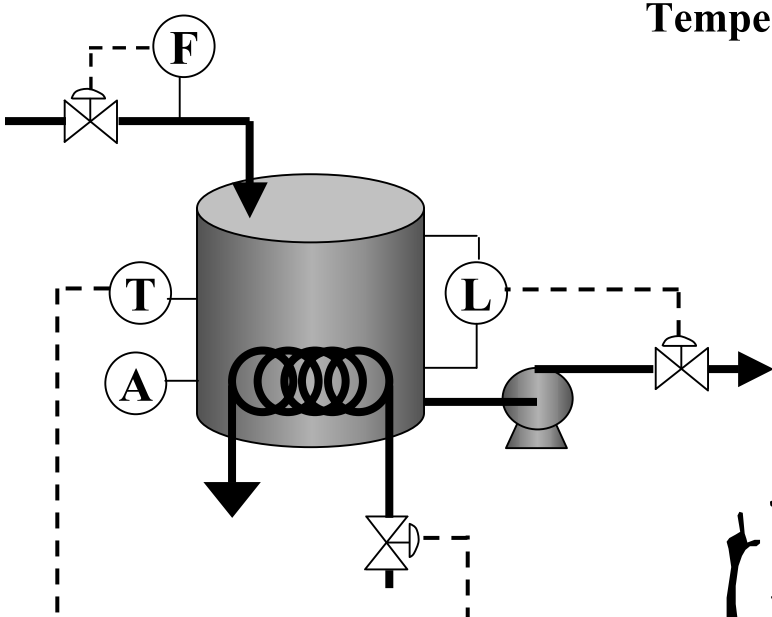
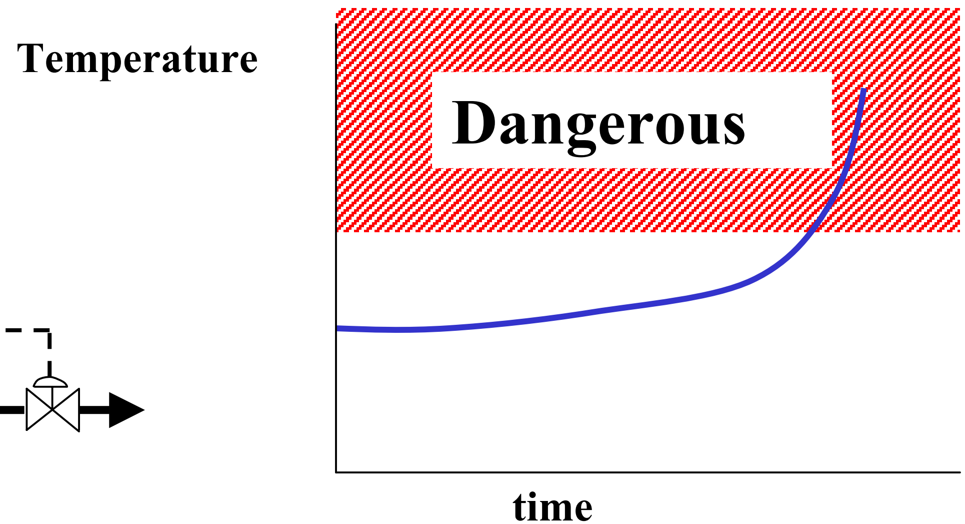
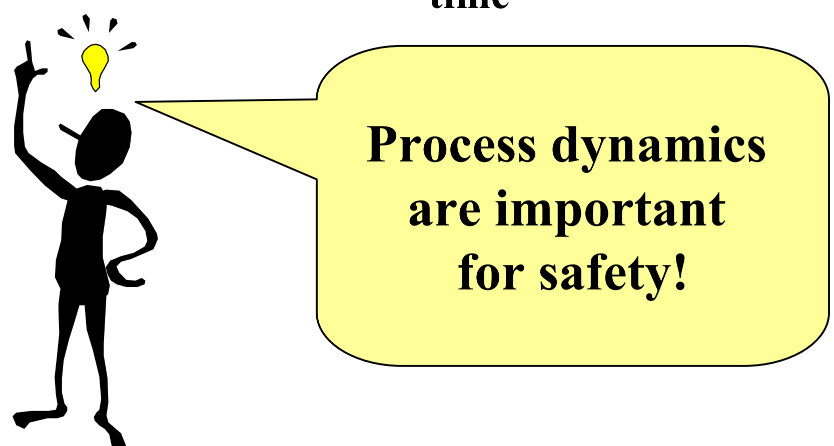




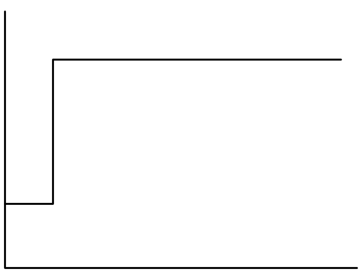


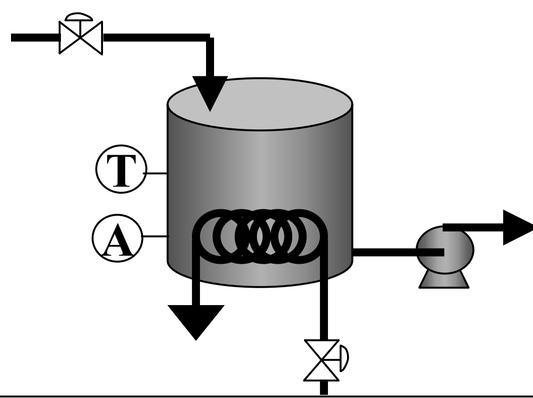
WHY WE DEVELOP MATHEMATICAL MODELS?

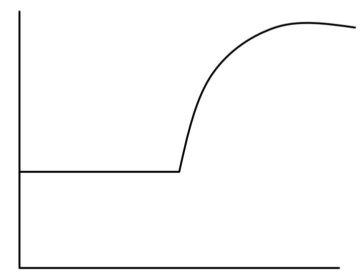
Input change, e.g., step in coolant flow rate

Process

Effect on output variable







How does the process influence the response?

- **How far?**
- **How fast**
- **“Shape”**

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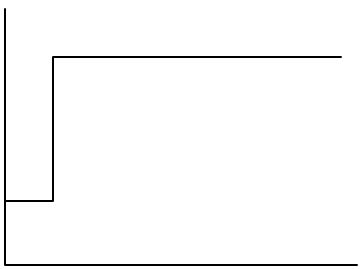
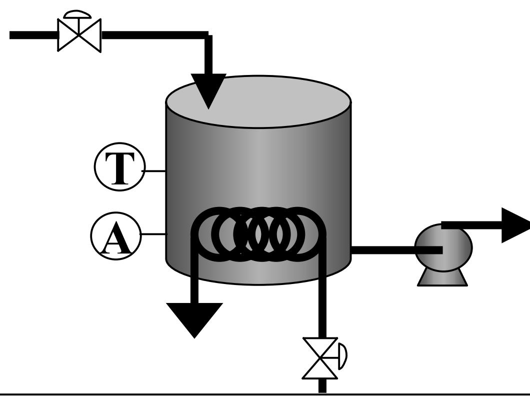
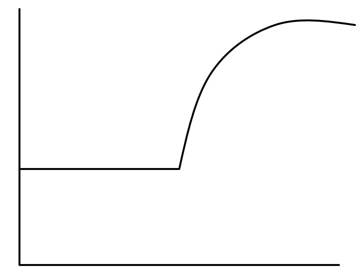
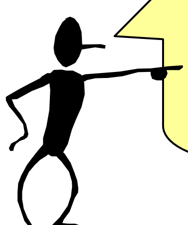








Math models help us answer these questions!

How does the process influence the response?

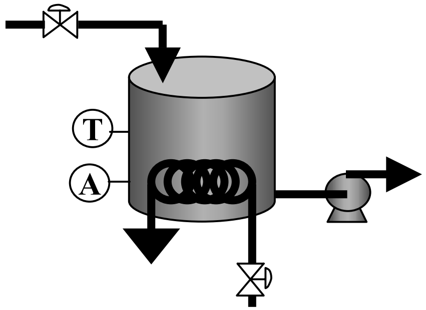
- **How far?**
- **How fast**
- **“Shape”**

SIX-STEP MODELLING PROCEDURE

1. Define Goals
2. Prepare information
3. Formulate the model
4. Determine the solution
5. Analyze Results
6. Validate the model

We apply this procedure

- to many physical systems
- overall material balance
- component material balance
- energy balances



SIX-STEP MODELLING PROCEDURE

1. Define Goals
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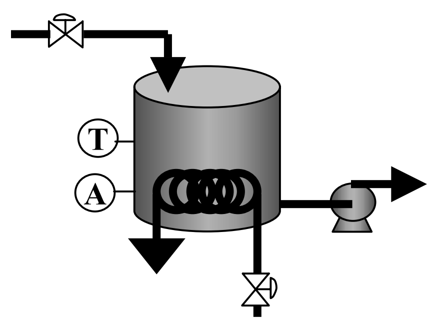
- What decision?
- What variable?
- Location



Examples of variable selection

liquid level	→	total mass in liquid
pressure	→	total moles in vapor
temperature	→	energy balance
concentration	→	component mass

SIX-STEP MODELLING PROCEDURE

1. Define Goals
2. Prepare information
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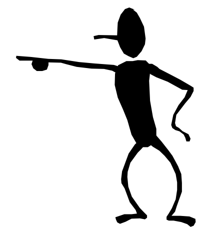
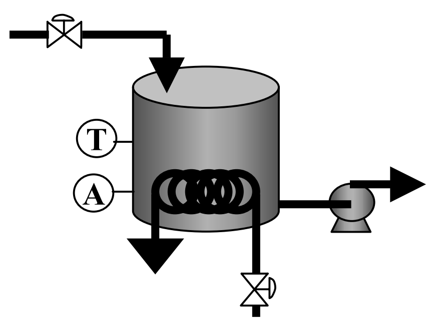
6. Validate the model

- Sketch process
- Collect data
- State assumptions
- Define system

Key property of a “system”?





SIX-STEP MODELLING PROCEDURE

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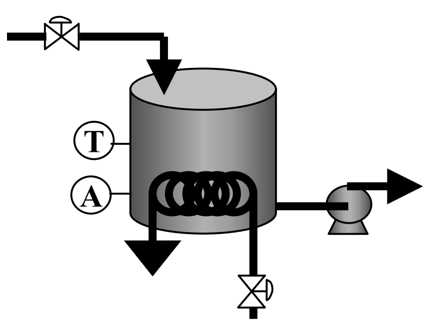
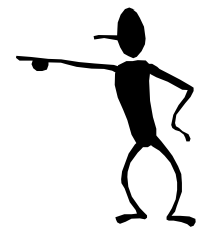


Key property of a “system”?



Variable(s) are the same for any location within the system!

SIX-STEP MODELLING PROCEDURE

1. Define Goals
2. Prepare information
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CONSERVATION BALANCES

Overall Material

$$\{\text{Accumulation of mass}\} = \{\text{mass in}\} - \{\text{mass out}\}$$

Component Material

$$\begin{Bmatrix}\text{Accumulation of} \\ \text{component mass}\end{Bmatrix} = \begin{Bmatrix}\text{component} \\ \text{mass in}\end{Bmatrix} - \begin{Bmatrix}\text{component} \\ \text{mass out}\end{Bmatrix} + \begin{Bmatrix}\text{generation of} \\ \text{component mass}\end{Bmatrix}$$

Energy*

$$\begin{Bmatrix}\text{Accumulation} \\ U + PE + KE\end{Bmatrix} = \{H + PE + KE\}_{in} - \{H + PE + KE\}_{out} + Q - W_s$$

* Assumes that the system volume does not change

SIX-STEP MODELLING PROCEDURE

1. Define Goals
2. Prepare information
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- What type of equations do we use first?

  Conservation balances for key variable

- How many equations do we need?

  Degrees of freedom = NV - NE = 0

- What after conservation balances?

  Constitutive equations, e.g.,

  $Q = h\,A\,(\Delta T)$

  $r_A = k_0\,e^{-E/RT}$

  Not fundamental, based on empirical data

SIX-STEP MODELLING PROCEDURE

1. Define Goals
2. Prepare information
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Our dynamic models will involve differential (and algebraic) equations because of the accumulation terms.

$$V\frac{dC_A}{dt} = F(C_{A0} - C_A) - VkC_A$$

With initial conditions

$C_A = 3.2$ kg-mole/m^3 at $t = 0$

And some change to an input variable, the "forcing function", e.g.,

$C_{A0} = f(t) = 2.1\ t$ (ramp function)

SIX-STEP MODELLING PROCEDURE

1. Define Goals
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We will solve simple models analytically to provide excellent relationship between process and dynamic response, e.g.,

$$C_A(t) = C_A(t)\Big|_{t=0} + (\Delta C_{A0})K(1 - e^{-t/\tau})$$

$$\text{for } t \succ 0$$

Many results will have the same form! We want to know how the process influences K and τ, e.g.,

$$K = \frac{F}{F + kV} \qquad \tau = \frac{V}{F + Vk}$$

SIX-STEP MODELLING PROCEDURE

1. Define Goals
2. Prepare information
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We will solve complex models numerically, e.g.,

$$V \frac{dC_A}{dt} = F(C_{A0} - C_A) - VkC_A^2$$

Using a difference approximation for the derivative, we can derive the Euler method.

$$C_{A_n} = C_{A_{n-1}} + (\Delta t)\left[\frac{F(C_{A0} - C_A) - VkC_A^2}{V}\right]_{n-1}$$

Other methods include Runge-Kutta and Adams.

SIX-STEP MODELLING PROCEDURE

1. Define Goals
2. Prepare information
3. Formulate the model
4. Determine the solution
5. Analyze Results
6. Validate the model

- Check results for correctness
  - sign and shape as expected
  - obeys assumptions
  - negligible numerical errors
- Plot results
- Evaluate sensitivity & accuracy

- Compare with empirical data

SIX-STEP MODELLING PROCEDURE

1. Define Goals
2. Prepare information
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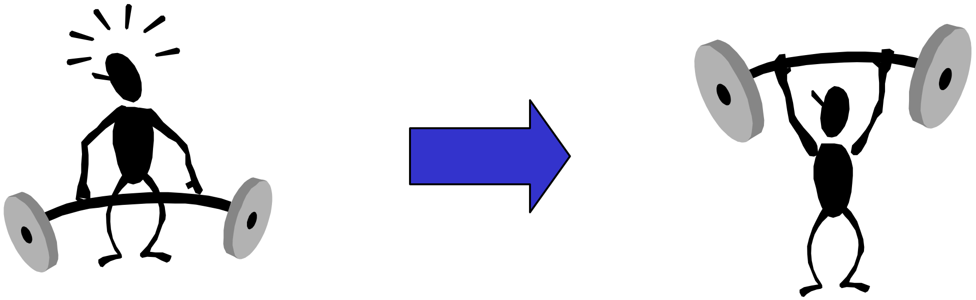
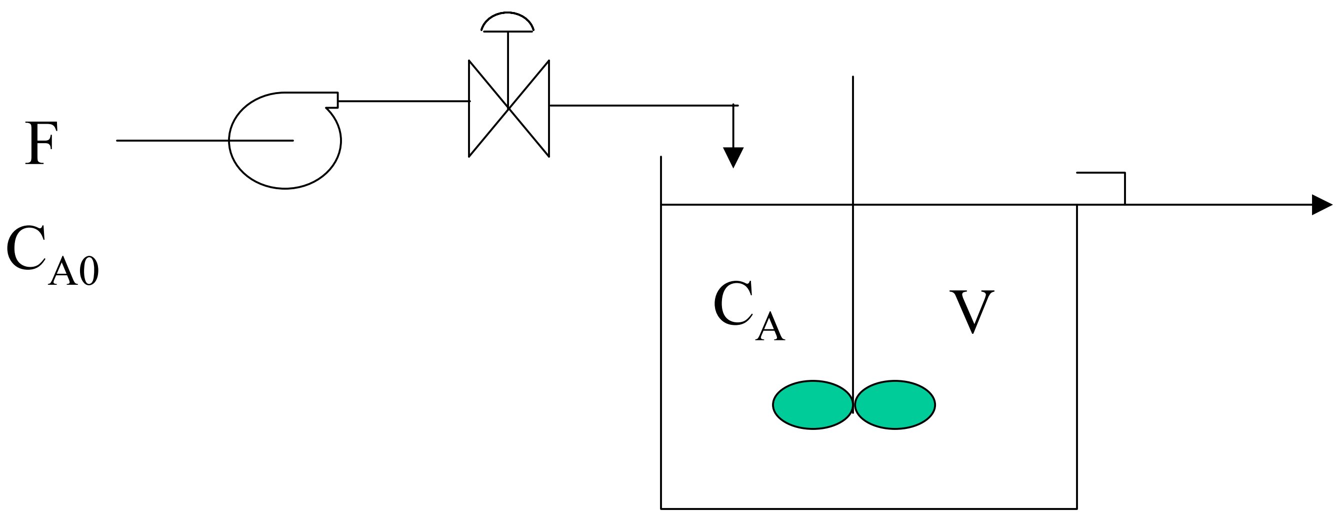
Let's practice modelling until we are ready for the Modelling Olympics!



Please remember that modelling is not a spectator sport! You have to practice (a lot)!

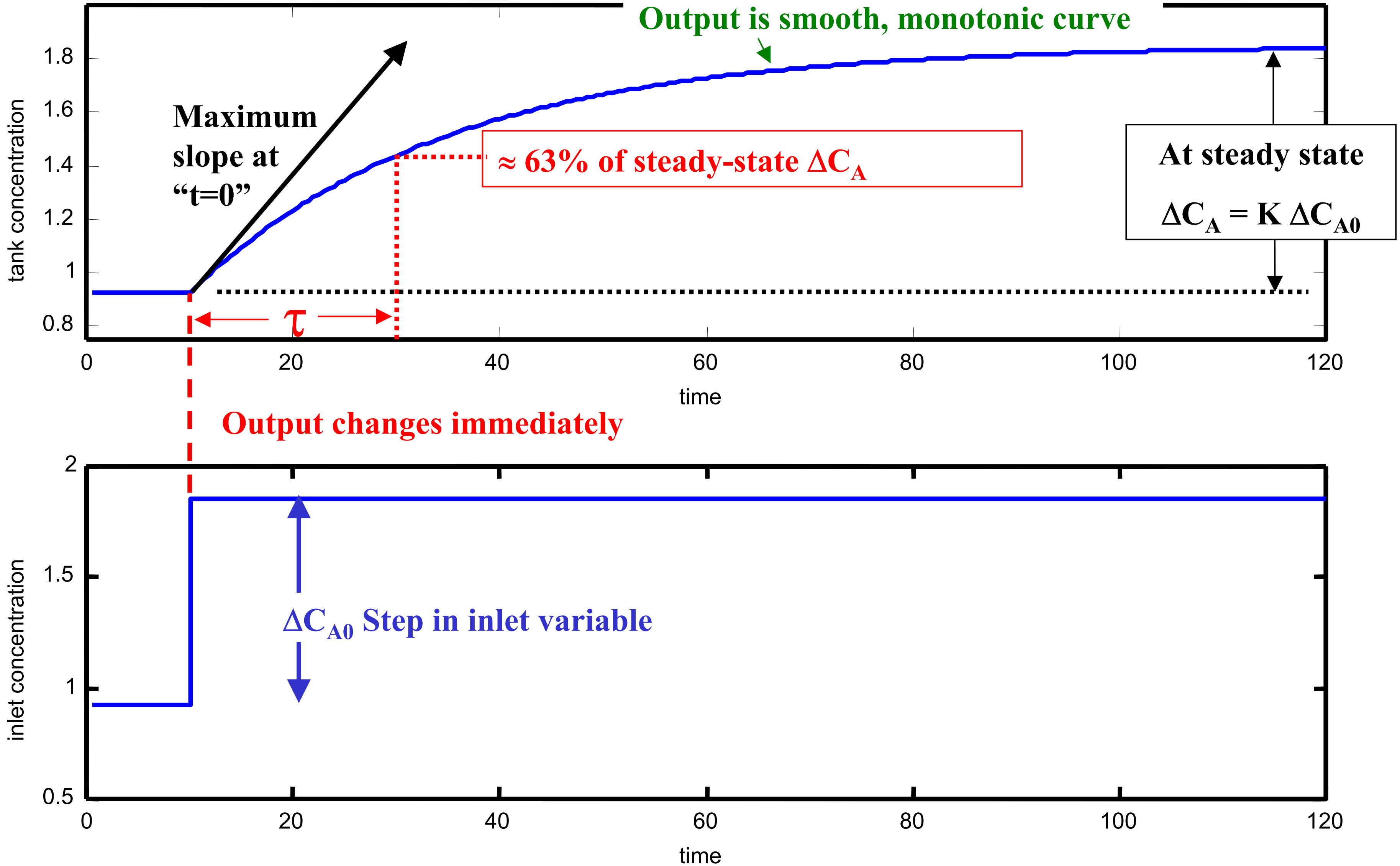
MODELLING EXAMPLE 1. MIXING TANK

Textbook Example 3.1: The mixing tank in the figure has been operating for a long time with a feed concentration of 0.925 kg-mole/m^3. The feed composition experiences a step to 1.85 kg-mole/m^3. All other variables are constant. Determine the dynamic response.



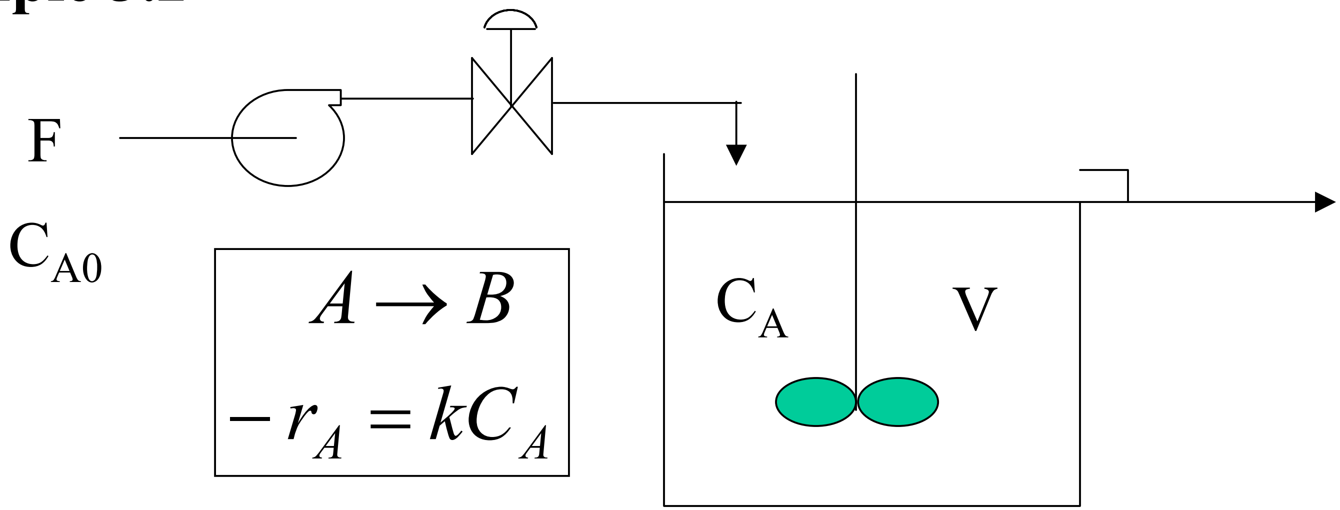
(We'll solve this in class.)

Let's understand this response, because we will see it over and over!



MODELLING EXAMPLE 2. CSTR

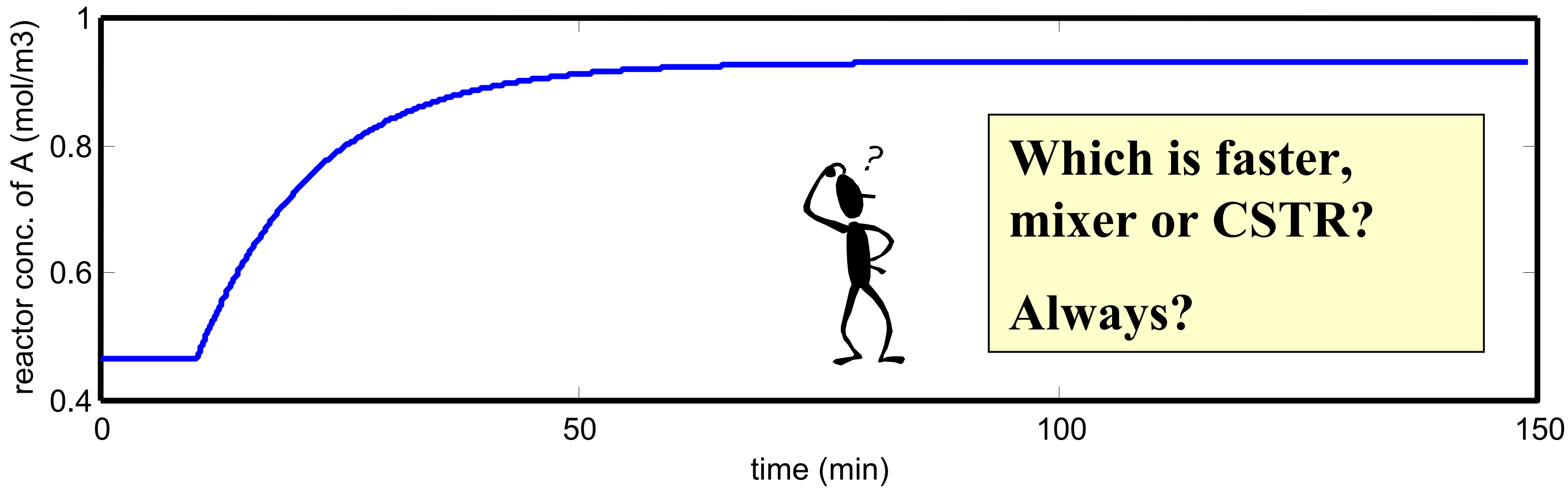
The isothermal, CSTR in the figure has been operating for a long time with a feed concentration of 0.925 kg-mole/m^3. The feed composition experiences a step to 1.85 kg-mole/m^3. All other variables are constant. Determine the dynamic response of C_A. Same parameters as textbook Example 3.2

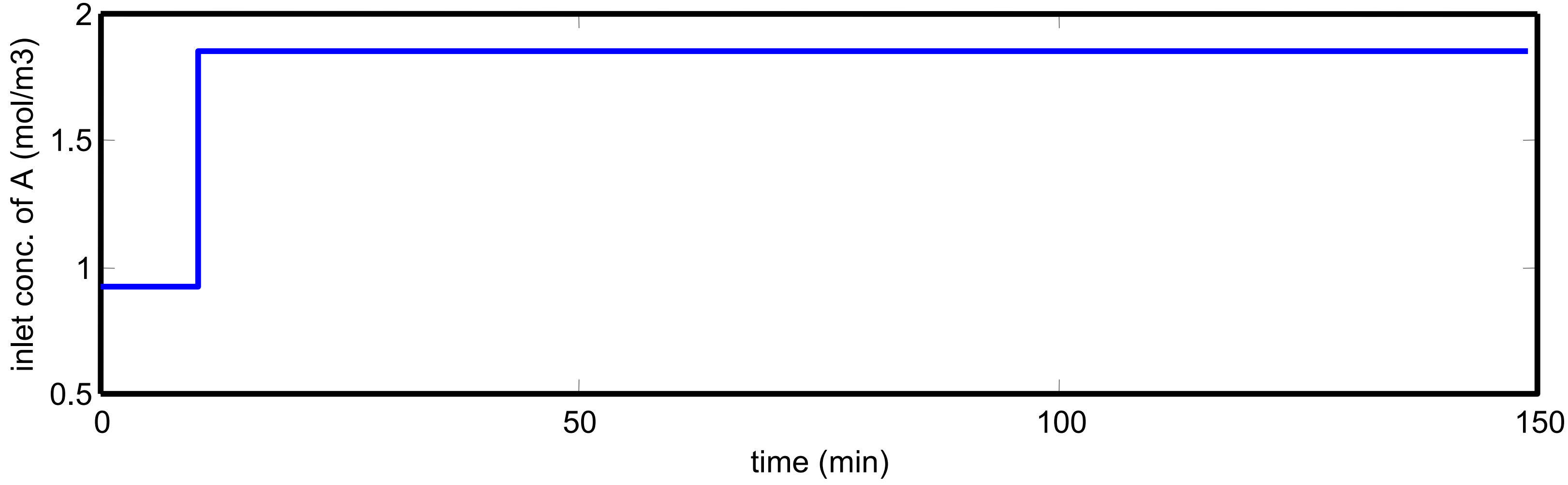


(We'll solve this in class.)

MODELLING EXAMPLE 2. CSTR

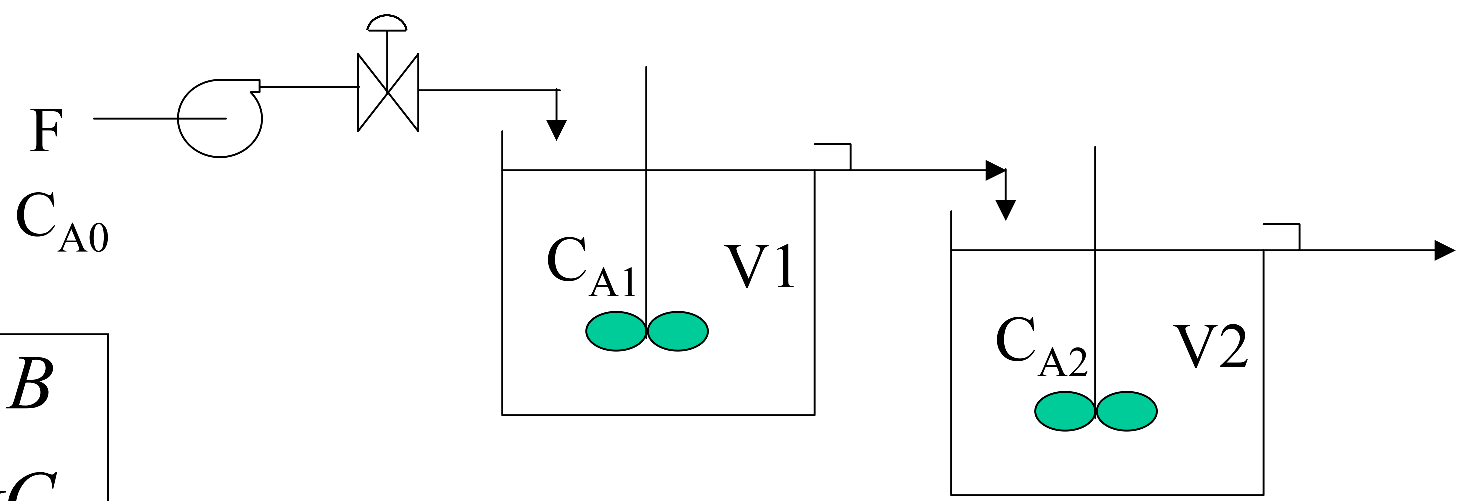
Annotate with key features similar to Example 1





MODELLING EXAMPLE 2. TWO CSTRs

Two isothermal CSTRs are initially at steady state and experience a step change to the feed composition to the first tank. Formulate the model for C_{A2}. Be especially careful when defining the system!



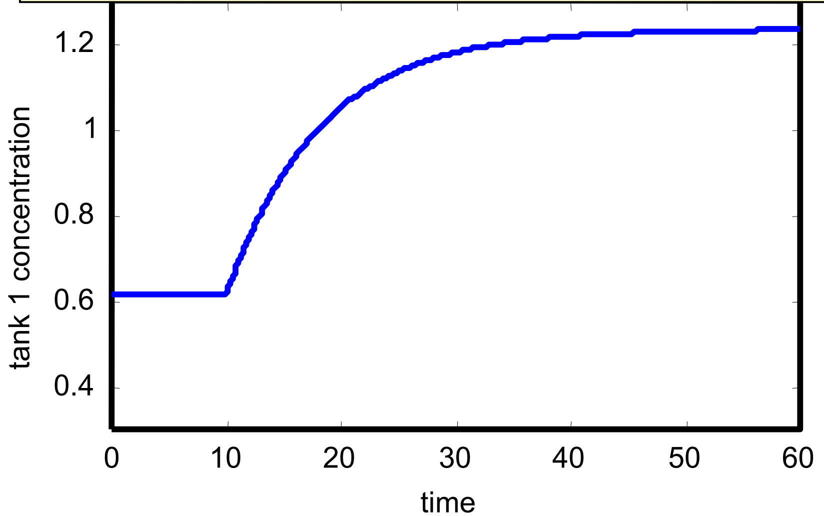
$$A \rightarrow B$$

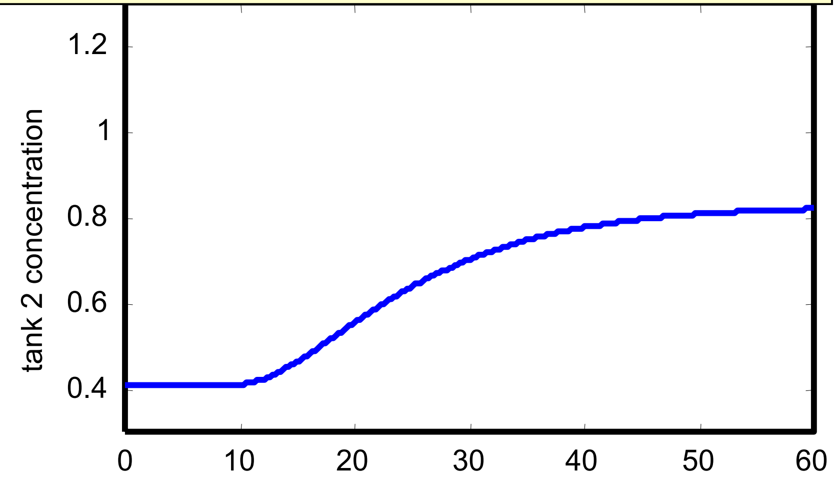
$$-r_A = kC_A$$

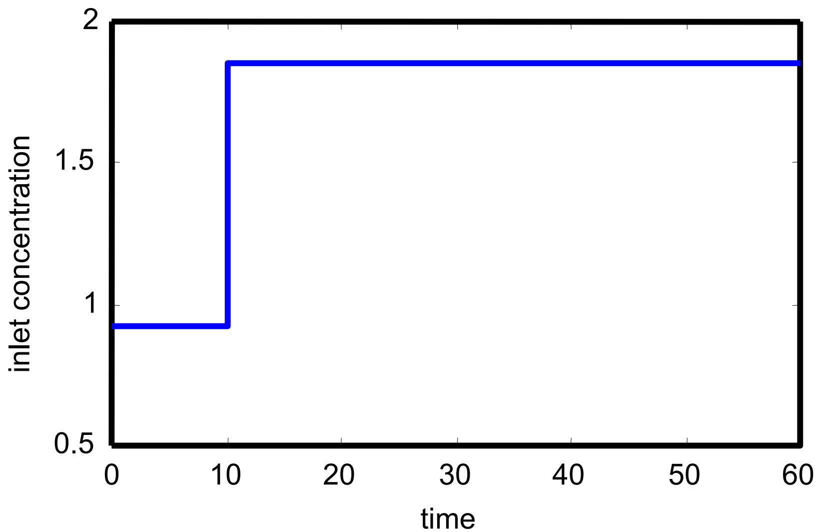
(We'll solve this in class.)

MODELLING EXAMPLE 3. TWO CSTRs

Annotate with key features similar to Example 1







SIX-STEP MODELLING PROCEDURE

1. Define Goals
2. Prepare information
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4. Determine the solution
5. Analyze Results
6. Validate the model

We can solve only a few models analytically - those that are linear (except for a few exceptions).

We could solve numerically.

We want to gain the **INSIGHT** from learning how K (s-s gain) and τ's (time constants) depend on the process design and operation.

Therefore, we linearize the models, even though we will not achieve an exact solution!

LINEARIZATION

Expand in Taylor Series and retain only constant and linear terms. We have an approximation.

This is the only variable

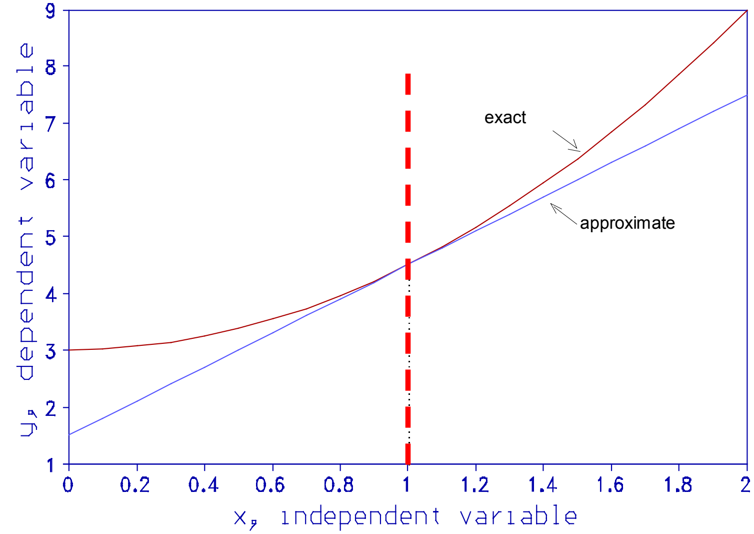
$$F(x) = \underbrace{F(x_s) + \left.\frac{dF}{dx}\right|_{x_s}}_{\text{Remember that these terms are constant because they are evaluated at } x_s} \overbrace{(x - x_s)}^{\text{This is the only variable}} + \cancel{\frac{1}{2!}\left.\frac{d^2F}{dx^2}\right|_{x_s}(x - x_s)^2 + R}$$

Remember that these terms are constant because they are evaluated at x_s

We define the deviation variable: $x' = (x - x_s)$

LINEARIZATION

$y = 1.5\,x^2 + 3$ about $x = 1$



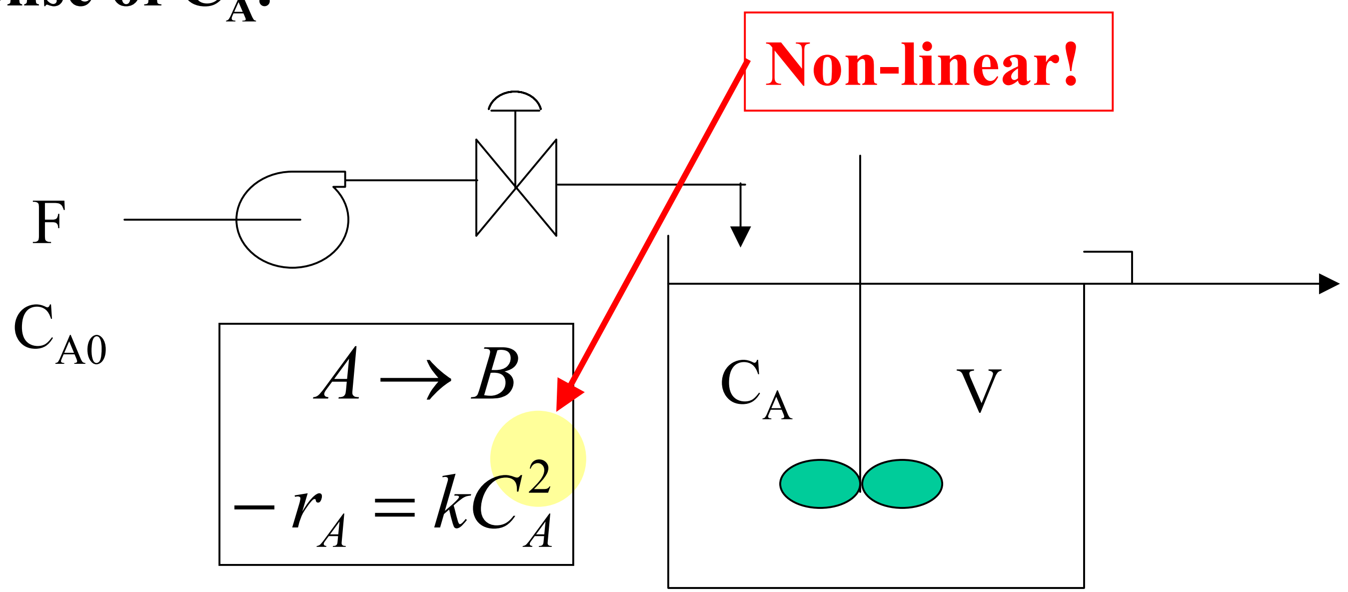
We must evaluate the approximation. It depends on

- **non-linearity**
- **distance of x from x_s**

Because process control maintains variables near desired values, the linearized analysis is often (but, not always) valid.

MODELLING EXAMPLE 4. N-L CSTR

Textbook Example 3.5: The isothermal, CSTR in the figure has been operating for a long time with a constant feed concentration. The feed composition experiences a step. All other variables are constant. Determine the dynamic response of C_A.



(We'll solve this in class.)

MODELLING EXAMPLE 4. N-L CSTR

We solve the linearized model analytically and the non-linear numerically.

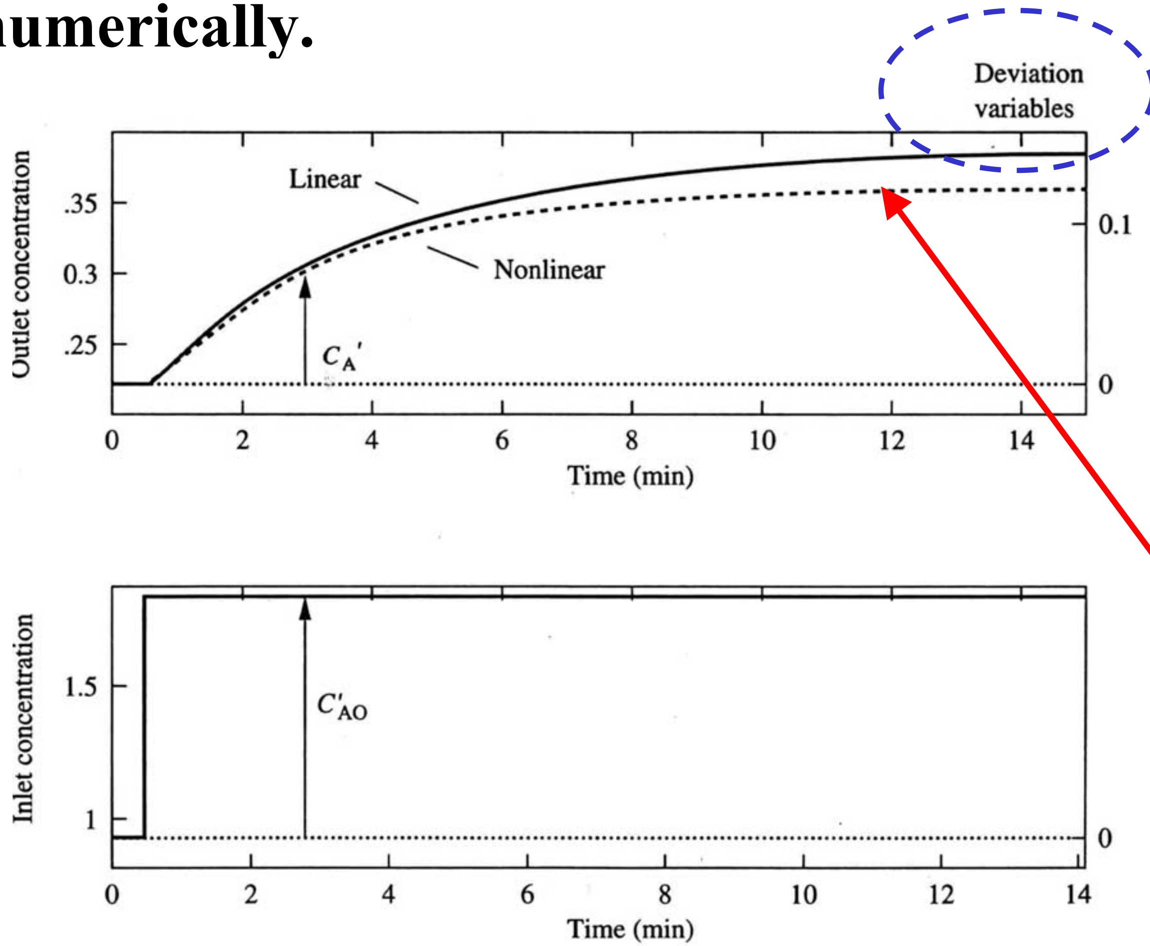


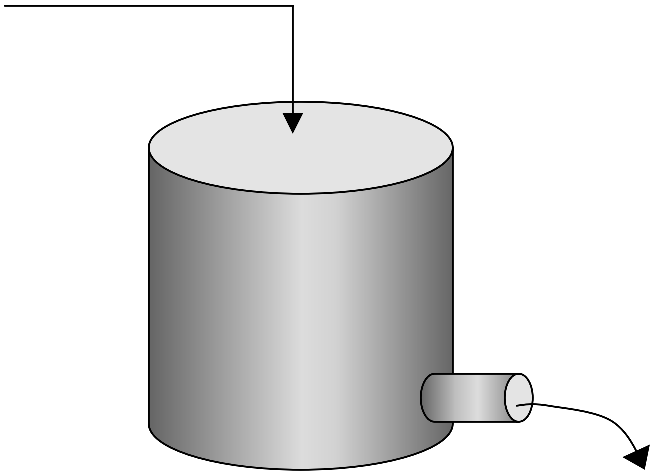
FIGURE 3.12

Deviation variables do not change the answer, just translate the values

In this case, the linearized approximation is close to the "exact"non-linear solution.

MODELLING EXAMPLE 4. DRAINING TANK

The tank with a drain has a continuous flow in and out. It has achieved initial steady state when a step decrease occurs to the flow in. Determine the level as a function of time.



Solve the non-linear and linearized models.

MODELLING EXAMPLE 4. DRAINING TANK

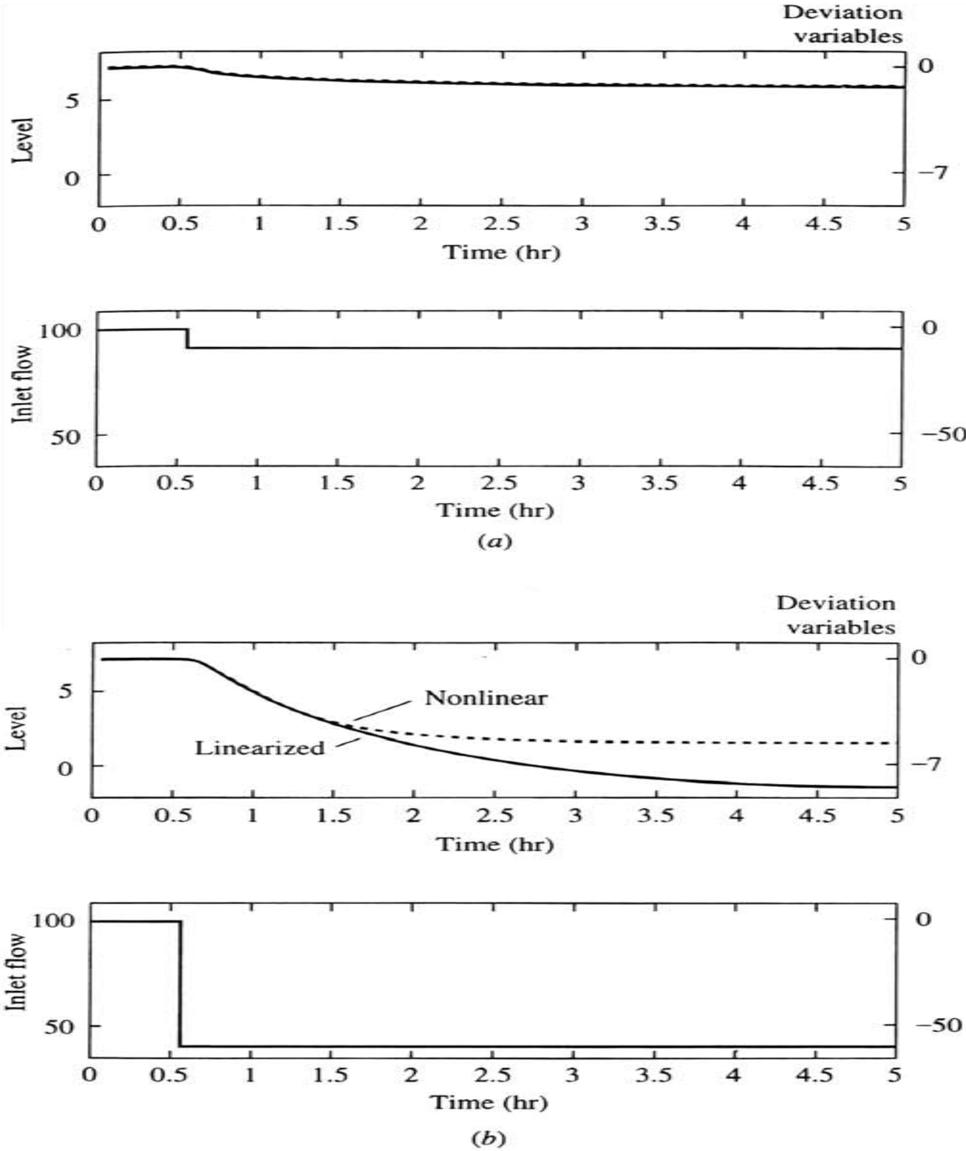


FIGURE 3.14

Small flow change: linearized approximation is good

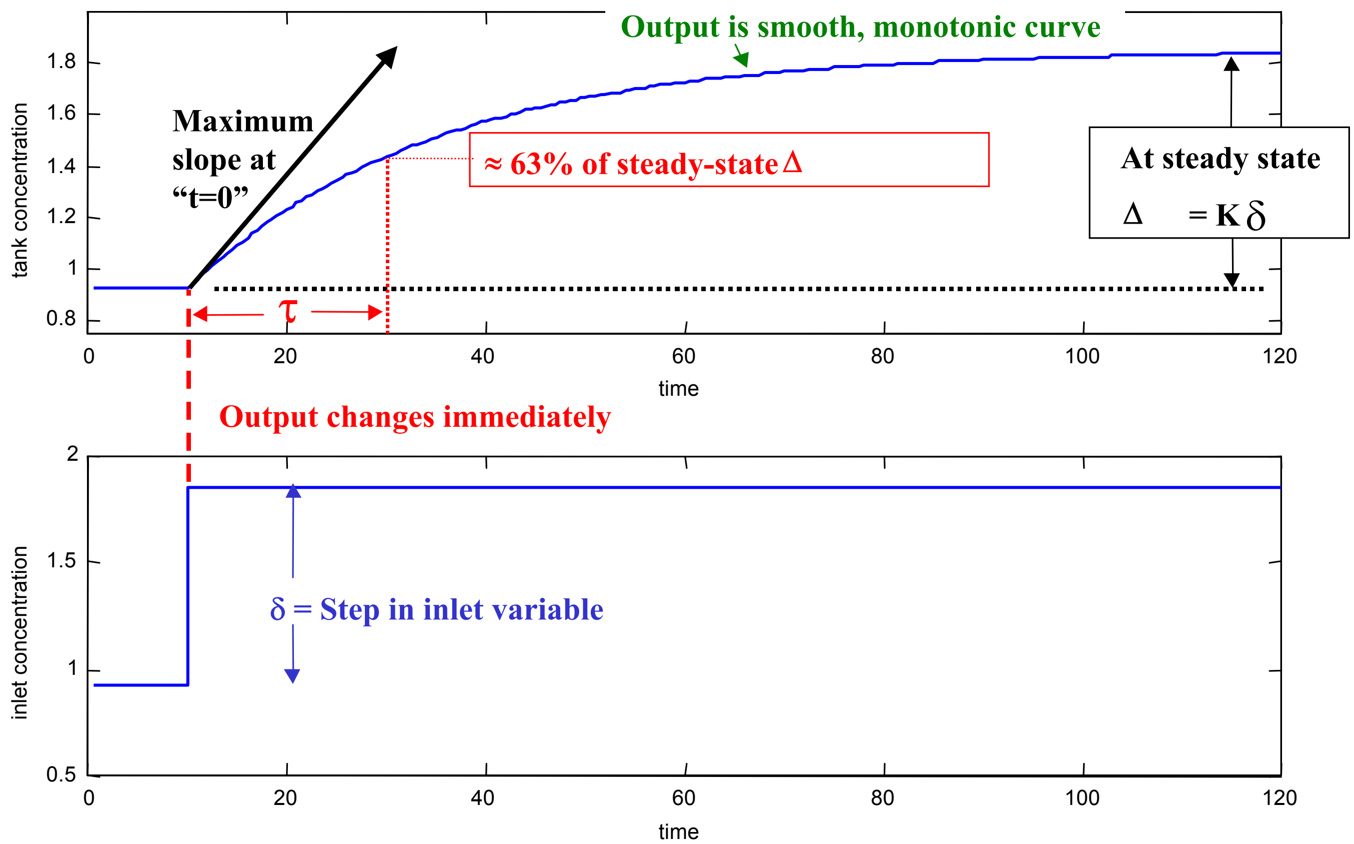
Large flow change: linearized model is poor – the answer is physically impossible! (Why?)

DYNAMIC MODELLING

We learned first-order systems have the same output "shape".

$$\tau \frac{dY}{dt} + Y = K[f(t))] \quad \text{with } f(t) \text{ the input or forcing}$$

Sample response to a step input



DYNAMIC MODELLING

The emphasis on analytical relationships is directed to understanding the key parameters. In the examples, you learned what affected the gain and time constant.

K: Steady-state Gain

- **sign**
- **magnitude (don't forget the units)**
- **how depends on design (e.g., V) and operation (e.g., F)**

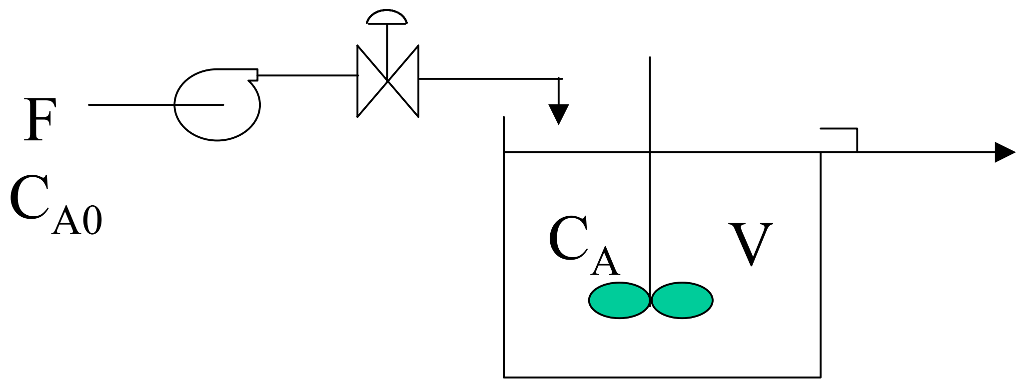
τ:Time Constant

- **sign (positive is stable)**
- **magnitude (don't forget the units)**
- **how depends on design (e.g., V) and operation (e.g., F)**

DYNAMIC MODELLING: WORKSHOP 1

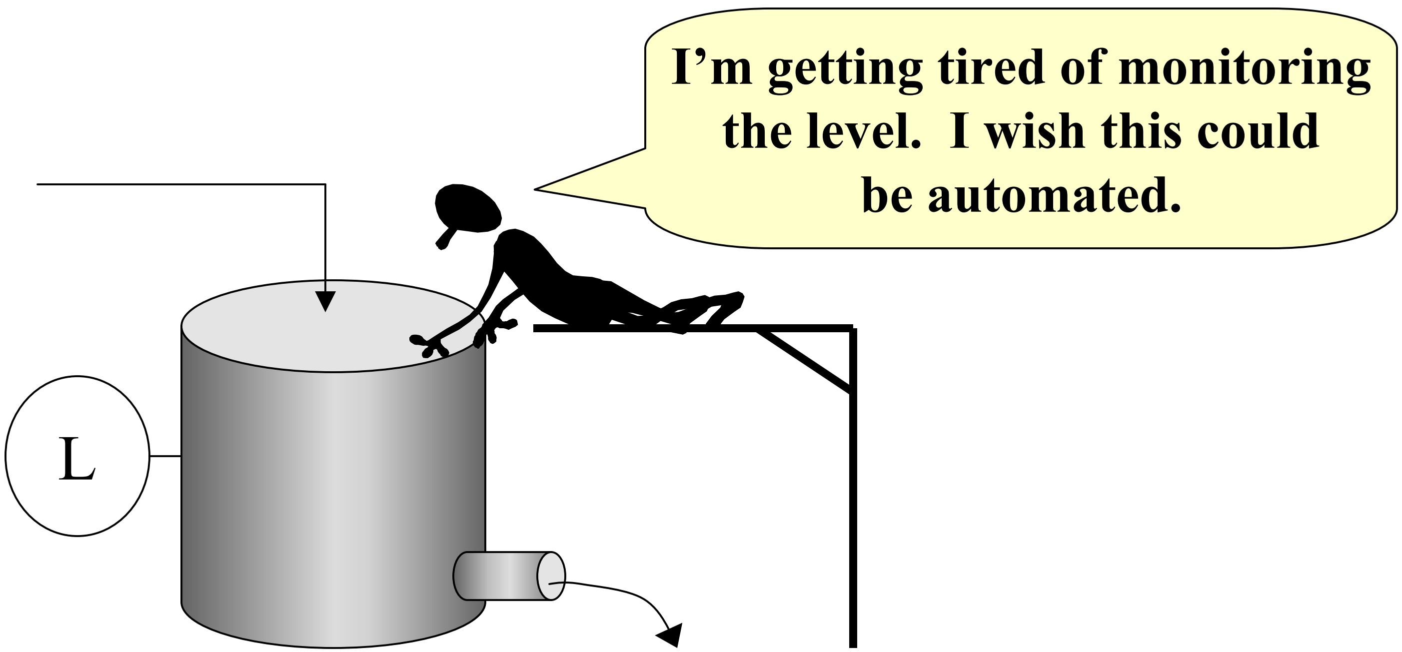
For *each* of the three processes we modelled, determine how the gain and time constant depend on V, F, T and C_{A0}.

- **Mixing tank**
- **linear CSTR**
- **CSTR with second order reaction**



DYNAMIC MODELLING: WORKSHOP 2

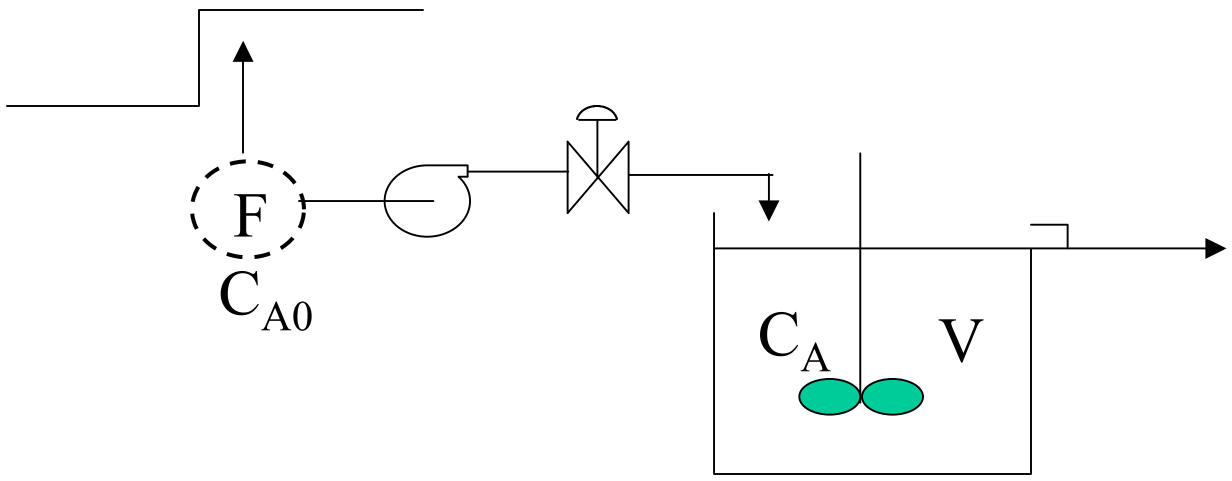
Describe three different level sensors for measuring liquid height in the draining tank. For each, determine whether the measurement can be converted to an electronic signal and transmitted to a computer for display and control.



DYNAMIC MODELLING: WORKSHOP 3

Model the dynamic response of component A (CA) for a step change in the inlet flow rate with inlet concentration constant. Consider two systems separately.

- **Mixing tank**
- **CSTR with first order reaction**



DYNAMIC MODELLING: WORKSHOP 4

The parameters we use in mathematical models are never known exactly. For several models solved in the textbook, evaluate the effect of the solution of errors in parameters.

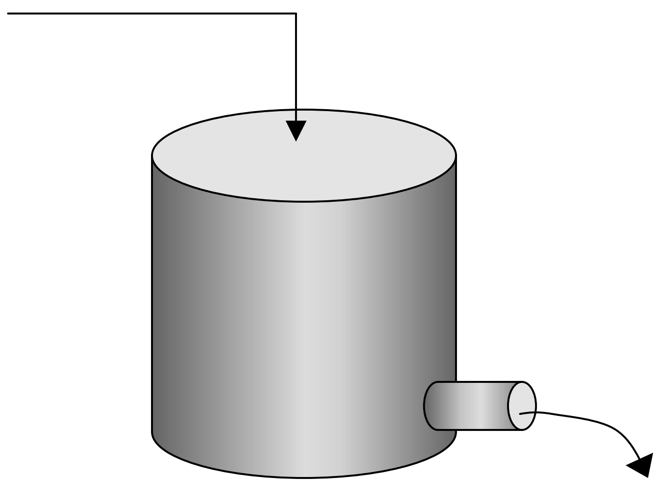
- **± 20% in reaction rate constant k**
- **± 20% in heat transfer coefficient**
- **± 5% in flow rate and tank volume**

How would you consider errors in several parameters in the same problem?

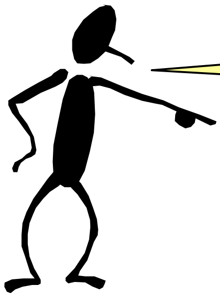
Check your responses by simulating using the MATLAB m-files in the Software Laboratory.

DYNAMIC MODELLING: WORKSHOP 5

Determine the equations that are solved for the Euler numerical solution for the dynamic response of draining tank problem. Also, give an estimate of a good initial value for the integration time step, Δt, and explain your recommendation.

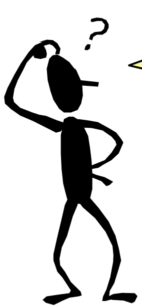


CHAPTER 3 : MATH. MODELLING



How are we doing?

- **Formulate dynamic models based on fundamental balances**
- **Solve simple first-order linear dynamic models**
- **Determine how key aspects of dynamics depend on process design and operation**



Lot’s of improvement, but we need some more study!

- **Read the textbook**
- **Review the notes, especially learning goals and workshop**
- **Try out the self-study suggestions**
- **Naturally, we’ll have an assignment!**

CHAPTER 3: LEARNING RESOURCES

- **<u>SITE PC-EDUCATION WEB</u>**

  - Instrumentation Notes

  - Interactive Learning Module (Chapter 3)

  - Tutorials (Chapter 3)

  - M-files in the Software Laboratory (Chapter 3)

- **Read the sections on dynamic modelling in previous textbooks**

  - Felder and Rousseau, Fogler, Incropera & Dewitt

- **Other textbooks with solved problems**

  - See the course outline and books on reserve in Thode

CHAPTER 3:
SUGGESTIONS FOR SELF-STUDY

1. Discuss why we require that the degrees of freedom for a model must be zero. Are there exceptions?

2. Give examples of constitutive equations from prior chemical engineering courses. For each, describe how we determine the value for the parameter. How accurate is the value?

3. Prepare one question of each type and share with your study group: T/F, multiple choice, and modelling.

4. Using the MATLAB m-files in the Software Laboratory, determine the effect of input step magnitude on linearized model accuracy for the CSTR with second-order reaction.

CHAPTER 3:
SUGGESTIONS FOR SELF-STUDY

5. For what combination of physical parameters will a first order dynamic model predict the following?

- an oscillatory response to a step input
- an output that increases without limit
- an output that changes very slowly

6. Prepare a fresh cup of hot coffee or tea. Measure the temperature and record the temperature and time until the temperature approaches ambient.

- Plot the data.
- Discuss the shape of the temperature plot.
- Can you describe it by a response by a key parameter?
- Derive a mathematical model and compare with your experimental results