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
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 a bump?

Dynamic performance depends more on the vehicle than the driver!
Do the Bus and bicycle have different dynamics?

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

Dynamic performance depends more on the vehicle than the driver!

The process dynamics are more important than the computer control!
Feed material is delivered periodically, but the process requires a continuous feed flow. How large should the tank volume be?
Feed material is delivered periodically, but the process requires a continuous feed flow. How large should the tank volume be?

We must provide process flexibility for good dynamic performance!
WHY WE NEED DYNAMIC MODELS

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

Process dynamics are important for safety!
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”
WHY WE DEVELOP MATHEMATICAL MODELS?

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

Effect on output variable

Process

• How far?
• How fast
• “Shape”

Math models help us answer these questions!

How does the process influence the response?
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
2. Prepare information
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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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- Sketch process
- Collect data
- State assumptions
- Define system

Key property of a “system”?
SIX-STEP MODELLING PROCEDURE

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

Key property of a “system”? Variable(s) are the same for any location within the system!
**SIX-STEP MODELLING PROCEDURE**

1. Define Goals
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**CONSERVATION BALANCES**

**Overall Material**

\[ \{ \text{Accumulation of mass} \} = \{ \text{mass in} \} - \{ \text{mass out} \} \]

**Component Material**

\[ \{ \text{Accumulation of component mass} \} = \{ \text{component mass in} \} - \{ \text{component mass out} \} + \{ \text{generation of component mass} \} \]

**Energy**

\[ \{ \text{Accumulation of } U + \text{PE} + \text{KE} \} = \{ H + \text{PE} + \text{KE} \}_{\text{in}} - \{ H + \text{PE} + \text{KE} \}_{\text{out}} + Q - W_s \]

* 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

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Our dynamic models will involve differential (and algebraic) equations because of the accumulation terms.

\[
V \frac{dC_A}{dt} = F(C_{A0} - C_A) - V k C_A
\]

With initial conditions

\[
C_A = 3.2 \text{ kg-mole/m}^3 \text{ at } t = 0
\]

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

\[
C_{A0} = f(t) = 2.1 \text{ t} \text{ (ramp function)}
\]
SIX-STEP MODELLING PROCEDURE

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

\[ C_A(t) = C_A(t)igg|_{t=0} + (\Delta C_{A0})K(1 - e^{-t/\tau}) \]

for \( t \succ 0 \)

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

\[ K = \frac{F}{F + kV} \quad \tau = \frac{V}{F + Vk} \]
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

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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)!
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/m³. The feed composition experiences a step to 1.85 kg-mole/m³. 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!

Output is smooth, monotonic curve

Maximum slope at “t=0”

Output changes immediately

At steady state

\[ \Delta C_A = K \Delta C_{A0} \]

\[ \approx 63\% \text{ of steady-state } \Delta C_A \]

\[ \tau \approx 63\% \text{ of steady-state } \Delta C_A \]
The isothermal, CSTR in the figure has been operating for a long time with a feed concentration of 0.925 kg-mole/m³. The feed composition experiences a step to 1.85 kg-mole/m³. All other variables are constant. Determine the dynamic response of $C_A$. Same parameters as textbook Example 3.2

\[ \dot{r}_A = kC_A \]

(We’ll solve this in class.)
MODELLING EXAMPLE 2. CSTR

Annotate with key features similar to Example 1

Which is faster, mixer or CSTR? Always?
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 $C_{A_2}$. 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
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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.

\[ F(x) = F(x_s) + \frac{dF}{dx}\bigg|_{x_s}(x - x_s) + \frac{1}{2!} \frac{d^2F}{dx^2}\bigg|_{x_s}(x - x_s)^2 + R \]

This is the only variable

Remember that these terms are constant because they are evaluated at \( x_s \)

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

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.

\[ y = 1.5x^2 + 3 \text{ about } x = 1 \]
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.

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

Small flow change: linearized approximation is good

Large flow change: linearized model is poor – the answer is physically impossible! (Why?)
We learned first-order systems have the same output “shape”.

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

Sample response to a step input

Maximum slope at \( t=0 \)

Output is smooth, monotonic curve

Output changes immediately

At steady state

\[ \Delta = K\delta \]

\( \approx 63\% \) of steady-state \( \Delta \)
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)
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
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.

I’m getting tired of monitoring the level. I wish this could be automated.
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
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.
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, $\Delta t$, 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

• SITE PC-EDUCATION WEB
  - 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
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