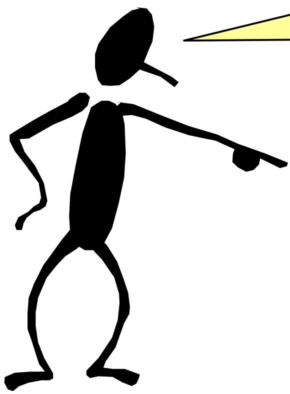
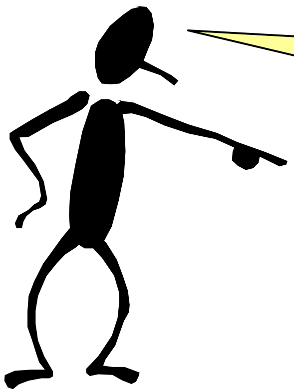
CHAPTER 6: EMPIRICAL MODEL IDENTIFICATION



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

- **Design and implement a good experiment**
- **Perform the graphical calculations**
- **Perform the statistical calculations**
- **Combine fundamental and empirical modelling for chemical process systems**

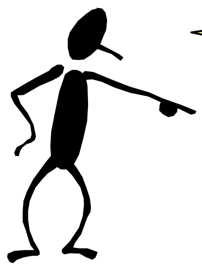
CHAPTER 6: EMPIRICAL MODEL IDENTIFICATION



Outline of the lesson.

- **Experimental design for model building**
- **Process reaction curve (graphical)**
- **Statistical parameter estimation**
- **Workshop**

CHAPTER 6: EMPIRICAL MODELLING

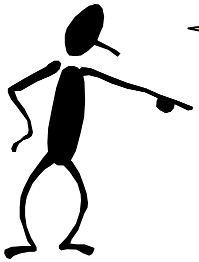


We have invested a lot of effort to learn fundamental modelling. Why are we now learning about an empirical approach?

TRUE/FALSE QUESTIONS

- **We have all data needed to develop a fundamental model of a complex process**
- **We have the time to develop a fundamental model of a complex process**
- **Experiments are easy to perform in a chemical process**
- **We need very accurate models for control engineering**

CHAPTER 6: EMPIRICAL MODELLING



We have invested a lot of effort to learn fundamental modelling. Why are we now learning about an empirical approach?

TRUE/FALSE QUESTIONS

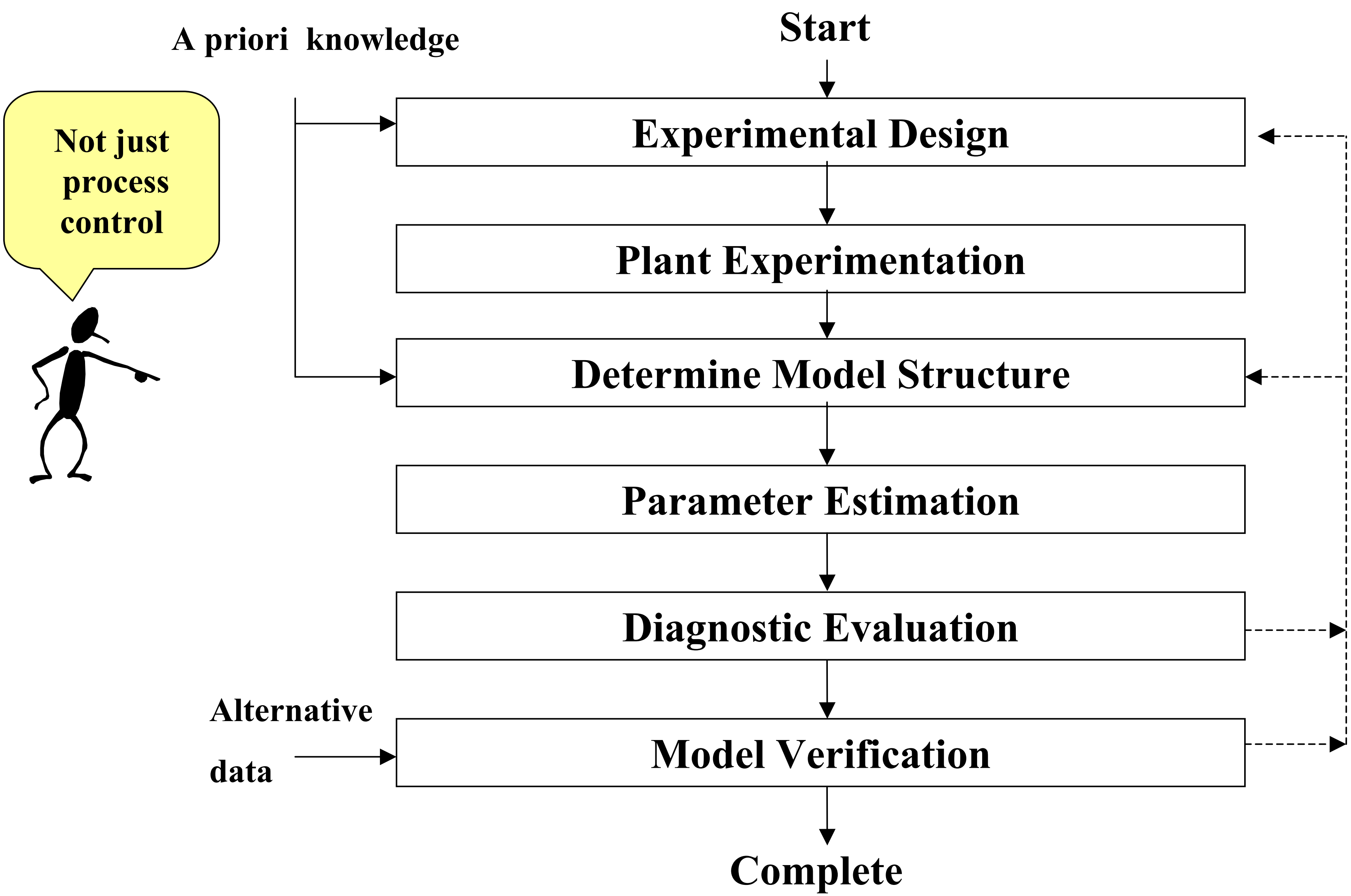
false We have all data needed to develop a fundamental model of a complex process

false We have the time to develop a fundamental model of a complex process

false Experiments are easy to perform in a chemical process

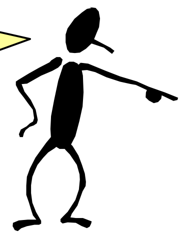
false We need very accurate models for control engineering

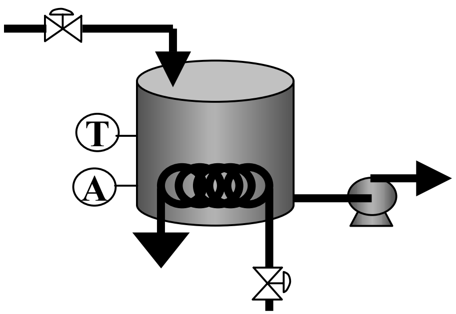
EMPIRICAL MODEL BUILDING PROCEDURE

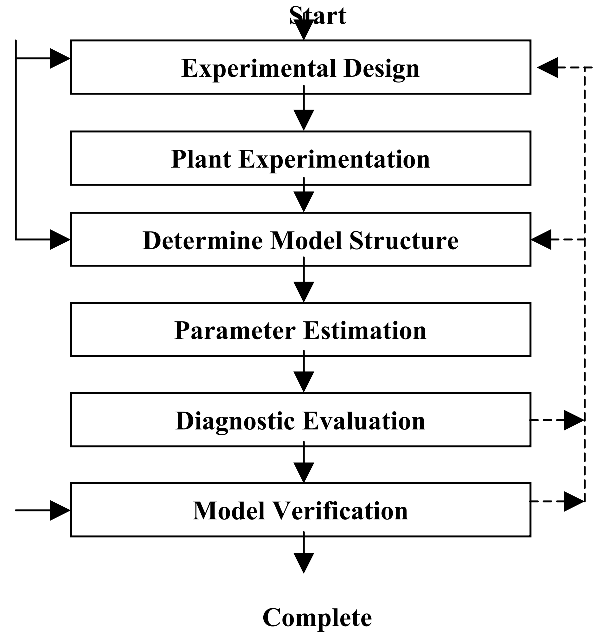


EMPIRICAL MODEL BUILDING PROCEDURE

**Looks very general; it is!
However, we still need to
understand the process!**







- **Changing the temperature 10 K in a ethane pyrolysis reactor is allowed.**
- **Changing the temperature in a bio-reactor could kill micro-organisms**

EMPIRICAL MODEL BUILDING PROCEDURE

Start

Experimental Design

Plant Experimentation

Determine Model Structure

Parameter Estimation

Diagnostic Evaluation

Model Verification

Complete

- Base case operating conditions
- Definition of perturbation
- Measures
- Duration

- Safely
- Small effect on product quality
- Small effect of profit

- We will stick with linear.
- What order, dead time, etc?

EMPIRICAL MODEL BUILDING PROCEDURE

Start

↓

Experimental Design

↓

Plant Experimentation

↓

Determine Model Structure

↓

Parameter Estimation → • Gain, time constant, dead time ...

↓

Diagnostic Evaluation → • Does the model fit the data used to evaluate the parameters?

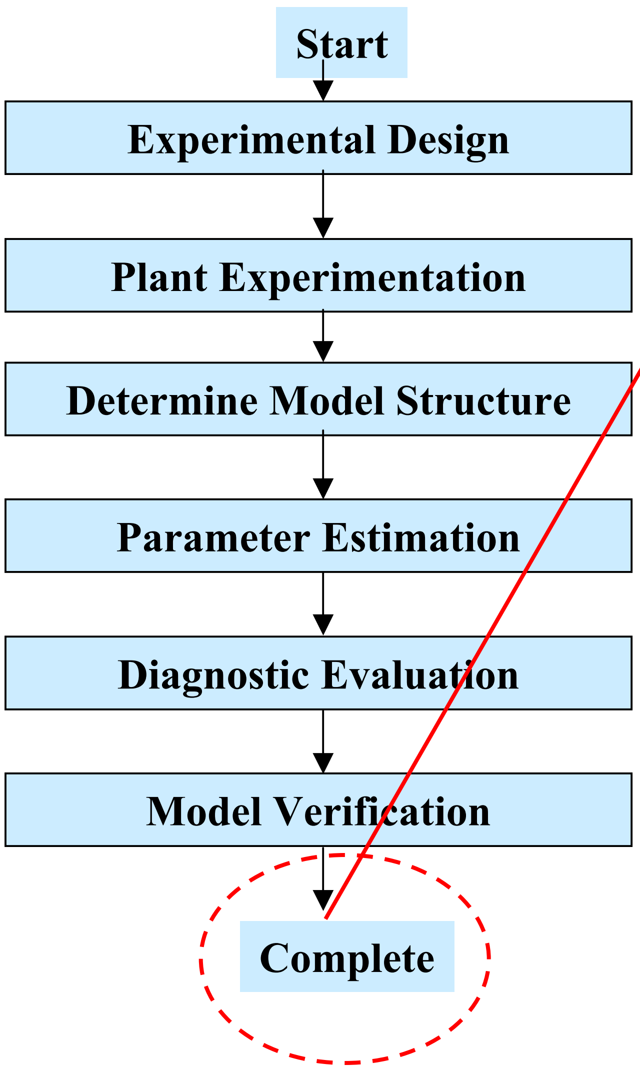
↓

Model Verification → • Does the model fit a new set of data not used in parameter estimation.

↓

Complete

EMPIRICAL MODEL BUILDING PROCEDURE



- **What is our goal?**

  We seek models good enough for control design, controller tuning, and process design.

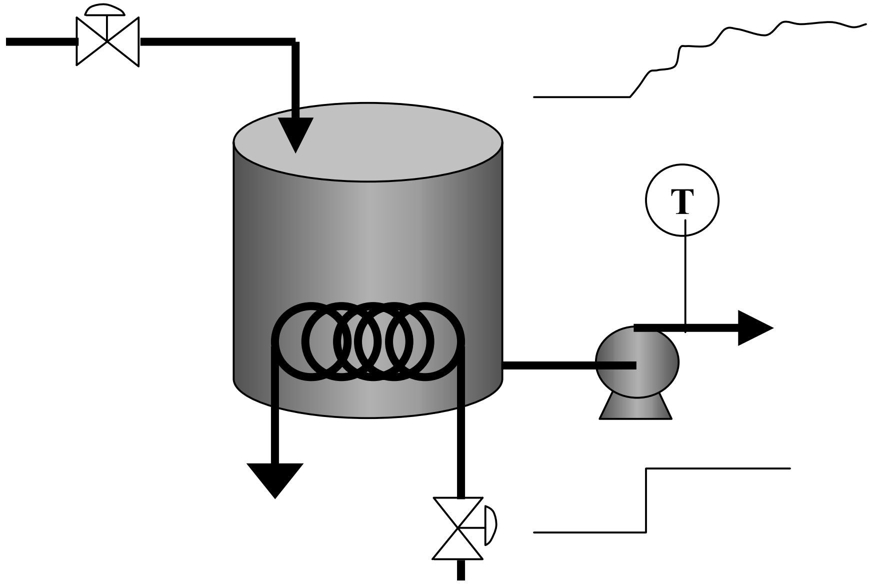
- **How do we know?**

  We'll have to trust the book and instructor for now. <u>But, we will check often in the future!</u>

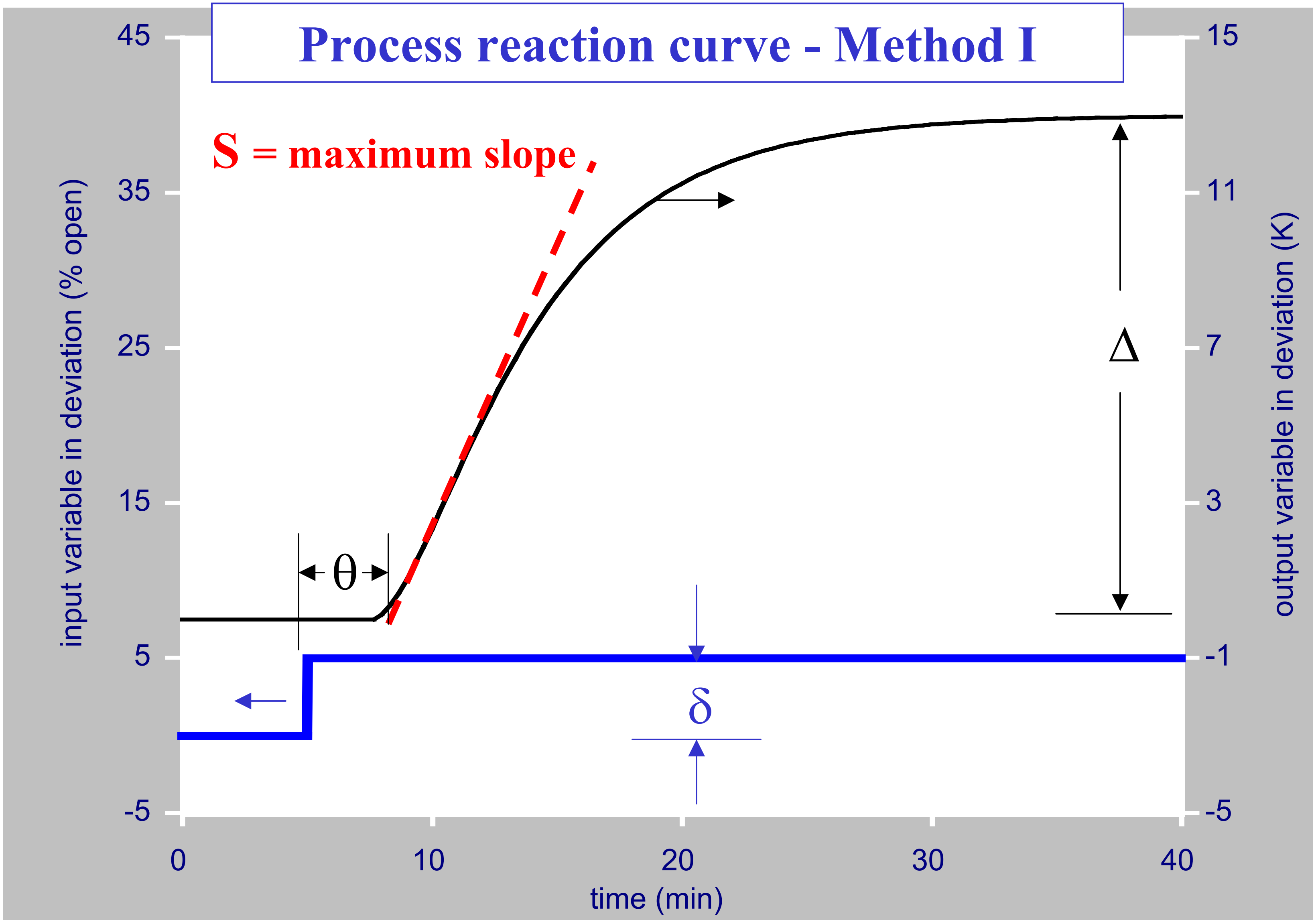
EMPIRICAL MODEL BUILDING PROCEDURE

Process reaction curve - The simplest and most often used method. Gives nice visual interpretation as well.

1. Start at steady state
2. Single step to input
3. Collect data until steady state
4. Perform calculations

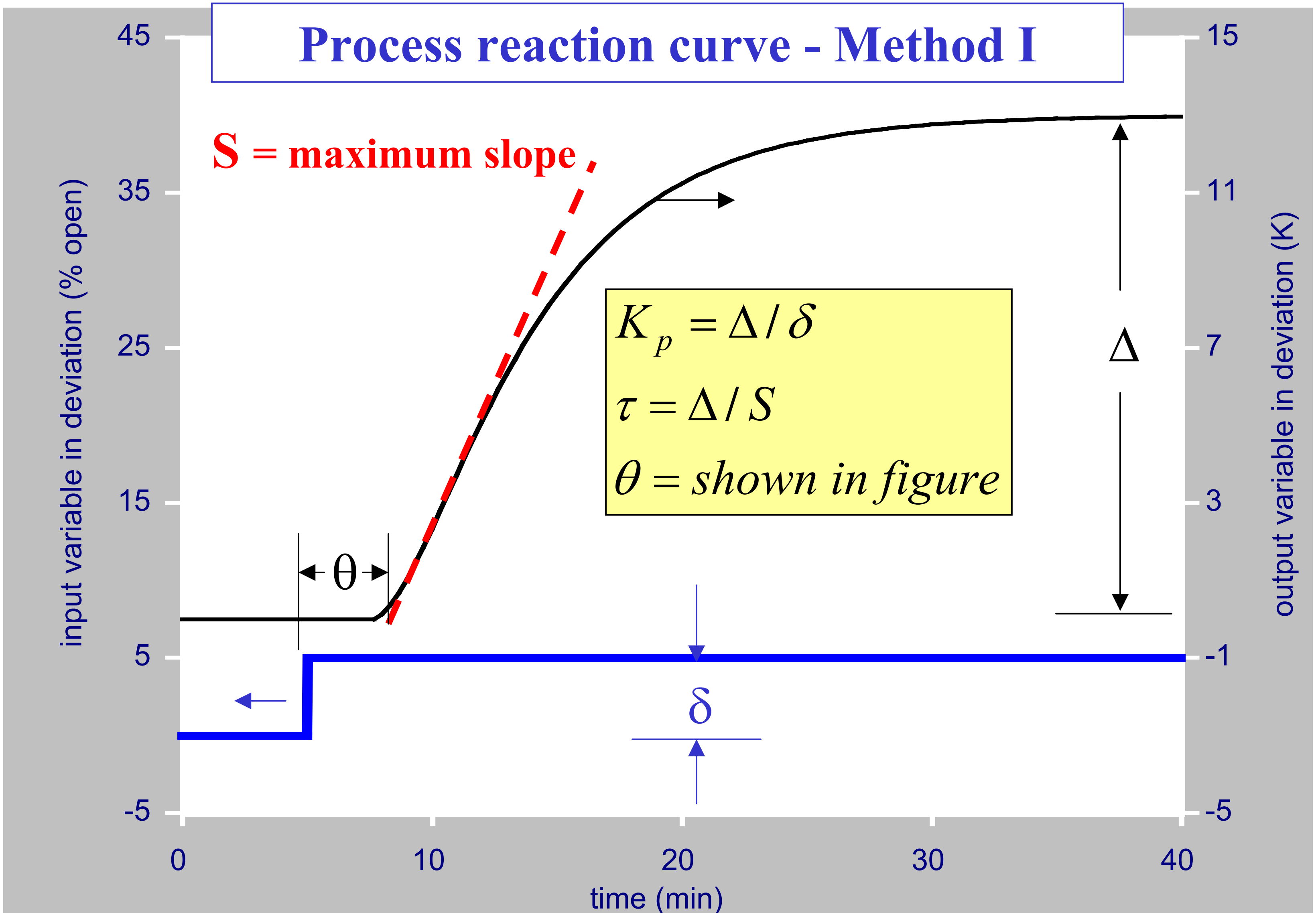


EMPIRICAL MODEL BUILDING PROCEDURE



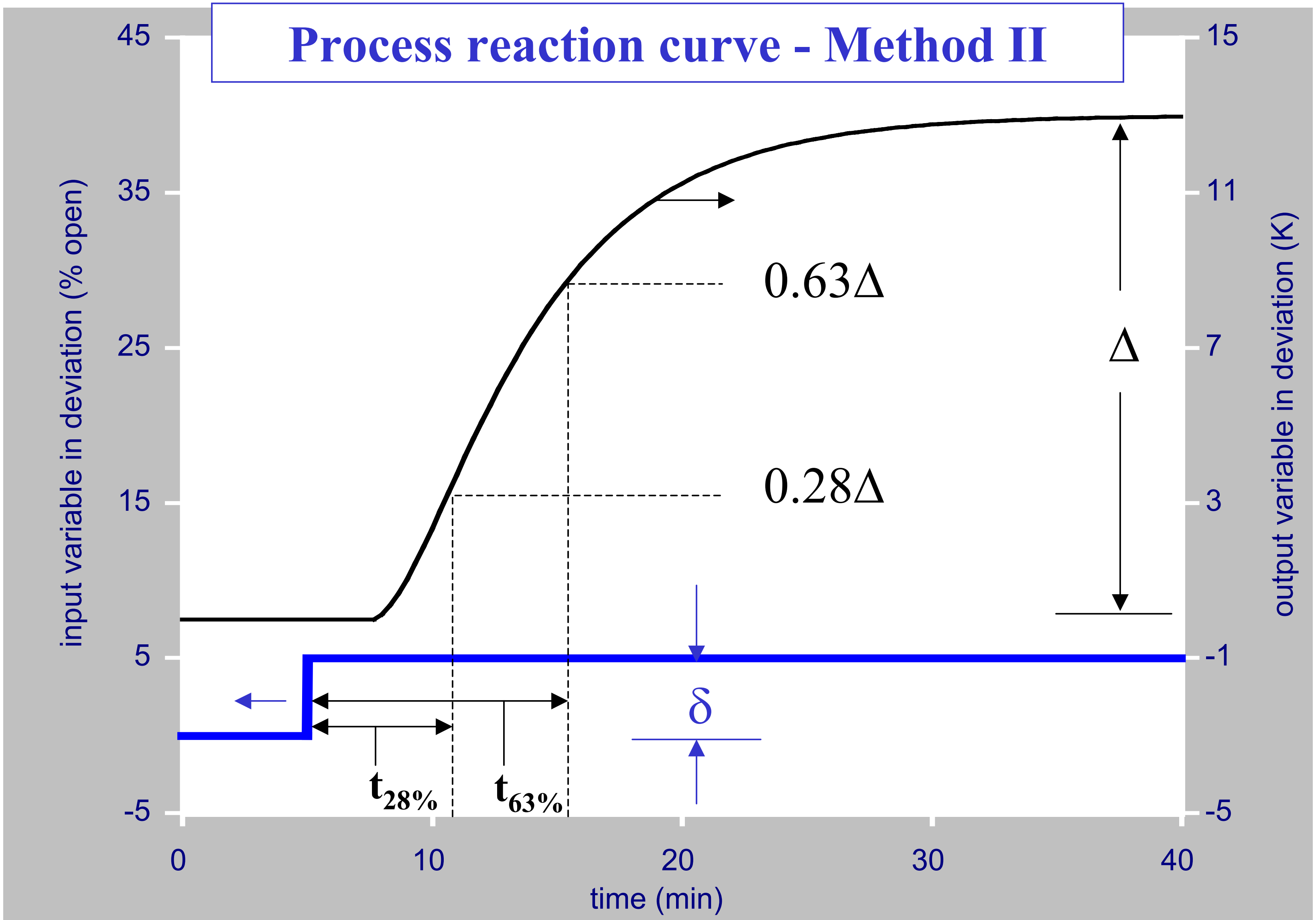
Data is plotted in deviation variables

EMPIRICAL MODEL BUILDING PROCEDURE



Data is plotted in deviation variables

EMPIRICAL MODEL BUILDING PROCEDURE



Data is plotted in deviation variables

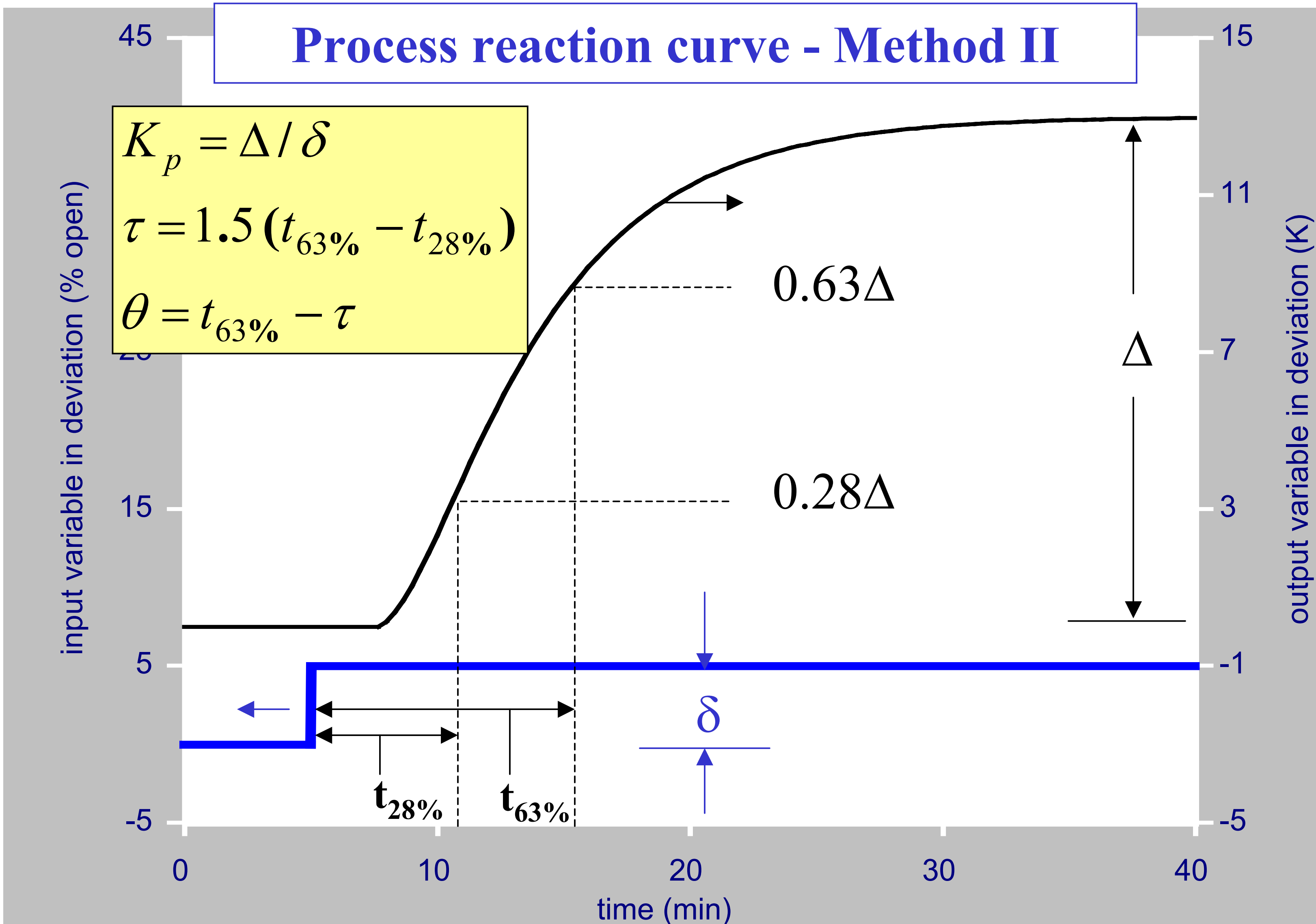
EMPIRICAL MODEL BUILDING PROCEDURE

Process reaction curve - Method II

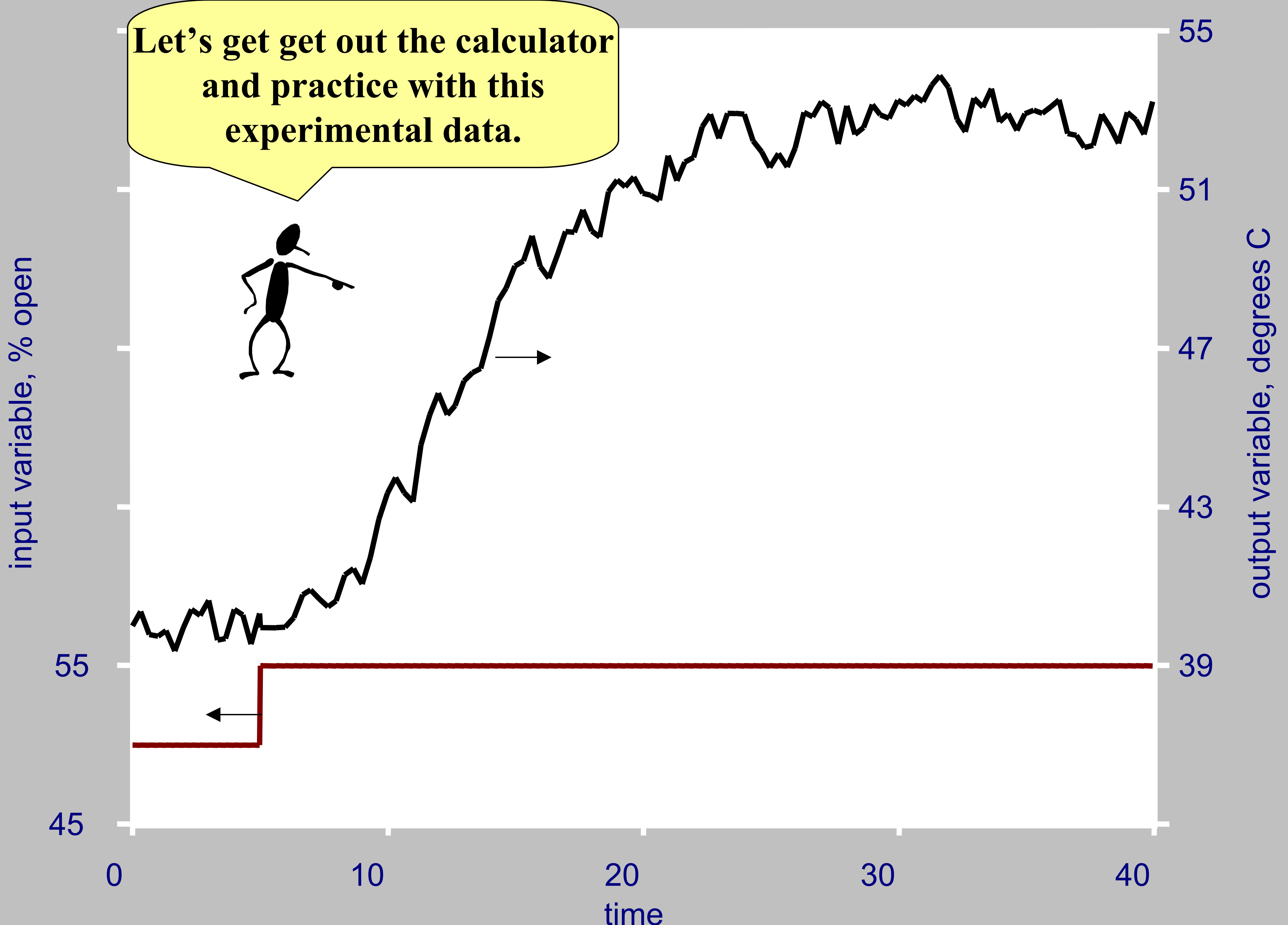
$$K_p = \Delta / \delta$$

$$\tau = 1.5\,(t_{63\%} - t_{28\%})$$

$$\theta = t_{63\%} - \tau$$



Data is plotted in deviation variables



Let's get get out the calculator and practice with this experimental data.
input variable, % open
output variable, degrees C
time
45
55
0
10
20
30
40
39
43
47
51
55

EMPIRICAL MODEL BUILDING PROCEDURE

Process reaction curve - Methods I and II

The same experiment in either method!

Method I

- Developed first
- Prone to errors because of evaluation of maximum slope

Method II

- Developed in 1960's
- Simple calculations

EMPIRICAL MODEL BUILDING PROCEDURE

Process reaction curve - Methods I and II

The same experiment in either method!

Method I

- **Developed first**
- **Prone to errors because of evaluation of maximum slope**

Method II

- **Developed in 1960's**
- **Simple calculations**

Recommended

EMPIRICAL MODEL BUILDING PROCEDURE

Process reaction curve

Start

Experimental Design

Plant Experimentation

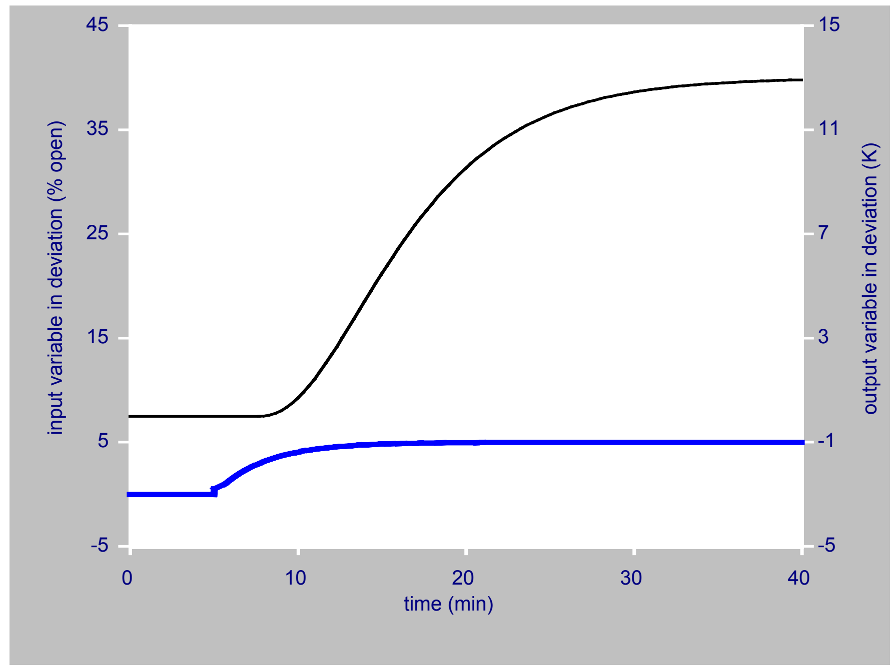
Determine Model Structure

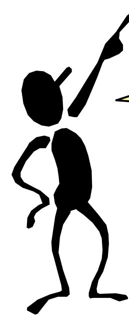
Parameter Estimation

Diagnostic Evaluation

Model Verification

Complete

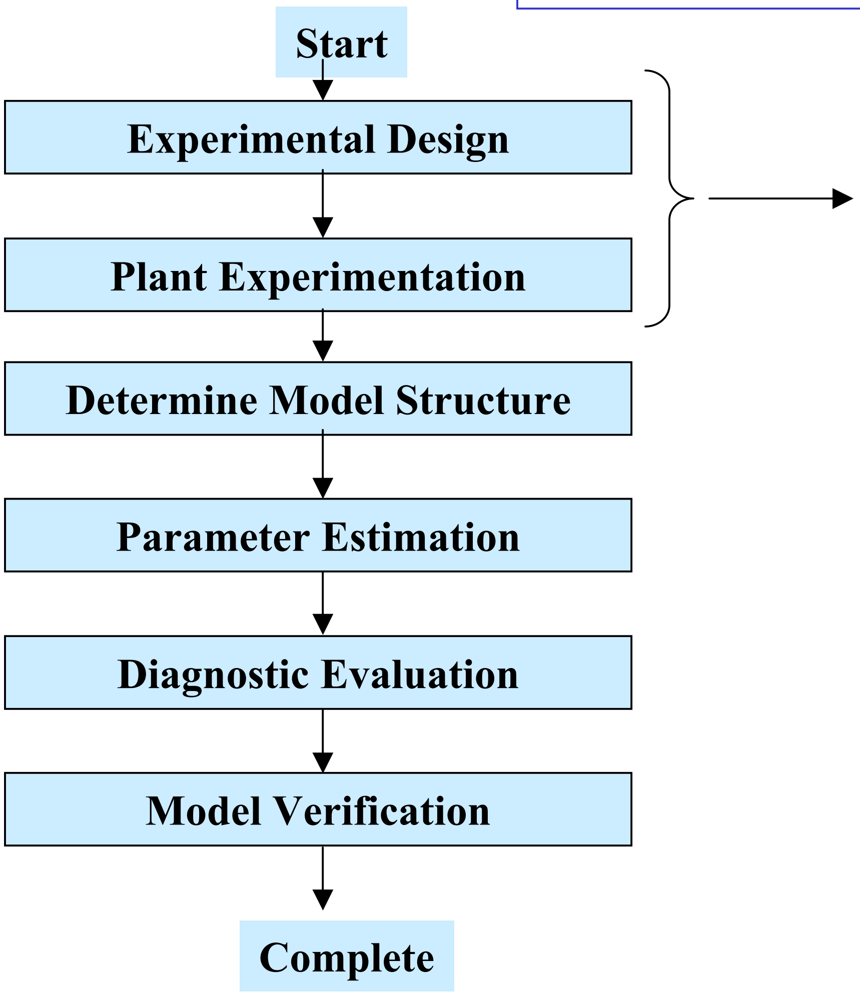


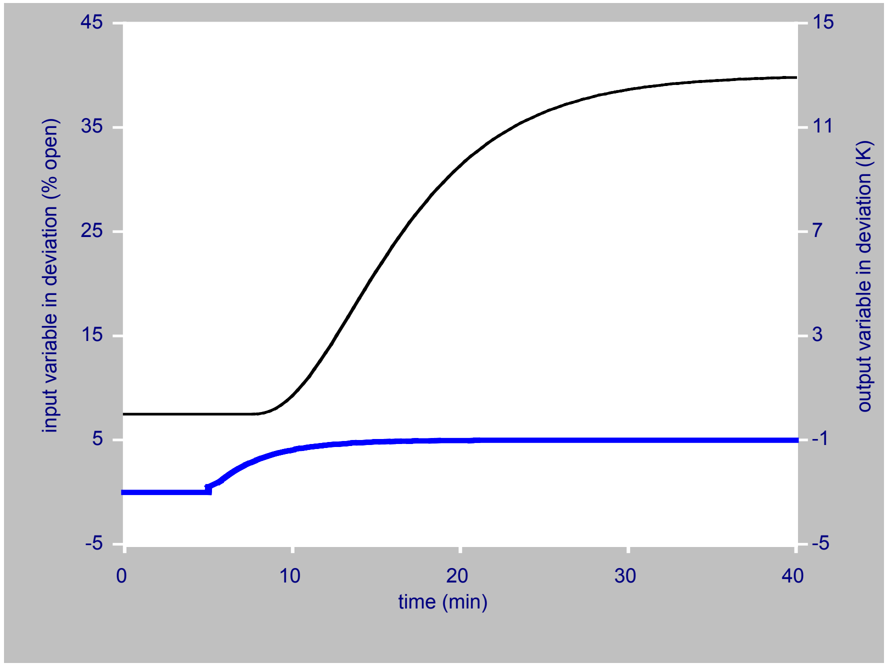


Is this a well designed experiment?

EMPIRICAL MODEL BUILDING PROCEDURE

Process reaction curve





EMPIRICAL MODEL BUILDING PROCEDURE

Process reaction curve

Start

Experimental Design

Plant Experimentation

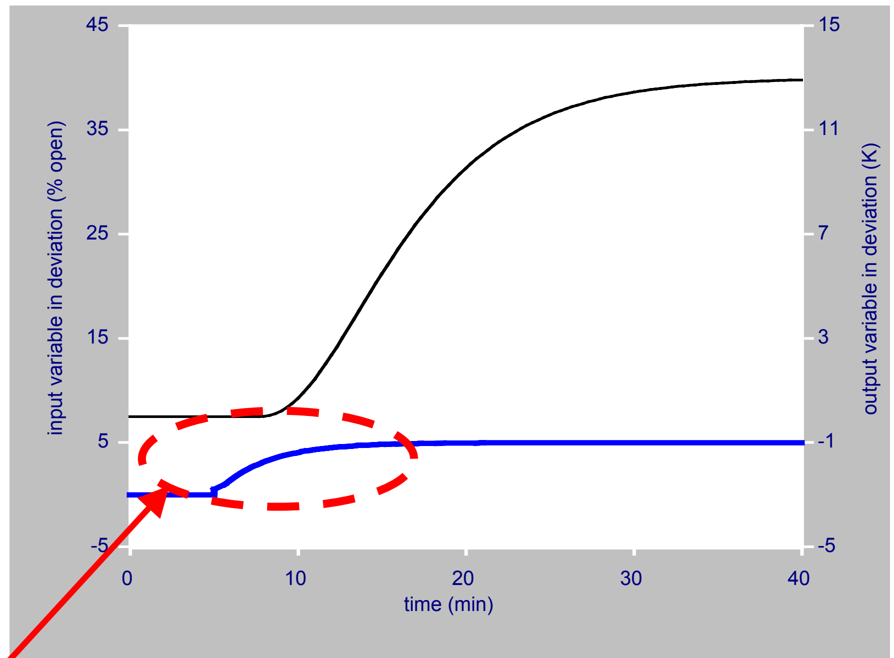
Determine Model Structure

Parameter Estimation

Diagnostic Evaluation

Model Verification

Complete



Input should be close to a perfect step; <u>this was basis of equations</u>. If not, cannot use data for process reaction curve.

EMPIRICAL MODEL BUILDING PROCEDURE

Start

Experimental Design

Plant Experimentation

Determine Model Structure

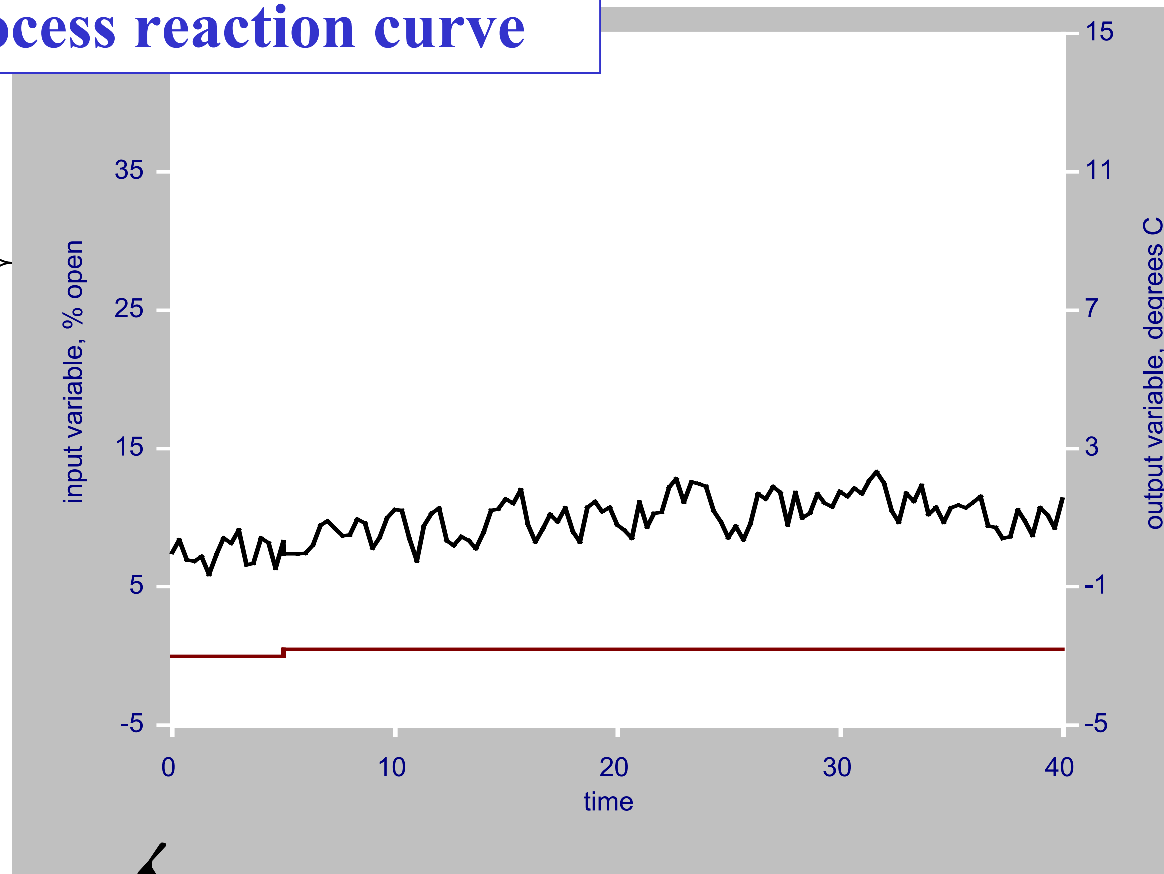
Parameter Estimation

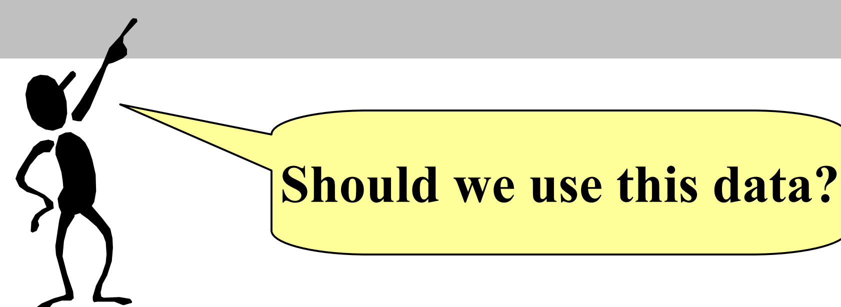
Diagnostic Evaluation

Model Verification

Complete

Process reaction curve





EMPIRICAL MODEL BUILDING PROCEDURE

Start

Experimental Design

Plant Experimentation

Determine Model Structure

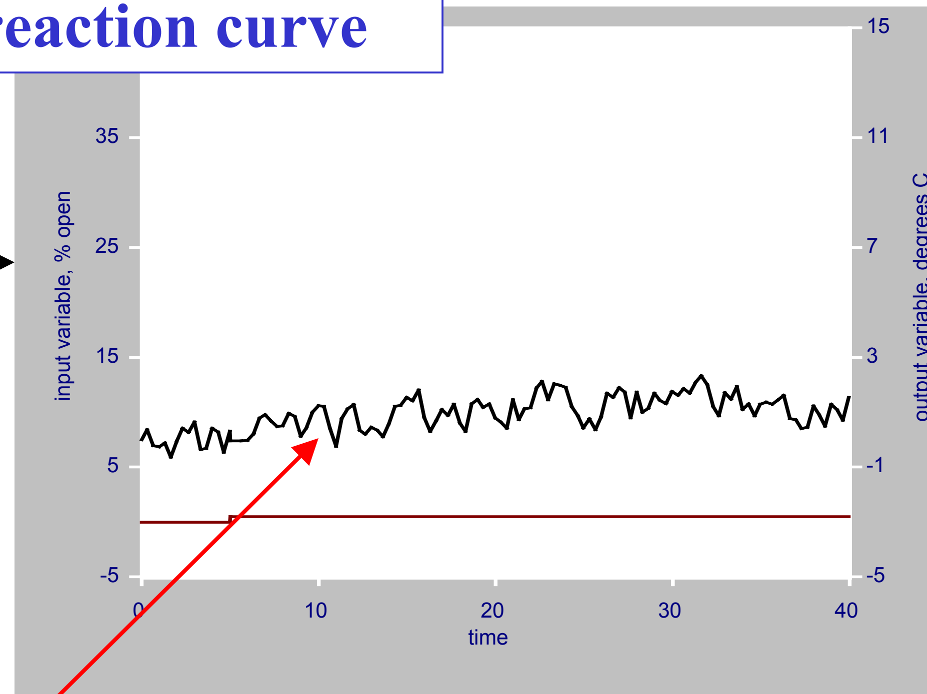
Parameter Estimation

Diagnostic Evaluation

Model Verification

Complete

Process reaction curve



The output must be "moved" enough. Rule of thumb:

Signal/noise > 5

EMPIRICAL MODEL BUILDING PROCEDURE

Process reaction curve

Start

↓

Experimental Design

↓

Plant Experimentation

↓

Determine Model Structure

↓

Parameter Estimation

↓

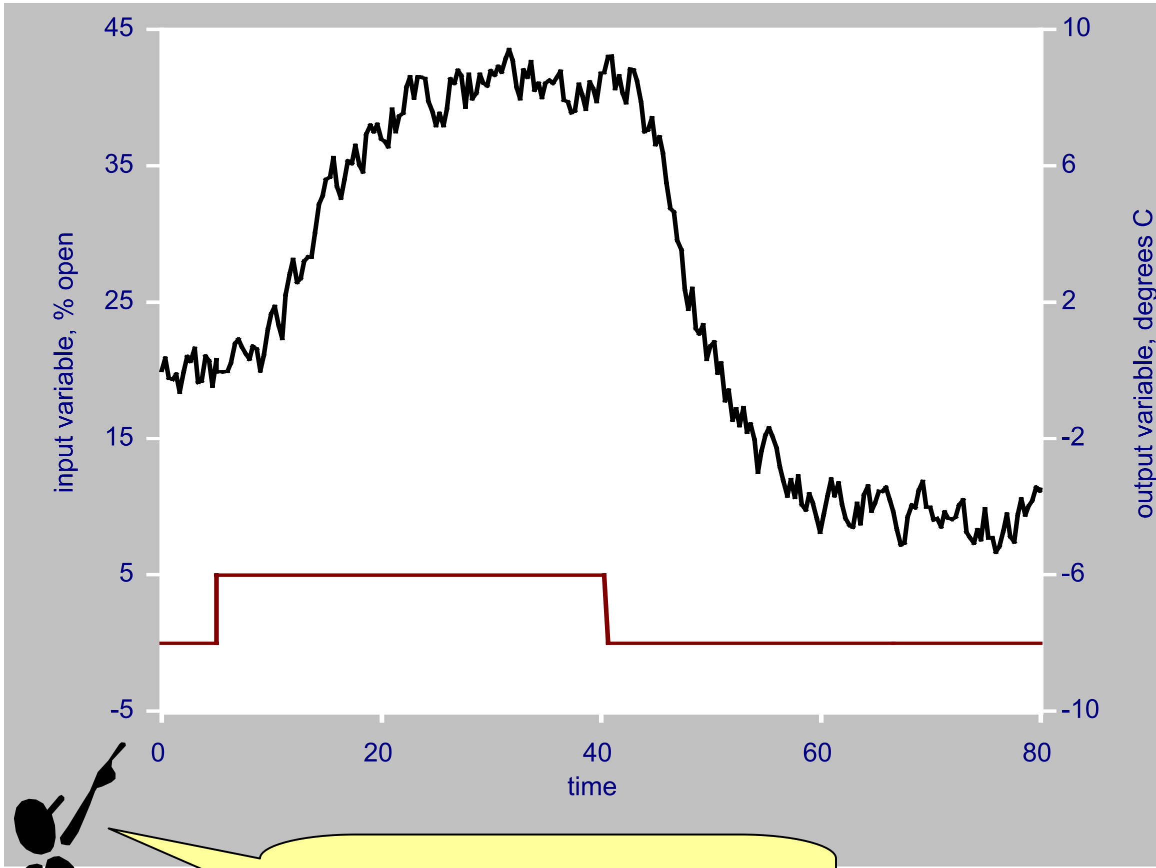
Diagnostic Evaluation

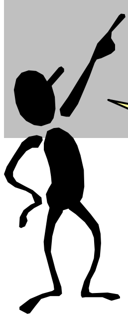
↓

Model Verification

↓

Complete





Should we use this data?

EMPIRICAL MODEL BUILDING PROCEDURE

Start

Experimental Design

Plant Experimentation

Determine Model Structure

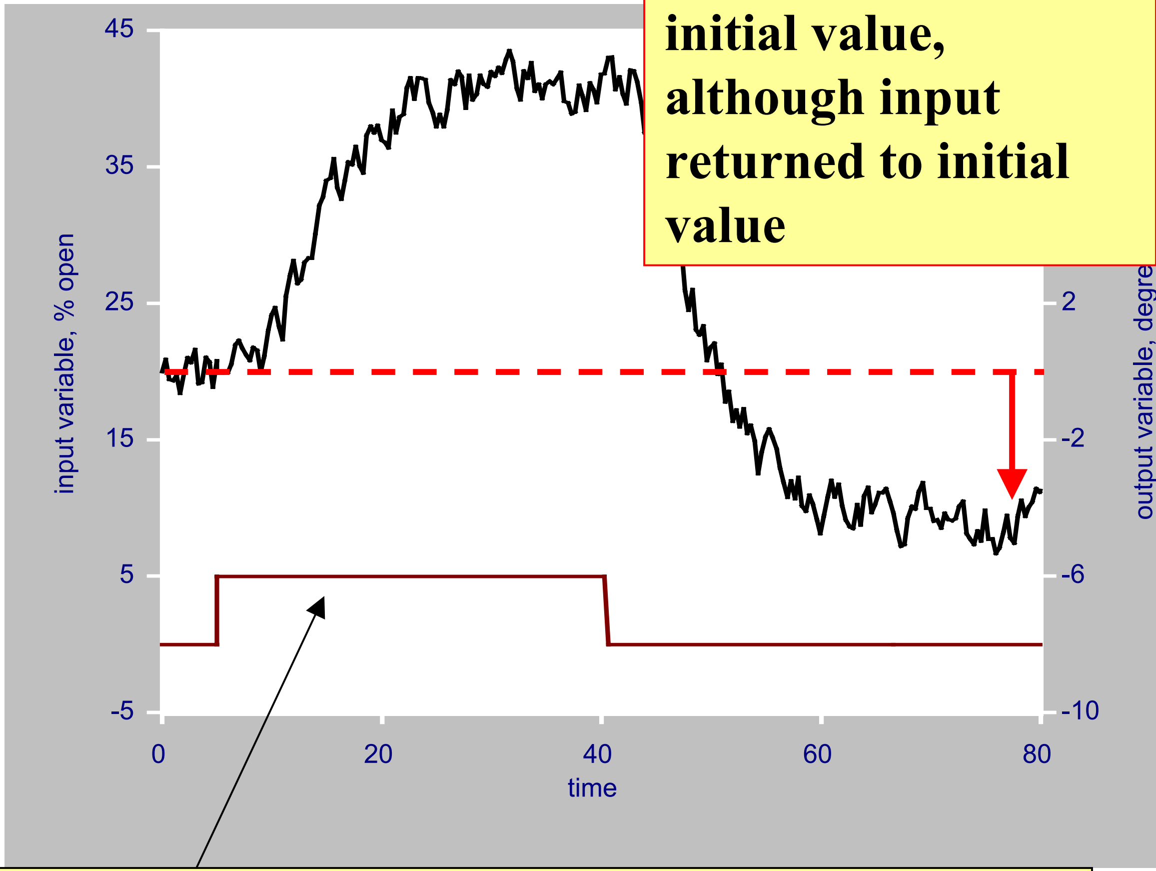
Parameter Estimation

Diagnostic Evaluation

Model Verification

Complete

Process reaction curve



Output did not return close to the initial value, although input returned to initial value

This is a good experimental design; it checks for disturbances

EMPIRICAL MODEL BUILDING PROCEDURE

Process reaction curve

Start

↓

Experimental Design

↓

Plant Experimentation

↓

Determine Model Structure

↓

Parameter Estimation

↓

Diagnostic Evaluation

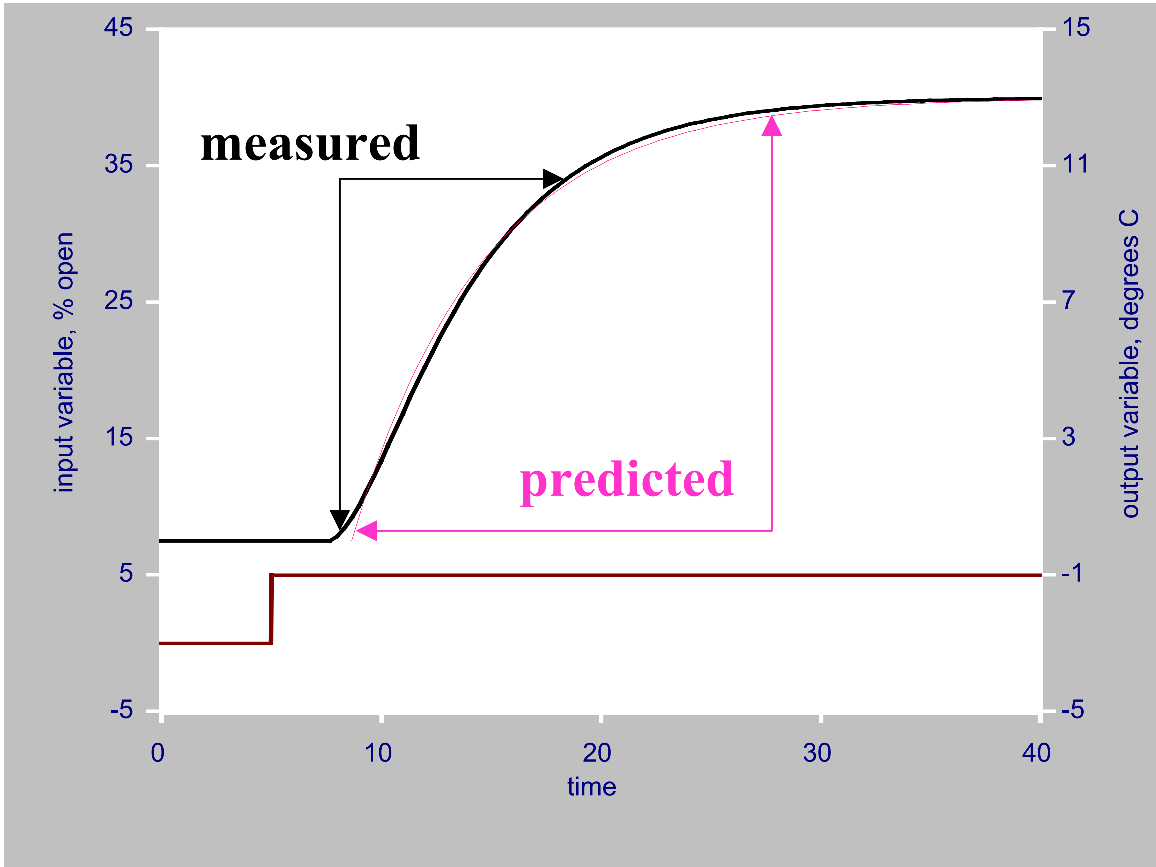
↓

Model Verification

↓

Complete

Plot measured vs predicted



EMPIRICAL MODEL BUILDING PROCEDURE

Statistical method

Provides much more general approach that is not restricted to

- **step input**
- **first order with dead time model**
- **single experiment**
- **“large” perturbation**
- **attaining steady-state at end of experiment**

Requires

- **more complex calculations**

EMPIRICAL MODEL BUILDING PROCEDURE

Statistical method

- The basic idea is to formulate the model so that regression can be used to evaluate the parameters.
- We will do this for a first order plus dead time model, although the method is much more general.
- How do we do this for the model below?

$$\tau \frac{dY(t)}{dt} + Y(t) = K_p \, X(t-\theta) \qquad \frac{Y(s)}{X(s)} = \frac{K_p e^{-\theta s}}{\tau \mathbf{s} + \mathbf{1}}$$

EMPIRICAL MODEL BUILDING PROCEDURE

Statistical method

We have discrete measurements, so let's express the model as a difference equation, with the next prediction based on current and past measurements.

$$\left(Y'_{i+1}\right)_{predicted} = a\left(Y'_{i}\right)_{measured} + b\left(X'_{i-\Gamma}\right)_{measured}$$

$$a = e^{-\Delta t/\tau}$$

$$b = K_p(1 - e^{-\Delta t/\tau})$$

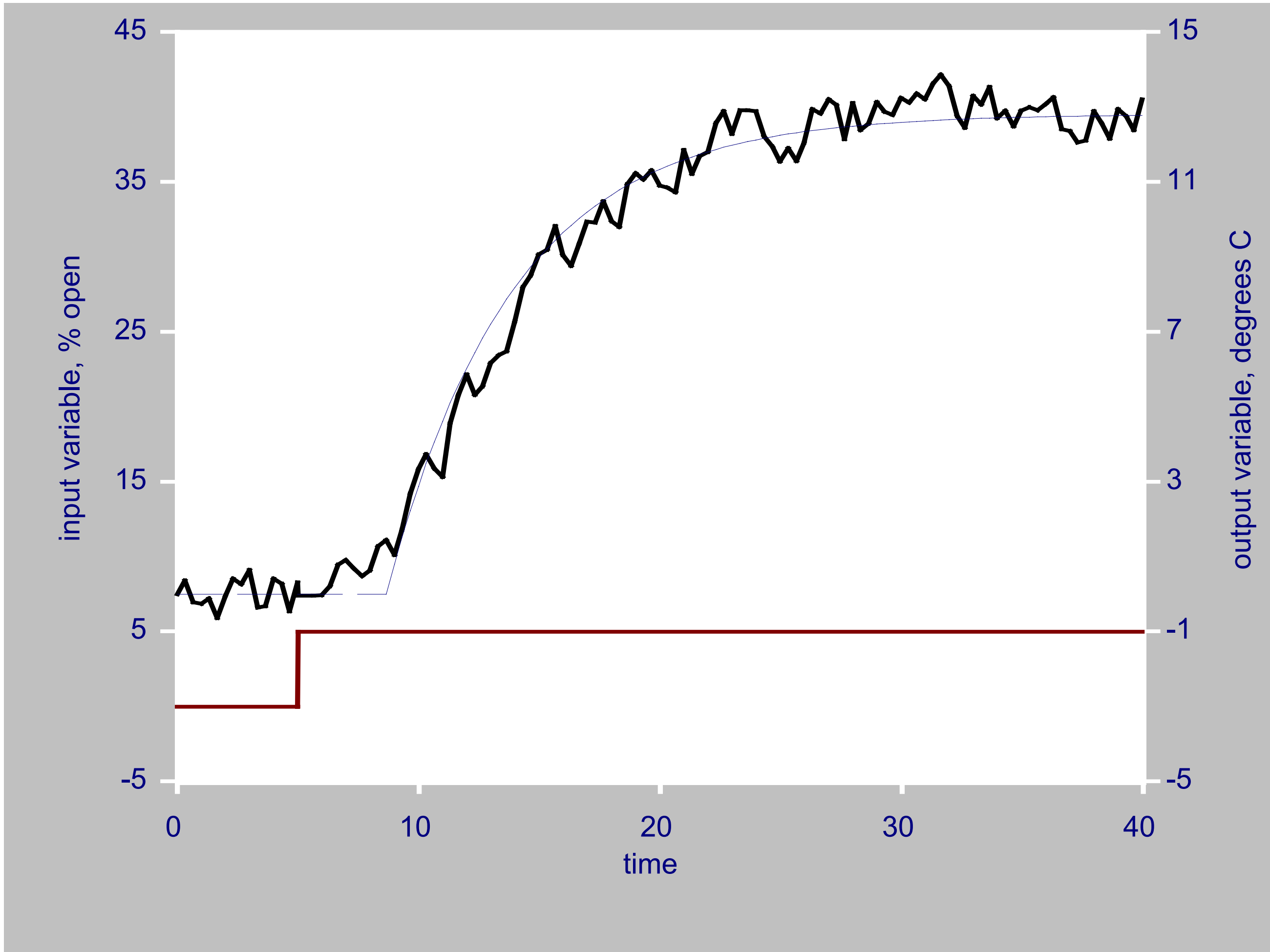
$$\Gamma = \theta / \Delta t$$

EMPIRICAL MODEL BUILDING PROCEDURE

$$\min \sum_i \left[\left(Y_i'\right)_{predicted} - \left(Y_i'\right)_{measured} \right]^2$$

Now, we can solve a standard regression problem to minimize the sum of squares of deviation between prediction and measurements.

Details are in the book.



EMPIRICAL MODEL BUILDING PROCEDURE

Statistical method

Start

Experimental Design

Plant Experimentation

Determine Model Structure

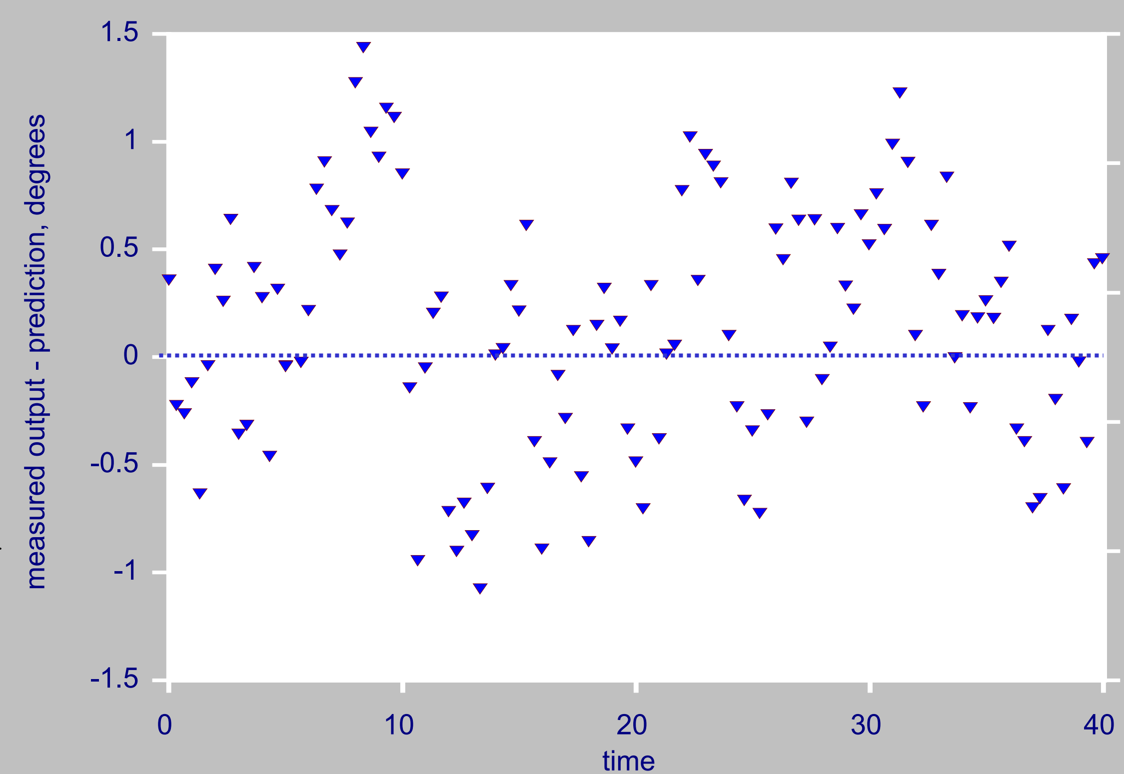
Parameter Estimation

Diagnostic Evaluation

Model Verification

Complete

$$\left[\left(Y_i'\right)_{predicted} - \left(Y_i'\right)_{measured}\right]$$ **Random?**



Plotted for every measurement (sample)

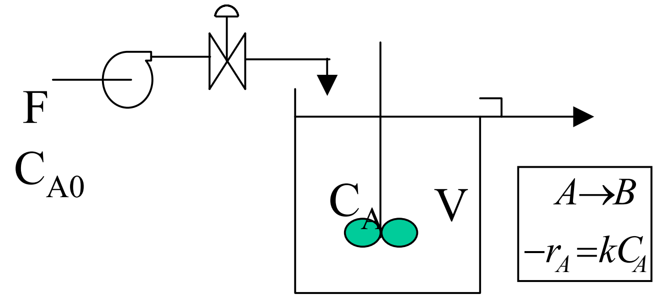
EMPIRICAL MODEL BUILDING PROCEDURE

We performed a process reaction curve for the isothermal CSTR with first order reaction. The dynamic parameters are

$$K_p = \frac{\Delta C_A}{\Delta C_{A0}} = 0.50 \ \frac{kmol/m^3}{kmol/m^3}$$

$$\tau = 12.4 \ \text{min}$$

Recently, we changed the feed flow rate by -40% and reached a new steady-state. What are the $C_{A0} \rightarrow C_A$ dynamics now?

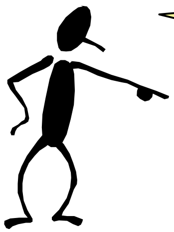


$$V \frac{dC'_A}{dt} = F(C'_{A0} - C'_A) - VkC'_A$$

$$\tau \frac{dC'_A}{dt} + C'_A = KC'_{A0}$$

$$\textbf{with } \tau = \frac{\mathbf{V}}{\mathbf{F + kV}} \ \textbf{ and K} = \frac{\mathbf{F}}{\mathbf{F + kV}}$$

EMPIRICAL MODEL BUILDING PROCEDURE



Match the method to the application.

Feature	Process reaction curve	Statistical method
Input magnitude	Signal/noise > 5	Can be much smaller
Experiment duration	Reach steady state	Steady state not required
Input change shape	Nearly perfect step	Arbitrary, sufficient "information" required
Model structure	First order with dead time	General linear dynamic model
Accuracy with unmeasured disturbances	Poor with significant disturbance	Poor with significant disturbance
Diagnostics	Plot prediction vs data	Plot residuals
Calculations	simple	Requires spreadsheet or other computer program

EMPIRICAL MODEL BUILDING

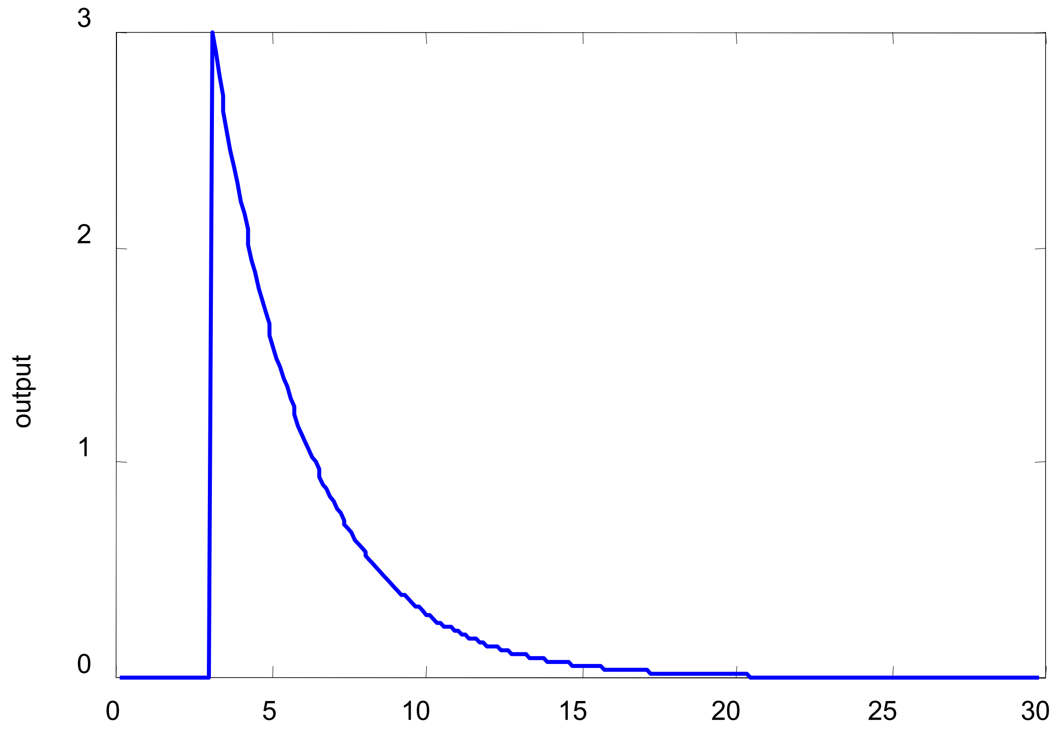
How accurate are empirical models?

- Linear approximations of non-linear processes
- Noise and unmeasured disturbances influence data
- Lack of consistency in graphical method
- lack of perfect implementation of valve change
- sensor errors

Let's say that each parameter has an error $\pm$ 20%. Is that good enough for future applications?

CHAPTER 6: EMPIRCAL MODELLING WORKSHOP 1

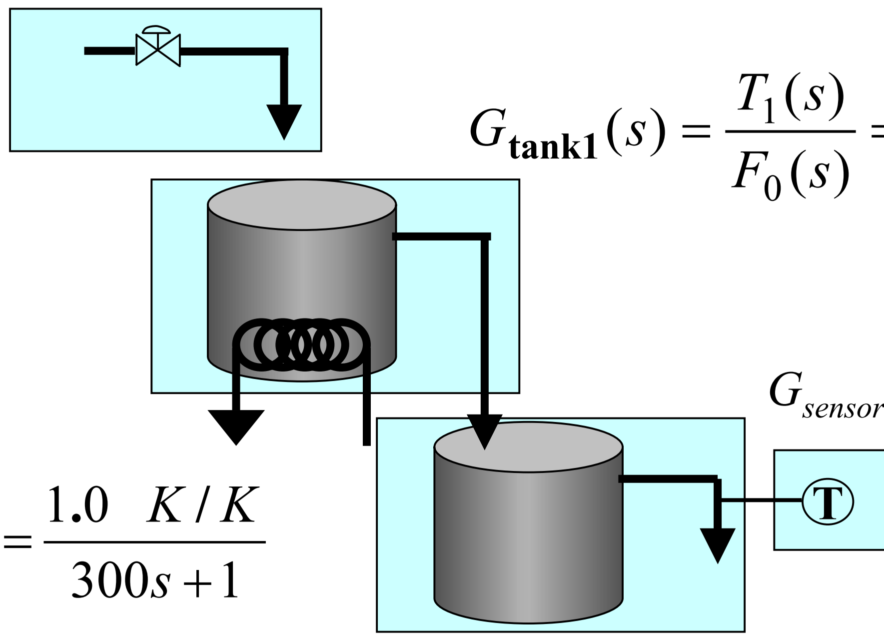
We introduced an impulse to the process at t=0. Develop and apply a graphical method to determine a dynamic model of the process.



CHAPTER 6: EMPIRCAL MODELLING WORKSHOP 2

State whether we can use a first order with dead time model for the following process. Explain your answer.

$$G_{valve}(s) = \frac{F_0(s)}{v(s)} = .10 \ \frac{m^3/s}{\% \ open}$$



$$G_{\mathbf{tank1}}(s) = \frac{T_1(s)}{F_0(s)} = \frac{-1.2 \quad K / m^3/s}{250s + 1}$$

$$G_{sensor}(s) = \frac{T_{measured}(s)}{T_2(s)} = \frac{1.0 \quad K/K}{10s + 1}$$

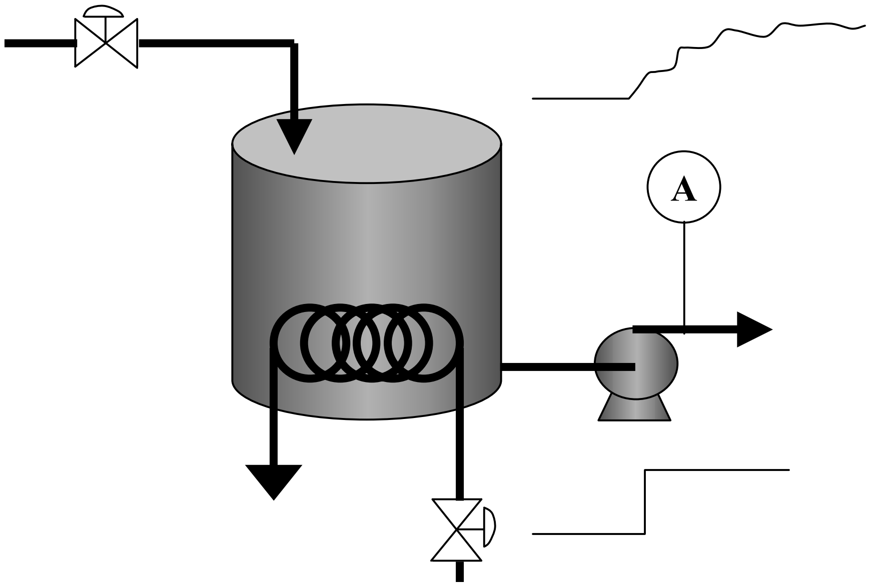
$$G_{\mathbf{tank2}}(s) = \frac{T_2(s)}{T_1(s)} = \frac{1.0 \quad K/K}{300s + 1}$$

(Time in seconds)

CHAPTER 6: EMPIRCAL MODELLING WORKSHOP 3

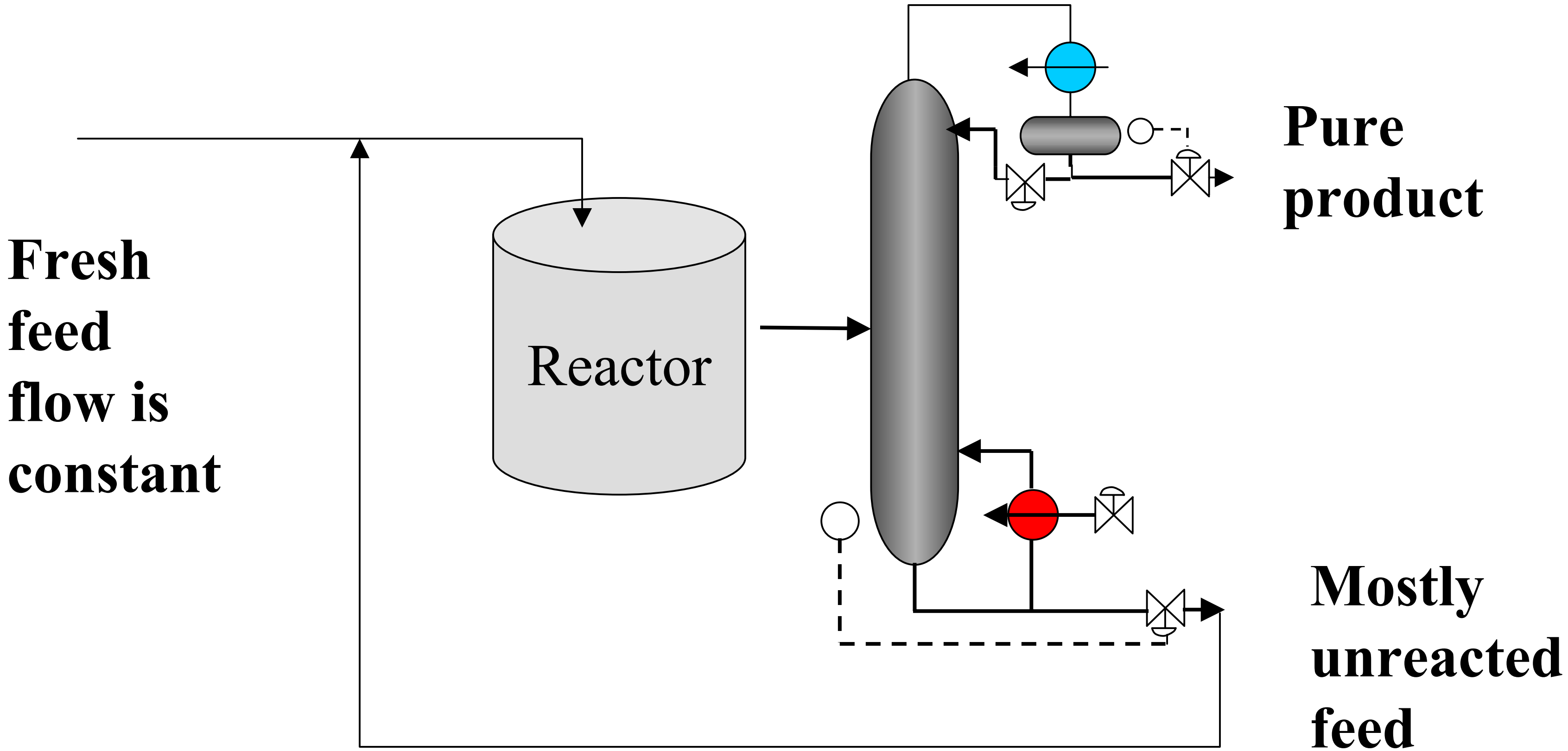
We are familiar with analyzers from courses on analytical chemistry. In an industrial application, we can extract samples and transport them to a laboratory for measurement.

What equipment is required so that could we can achieve faster measurements for use in feedback control?

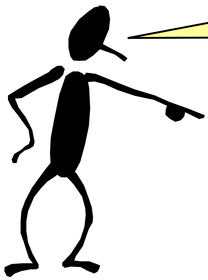


CHAPTER 6: EMPIRCAL MODELLING WORKSHOP 4

We are performing an experiment, changing the reflux flow and measuring the purity of the distillate. Discuss the processes that will affect the empirical dynamic model.

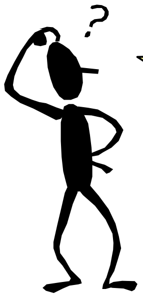


CHAPTER 6: EMPIRICAL MODEL IDENTIFICATION



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

- Design and implement a good experiment
- Perform the graphical calculations
- Perform the statistical calculations
- Combine fundamental and empirical modelling for chemical process systems



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 6: LEARNING RESOURCES

- <u>SITE PC-EDUCATION WEB</u>
  - Instrumentation Notes
  - Interactive Learning Module (Chapter 6)
  - Tutorials (Chapter 6)
- Software Laboratory
  - S_LOOP program to simulate experimental step data, with noise if desired
- Intermediate reference on statistical method

  - Brosilow, C. and B. Joseph, Techniques of Model-Based Control, Prentice-Hall, Upper Saddle River, 2002 (Chapters 15 & 16).

CHAPTER 6: SUGGESTIONS FOR SELF-STUDY

1. **Find a process reaction curve plotted in Chapters 1-5 in the textbook. Fit using a graphical method.**

   Discuss how the parameters would change if the experiment were repeated at a flow 1/2 the original value.

2. **Estimate the range of dynamics that we expect from**
   a. flow in a pipe
   b. heat exchangers
   c. levels in reflux drums
   d. distillation composition
   e. distillation pressure

3. **Develop an Excel spreadsheet to estimate the parameters in a first order dynamic model.**