



Aalto University

# Process dynamics and control

CHEM-E7190 (was E7140) | 2023

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Chemical and Metallurgical Engineering  
School of Chemical Engineering

# Overview

We study the mathematical principles and basic computational tools of state-feedback and optimal control theory to manipulate the dynamic behaviour of process systems



- ~> Understanding of feedback control
- ~> Examples from process systems
- (Catchy image from the internet)

The approach is general with application domains in many (bio)-chemical technologies

## Overview (cont.)



### Process control and automation at Aalto University

#### Francesco Corona

- ~> Professor of process control and automation
  - Once and future chemical engineer
  - Camouflaged as computer scientist

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Research and teaching about **computational** and **inferential thinking** of process systems

~> **Automatic control and machine learning**

- **Three + one doctoral students**
- **Nine + one master's student**

~> Production planning and optimisation



Formal methods from automatic control, statistics, and optimisation, plus applications

## Overview (cont.)

- ↪ Dynamic process modelling and state-space representations
  - ↪ Introduction to state-feedback and optimal control
  - ↪ Introduction to state estimation
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### Outcome 1

- How to write and analyse a mathematical description of a control process system
- ↪ Model expressed as a set of (ordinary and/or partial) differential equations

### Outcome 2

- How to design/synthesise controllers to manipulate/drive the process system
- ↪ Design/synthesis of controllers is based on optimal state-feedback

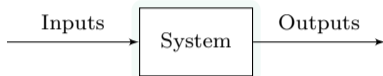
### Outcome 3

- How to design state estimators to reconstruct the process state from data
- ↪ Design/synthesis also based on optimal state-estimation

# Trajectory

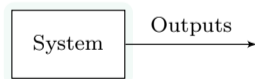
## Input-output (I/O) process modelling of process systems

- I Control variables and disturbances
- O Measurement variables, the data
- ↪ The system evolves in time
- ↪ (System/model/process)



## Ordinary differential equations and matrix algebra

- Force-free response (no inputs)
- Numerical integration
- ↪ Stability

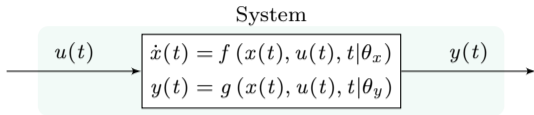


# Trajectory (cont.)

## State-space (SS) process modelling

I/O Inputs  $u$ , outputs  $y$

S State variables  $x$



The dynamics of the state variables are expressed by a function  $f$  (the process model)

- Function  $f$  returns  $\dot{x}(t)$  at time  $t$ , given  $x(t)$ ,  $u(t)$ , and  $t$

How state variables are transformed into measurements, function  $g$  (instruments model)

- Function  $g$  returns  $y(t)$ , at time  $t$ , given the values  $x(t)$ ,  $u(t)$  (and  $t$ )

Functions  $f$  often derived from classical process modelling: **Mass and energy balances**

$$\underbrace{[\text{Stuff in}] - [\text{Stuff out}] + \dots - [\text{Stuff generated/consumed}]}_{f(x, u, t)} = \underbrace{[\text{Stuff accumulated}]}_{\dot{x}}$$

Functions  $g$  often determined by the automation system: **Sensors and lab analysis**

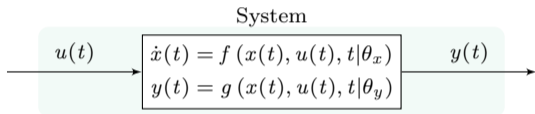
## Trajectory (cont.)

We understand dynamic systems as processes that are evolving in time and that can be represented using states that allow to determine the future behaviour of the system

I/O Controls  $u$ , outputs  $y$

S State variables  $x$

P Parameters  $\theta_{x,y}$

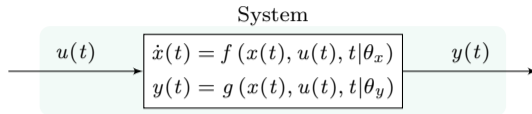


The dynamical system can be controlled by a suitable choice of inputs denoted controls

- The control actions should be chosen optimally, in some sense
- The control actions must always satisfy certain constraints

This course is about methods and solutions to determine the optimal control actions

## Trajectory (cont.)



One fundamental element of dynamical systems is represented by state  $x(t)$  at time  $t$

↪ The state space  $\mathcal{X}$  is the set of all possible values of the state

- The state-space can be continuous, like the usual  $\mathcal{R}^{N_x}$
- It can be a discrete countable set such that  $|\mathcal{X}| = N_{\mathcal{X}}$
- It can be hybrid, with continuous and discrete states

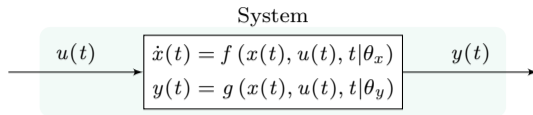
The other main element of dynamical systems is represented by controls  $u(t)$  at time  $t$

↪ The control/action space  $\mathcal{U}$  is the set of all possible controls

- The control-space can be continuous, like the usual  $\mathcal{R}^{N_u}$
- It can be a discrete countable set such that  $|\mathcal{U}| = N_{\mathcal{U}}$
- It can be hybrid, with continuous and discrete actions



## Trajectory (cont.)



The dynamics of the state variables are represented by some nonlinear function  $f$

- Function  $f$  returns  $\dot{x}(t)$  at time  $t$ , given the values  $x(t)$  and  $u(t)$ , and  $t$
- Function  $f$  is parameterised, all parameters are in the vector  $\theta_x$

How the state variables are transformed into measurements, nonlinear function  $g$

- Function  $g$  returns  $y(t)$  at time  $t$ , given the values  $x(t)$  and  $u(t)$ , and  $t$
- Function  $g$  is parameterised, all parameters are in the vector  $\theta_y$

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Knowledge of the **initial state**  $x(t_0)$  and of the **control trajectory**  $u(t)$  over some time interval such that  $t \in [t_0, T]$  allows to determine the **state trajectory**  $x(t)$  for  $t \in [t_0, T]$

- The system model with a certain evolution is of the deterministic kind
- Stochastic models describe evolutions that are known statistically

## Trajectory (cont.)

In general, functions  $f$  and  $g$  may change in time ( $f$  and  $g$  will change with time  $t$ )

- Typical of process subjected under varying configurations or obsolescence
- It is an important topic, but we will not discuss those explicitly

In the course we will only consider time-invariant systems,

$$\rightsquigarrow \dot{x}(t) = f(x(t), u(t), t | \theta_x)$$

$$\rightsquigarrow y(t) = g(x(t), u(t), t | \theta_y)$$

## Trajectory (cont.)

Chemical kinetics are concerned with understanding the evolution of reaction systems

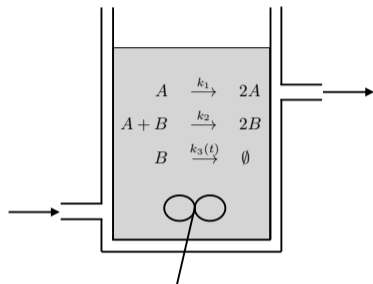
- The system is specified by a set of coupled chemical reactions

Chemical kinetics induce a set of ordinary differential equations

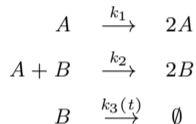
- These equations define the dynamics of the system

## Trajectory (cont.)

## Example



The Lotka-Volterra system is usually used to capture interactions between competing (not only) chemical species



Assume that we are able to manipulate the rate at which component  $B$  is removed

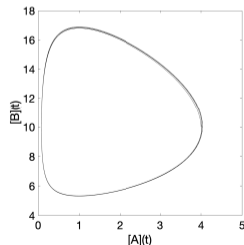
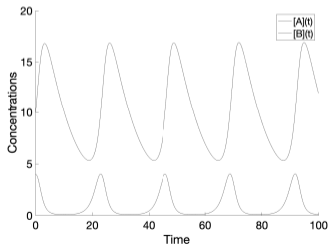
Also assume that the system is closed, there is no inflow and outflow

$$\begin{bmatrix} \frac{d[A](t)}{dt} \\ \frac{d[B](t)}{dt} \end{bmatrix} = \begin{bmatrix} k_1[A](t) - k_2[A](t)[B](t) \\ k_2[A](t)[B](t) - k_3(t)[B](t) \end{bmatrix}$$

## Trajectory (cont.)

$$\underbrace{\begin{bmatrix} \frac{d[A](t)}{dt} \\ \frac{d[B](t)}{dt} \end{bmatrix}}_{\dot{x}(t)} = \underbrace{\begin{bmatrix} k_1[A](t) - k_2[A](t)[B](t) \\ k_2[A](t)[B](t) - k_3(t)[B](t) \end{bmatrix}}_{f(x(t), u(t) | \theta_x)}$$

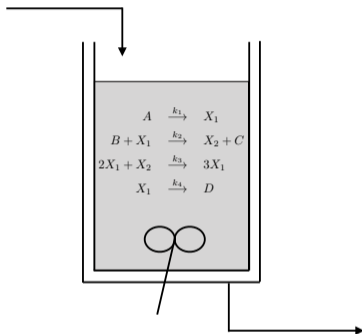
- Two state variables  $x(t) = (x_1(t), x_2(t)) = ([A](t), [B](t))$
- Two control variables  $u(t) = u_1(t) = k_3(t)$
- Two parameters  $\theta_x = (k_1, k_2)$



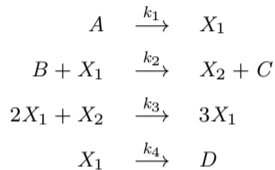
The evolution, for an initial condition  $x(0) = x_0$  and sequence of inputs  $u(0 \rightsquigarrow T)$  □

## Trajectory (cont.)

## Example



The Brusselator is a theoretical model for certain auto-catalytic reactions



The reaction components ( $X_1, X_2$ ) are a pair of intermediate chemical species

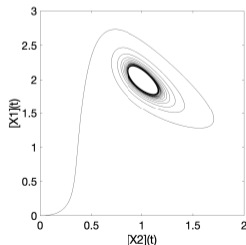
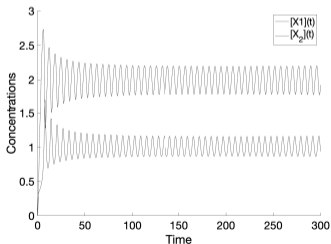
Assuming that the concentration species  $A$  and  $B$  (and  $C$  and  $D$ ) can be manipulated

$$\begin{bmatrix} \frac{d[X_1](t)}{dt} \\ \frac{d[X_2](t)}{dt} \end{bmatrix} = \begin{bmatrix} k_2 (a(t) - b(t)[X_1](t)) + k_3 ([X_1]^2(t)[X_2](t)) - k_4[X_1](t) \\ k_2 (b(t)[X_1](t)) - k_3 ([X_1]^2(t)[X_2](t)) \end{bmatrix}$$

## Trajectory (cont.)

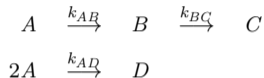
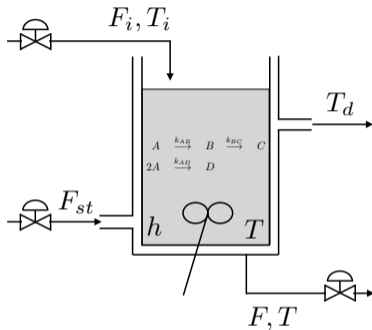
$$\underbrace{\begin{bmatrix} \frac{d[X_1](t)}{dt} \\ \frac{d[X_2](t)}{dt} \end{bmatrix}}_{\dot{x}(t)} = \underbrace{\begin{bmatrix} k_2 (a(t) - b(t)[X_1](t)) + k_3 ([X_1]^2(t)[X_2](t)) - k_4[X_1](t) \\ k_2 (b(t)[X_1](t)) - k_3 ([X_1]^2(t)[X_2](t)) \end{bmatrix}}_{f(x(t), u(t) | \theta_x)}$$

- Two state variables  $x(t) = (x_1(t), x_2(t)) = ([X_1](t), [X_2](t))$
- Two control variables  $u(t) = (u_1(t), u_2(t)) = (a(t), b(t))$
- Four parameters  $\theta_x = (k_1, k_2, k_3, k_4)$



The evolution, for an initial condition  $x(0) = x_0$  and sequence of inputs  $u(0 \rightsquigarrow T)$  □

## Example



A non-isothermal CSTR (Van de Vusse)

$$\frac{d\rho_A}{dt} = q(\rho_{\text{in}}^{(A)} - \rho_A) - (k_{AB}(T)\rho_A + k_{AD}(T)\rho_A^2)$$

$$\frac{d\rho_B}{dt} = -q\rho_B + k_{AB}(T)\rho_A - k_{BC}(T)\rho_B$$

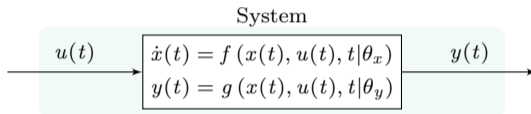
$$\frac{dT}{dt} = q(T_{\text{in}} - T) + \frac{k_W A_r}{\rho C_p V_r} (T_d - T) - \frac{1}{\rho C_p} (k_{AB}(T)\rho_A \Delta H_{AB} + k_{BC}\rho_B \Delta H_{BC} + k_{AD}(T)\rho_A^2 \Delta H_{AC})$$

$$\frac{dT_d}{dt} = \frac{1}{m_K C_{pK}} Q + \frac{k_W A_r}{m_K C_{pK}} (T - T_d)$$



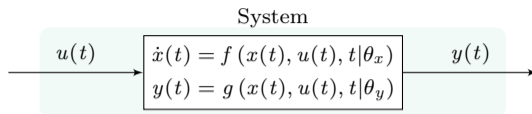
## Trajectory (cont.)

By definition, the system/model itself is an approximation of the physical process



- ↪ Oftentimes, we will need to accept even more approximations
- Oftentimes, this is a necessary step to be able to proceed
  - Otherwise, the mathematics would be too complicated

## Trajectory (cont.)



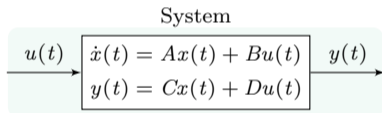
### Approximated process dynamics (linear and time-invariant)

- Function  $f$  becomes two matrices

$$f(x(t), u(t)) \approx Ax(t) + Bu(t)$$

- Function  $g$  becomes two matrices

$$g(x(t), u(t)) \approx Cx(t) + Du(t)$$



### Linearisation of nonlinearities around steady-states

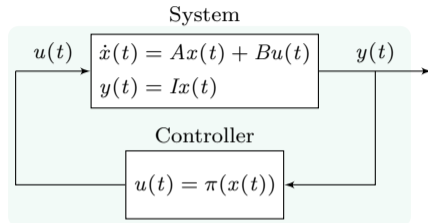
- ↪ First-order Taylor approximations
- ↪ The work-horse of modernity
- ↪ Leading tech, since 1700's

## Trajectory (cont.)

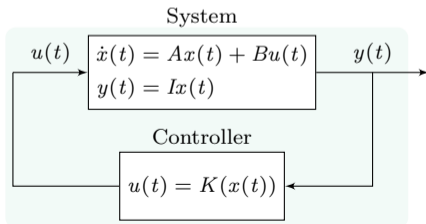
### From (approximated, linear) process dynamics to state-feedback control

We will make some initial assumptions

- We can measure the states  $x(t)$
- We define control actions  $u(t)$
- ⇒ The (static) controller,  $\pi$
- ⇒ Controllability



### State-feedback optimal control (again linear dynamics, plus quadratic costs)



We introduce performance measures

- Control accuracy

$$\|x(t) - x_{\text{target}}\|_Q^2$$

- Control effort

$$\|u(t) - u_{\text{reference}}\|_R^2$$

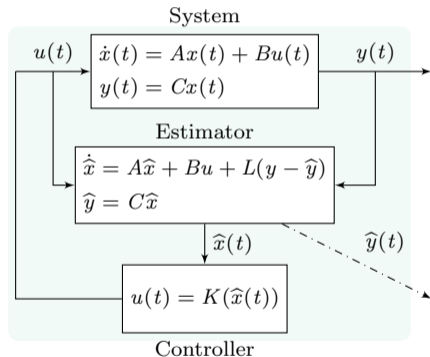
## Trajectory (cont.)

### Optimal state-feedback, estimation, and control (again, linear and quadratic)

We will relax some initial assumptions

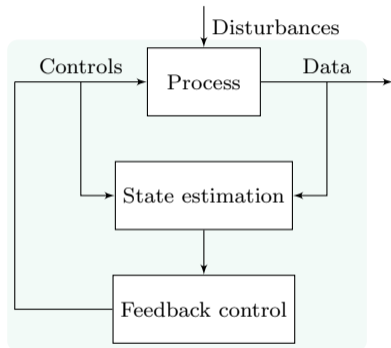
- Cannot measure the states  $x(t)$
- Must estimate them, from data
- ↪ The estimator,  $\varphi$
- ↪ Observability

We then define control actions,  $u(t)$



## Trajectory (cont.)

### Optimal state-feedback, estimation, and control (the general framework)



A general structure, each block can be treated using different technologies

- First-principles (physics)
- Empirical (data-derived)

It scales (it can be solved) reasonably well with the process size (complexity)

**Process control** is a field about methods for sensing, learning, reasoning, and actuating

## Trajectory (cont.)

**Sensing**, 'observing, getting measurements'

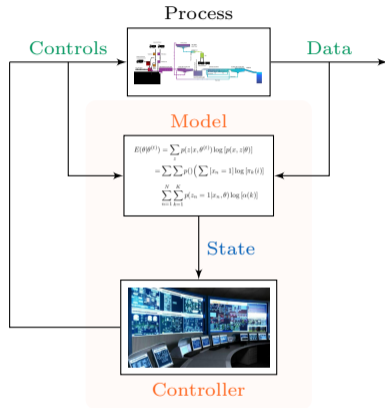
**Learning**, 'making statistical inferences'

**Reasoning**, 'making optimal decisions'

**Actuating**, 'implementing decisions'

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**Process control** is applied **automatic control**, **optimisation**, and **statistics** to **(bio-)chem eng**



Key factor is that the approach needs to be automatic, interpretable, general and efficient

- Full-scale industrial and environmental systems (that is, constraints)

## Why should I care? An example: Control4Reuse

Present wastewater treatment technologies are designed to produce a disposable WW

- Discharged wastewater is expected to be poor in solids and nutrients
- Low carbon (C), nitrogen (N) and phosphorus (P) concentration

Increasing water scarcity requires us to reuse treated WW, a non conventional resource

- At present there exists no standardised solution for urban WWTPs that explicitly aim at delivering a treated wastewater that fulfils the requirements for reuse
- ~> In agriculture, high N and P contents and absence of micro-pollutants, pathogens and antibiotic resistant bacteria (ARB), and antibiotic resistance genes (ARG)

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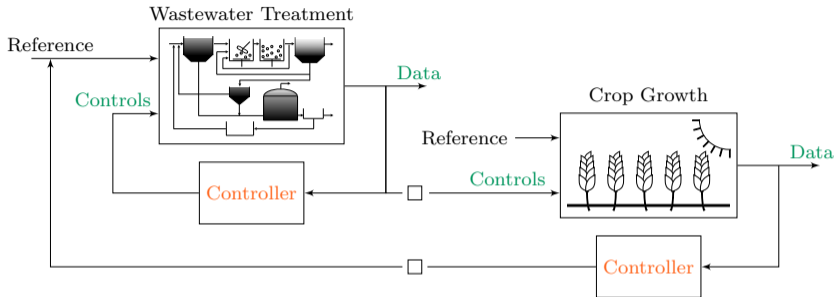
Most of water withdrawal goes to agriculture

**Can we operate a large-scale WWTP to produce reuse water of different grades, on demand?**



Wastewater not as a waste but as a resource

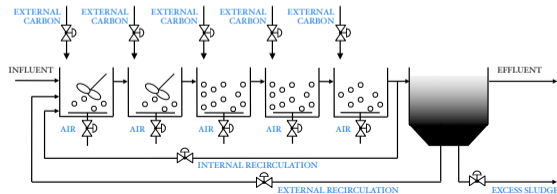
## Control4Reuse (cont.)



### The Benchmark Simulation Model no. 1 (BSM1)

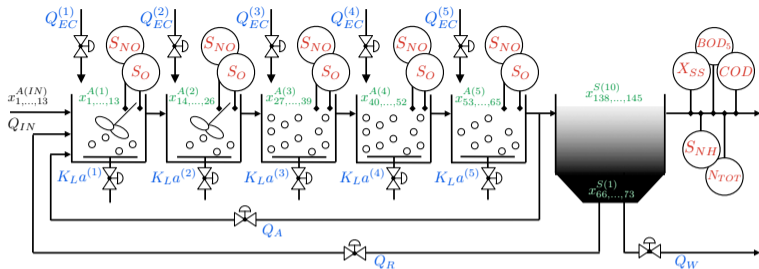
- ~ 5 bio-reactors (ASMs)
- ~ 1 settler ('TAKACS')

### The Benchmark Simulation Model no. 2 (BSM2)



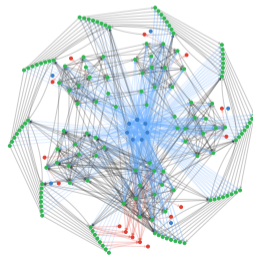


## Control4Reuse (cont.)



Analysis of the dynamics and control flexibility of activated sludge plants

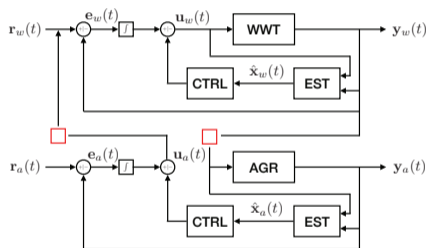
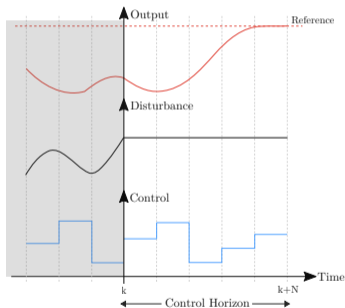
- ~ Full-state controllability
- ~ Full-state observability
- ~ Online optimal control



Neto et al. in ECC + IFAC (2020),  
ADCHEM (2021), DYCOPS + JPC (2022)

## Control4Reuse (cont.)

- ~> ASPs are controllable but unobservable, in a structural sense
- ~> ASPs are uncontrollable and unobservable in a classical sense



~> A cascade of optimal controllers

There will be a guest seminar on how to control wastewater treatment plants for reuse

# Overview

CHEM-E7190 is a set of **lectures (approx. 24h)** and **exercises (approx. 24h)**

↪ The objective is to provide a modern view on process control

**To pass CHEM-E7190 you must pass the exam (65% of the total points)**

**The remaining points (35%) can be collected from the exercises**

*We encourage you to collaborate in figuring out answers and help others solve the problems, yet we ask you to submit your work individually and to explicitly acknowledge those with whom you collaborated. We are assuming that you take the responsibility to make sure you personally understand the solution to work arising from collaboration*