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Automated Control Strategies for Chemical Reactors

PhD Filippo Sanfilippo [1,2]

[1] Department of Maritime Technology and Operations, Aalesund University College, Postboks 1517, 6025 Aalesund, Norway,
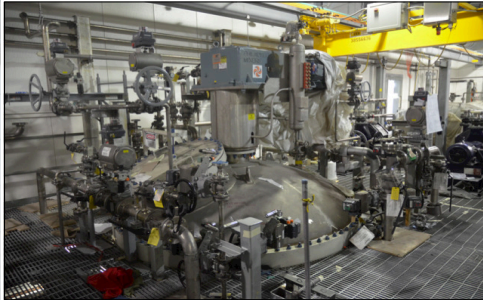fisa@hials.no,
http://filipposanfilippo.inspitivity.com/

[2] Department of Engineering Cybernetics, Norwegian University of Science and Technology, 7491 Trondheim, Norway

Trial Lecture

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Reaction types
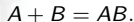Reactors Classification
Control Challenges

Introduction

### What is a *chemical reactor*?

- In chemical engineering, a vessel designed to contain chemical reactions.
- *Chemical reaction engineering* is the branch of chemical engineering which deals with chemical reactors and their design.
- Chemical engineers design reactors to maximize efficiency.

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Reaction Types

- Direct Combination or Synthesis Reaction:

$$A + B = AB.$$

- Chemical Decomposition or Analysis Reaction:

$$AB = A + B.$$
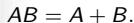
- Single Displacement or Substitution Reaction:

$$A + BC = AC + B.$$
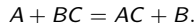
- Metathesis or Double Displacement Reaction:
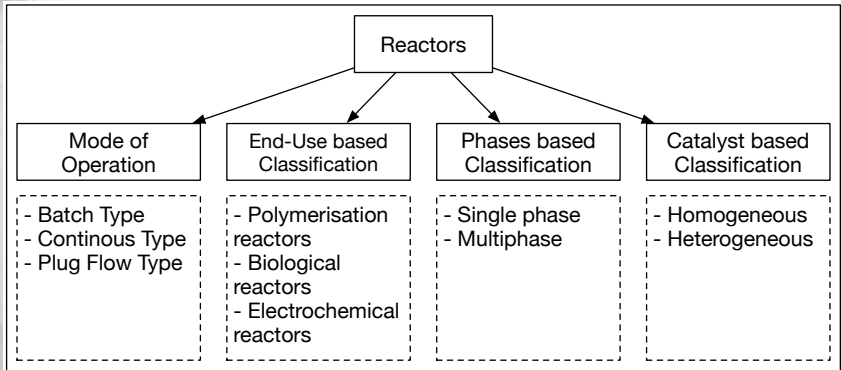
$$AB + CD = CB.$$

- NOTE: side reaction!!

$$A + B = C, A + C = D.$$

In addition to the basic data, include::

- a heat and mass transfer characteristics;
- physical, chemical and thermodynamic properties of components;
- corrosion-erosion characteristics of any potential hazard.

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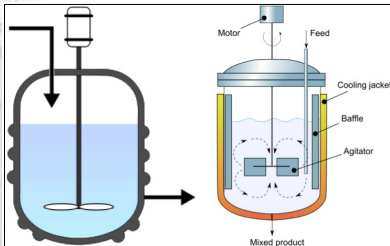Reactors Classification
Control Challenges

Batch Reactor

Batch reactors are widely used in the process industries:

- typically a tank with an agitator and integral heating/cooling system;
- vessels of this type are used for a variety of process operations such as solids dissolution, product mixing, chemical reactions, batch distillation, ...;
- usually fabricated in steel, stainless steel, glass-lined steel, glass or exotic alloy;
- liquids and solids are usually charged via connections in the top cover of the reactor. Vapors and gases also discharge through connections in the top. Liquids are usually discharged out of the bottom.

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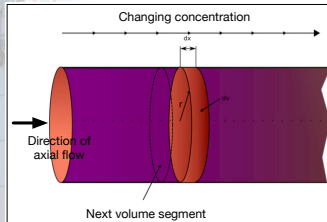Control Challenges

Continuous Stirred-Tank Reactor

- Continuous reactors are generally smaller than batch reactors and handle the product as a flowing stream.
- They may be designed as pipes with or without baffles or a series of interconnected stages.

The continuous flow stirred-tank reactor (CSTR) is a common ideal reactor type:

- approximated as a Continuous Ideally Stirred-Tank Reactor (CISTR);
- CISTRs assume perfect mixing (the output composition is identical to composition of the material inside the reactor);
- often used to simplify engineering calculations and can be used to describe research reactors. In practice it can only be approached, in particular in industrial size reactors.

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Plug Flow Reactor Model

The plug flow reactor model (PFR):

- chemical reactions in continuous, flowing systems of cylindrical geometry;
- used to predict the behavior of chemical reactors of such design, so that key reactor variables can be estimated;
- fluid going through a PFR may be modeled as a series of infinitely thin coherent "plugs", each with a uniform composition, traveling in the axial direction of the reactor, with each plug having a different composition from the ones before and after it.

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Control Challenges

Endothermic/Exothermic reactions:

- chemical reactions occurring in a reactor may be exothermic, meaning giving off heat, or endothermic, meaning absorbing heat;
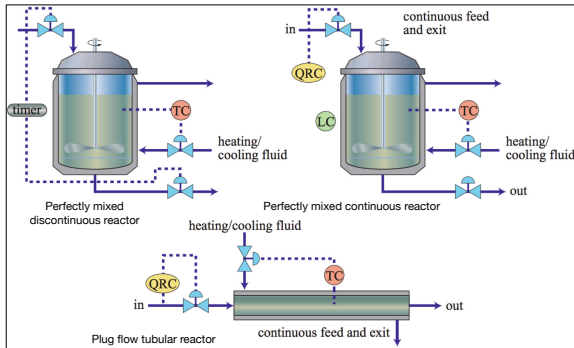
Design challenges:

- a chemical reactor vessel may have a cooling or heating jacket or cooling or heating coils (tubes) wrapped around the outside of its vessel wall to cool down or heat up the contents.
- exothermic behaviour may cause the reaction to become unstable and consequently poses safety concern to the plant personnel.

Control challenges:

- heat is needed to speed up the reaction rate so that the overall process cycle time can be reduced whereas the cooling is employed to cool down the reactor in order to reduce excessive heat.

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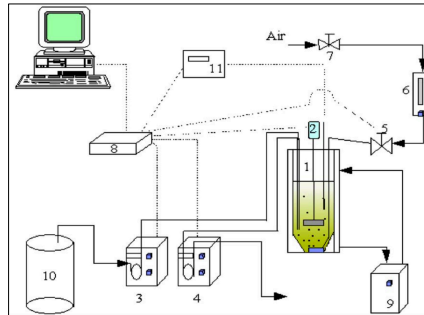Required Instrumentation

Required Instrumentation

TC, temperature gauge-controller; QRC, flow rate recorder-controller; LC, level controller; timer, for valves opening/closure[1].

[1] U Romano. "Encyclopaedia of hydrocarbons". In: *Instruments, Process Engineering Aspects, Volume V, Istituto della enciclopedia italiana Fondata da Giovanni Treccani Spa* (2009).

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Required Instrumentation

Instrumentation Example

(1) Reactor, (2) mixer, (3) filling pump, (4) decantation pump, (5) solenoid valve, (6) flow meter, (7) pressure regulation valve, (8) data acquisition card, (9) temperature controller, (10) feeding tank and (11) oxygen meter[2].

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[2] Germán Buitrón et al. "Evaluation of two control strategies for a sequencing batch reactor degrading high concentration peaks of 4-chlorophenol". In: *Water research* 39.6 (2005), pp. 1015–1024.

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A Continuous Stirred Tank Reactor (CSTR)

SISO Vs MIMO:

- processes with only one output being controlled by a single manipulated variable are single-input single-output (SISO) systems;
- however, most unit operations have more than one control loop;
- systems with more than one control loop are known as multi-input multi-output (MIMO) or multivariable systems.
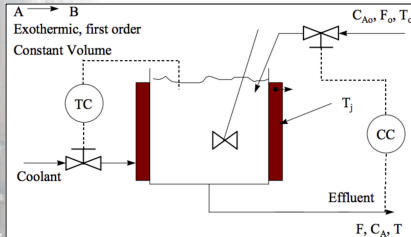

A continuous stirred tank reactor will be used as the motivating example:

- to introduce the basic concepts of multivariable control;
- to highlight the phenomenon of loop interactions;
- to introduce alternative control strategies.

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A Continuous Stirred Tank Reactor (CSTR)

Variables of interest:

- product composition;
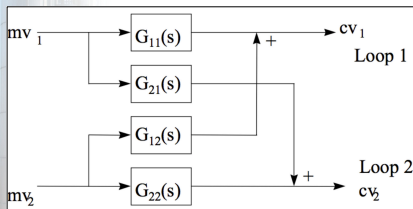- temperature of the reacting mass.
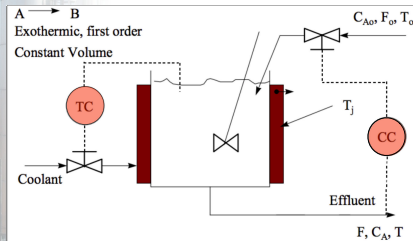
A composition control loop and a temperature control loop:

- feed to the reactor is used to manipulate product composition;
- temperature is controlled by adding (removing) energy via heating (cooling) coils or jackets.

"TC" represents a temperature controller, the mv for this loop being coolant flowrate to the jacket. "CC" represents the composition controller, the mv being reactant feedrate. NOTE: loop interaction must be considered when developing a control strategy!
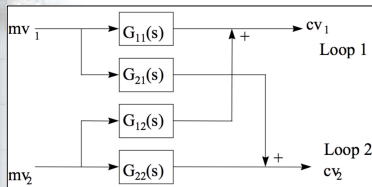
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Input-Output Multivariable System Models

(2 x 2) Multivariable model structure:

- $G_{11}(s)$ represents the forward path dynamics between mv_1 and cv_1;
- $G_{22}(s)$ describes how cv_2 responds after a change in mv_2;
- the interaction effects are modelled using transfer functions $G_{21}(s)$ and $G_{12}(s)$.

- mv_1 is the coolant flowrate, while mv_2 is the flowrate of the reactant.
- the output cv_1 is the reactor temperature while the output cv_2 is the effluent concentration.

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The Mathematical Model in Matrix-Vector Notation

$$G_p(s) = \frac{k_p e^{s\theta}}{\tau_p s + 1},$$

where k_p is a process gain, τ_p the process time constant and θ the process time delay. NOTE that each block will have different parameters that must be determined.

$$cv_1 = G_{11} mv_1 + G12 mv_2,$$

$$cv_2 = G_{21} mv_1 + G22 mv_2.$$

These equations may be expressed in matrix-vector notation:

$$\mathbf{cv} = \mathbf{Gmv},$$

where $\mathbf{cv} = [cv_1, cv_2]^T$,
$\mathbf{mv} = [mv_1, mv_2]^T$, and
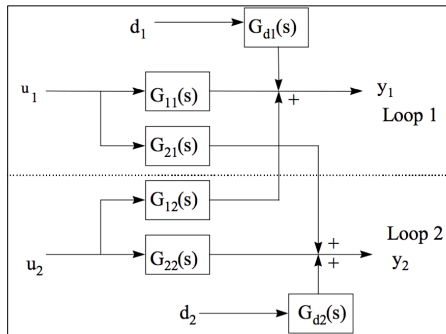$\mathbf{G} = \left[\begin{array}{cc} G_{11} & G_{12} \\ G_{21} & G_{22} \end{array} \right].$

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Incorporation of Load Disturbance Terms into the Systems Model

Processes are influenced by external factors such as changes in ambient conditions, changes in the quality of raw materials, changes in the operating environment and so on.

$$\mathbf{cv} = \mathbf{Gmv} + \mathbf{G}_d\mathbf{dv},$$

where $\mathbf{G}_d = \begin{bmatrix} G_{d1} & 0 \\ 0 & G_{d2} \end{bmatrix}$ and $\mathbf{dv} = \begin{bmatrix} dv_1 & dv_2 \end{bmatrix}$.

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Multivariable Control: An introduction
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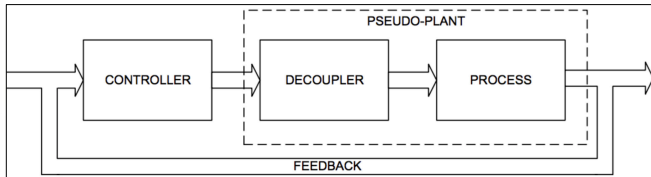**Statement of the Interaction Problem**

Statement of the Interaction Problem

With multivariable systems, where loop interactions exist, configuration of two single loop controllers could cause system instability, or at the very least result in poor control performance[3].

Interaction problems can be overcome by:

- choosing a manipulated variable/controlled variable pairing so that system interactions are minimised.
- the design a multivariable controller that achieves non interacting control.

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[3] F. G. Shinskey. *Process control systems*. McGraw-Hill, 1979.

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Machine Learning Procedures for Multivariable Control
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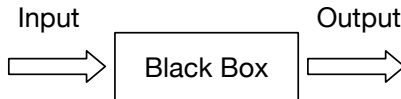
Machine Learning Procedures for Multivariable Control

Traditional methods based on PID controllers:

- in industry, PID controller is still widely implemented due to its simplicity;
- although the parameters of a PID controller can be obtained by using some conventional tuning methods, it still needs an operator to manual re-tune the settings;
- the optimum results are seldom obtained due to the need of operator's experiences.

Artificial intelligence (AI) techniques are introduced:

- reduce the dependency on human operator;
- the system is be able to automatically learn the properties of the controlled reactor.

Input → Black Box → Output

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Machine Learning Procedures for Multivariable Control
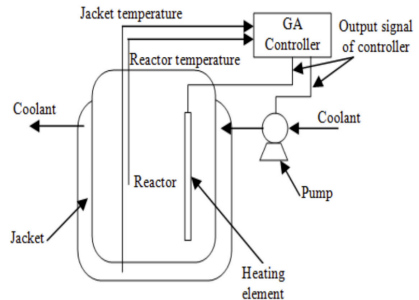GA based Multivariable Control for Exothermic Batch Process

Genetic Algorithm based Multivariable Control for Exothermic Batch Process: Control Strategy

- An exothermic process is an highly nonlinear and complex process.
- Large amount of heat will be released during the chemical reaction. As a result of the exothermic behaviour, the reaction may become unstable and consequently poses safety concern.

A genetic algorithm (GA) to control the reaction temperature and to balance the production needs with safety:

- GA exploits probabilistic search method to optimise the specific objective function.
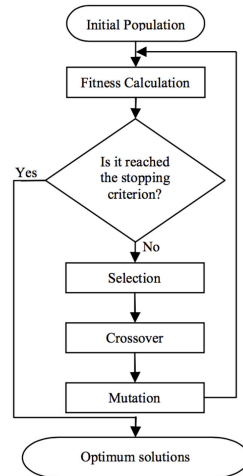

[4]

[4] Min Keng Tan et al. "Genetic Algorithm Based Multivariable Control for Exothermic Batch Process". In: *Proc. of the Fourth IEEE International Conference on Computational Intelligence, Communication Systems and Networks (CICSyN)*. 2012, pp. 32–37.

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Machine Learning Procedures for Multivariable Control
GA based Multivariable Control for Exothermic Batch Process

Genetic Algorithm based Multivariable Control for Exothermic Batch Process: Initialisation

Initialisation:

- potential solutions (chromosomes) are randomly generated;

- the range of heater power is from 0 kW to 300 kW, whereas the range of coolant flow rate is from 0 liter/s to 1 liter/s;

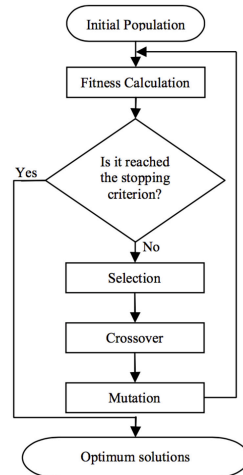- 50 population size of GA is enough for this study.

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Machine Learning Procedures for Multivariable Control
GA based Multivariable Control for Exothermic Batch Process

Genetic Algorithm based Multivariable Control for Exothermic Batch Process: Fitness Evaluation

Fitness Evaluation:

- the fitness evaluation function interprets the chromosomes in term of physical representation and evaluates its fitness based on desired objective;

-
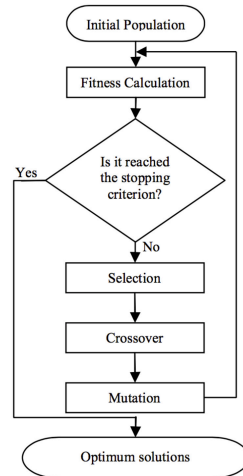$$J = \frac{1}{|T_{ref} - T_r|},$$

where J is the fitness value of each chromosome, T_{ref} is the reference temperature and T_r is the current temperature;

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Genetic Algorithm based Multivariable Control for Exothermic Batch Process: Selection

Selection:

- all the chromosomes are sorted according to their fitness, from worst to best (the fittest chromosome will have higher ranking);
- roulette-wheel mechanism;
- the cumulative fitness of each chromosome is calculated by adding the individual ranked;
- the selection probability is generated by multiply the total cumulative fitness with 50 random generated numbers. If the probability is within the cumulative fitness range of each individual, then the chromosome will be selected to the matching pool.

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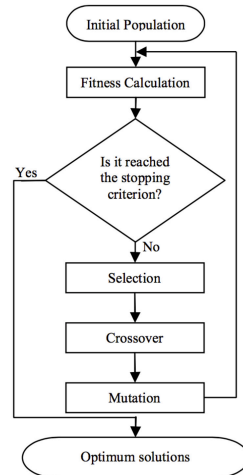# Genetic Algorithm based Multivariable Control for Exothermic Batch Process: Crossover

Crossover:

- two chromosomes (parents) are randomly picked up from matching pool;
- some portions of the parents will exchange between each other and create two new chromosomes (offspring);

-
$$x_{01} = \beta x_{p1} + (1 - \beta)x_{p2},$$
$$x_{02} = (1 - \beta)x_{p1} + \beta x_{p2},$$

where x_{0i} is offspring i, x_{pi} is parent i and β is a random number.

- 10% elitism.

Initial Population → Fitness Calculation → Is it reached the stopping criterion? — Yes → Optimum solutions; No → Selection → Crossover → Mutation → (loop back to Fitness Calculation)

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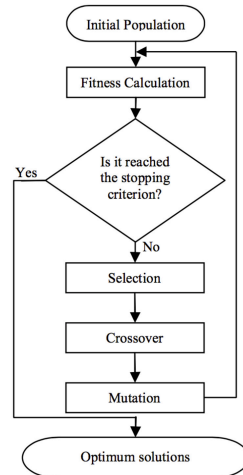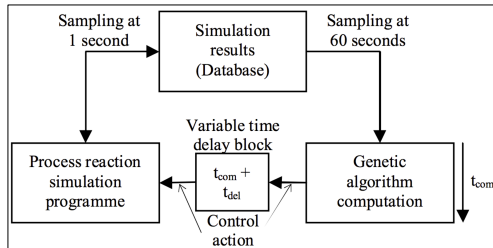GA based Multivariable Control for Exothermic Batch Process

Genetic Algorithm based Multivariable Control for Exothermic Batch Process: Mutation

Mutation:

- each chromosomes is subject to random changes;
- the mutation operator helps to prevent the searching trap in local maxima.
- however, the mutation probability should be kept low to prevent the loss of too many fit chromosomes and affect the convergence;
- the mutation rate is set to 0.01.

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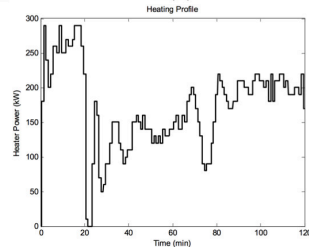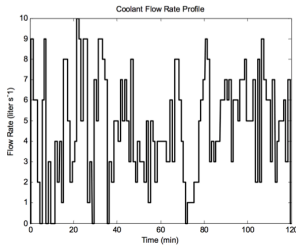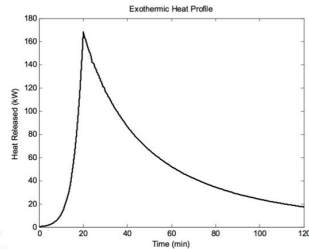GA based Multivariable Control for Exothermic Batch Process
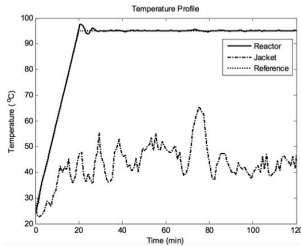
Genetic Algorithm based Multivariable Control for Exothermic Batch Process: Simulation

- During the computation of GA algorithm, the process simulation is continuing run.
- Measurement errors are always present in practical due to the sensor accuracy and precision. This situation is included in this work by adding noises to all the simulated temperature measurements.

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Genetic Algorithm based Multivariable Control for Exothermic Batch Process: Results

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Cleaning and Maintenance Challenges
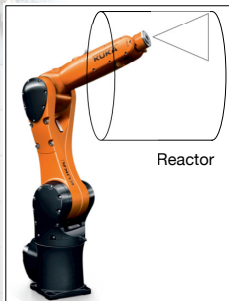Robotic Arms
Snake Robots

Cleaning and Maintenance Challenges

- Challenging operating environment.
- Automated clean-in-place systems clean more thoroughly than other methods, dramatically reducing or eliminating risk of cross-contamination caused by product or cleaning-chemical residue.

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Cleaning and Maintenance Challenges
Robotic Arms
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Robotic Arms for Reactor Inspection and Cleaning

[5,6]

[5] Filippo Sanfilippo et al. "JOpenShowVar: an Open-Source Cross-Platform Communication Interface to Kuka Robots". In: *Proc. of the IEEE International Conference on Information and Automation (ICIA), Hailar, China.* 2014, pp. 1154–1159.

[6] Filippo Sanfilippo et al. "JOpenShowVar: a Flexible Communication Interface for Controlling Kuka Industrial Robots". In: *IEEE Robotics & Automation Magazine* (2015). Manuscript accepted for publication.

Snake Robots for Reactor Inspection and Cleaning

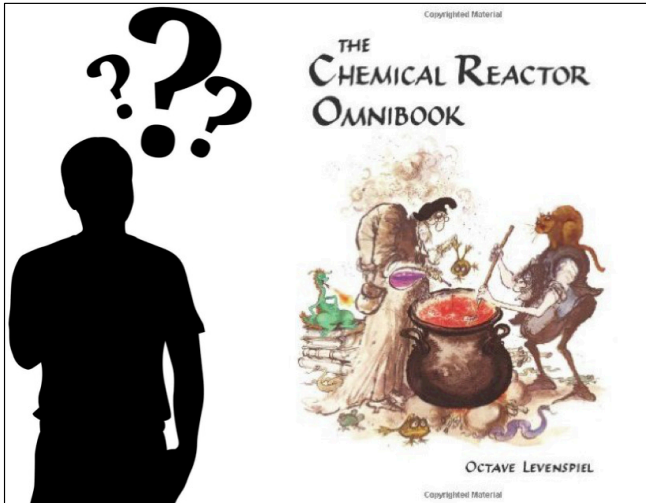- Snake robots may be use for inspection and cleaning operations[7].

[7] Pal Liljebäck et al. *Snake Robots: Modelling, Mechatronics, and Control.* Springer Science & Business Media, 2012.

Conclusions

A brief overview of automated control strategies for reactors:

- reaction types and reactors classification;
- fundamental challenges;
- required instrumentation;
- control principles and multivariable system models;
- alternative control strategies;
- cleaning and maintenance;

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Thank you for your attention!

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[1] U Romano. "Encyclopaedia of hydrocarbons". In: *Instruments, Process Engineering Aspects, Volume V, Istituto della enciclopedia italiana Fondata da Giovanni Treccani Spa* (2009).

[2] Germán Buitrón et al. "Evaluation of two control strategies for a sequencing batch reactor degrading high concentration peaks of 4-chlorophenol". In: *Water research* 39.6 (2005), pp. 1015–1024.

[3] F. G. Shinskey. *Process control systems*. McGraw-Hill, 1979.

[4] Min Keng Tan et al. "Genetic Algorithm Based Multivariable Control for Exothermic Batch Process". In: *Proc. of the Fourth IEEE International Conference on Computational Intelligence, Communication Systems and Networks (CICSyN)*. 2012, pp. 32–37.

[5] Filippo Sanfilippo et al. "JOpenShowVar: an Open-Source Cross-Platform Communication Interface to Kuka Robots". In: *Proc. of the IEEE International Conference on Information and Automation (ICIA), Hailar, China*. 2014, pp. 1154–1159.

[6] Filippo Sanfilippo et al. "JOpenShowVar: a Flexible Communication Interface for Controlling Kuka Industrial Robots". In: *IEEE Robotics & Automation Magazine* (2015). Manuscript accepted for publication.

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Springer Science & Business Media, 2012.