Introduction to process dynamics and control

Davide Manca

Lesson 1 of "Dynamics and Control of Chemical Processes" – Master Degree in Chemical Engineering

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Why should we control both chemical and industrial processes?

1) SAFETY

of field operators and civilians/residents. Equipment integrity. Run the plant under nominal conditions (*i.e.* design specification).

2) ENVIRONMENTAL REGULATIONS

European Community directives, national laws. Analysis and control of the plant interaction with the environment. Gas and liquid emissions control.

3) PRODUCTION SPECIFICATIONS

Quantity (production rate) and quality (purity) specifications. Specifications on by-products (if they are valuable).

Why should we control both chemical and industrial processes?

4) OPERATIONAL CONSTRAINTS

on the different process units.
For example: pumps suction head, tank maximum level, reactor pressure, flows in the distillation column, heat supply to a furnace, etc.

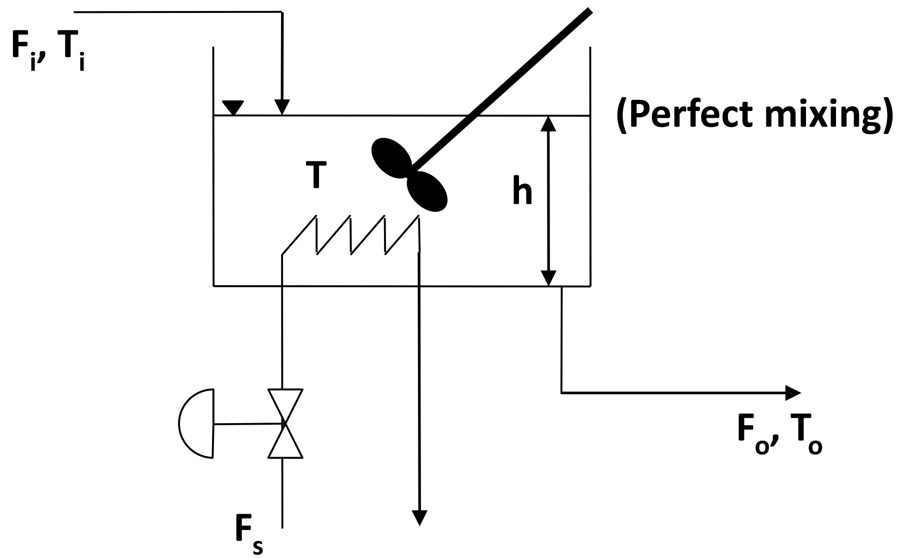
5) ECONOMICS

The plants must operate according to the market demands, taking into account the raw material and utility costs and products prices.

Control system tasks:

- Disturbance rejection
- Process stability
- Process optimization

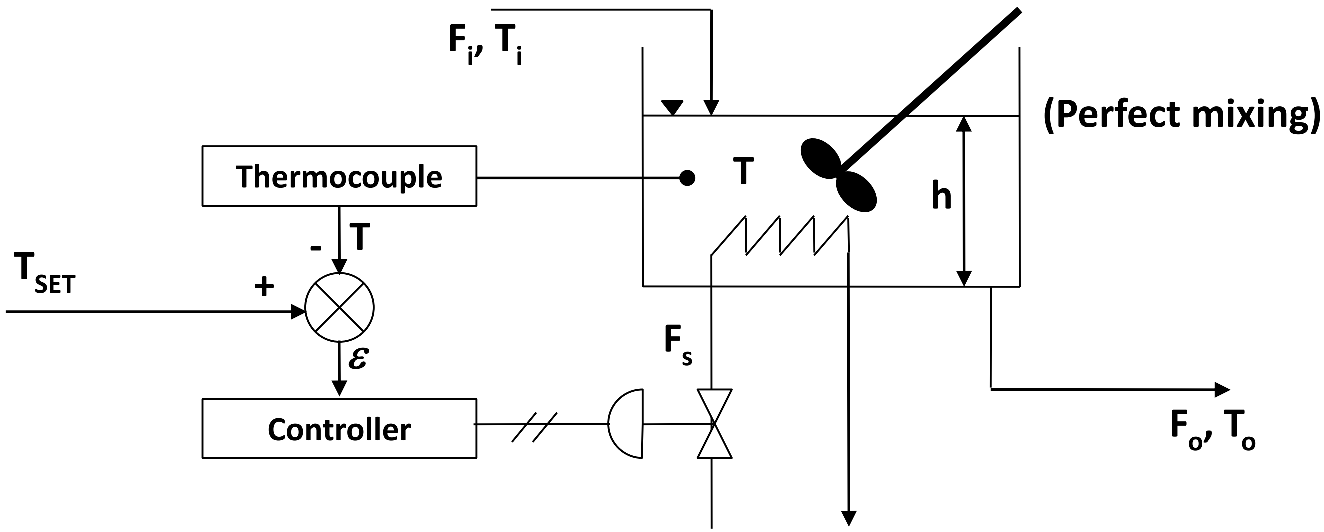
Disturbances rejection



The target is to keep CONSTANT the outlet Temperature T ($T=T_o$) and the Volume V (or equivalently the level h, h=const.) in presence of external disturbances on F_i e T_i. It is not possible to set F_s and leave the system without control because the disturbances on F_i and T_i will affect T_o and h. Even if F_i and T_i were constant, other disturbances such as fouling on the heat exchanger tubes or changes of F_s might affect T_o.

Disturbances rejection

It is possible to set up a feedback control on T_o (=T, due to the perfect mixing)



If $\varepsilon > 0$ the controller OPENS the steam valve

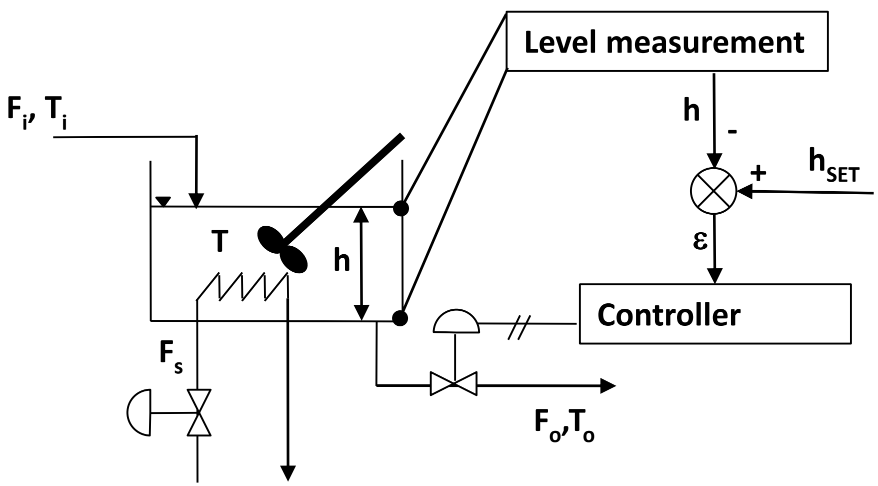
Se $\varepsilon < 0$ the controller CLOSES the steam valve

Se $\varepsilon = 0$ the controller does NOT move the steam valve (it leaves the valve in its position)

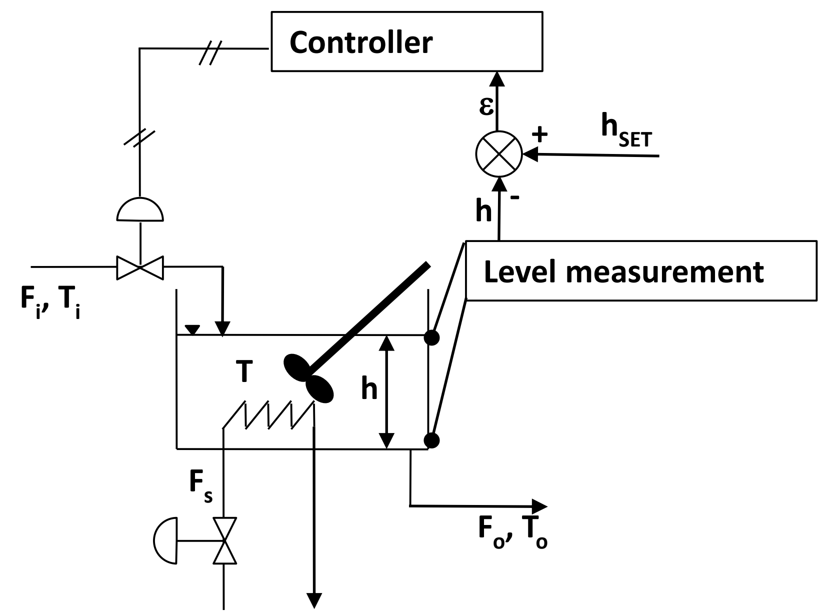
Disturbances rejection

In order to control the tank volume, *i.e.* the *h* level, two different alternatives of feedback control can be implemented: regulate the valve on the flow-rate F_o (alternative A) or the valve on the feed flow-rate F_i (alternative B).

FEEDBACK LEVEL CONTROL (alternative A)



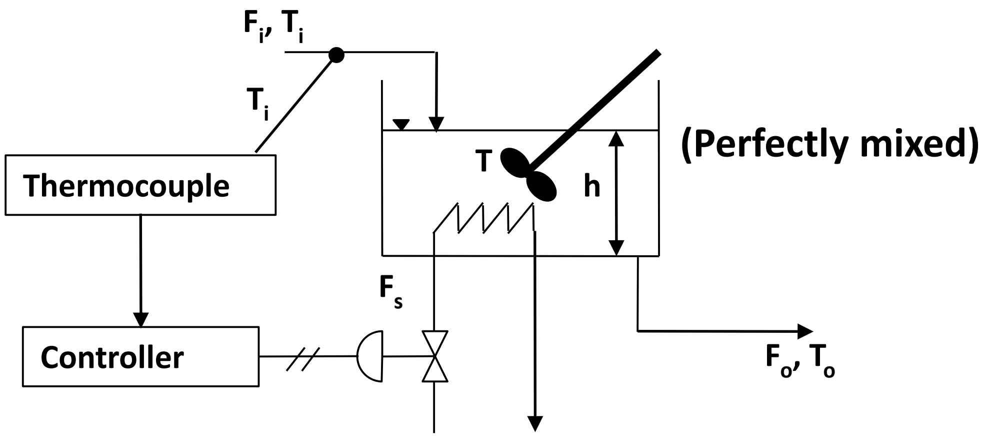
FEEDBACK LEVEL CONTROL (alternative B)



Disturbances rejection

A different control approach consists in adopting a FEEDFORWARD control, instead of a FEEDBACK one, based on anticipating the control action before the external disturbance affects the system.

FEEDFORWARD TEMPERATURE CONTROL (the controlled variable is $T = T_o$)



The control system must feature an advanced logic (*i.e.* based on the process model) and be capable to predict the system response to a measured (measurable) and modeled disturbance.

However, if the control system does NOT detect or model a disturbance (for example the fouling of the heat exchanger coil) it will NOT be possible to adjust the controlled variable (*i.e.* the product temperature).

Process stability

Given the exothermic reaction A→B occurring in a CSTR with jacket cooling by a liquid coolant:

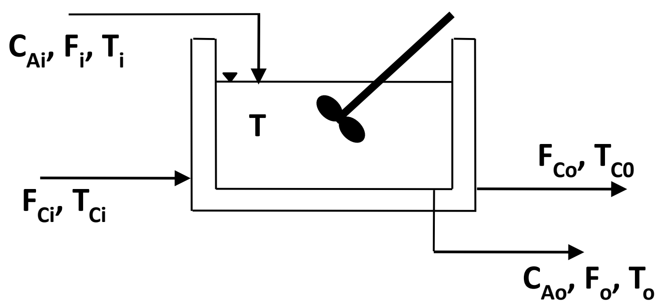
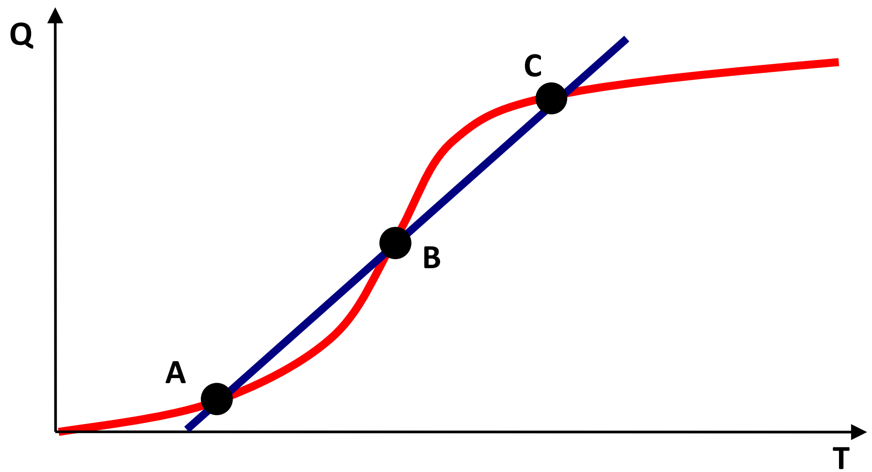


Diagram of the thermal power provided by the reaction (red curve) and the power exchanged with the cooling jacket (blue curve) as a function of the reaction temperature:



The **sigmoid curve** is the heat released by the exothermic reaction.

The **straight line** is the heat exchanged with the coolant.

Process stability

Point **A** is usually a shut-down or low yield point.

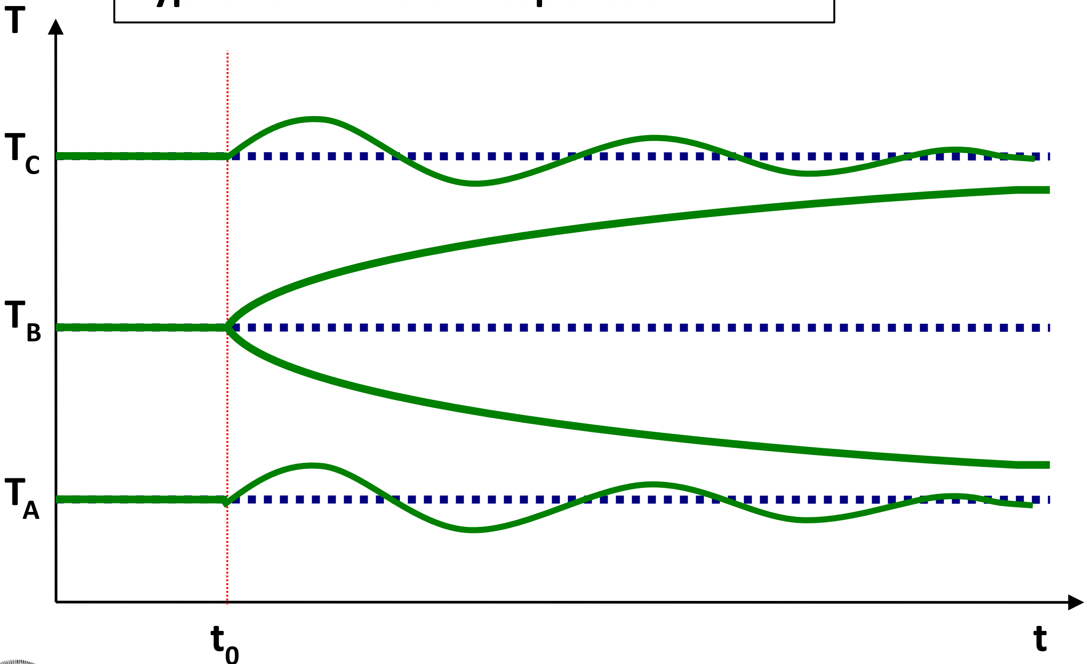
Point **C** is usually not feasible for a number of factors as: the catalyst, the reactor material, or due to the low reaction selectivity.

Point **B** is usually the best point where to run the process BUT it is unstable.

⇒ **A** and **C** are STABLE

⇒ **B** is UNSTABLE

Typical OPEN LOOP responses

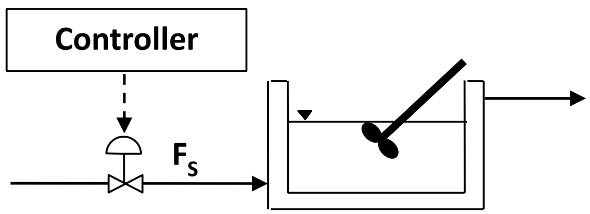


In presence of disturbances, for example on the heat subtracted by the coolant, points **A** and **C** are stable, while **B** diverges to **A** or **C**.

It is often necessary to operate at **B** that is unstable, and so a control system is needed, in order to keep the reactor operating at point **B**.

Process optimization, Optimal control

Consider a discontinuous reactor (batch) characterized by two endothermic consecutive reactions: A→B→C where B is the product and C is the by-product. The heat is provided by steam.



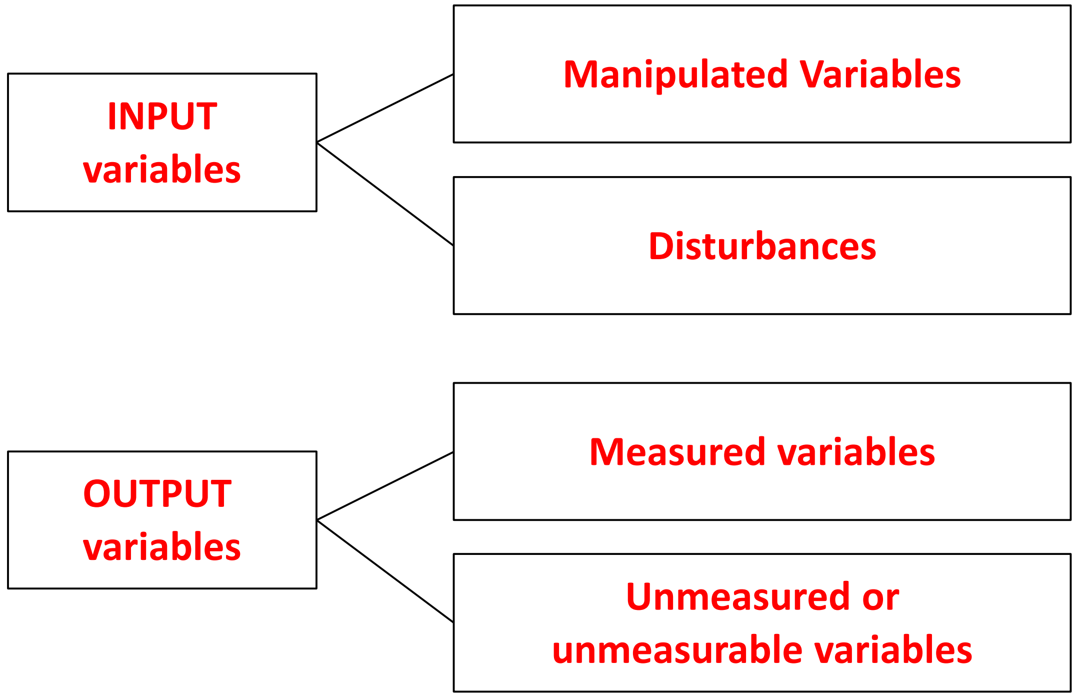
Find the steam flow-rate F_s that gives the maximum profit Φ :

$$\text{Max } \Phi = \text{Revenues from selling B} - \left[\int_0^{t_{TOT}} F_s(t)\,dt\right] - \text{Expenses to buy A}$$

The value of $F_s(t)$ must be in the range $[F_s^{min}(t), \ldots, F_s^{max}(t)]$ and the problem consists in determining the optimal trajectory (optimal control).

In this approach the system does not reject any disturbances. Instead, it controls the process according to some economics. Note that as the time passes more B is produced and so the risk to produce C massively is higher. If F_s is too high, then there is the risk that most or all the amount of B produced is converted to C (*i.e.* low selectivity).

Process variables classification



INPUT variables denote the effect of the surroundings on the process.

OUTPUT variables denote the effect of the process on the surroundings.

In addition, there are both PROCESS and INTERNAL variables that describe the features of the single process units of the plant.

Process variables classification

MEASURED variables can be measured DIRECTLY (for example pressure or temperature) or INDIRECTLY (for example the temperature of the third tray of a distillation column in order to know the purity x_i of the bottom product).

Often the INFERENTIAL measurement is necessary because the direct one is not feasible or it is too slow or too expensive.

Another aspect is related to the data reconciliation intended as MODEL IDENTIFICATION or COAPTATION, see also SOFT SENSOR.

Process variables classification

The structure or the control configuration describes the connection between the manipulated variables and the controlled ones.

The structure can be either SISO or MIMO. In case of MIMO, the control structure is not necessarily square but it may be rectangular. In general the number of manipulated variables is higher than the number of controlled ones.

Available control structures

- **DIRECT FEEDBACK**
- **INFERENTIAL FEEDBACK**
- **FEEDFORWARD**

DIRECT FEEDBACK measures controlled variables and adjusts the manipulated ones.

INFERENTIAL FEEDBACK cannot measure the controlled variables and so it measures other variables inferring the value of the controlled variables and adjusts the manipulated ones.

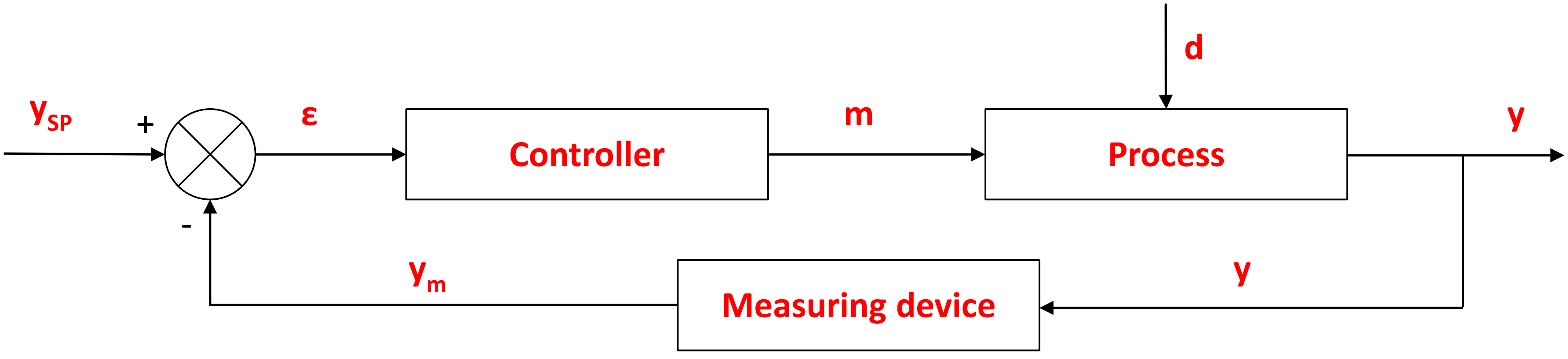
FEEDFORWARD measures disturbances and adjusts manipulated variables.

Hardware of a Process Control System

In every control structure it is possible to distinguish:

- The chemical process constituted by the operating units and their connections
- The measuring instruments and sensors:
    - Thermocouples, IR probes, …
    - Level and Pressure measurement devices , …
    - Flow meters, Pitometer, Venturi meter, …
    - Gas chromatograph, NIR, FTIR, …
- Transducers converting the measurement in a transmittable signal;
- Transmission lines, transmission bus and transmission protocols;
- The CONTROLLER is the CPU elaborating the control philosophy;
- The FINAL CONTROL ELEMENT (usually an automated valve) implements the calculated commands, decided and sent by the controller;
- Recording elements (historical trends, data retrieval, data analysis, ...).

Structure and typology of feedback controllers



y_m is the controlled variable, the value of which is measured or determined by the measuring instrument. Usually y corresponds to y_m. Conversely, the inferential control measure y and determines (*i.e.* infers) y_m, which is the real variable to be controlled.

Usually there are:

- FC = flow control
- PC = pressure control
- LC = level control
- TC = temperature control
- CC = composition control

Proportional control

For each controller type, it is defined ε = y_{SP}- y_m , there is the following time dependence:

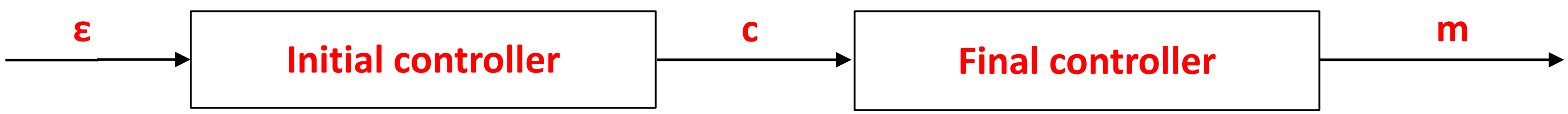
ε(t) = y_{SP}-y_m(t), or more generally: ε(t) = y_{SP}(t) - y_m(t).

The proportional control is characterized by:

$$c(t) = K_C \varepsilon(t) + c_S$$

where K_C is the proportional gain.

Note that the control has an articulate structure:



m = MANIPULATED variable

c = ACTUATION signal

Proportional – integral control

$$c(t) = K_C \varepsilon(t) + \frac{K_C}{\tau_I} \int_0^t \varepsilon(t)\,dt + c_S$$

τ_I = integral constant

Proportional, integral, and derivative control

$$c(t) = K_C \varepsilon(t) + \frac{K_C}{\tau_I} \int_0^t \varepsilon(t)\,dt + K_C \tau_D \frac{d\varepsilon(t)}{dt} + c_S$$

τ_D = derivative constant

Proportional, integral and derivative control

NOTES:

- c_S is defined as the BIAS of the controller and it is its action when the system is working exactly at the set point.
- Usually $K_C \in 0.002, \dots 1$ and $\tau_I \in 0.1, \dots 50$ min
- The action of the proportional control (P) cannot remove the offset.
- The integral action of the PI can remove even small deviations of y respect to y_{SP}.
- A possible disadvantage of the PI controller consists in the fact that sometimes errors are too slow to be eliminated, so that the control action becomes more and more higher until the valve is COMPLETELY open or closed. This situation is called INTEGRAL WINDUP.
- The derivative contribution (D) of the PID anticipates the action.
- In the derivative controller there is the risk of DERIVATIVE RINGING when there is a significant presence of background noise.

Tuning of the PID constants

Simple criteria exist, using the following parameters :

- Overshoot
- Rise time
- Settling time
- Decay ratio
- Frequency of oscillation

There are also **integral criteria** minimizing the integral of the error, defined as:

- ISE: Integral Square Error: $$ISE = \int_0^\infty \left[\varepsilon(t)\right]^2 dt$$
- IAE: Integral of the Absolute Error: $$IAE = \int_0^\infty \left|\varepsilon(t)\right| dt$$
- ITAE: Integral of the Time-Weighted Absolute Error: $$ITAE = \int_0^\infty t\left|\varepsilon(t)\right| dt$$

Tuning of the PID constants

ISE is suitable to eliminate relevant errors.

IAE is suitable to eliminate errors of the same entity.

ITAE is suitable to eliminate small errors persisting even for long times.

The following numerical problem must be solved:

$$Min_{K_C \tau_I \tau_D} \Psi \qquad \text{con} \qquad \Psi = \begin{cases} \text{ISE} \\ \text{IAE} \\ \text{ITAE} \end{cases}$$

Parameter control synthesis with:

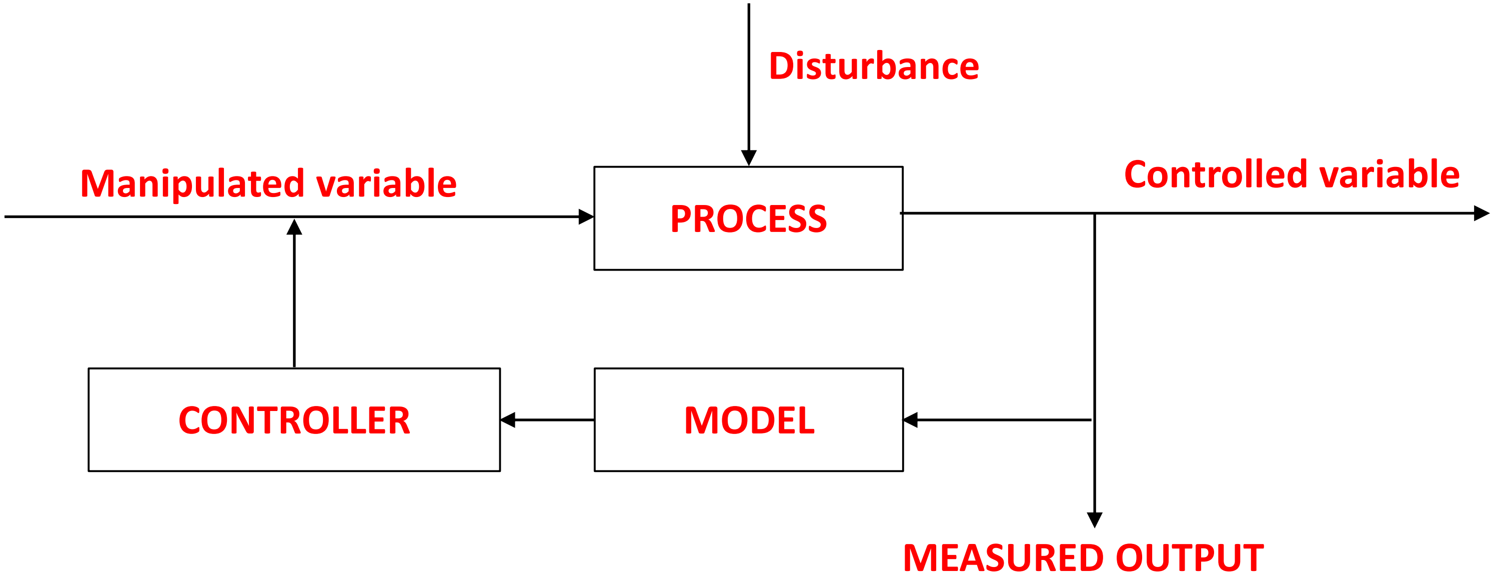
- COHEN-COON method: analysis of the response of the system to a *step change* on *c* variable (Controller activation signal). Response usually equivalent to the one of a <u>first order</u> system with delay;

- ZIEGLER-NICHOLS method: system response in <u>FREQUENCY</u>. The system is progressively taken to a continuous and stable limit of oscillation. This is achieved by implementing a sinewave disturbance on the *c* variable (ACTIVATION signal of the controller).

Process dynamics modeling

Dynamic modeling of a process or a whole process is necessary in:

- FEEDBACK CONTROL for the control loop synthesis (tuning of K_C, τ_I and τ_D);
- FEEDFORWARD CONTROL;
- INFERENTIAL CONTROL.



Dynamic model

$$\frac{d\psi}{dt} = \mathrm{F}_{\Psi}^{IN} - F_{\Psi}^{OUT} + \psi_{GEN} - \psi_{CONS}$$

GEN = generated

CONS = consumed

Sign convention (+) if inbound (*i.e.* it enters)

Ψ is one of the following

- Total mass
- Single component mass
- Total energy
- Momentum

- **GLOBAL MATERIAL BALANCE**

$$\frac{d\left(\rho v\right)}{dt} = \sum_{i=1}^{NIN} \rho_i F_i^{IN} - \sum_{i=1}^{NOUT} \rho_i F_i^{OUT}$$

- **MASS BALANCE ON COMPONENT A**

$$\frac{dn_A}{dt} = \frac{dc_A V}{dt} = \sum_{i=1}^{NIN} c_{A_i}^{IN} F_i^{IN} - \sum_{i=1}^{NOUT} c_{A_i}^{OUT} F_i^{OUT} \pm r_A V$$

- **ENERGY BALANCE**

$$\frac{dE}{dt} = \frac{d\left(U + K + P\right)}{dt} = \sum_{i=1}^{NIN} \rho_i^{IN} F_i^{IN} h_i^{IN} - \sum_{i=1}^{NOUT} \rho_i^{OUT} F_i^{OUT} h_i^{OUT} \pm Q \pm W_S$$

Dynamic model

For fixed units: $\frac{dK}{dt} = 0$ and $\frac{dP}{dt} = 0,$ so $\frac{dE}{dt} = \frac{dU}{dt}$

For liquid systems: $\frac{dU}{dt} \cong \frac{dH}{dt}$

As a first approximation: $H = \rho V c_p \left(T - T_{RIF}\right) = \rho A h c_p \left(T - T_{RIF}\right)$

Other contributions to the balance equations are:

- **Heat transfer equations** $Q = U\,A\,\Delta T$
- **Kinetic expressions** $r = K_0 e^{\left(-E_a/RT\right)} c_A$
- **Phase Equilibria equations**
- **Equations of state**

In case of dynamic simulation, we have to solve a DAE system, *i.e.* a Differential Algebraic Equation system:

$$\begin{cases} y' = f\left(y,t\right) \\ 0 = g\left(y,t\right) \end{cases}$$

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