Process Modelling

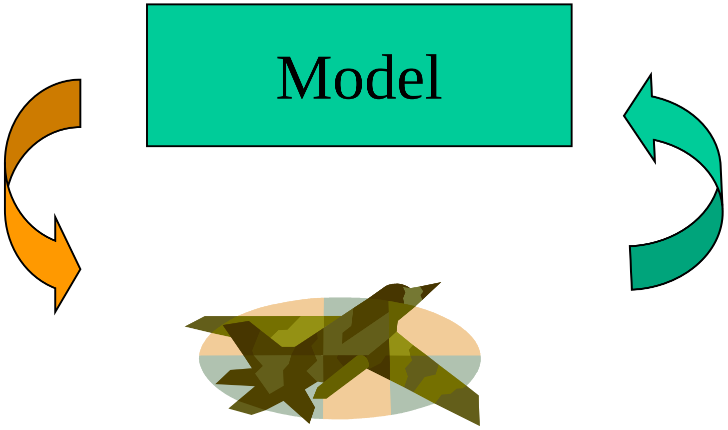
Prof. Cesar de Prada
Dpt. Systems Engineering and Automatic Control
University of Valladolid, Spain
prada@autom.uva.es
http://www.isa.cie.uva.es/~prada/

Outline

- Motivation
- Models
- Modelling methodology
- First principles models. Examples
- Linearized models
- States space models
- Impulse response models

Motivation

- Models are required to analyse the behaviour of a system and taking decisions about its functioning, not by experimenting all possible options, but in a systematic and more rational way



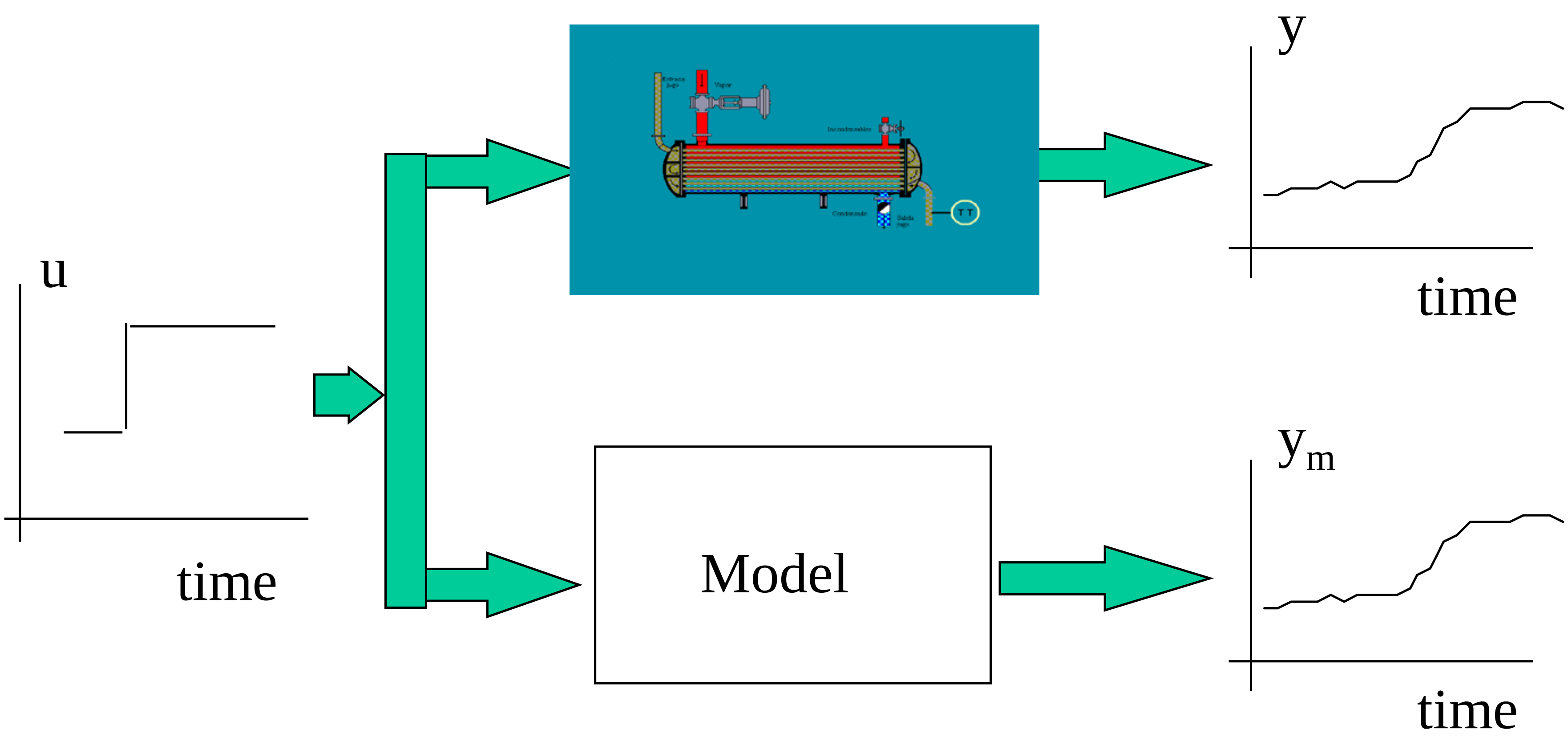
Models

- They are approximate representations of the real world
- Several types of models: Physical, qualitative, mathematical…
- Different applications: design, training, what happens if…?, decision making,…
- Abstraction: Only those aspects relevant to the problem considered are included in the model.
- How can be generated, solved, used, validated…?

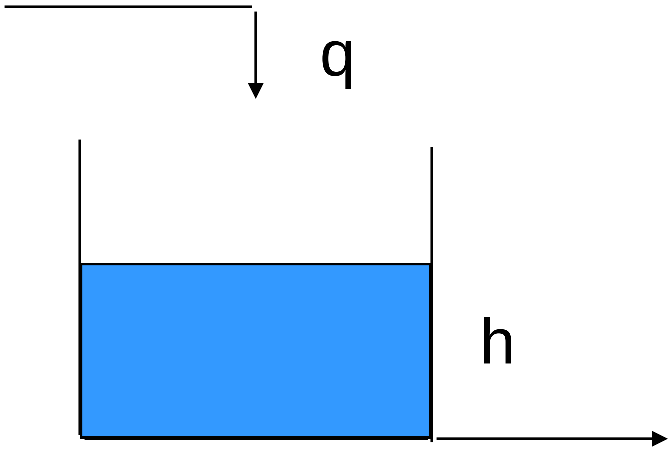
What is a mathematical model?

- Set of equations that describe in a sound way the behaviour of the system we are modelling.
- They are always approximations, not the real system
- Different models for different types of processes and aims
- Compromise between easy of use and fidelity in the representation of the reality

Adequate representation…



Continuous and discrete event processes



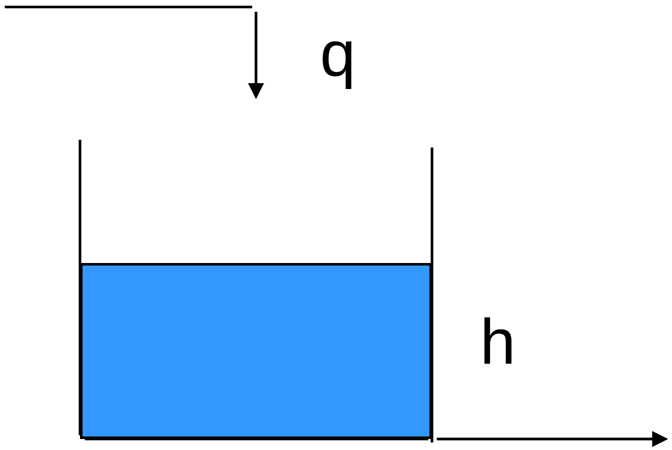
Continuous processes:
Its variables evolve continuously over time and can have any value within a given range

Discrete event systems:
Its variables only change at certain time instants and can have only an integer number of values

Continuous / Discrete events

- Continuous processes
  - They are described mainly by DAEs or PDEs.
  - Main interest: the trajectory of some variables
- Discrete events processes
  - They are describe mainly as sequences of activities.
  - Main interest: the statistical behaviour of some variables

Static and dynamic models



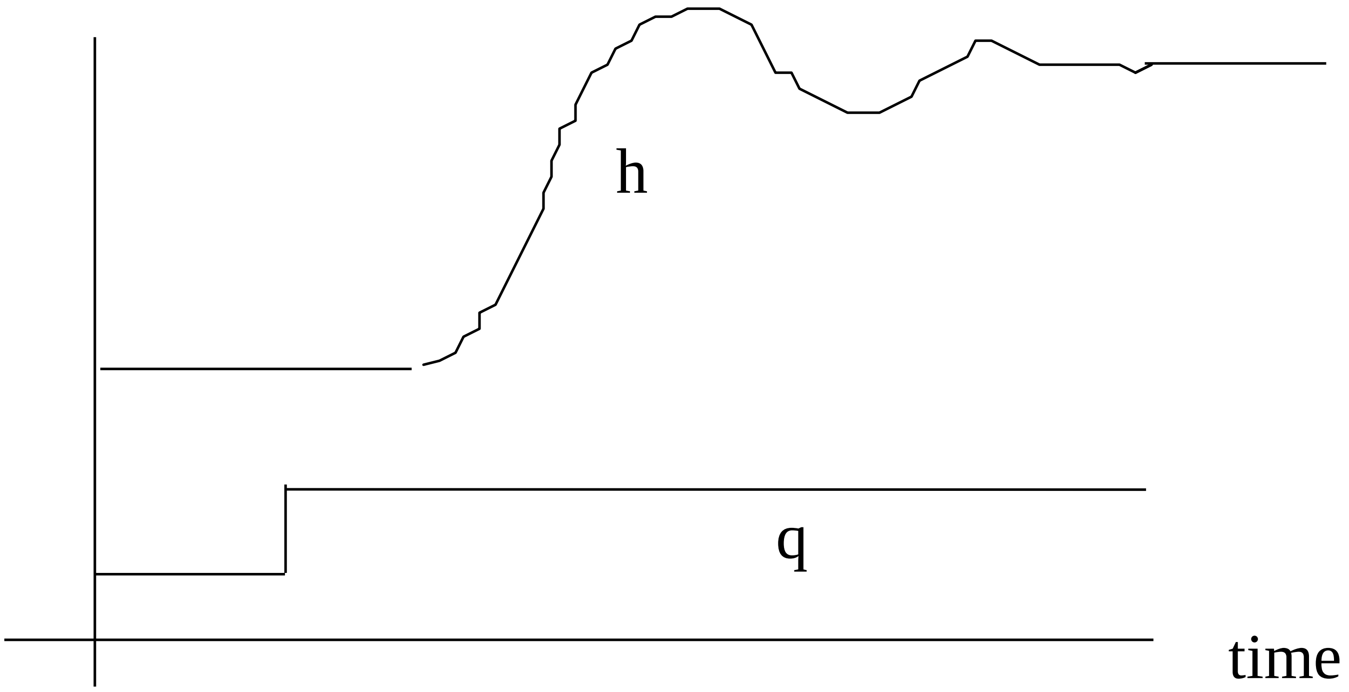
$$q = k\rho\sqrt{h}$$

Static model: It relates the values of the process variables at an equilibrium state

$$A\rho\frac{dh}{dt} = q - k\rho\sqrt{h}$$

Dynamic model: It relates the value of the process variables over time

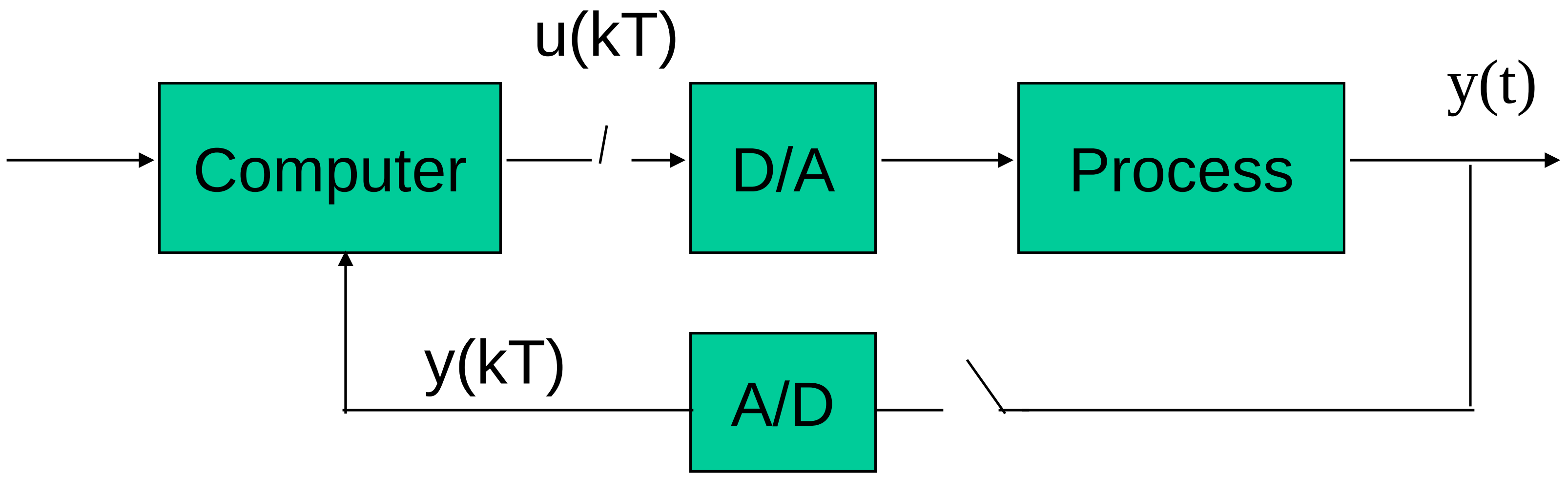
Dynamic response



Static and dynamic models

- Static models
  - They describe processes at equilibrium
  - They are described by algebraic equations (AE)
  - Typical application: Process design
- Dynamic models (in continuous time)
  - They describe the time evolution of the process
  - They are described by DAE and PDE
  - Wide range of applications: control, training,...

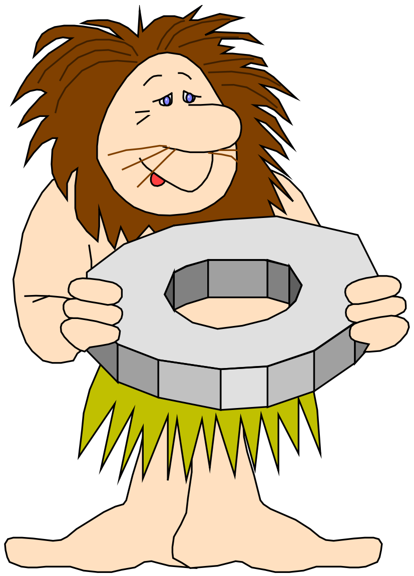
Other kind of dynamic systems



- discrete time models
- They relate the process variables at the sampling instants kT, k = 0, 1, 2, ,….
- Equations in differences: y((k+1)T) = f(y(kT), u(kT))

How to obtain a process model?

Using reasoning
and laws of nature



Using experimentation and
data from the process

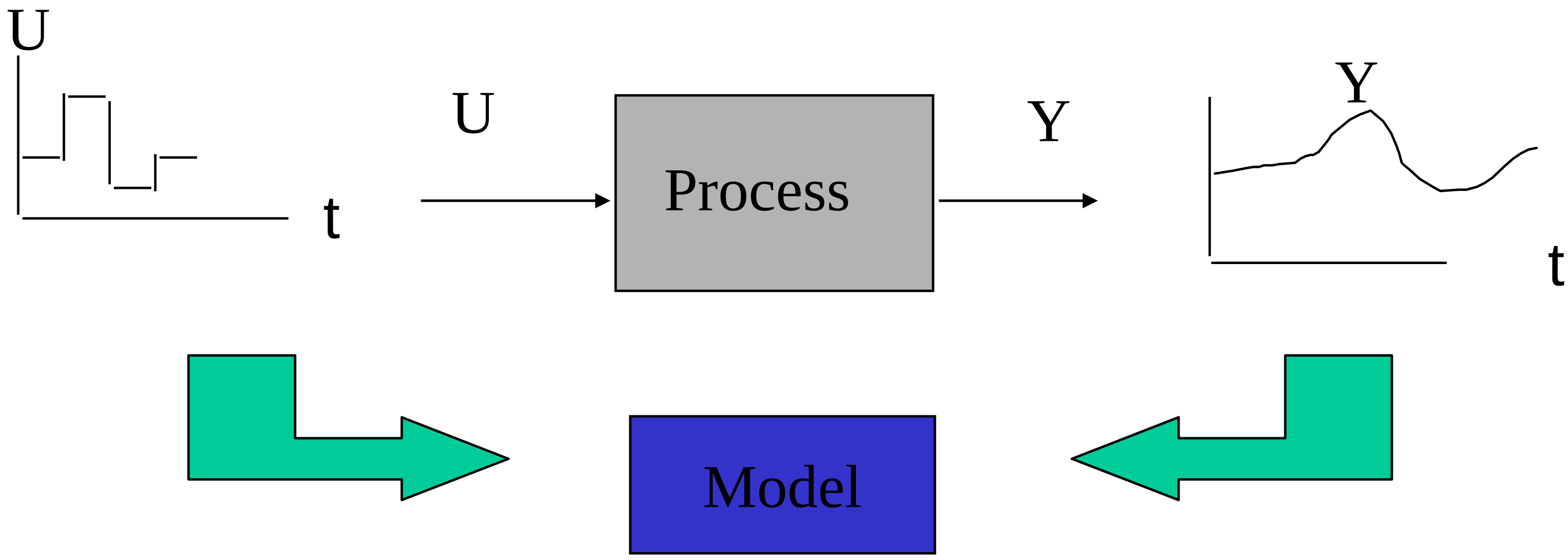
First principles models

- They are obtained from reasoning and the use of laws of nature: conservation of mass, energy or momentum as well as others from the application domain.
- They have a wide range of validity
- They require a deep knowledge of the process and the applicable laws from chemistry, physics, biology, etc.

Experimental models: Identification

The model is obtained from the information provided by a set of experiments.

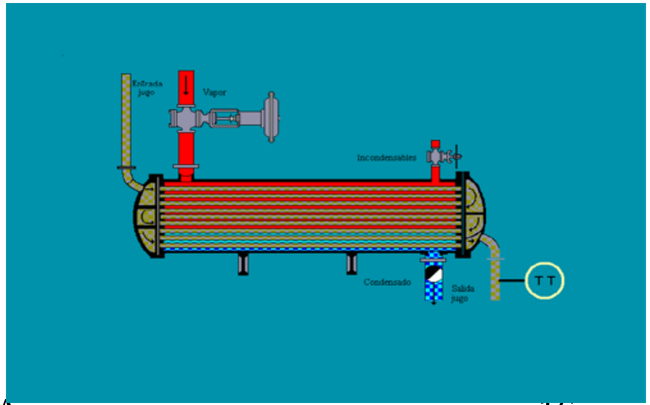
A model structure is postulated and its coefficients are computed using the data



First principles models

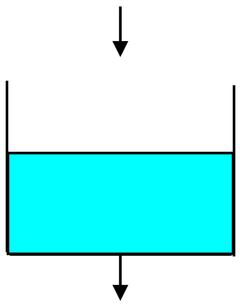
Modelling methodology:

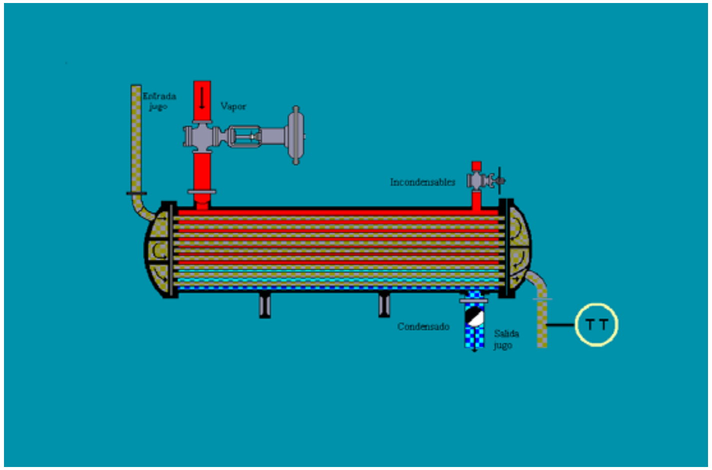
- Set the aims and range of application of the model
- Fix a set of hypothesis about its behaviour
- Formulate the mathematical equations using the appropriate laws of nature according to the hypothesis made
- Estimate the value of its parameters
- Validate the model



Many kinds of models

- Lumped parameters
- Distributed parameters
- Non-linear
- Linear
- In the time domain
- In the frequency domain
- ….





Mass conservation law

Mass accumulation in the system per unit time =

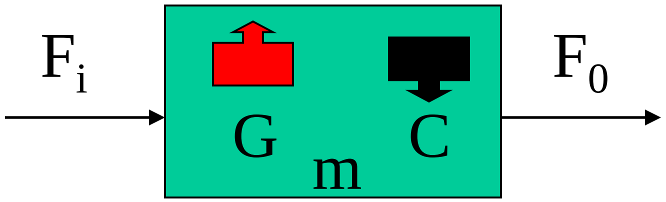
Incoming mass per unit time -

Outgoing mass per unit time -

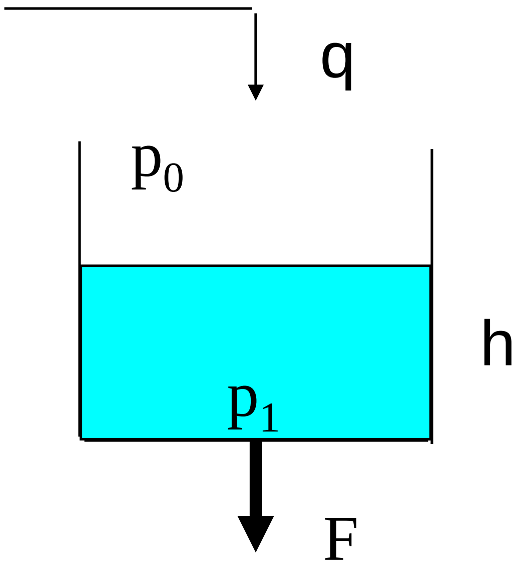
Mass generated inside the system per unit time -

Mass consumed inside the system per unit time -

$$\frac{dm}{dt} = F_i - F_0 + G - C$$



Example: Gravity drained tank



Mass conservation

Accumulation per unit time = Input flow q - outflow F

$$\frac{dm}{dt} = q\rho - F\rho$$

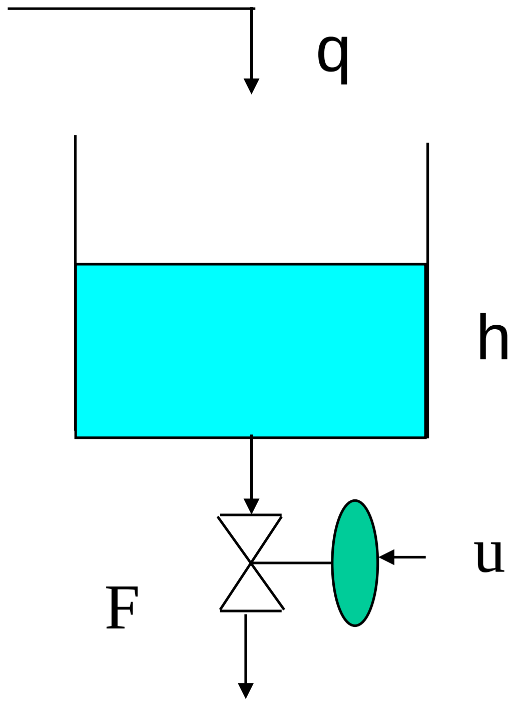
$$m = A\rho h \qquad F = Sv = Sk_1\sqrt{p_1 - p_0}$$

$$p_1 = p_0 + \rho g h \qquad F = k\sqrt{h}$$

$$A\rho\frac{dh}{dt} = q\rho - \rho k\sqrt{h}$$

m mass in the tank
A tank cross section
ρ density, k constant

Example: Gravity drained tank



Mass conservation

Accumulation per unit time = Input flow q - outflow F

$$\frac{dm}{dt} = q\rho - F\rho$$

$$m = A\rho h \qquad F = uk\sqrt{h}$$

$$A\frac{dh}{dt} = q - uk\sqrt{h}$$

$$V = Ah$$

Non-linear differencial equation

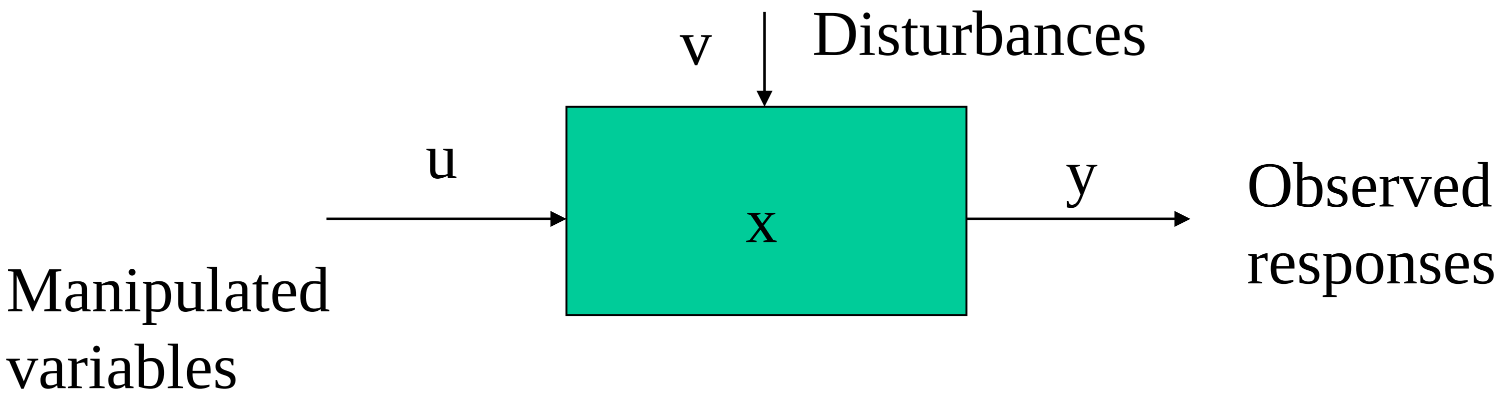
Algebraic equation

m mass in the tank
A tank cross section
ρ density, k constant
u valve opening

States space models

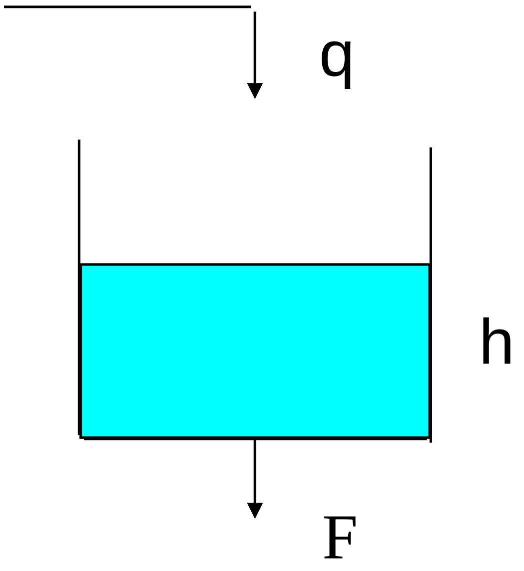
$$\frac{d\,x(t)}{dt} = f(x(t), u(t), v(t), t)$$

$$y(t) = g(x, u(t), v(t), t)$$



x states

Model simulation



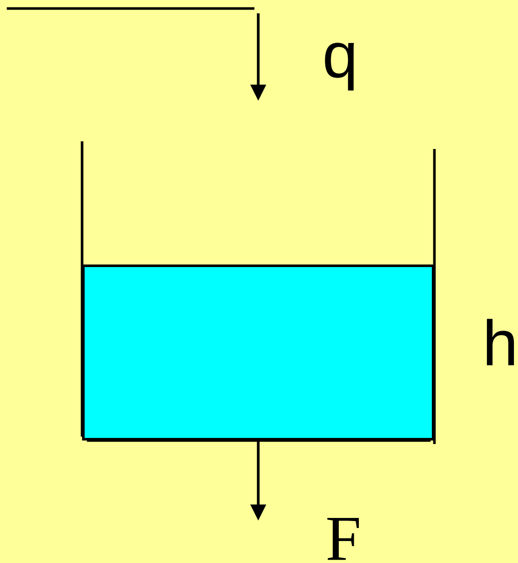
Integrating (numerically) the model, one can obtain the time evolution of the liquid volume as a function of q

$$\frac{dh}{dt} = \frac{1}{A} q - \frac{uk}{A}\sqrt{h} \qquad V = Ah$$

Euler integration formula

$$h(t+\Delta t) = h(t) + \left[\frac{1}{A} q(t) - \frac{u(t)k}{A}\sqrt{h(t)}\right]\Delta t$$

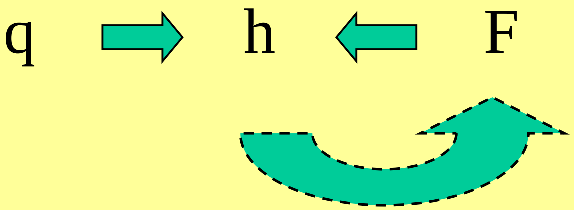
Causality



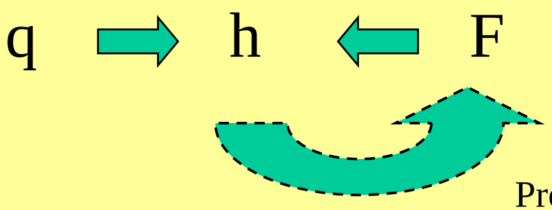
$$A\frac{dh}{dt} = q - F$$

$$F = k\sqrt{h}$$

Computational causality: the order in which the variables are computed

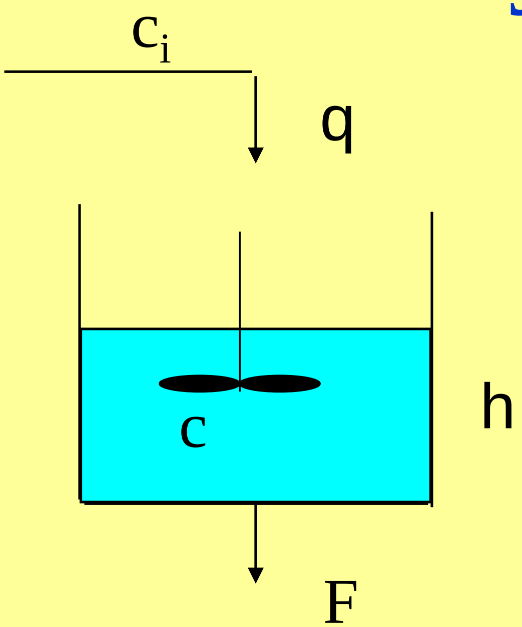


Physical causality: causes and effects

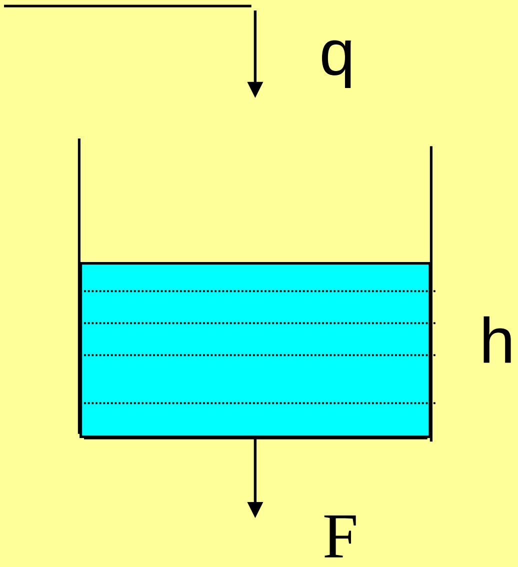


The intended use of the model (what happens if…, control,.., may impose the computational causality

Hypothesis



Perfect mixture



Plug flow

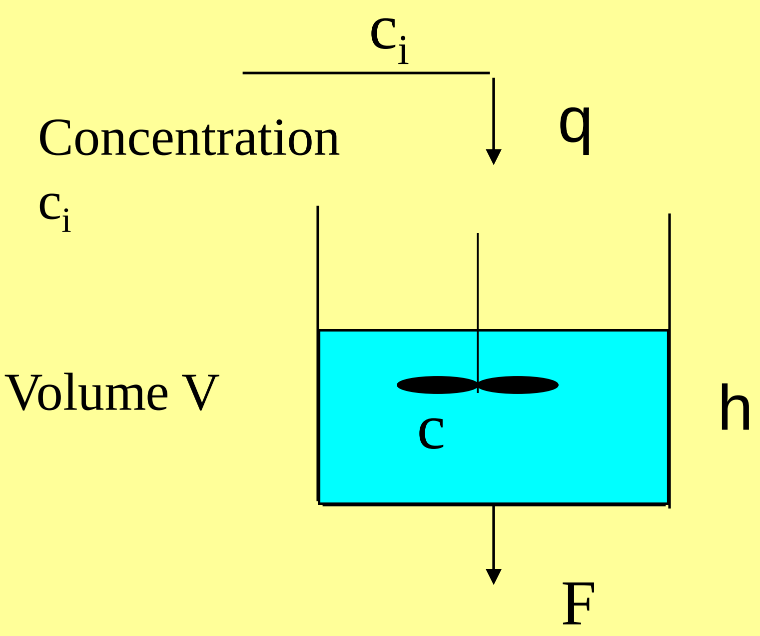
$$\frac{dVc}{dt} = qc_i - Fc$$

$$\frac{dV}{dt} = q - F \quad V = Ah$$

$$c(t) = c_i(t - \frac{h}{v}) = c_i(t - \frac{Ah}{Av}) = c_i(t - \frac{V}{F})$$

$$\frac{dV}{dt} = q - F \quad V = Ah$$

Formulation



Perfect mix

ρ constant

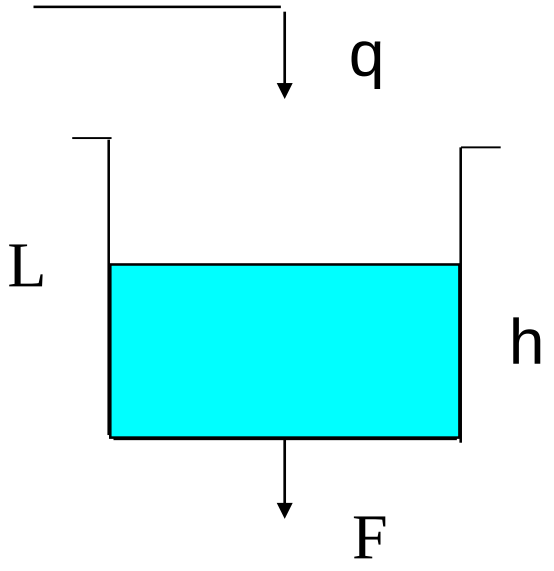
$$\left.\begin{aligned}\frac{d(Vc)}{dt} &= qc_i - Fc \\ \frac{dV}{dt} &= q - F\end{aligned}\right\} c = \frac{Vc}{V}$$

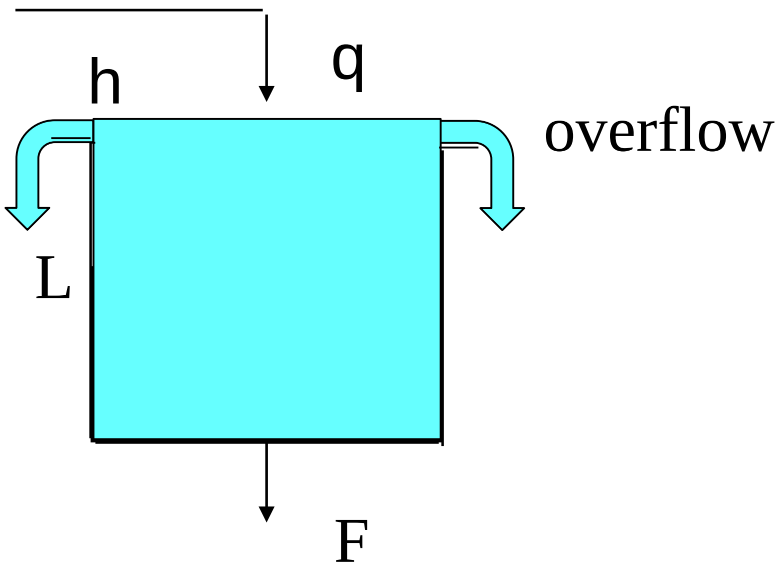
$$V\frac{dc}{dt} + c\frac{dV}{dt} = qc_i - Fc$$

$$V\frac{dc}{dt} + c(q - F) = qc_i - Fc$$

$$V\frac{dc}{dt} = q(c_i - c)$$

Physical constraints

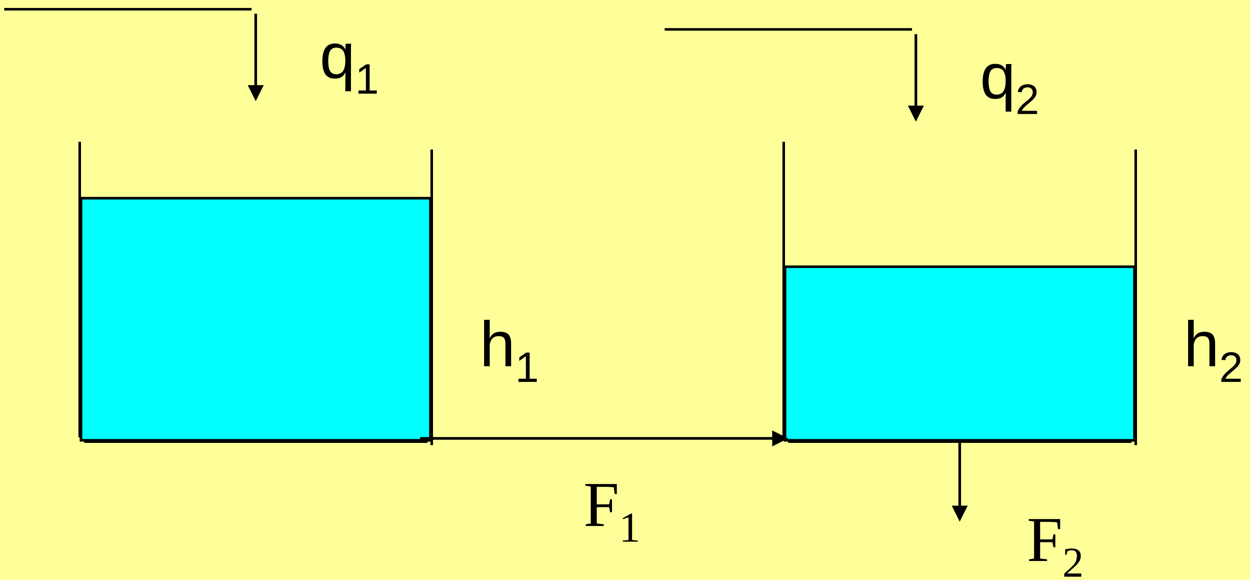




$$A\frac{dh}{dt} = q - uk\sqrt{h}$$

$$A\frac{dh}{dt} = q - uk\sqrt{h} - \alpha[\max(0, h - L)]^{2/3}$$

Numerical errors



Laws + constraints

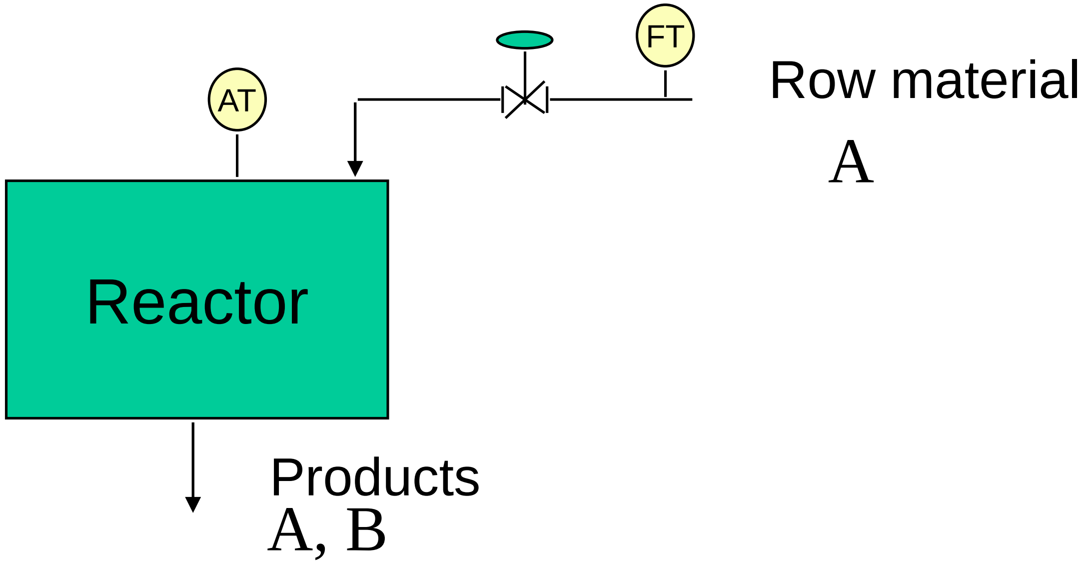
$$A_1 \frac{dh_1}{dt} = q_1 - F_1 \qquad A_2 \frac{dh_2}{dt} = q_2 + F_1 - F_2$$

$$F_1 = k_1 \sqrt{h_1 - h_2} \qquad h_1 < h_2 \, ? \qquad F_2 = k_2 \sqrt{h_2}$$

$$F_1 = k_1 \, \mathrm{sgn}(h_1 - h_2) \sqrt{|h_1 - h_2|} \qquad 0 \le h_i \le h_{max} \qquad q_i \ge 0$$

Isothermal chemical reactor

Reaction: $A \longrightarrow B$



Mathematical model

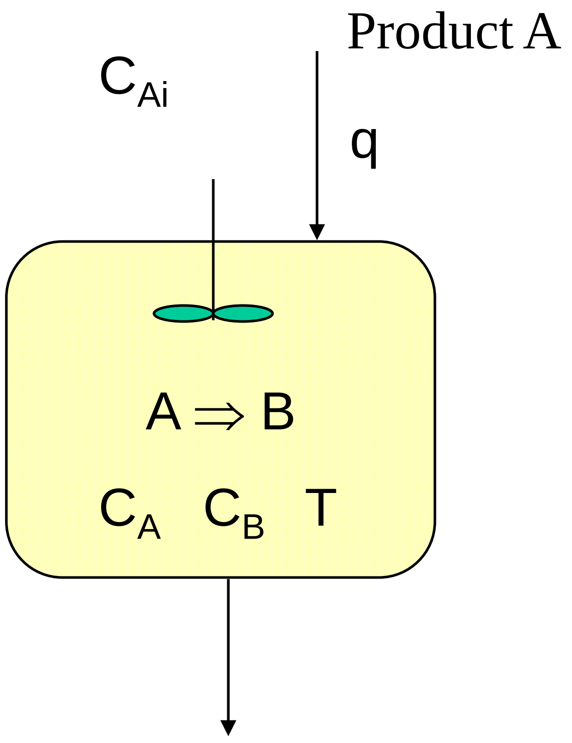
Hypothesis:

- perfect mix in the reactor
- Temperature T constant
- Volume V constant

$$V\frac{dc_A}{dt} = qc_{Ai} - qc_A - Vk_0 e^{-E/RT} c_A$$

$$V\frac{dc_B}{dt} = -qc_B + Vk_0 e^{-E/RT} c_A$$

Mass balances of products A and B



Example: CSTR Reactor

$$V\frac{dc_A}{dt} = q(c_{Ai} - c_A) - Vk_0 e^{-E/RT} c_A$$

$$V\rho c_p \frac{dT}{dt} = q\rho c_p (T_i - T) + Vk_0 c_A H - UA(T - T_r)$$

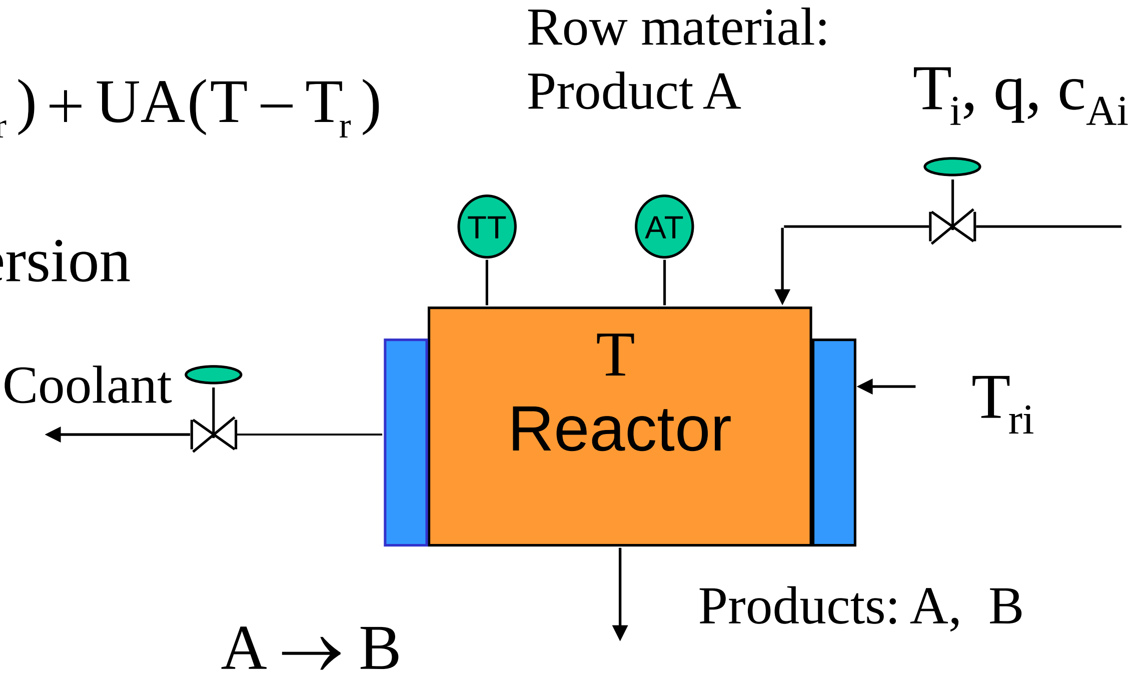
$$V_r \rho_r c_{pr} \frac{dT_r}{dt} = F_r \rho_r c_{pr} (T_{ri} - T_r) + UA(T - T_r)$$

$$c_A = c_{Ai}(1 - x) \quad x \ \text{conversion}$$

$$c_B = c_{Ai} - c_A = c_{Ai} x$$

$$V = \pi D^2 L / 4$$

$$A = \pi DL + \pi D^2 / 4$$



Bioreactor

x biomass
x substrate
p product
V volume

$$\frac{dVx}{dt} = \mu xV - \kappa Vx$$

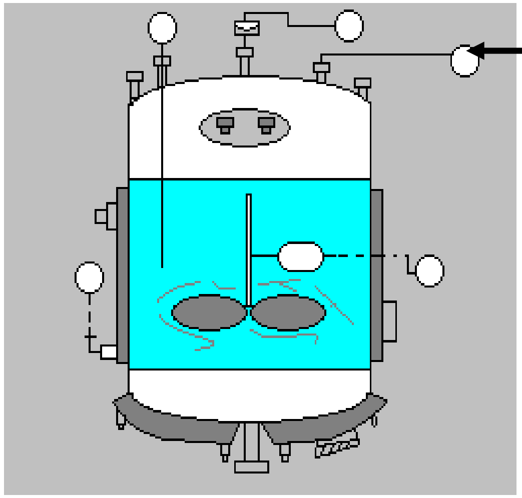
growing dead

$$\frac{dVs}{dt} = -\frac{\mu}{Y_x} xV - \frac{\sigma}{Y_p} xV + s_F F$$

Substrate consumption feed

$$\frac{dVp}{dt} = \sigma xV - K_H pV$$

$$\frac{dV}{dt} = F$$



$$\mu = \frac{\mu_x s}{s + K_x}$$

Monod

$$\sigma = \frac{\mu_p s}{K_p x + s + s^2 / K_I}$$

Haldane

Bioreactor

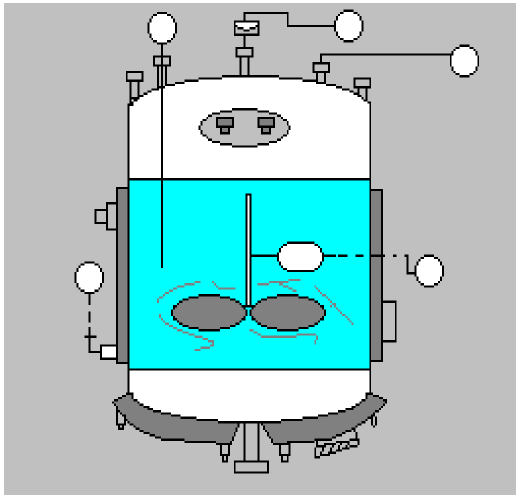
x biomass
x substrate
p product
V volume

$$V\frac{dx}{dt} + x\frac{dV}{dt} = \mu xV - \kappa xV$$

$$V\frac{ds}{dt} + s\frac{dV}{dt} = -\frac{\mu}{Y_x}xV - \frac{\sigma}{Y_p}xV + s_F F$$

$$V\frac{dp}{dt} + p\frac{dV}{dt} = \sigma xV - K_H pV$$

$$\frac{dV}{dt} = F$$



$$\mu = \frac{\mu_x s}{s + K_x} \qquad \sigma = \frac{\mu_p s}{K_p x + s + s^2 / K_I}$$

Bioreactor

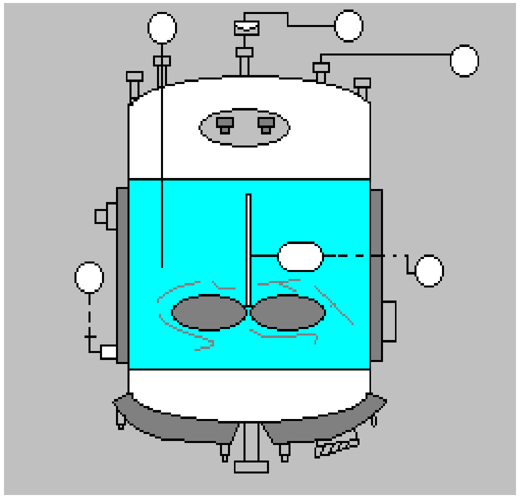
x biomass
x sustrate
p product
V volume

$$\frac{dx}{dt} = (\mu - \frac{F}{V} - \kappa)x$$

$$\frac{ds}{dt} = -(\frac{\mu}{Y_x} + \frac{\sigma}{Y_p})x + \frac{F}{V}(s_F - s)$$

$$\frac{dp}{dt} = \sigma x - (K_H + \frac{F}{V})p$$

$$\frac{dV}{dt} = F$$

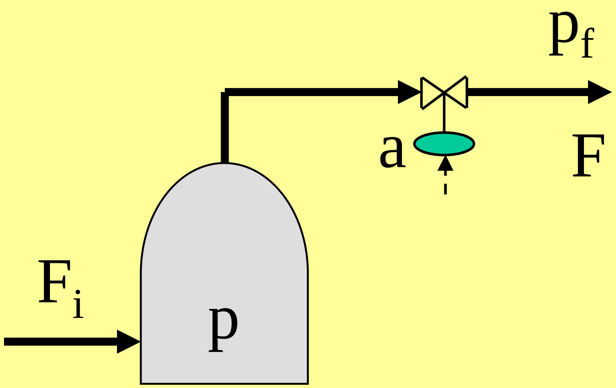


$$\mu = \frac{\mu_x s}{s + K_x}$$

$$\sigma = \frac{\mu_p s}{K_p x + s + s^2 / K_I}$$

Pressure in a container

$$\frac{dm}{dt} = F_i - F = F_i - aC_v\sqrt{p^2 - p_f^2}$$



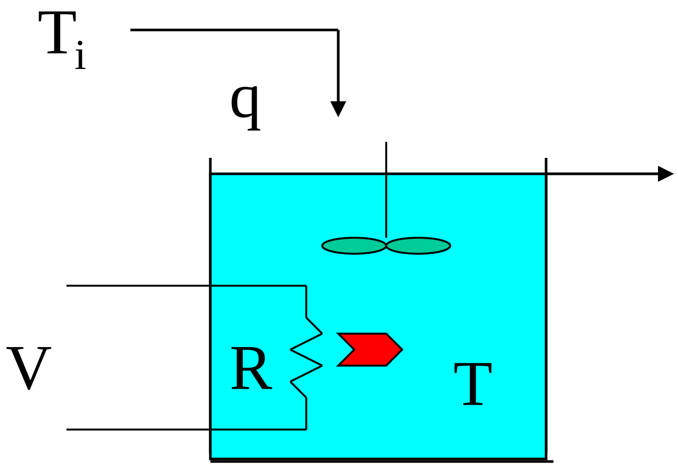
$$m = V\rho \qquad p = \frac{\rho}{M}RT \qquad \text{isothemal tank}$$

$$\frac{VM}{RT}\frac{dp}{dt} = F_i - aC_v\sqrt{p^2 - p_f^2}$$

Low pressure container

Constant composition

Energy conservation law



$$\frac{d(mH)}{dt} = q\rho H_i - q\rho H + \frac{V^2}{R}$$

$$\text{si} \quad H = c_e T \qquad m = Ah\rho$$

$$Ah\frac{dT}{dt} = q(T_i - T) + \frac{V^2}{\rho c_e R}$$

Non-linear differential equation

T temperature, V voltage
m mass of liquid in the tank
H enthalpy, c_e specific heat
A tank cross section
ρ density, R resistance

Hypothesis:

T uniform distribution
Perfect thermal isolation
Constant density

Liquid flow in a pipe

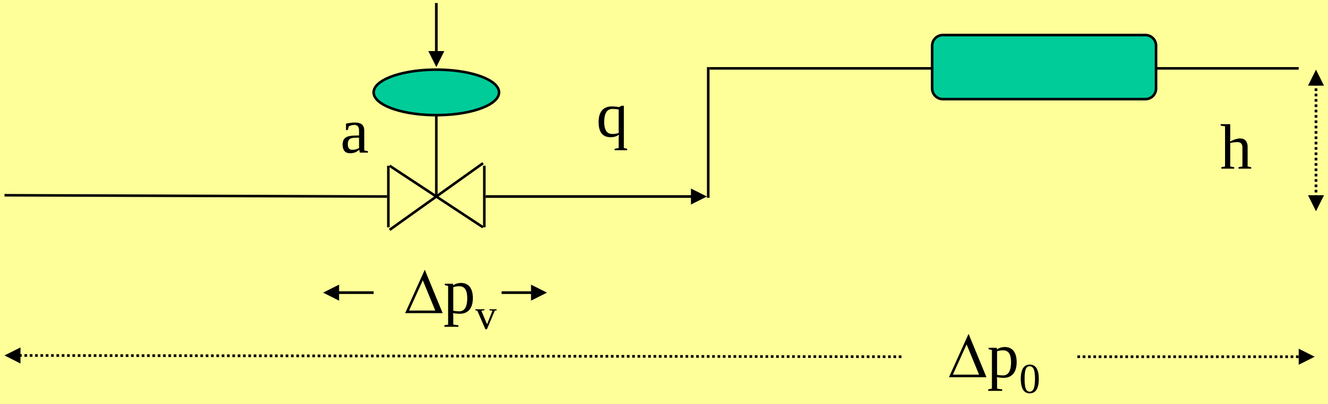
Momentum conservation law

$$\frac{d\,mv}{d\,t} = A\Delta p_0 - A\Delta p_v - AfL\rho v^2 - Ah\rho g$$

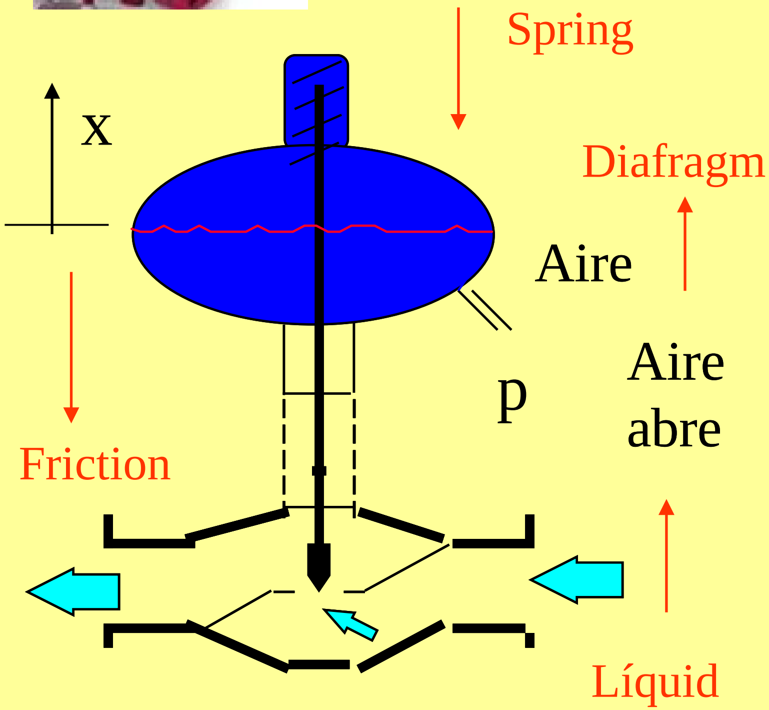
$$\Delta p_v = \frac{1}{a^2 C_v^2}\rho q^2 \qquad m = AL\rho \qquad q = Av$$

Non-linear differential equation

$$\frac{L}{A}\frac{d\,q}{d\,t} = \frac{\Delta p_0}{\rho} - \left(\frac{1}{a^2 C_v^2} + \frac{fL}{A^2}\right)q^2 - gh$$



Control valve (linear)



$$m\frac{d^2x}{dt^2} = (p - p_0)A + \Delta p_v S - kx - k_v \frac{dx}{dt}$$

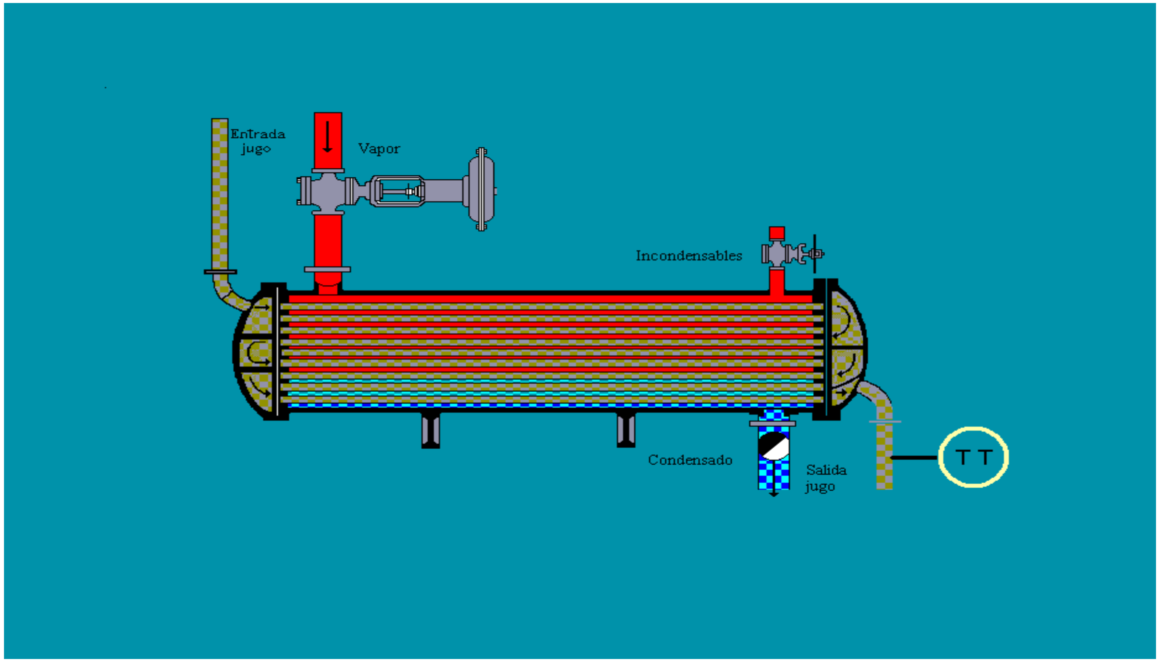
$$q = \frac{x}{L} C_v \sqrt{\frac{\Delta p_v}{\rho}}$$

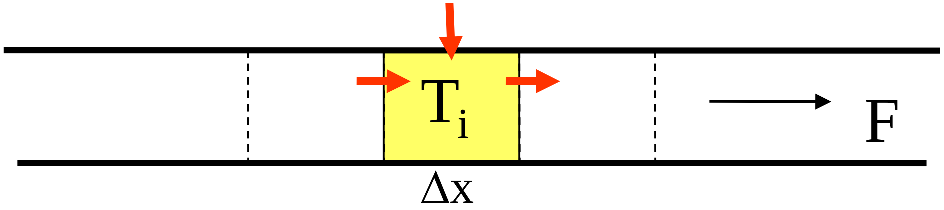
x position of stem from equilibrium position

L range of stem displacement

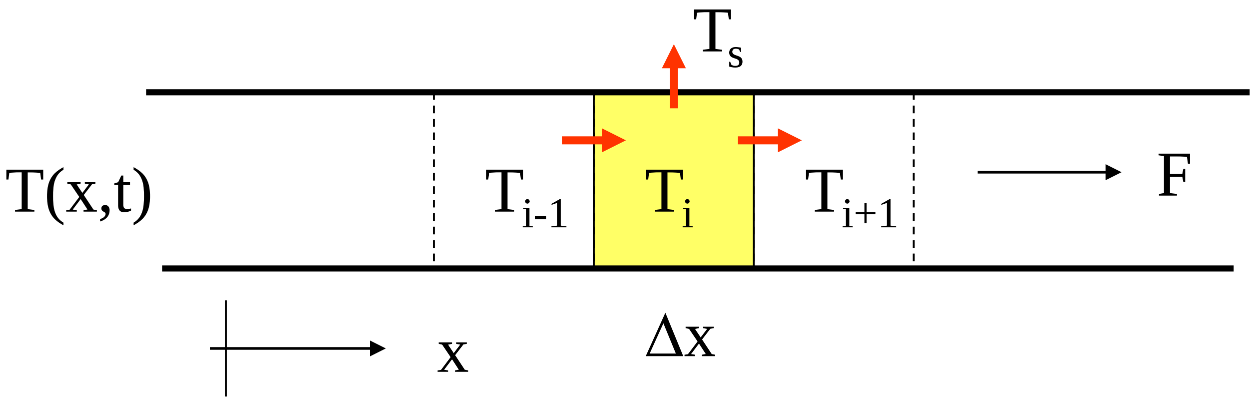
p air pressure

Distributed parameters processes





Distributed parameters process

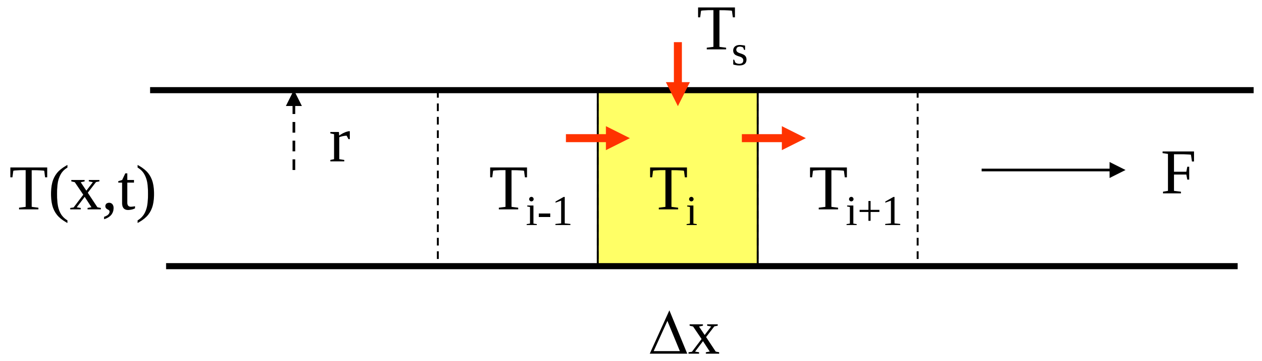


The pipe is divided into small volumes of width Δx where T can be assumed to be constant

Energy balance on every volume

Limit when $\Delta x \to 0$

Distributed parameters process



Energy balance

$$\frac{d\,\pi r^2 \Delta x \rho c_e T_i}{dt} = F\rho c_e T_{i-1} - F\rho c_e T_i + 2\pi r \Delta x U(T_s - T_i)$$

Partial differential equations

$$\frac{dT_i}{dt} = \frac{F}{\pi r^2}\frac{(T_{i-1} - T_i)}{\Delta x} + \frac{2U(T_s - T_i)}{r\rho c_e}$$

$$\lim_{\Delta x \to 0}\frac{dT_i}{dt} = \frac{F}{\pi r^2}\lim_{\Delta x \to 0}\frac{(T_{i-1} - T_i)}{\Delta x} + \lim_{\Delta x \to 0}\frac{2U(T_s - T_i)}{r\rho c_e}$$

$$\frac{\partial T(x,t)}{\partial t} = -\frac{F}{\pi r^2}\frac{\partial T(x,t)}{\partial x} + \frac{2U(T_s - T(x,t))}{r\rho c_e}$$

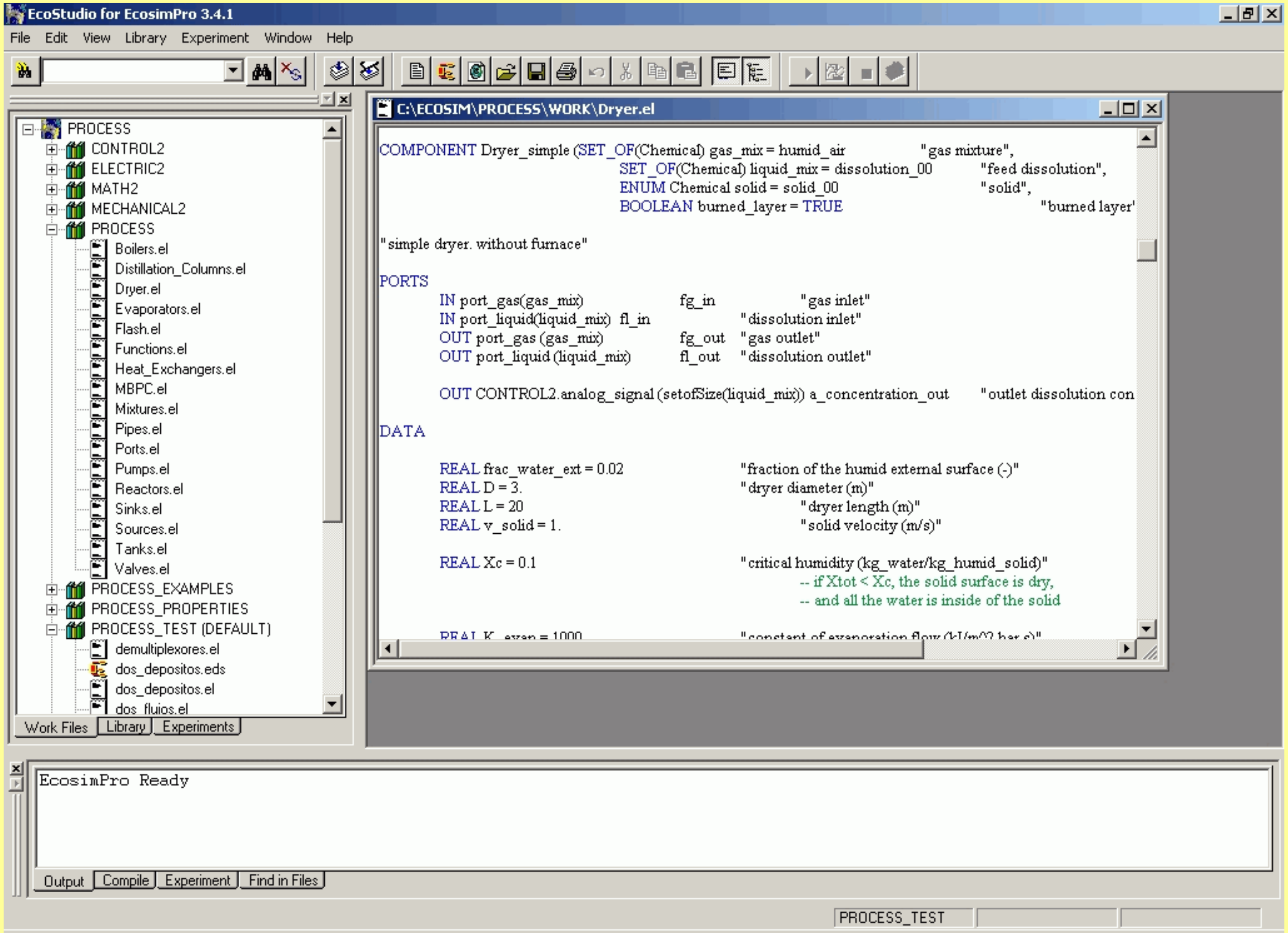
First principles models

- Described by sets of algebraic and differential equations, often non-linear.
- They can be used for a wide range of aims
- They have a wide range of validity within the one fix by the associated hypothesis
- They require a certain modelling background
- They may be difficult to operate with
- Quite often they are solved by simulation

Simulation: EcosimPro

- Facilitate the description of the model, and provides the methods to solve it
- Modelling / Simulation languages
- What happens if…?
- Based on object oriented software technologies
- Advanced numerical methods and functionalities
- ESA: European Space Agency
- C++ code generator with a development and execution environment
- Library / Component / Partition / Experiment
- Open system

EcosimPro


EcoStudio for EcosimPro 3.4.1
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MATH2
MECHANICAL2
PROCESS
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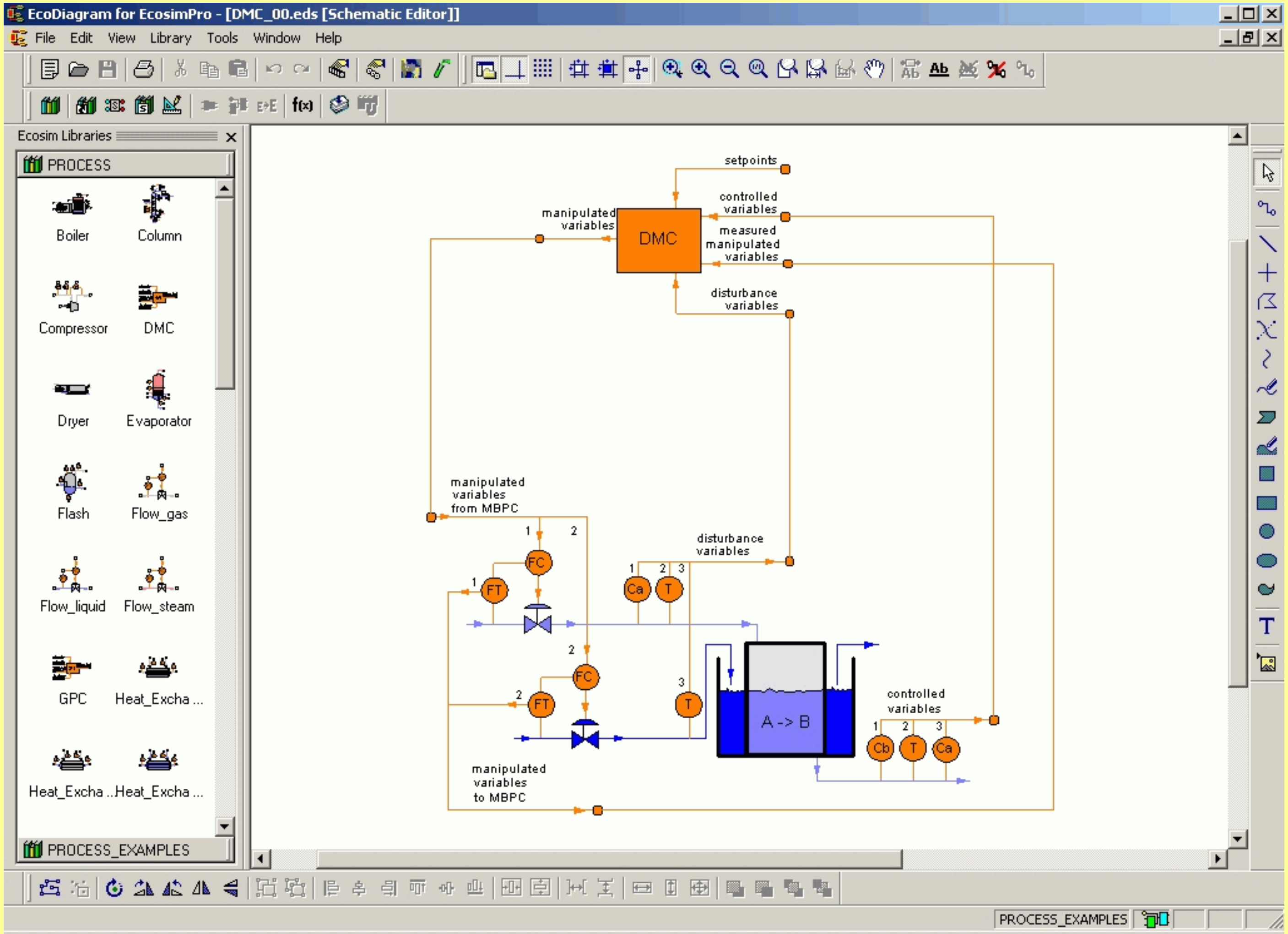
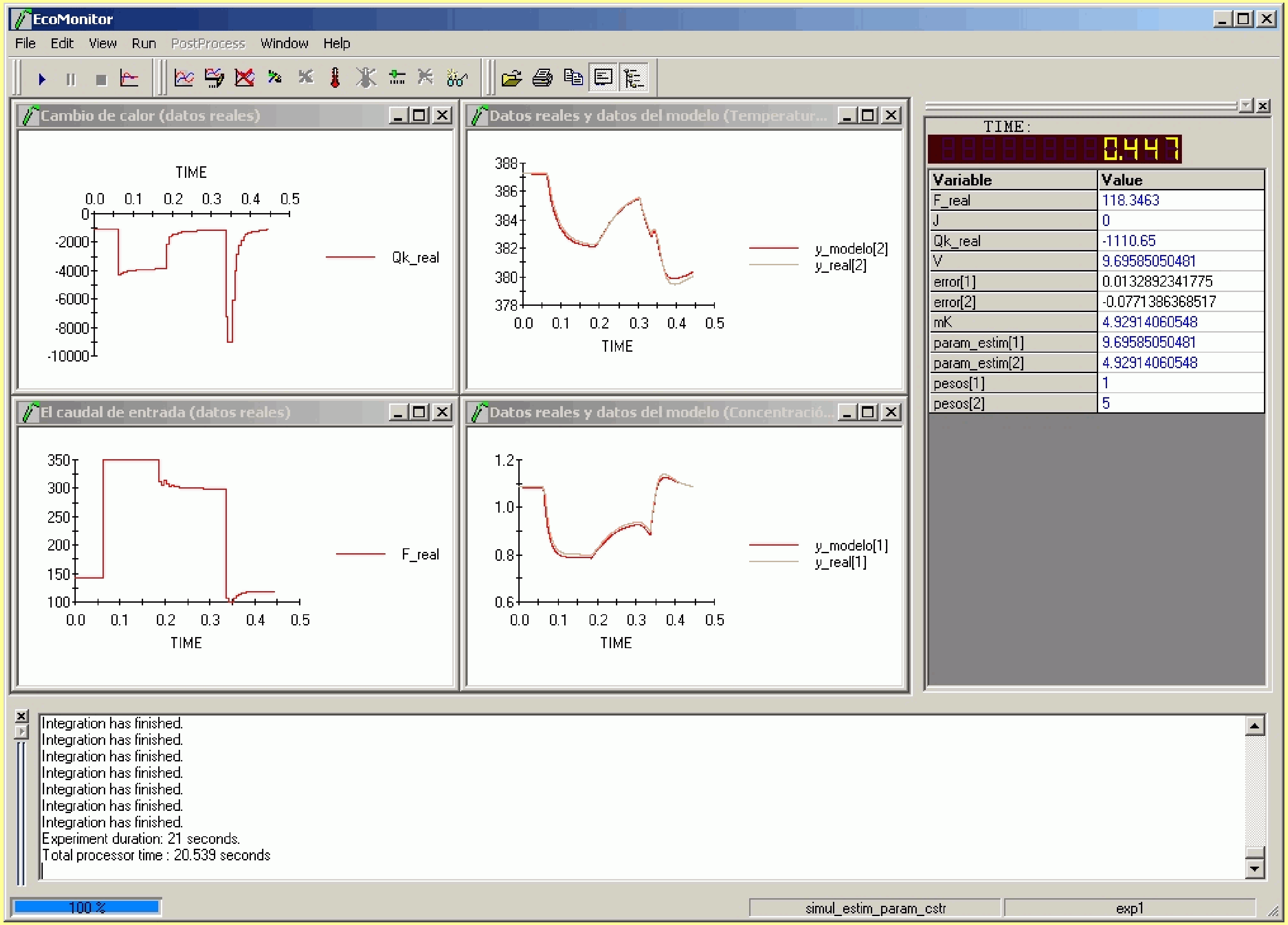
dos_depositos.el
Work Files
Library
Experiments
C:\ECOSIM\PROCESS\WORK\Dryer.el
COMPONENT Dryer_simple (SET_OF(Chemical) gas_mix = humid_air "gas mixture",
SET_OF(Chemical) liquid_mix = dissolution_00 "feed dissolution",
ENUM Chemical solid = solid_00 "solid",
BOOLEAN burned_layer = TRUE
"simple dryer. without furnace"
PORTS
IN port_gas(gas_mix) fg_in "gas inlet"
IN port_liquid(liquid_mix) fl_in "dissolution inlet"
OUT port_gas (gas_mix) fg_out "gas outlet"
OUT port_liquid (liquid_mix) fl_out "dissolution outlet"
OUT CONTROL2.analog_signal (setofSize(liquid_mix)) a_concentration_out
DATA
REAL frac_water_ext = 0.02 "fraction of the humid external surface (-)"
REAL D = 3. "dryer diameter (m)"
REAL L = 20 "dryer length (m)"
REAL v_solid = 1. "solid velocity (m/s)"
REAL Xc = 0.1 "critical humidity (kg_water/kg_humid_solid)"
-- if Xtot < Xc, the solid surface is dry,
-- and all the water is inside of the solid
EcosimPro Ready
Output
Compile
Experiment
Find in Files
PROCESS_TEST

Graphical environment



Simulation



EcoMonitor
File Edit View Run PostProcess Window Help
Cambio de calor (datos reales)
TIME
Qk_real
Datos reales y datos del modelo (Temperatur...
y_modelo[2]
y_real[2]
El caudal de entrada (datos reales)
F_real
Datos reales y datos del modelo (Concentració...
y_modelo[1]
y_real[1]
TIME:
0.447
Variable | Value
F_real | 118.3463
J | 0
Qk_real | -1110.65
V | 9.69585050481
error[1] | 0.0132892341775
error[2] | -0.0771386368517
mK | 4.92914060548
param_estim[1] | 9.69585050481
param_estim[2] | 4.92914060548
pesos[1] | 1
pesos[2] | 5
Integration has finished.
Integration has finished.
Integration has finished.
Integration has finished.
Integration has finished.
Integration has finished.
Integration has finished.
Experiment duration: 21 seconds.
Total processor time : 20.539 seconds
100 %
simul_estim_param_cstr
exp1

Model Linearization

- To facilitate the analysis and computations, we use a linear approximation of the non-linear equations
- Easier to operate, but with a limited validity range

$$A\frac{dh}{dt} = q - k\sqrt{h} \quad \Rightarrow \quad A\frac{d\Delta h}{dt} = \beta\Delta q - \alpha\Delta h$$

Linearization of a function f

Taylor series expansion in an operating point u_0, y_0, z_0, ….

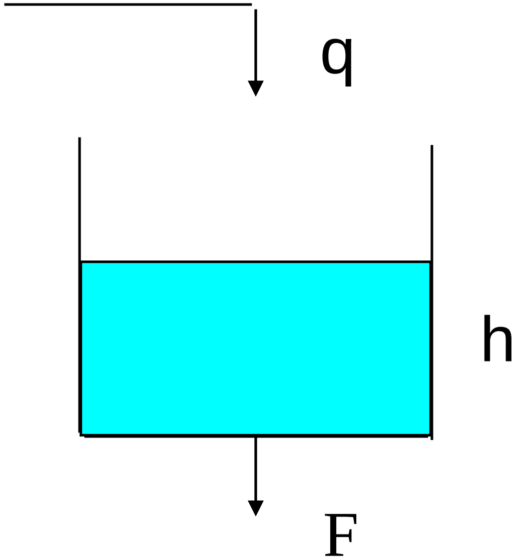
$$f(u,y,z)=0 \qquad f(u_0,y_0,z_0)=0$$

$$f(u,y,z)=f(u_0,y_0,z_0)+\left.\frac{\partial f}{\partial u}\right|_0 (u-u_0)+\left.\frac{\partial f}{\partial y}\right|_0 (y-y_0)+\left.\frac{\partial f}{\partial z}\right|_0 (z-z_0)+\ldots$$

$$\left.\frac{\partial f}{\partial u}\right|_0 \Delta u+\left.\frac{\partial f}{\partial y}\right|_0 \Delta y+\left.\frac{\partial f}{\partial z}\right|_0 \Delta z=0 \qquad \Delta u=u-u_0 \quad \Delta y=y-y_0 \quad \Delta z=z-z_0$$

Linear equation in the new variables Δu, Δy, Δz

Linearized model of the tank



$$A\frac{dh}{dt} - q + k\sqrt{h} = 0$$

$$f(\dot{h}, h, q) = 0 \qquad \dot{h}_0, h_0, q_0$$

$$\left.\frac{\partial f}{\partial \dot{h}}\right|_0 (\dot{h} - \dot{h}_0) + \left.\frac{\partial f}{\partial h}\right|_0 (h - h_0) + \left.\frac{\partial f}{\partial q}\right|_0 (q - q_0) = 0$$

$$\left.\frac{\partial f}{\partial \dot{h}}\right|_0 = A \qquad \left.\frac{\partial f}{\partial h}\right|_0 = \frac{k}{2\sqrt{h_0}} \qquad \left.\frac{\partial f}{\partial q}\right|_0 = -1$$

$$A\frac{d\Delta h}{dt} + \frac{k}{2\sqrt{h_0}}\Delta h - \Delta q = 0$$

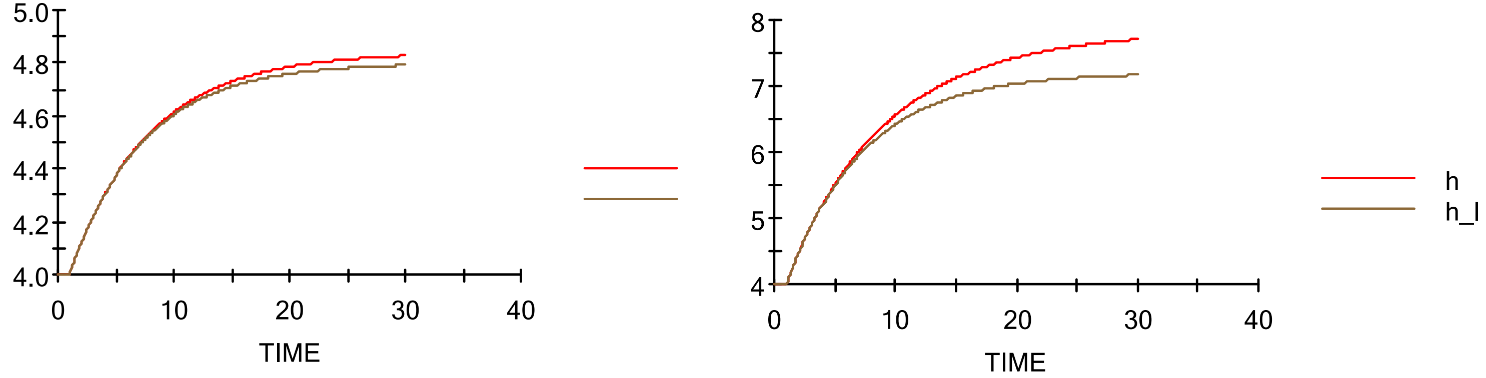
Deviation Variables

$\Delta h = h - h_0$

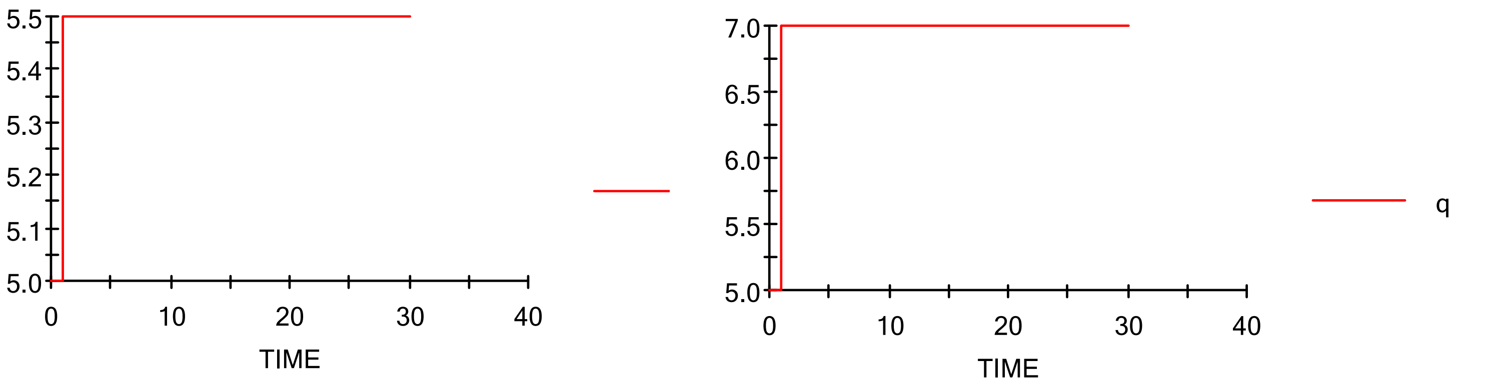
$\Delta q = q - q_0$

Linear differential equation

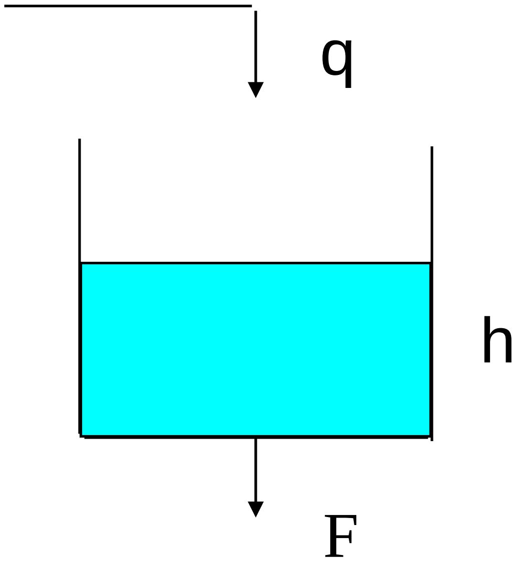
Simulation / Validation



Responses of the non-linear and linearized models for 2 step changes in q



Linearized model of the tank



$$A\frac{d\Delta h}{dt} + \frac{k}{2\sqrt{h_0}}\Delta h - \Delta q = 0$$

$$\frac{A2\sqrt{h_0}}{k}\frac{d\Delta h}{dt} + \Delta h = \frac{2\sqrt{h_0}}{k}\Delta q$$

$$\tau\frac{d\Delta h}{dt} + \Delta h = K\Delta q$$

$$\tau = \frac{A2\sqrt{h_0}}{k} \qquad K = \frac{2\sqrt{h_0}}{k}$$

Deviation Variables

$\Delta h = h - h_0$

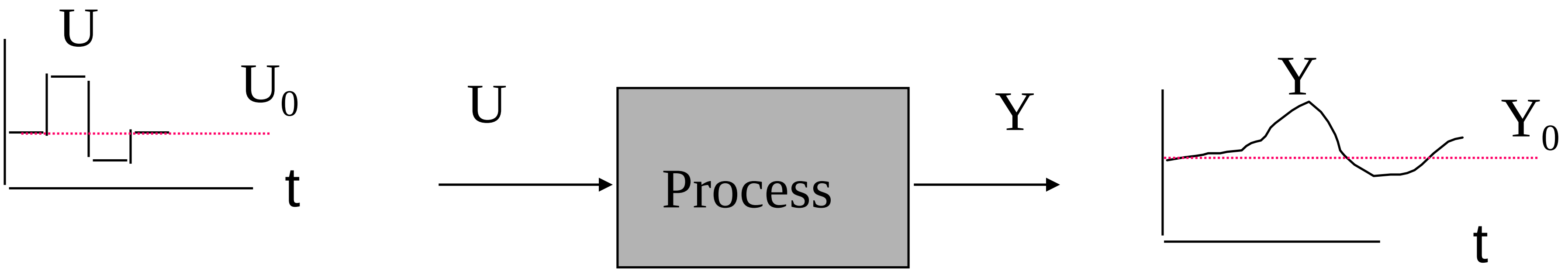
$\Delta q = q - q_0$

The value of the model coefficients depends on the linearization point

Linearized models

Variables u and y represent changes above and below the operation point U_0 , Y_0

$$u(t) = U(t) - U_0(t)$$
$$y(t) = Y(t) - Y_0(t)$$



The range of validity is constrained to a certain extent around the linearization point