8. Short introductions to: process equipment and design; biotechnology; process dynamics and control

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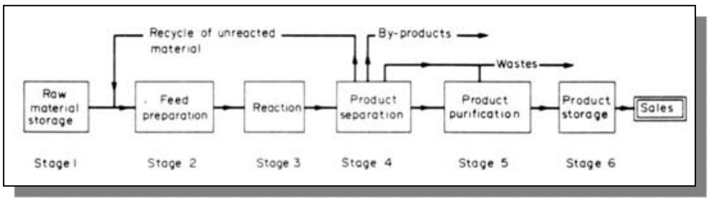
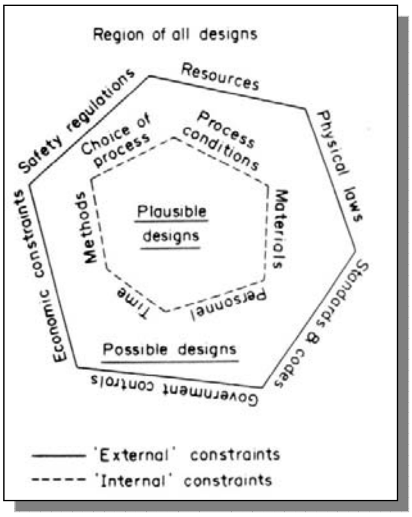
8.1 Process equipment and design

See also courses offered by
Laboratory for Process Design *("Anläggningsteknik")*

Chemical processes design



Schematic lay-out of a typical chemical process



Restrictions to the design of a chemical process

Pictures: CR93

Process design aspects

- Total process lay-out and design, includes
  - mass balances, energy balances, energy losses analysis
  - reactors and catalysts, biochemistry issues
  - unit operations *(sv: enhetsoperationer)* equipment: heat exchangers, separation processes, pumps/compressors, pipes and tubing, solids handling,......
  - electricity, steam/hot water, compressed air, cooling water, ...
  - location and site considerations
  - safety issues
  - process control
  - scale-up issues
  - mechanical aspects
  - raw material and product handling
  - waste and by-product handling
  - economic analysis, legal issues
  - sustainability, design-for-recycling

Picture: http://www.powtec.de/service_de.htm

with help from chemists, mechanical engineers, ...!!

Mass and energy balances

- Mass balance: for each mass stream, each non-reacting species and each element of periodic table

  in + production = out + consumption + accumulation
- Energy balance: in = out + accumulation

  ! Steady state: accumulation = 0

  1st Law of Thermodynamics: "Energy production" or "energy consumption" not possible !

  2nd Law of Thermodynamics: Entropy production ≥ 0

$$\text{energy streams : heat } \dot{Q}\text{, power } P = \dot{W},$$
$$\text{kinetic energy } \tfrac{1}{2}\dot{m}v^2\text{, potential energy } \dot{m}zg,$$
$$\text{enthalpy } \dot{H} = \dot{m}h = \dot{m}(u + pv) = \dot{U} + p\dot{V}$$
$$\text{entropy streams : } \dot{S}_{mass} = \dot{m}s,\ \dot{S}_{heat} = \frac{\dot{Q}}{T}$$

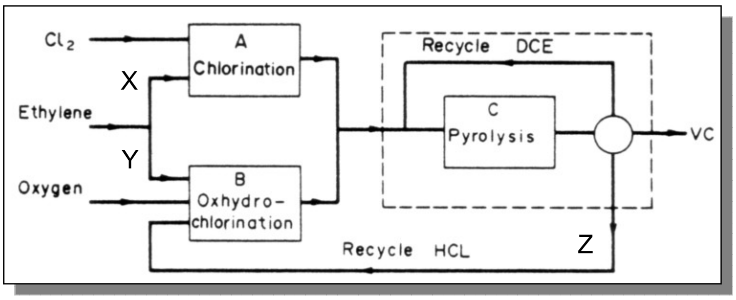
exothermic, fast chemistry* → *entropy production; high losses *especially at low temperatures**!***

Example: material balance vinyl chloride plant /1

- Production of vinyl chloride (VC, C_2H_3Cl) for polyvinyl chloride (PVC)
- Ethylene (ethene, $C_2^=$, C_2H_4) input is adjusted to balance the chlorination and oxychlorination processes

- Using the data → given, <u>calculate</u> flows (kmol/h) of $C_2^=$ to reactors A and B, and of dichloroethane (DCE) to reactor C, for 12500 kg/h VC production

Pictures: CR93



Block A, chlorination

$C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$, yield on ethylene 98 per cent

Block B, oxyhydrochlorination

$C_2H_4 + 2HCl + \tfrac{1}{2}O_2 \rightarrow C_2H_4Cl_2 + H_2O$, yields: on ethylene 95 per cent, on HCl 90 per cent

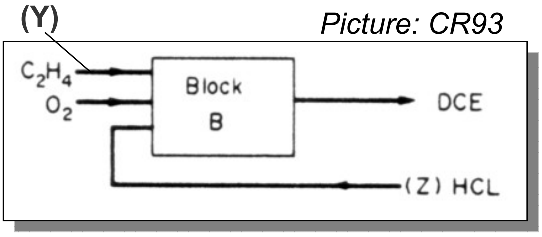
Block C, pyrolysis

$C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl$, yields: on DCE 99 per cent, on HCl 99·5 per cent

molar masses: HCl = 36.5 g/mol; VC = 62.5 g/mol; DCE = 99 g/mol

Example: material balance vinyl chloride plant /2

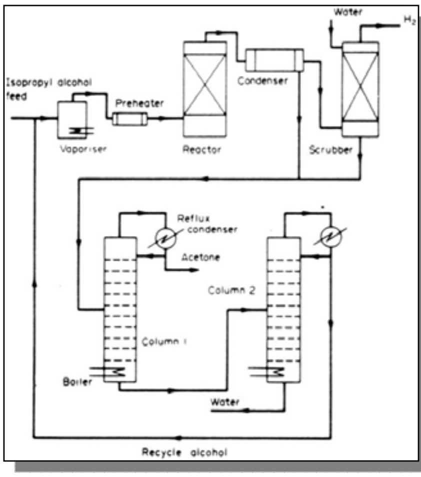
- 12500 kg/h VC production = 200 kmol/h
- With $C_2^=$ streams X into reactor A and Y into reactor B, and HCl recycle stream Z from reactor C: DCE production = 0.98·X+0.95·Y

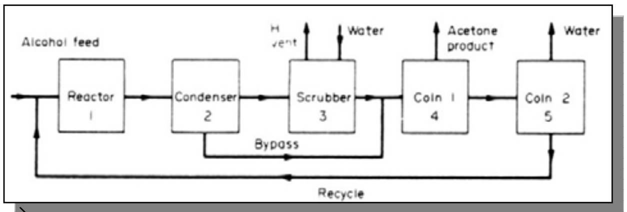


Picture: CR93

which is equal to HCl produced in C: Z = 0.995·(0.98·X+0.95·Y)   *)
- Based on HCl, the DCE yield is 90%: DCE produced in B = ½·0.9·Z
- Based on $C_2^=$ the DCE yield is 95%: DCE produced in B = 0.95·Y
  → this gives Z = 2·Y·0.95/0.9, substituted into *) gives Y = 0.837·X
- It is given that VC production = 99% of DCE production:
  → 0.99·(0.98·X+0.95·Y) = 200 kmol/h, with Y = 0.837·X gives finally : **X = 113.8 kmol/h; Y = 95.3 kmol/h, Z = 201.1 kmol/h**
- The overall VC yield based on $C_2^=$ is 200/(113.8+95.3) = 0.96 (96%)

Mass balances in matrix form /1

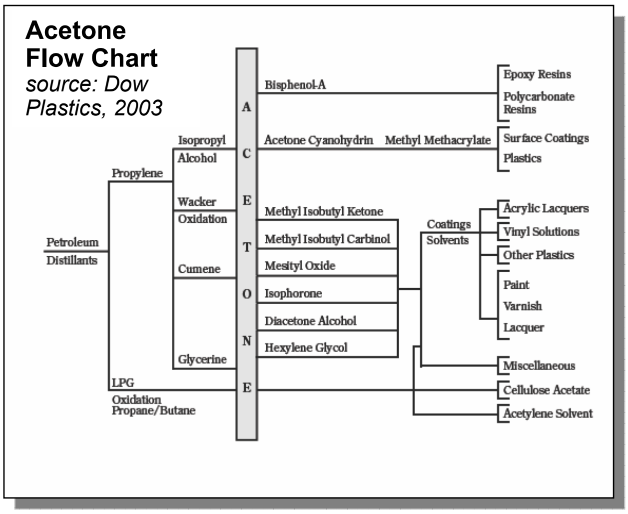




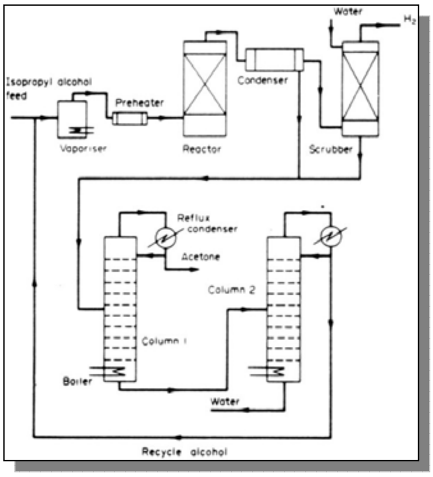
Pictures: CR93

Example: acetone production from isopropyl alcohol:

$C_3H_7OH \xrightarrow{+\ cat. +\ heat} (CH_3)_2CO + H_2$



Mass balances in matrix form /2

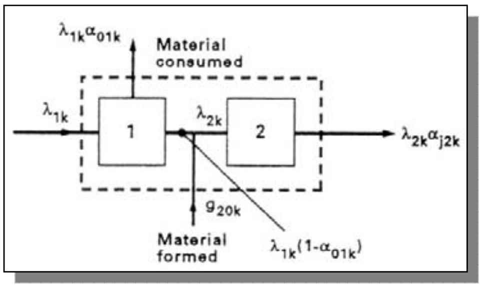


Example: acetone production from isopropyl alcohol:

$C_3H_7OH \xrightarrow{+\,cat. + \,heat} (CH_3)_2CO + H_2$

Pictures: CR93

For example, using split-fractions



Using so – called split - fractions in material balance equations :

i = unit number (-)

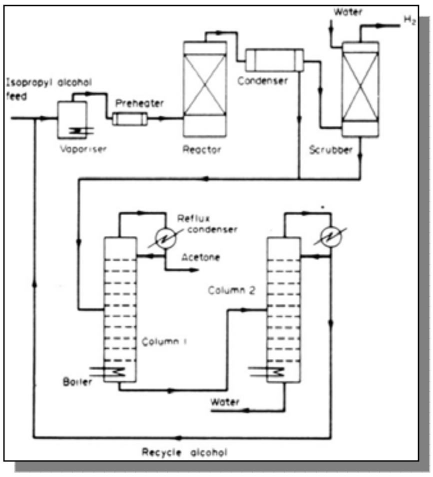
$\lambda_{i,k}$ = total flow of component k into unit i (mol/s or kg/s)

$\alpha_{j,i,k}$ = "split - fraction coefficient" = fraction of the flow of component k entering unit i, leaving into unit j (-)

$g_{i,0,k}$ = fresh feed of component k into unit i (mol/s or kg/s)

for example : flow of component k from i to j equals
$\lambda_{i,k} \cdot \alpha_{j,i,k}$ (mol/s or kg/s)

Mass balances in matrix form /3



Example: acetone production from isopropyl alcohol:

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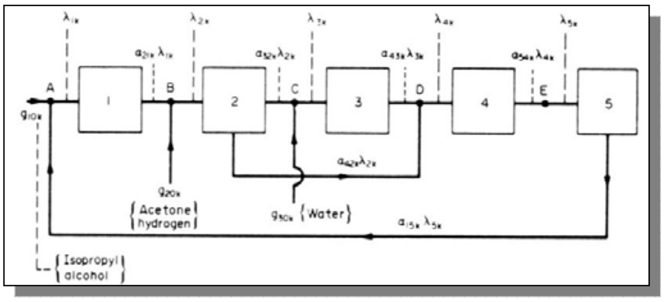
Pictures: CR93

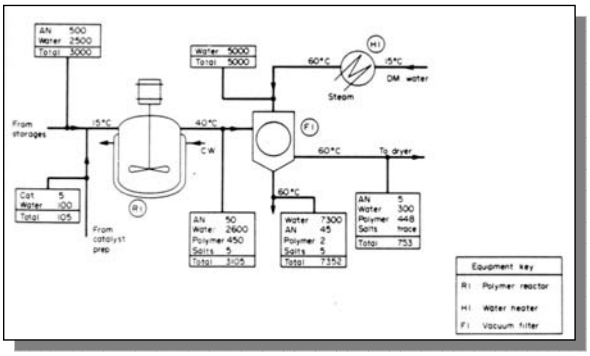


Flows, split-fractions and feeds

$$
\begin{array}{c|c}
 & i \rightarrow \quad 1 \qquad 2 \qquad 3 \qquad 4 \qquad 5 \\
j\downarrow & \\
\begin{array}{c}1\\2\\3\\4\\5\end{array} &
\begin{bmatrix}
1 & 0 & 0 & 0 & -\alpha_{15k} \\
-\alpha_{21k} & 1 & 0 & 0 & 0 \\
0 & -\alpha_{32k} & 1 & 0 & 0 \\
0 & -\alpha_{42k} & -\alpha_{43k} & 1 & 0 \\
0 & 0 & 0 & -\alpha_{54k} & 1
\end{bmatrix}
\times
\begin{bmatrix}
\lambda_{1k} \\ \lambda_{2k} \\ \lambda_{3k} \\ \lambda_{4k} \\ \lambda_{5k}
\end{bmatrix}
=
\begin{bmatrix}
g_{10k} \\ g_{20k} \\ g_{30k} \\ 0 \\ 0
\end{bmatrix}
\end{array}
$$

The set of equations for the system
e.g. $\lambda_{1k} - \alpha_{15k} \cdot \lambda_{5k} = g_{10k}$

Flow-sheeting, plant lay-out



An example flow-sheet for polymer production

Picture: CR93

- The process flow-sheet shows the equipment arrangement, stream connections, operating conditions, flow rates and often also compositions
- Based on the flow-sheet, the equipment, piping, instrumentation and plant *(sv: anläggning)* lay-out can be designed

Conceptual site lay-out of Shell/CNOOC at Nanhai (Guandong)

Picture: http://www.aitac.nl/plant/html/plantgallery.html

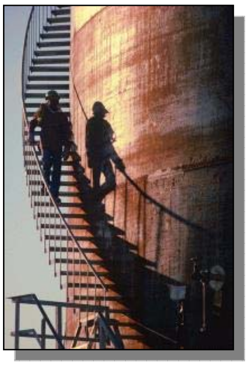
Process equipment /1

- Material transfer:
  - gases: compressors, blowers, fans
  - liquids: pumps
  - liquid/gas mixes: emulsion pumps
  - liquid/solid slurries: pumps, hydraulic conveying
  - solids: pneumatic conveying, mechanic conveying
- Raw material / product processing:
  - crushers, grinders, mixers, blenders, packaging
- Reactors: important aspects
  - phase contacting, mixing or plug flow, residence time distribution, batch or continuous, heat input or output, catalyst recovery, pressure

picture: http://www.materialanswers.com/fanalysis/reactor.htm

Process equipment /2

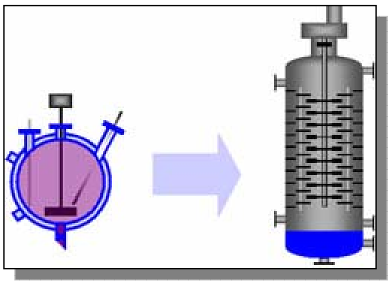
- Heat exchangers, condensers, evaporators, refrigerators, heat transfer networks (HENs)
- Furnaces, boilers, power utilities
- Separation & mixing processes:
  - distillation, absorption / desorption, extraction, ... in tray columns, packed tower columns, ...
  - devices for separating solids from liquids or gases
  - stirred vessels, other mixing and blending devices
- Process safety management
- Process control system

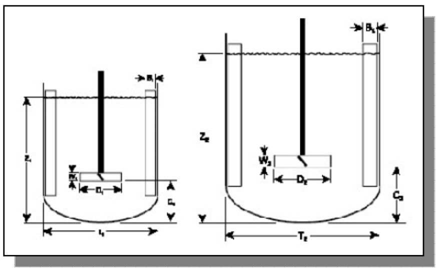


Picture:http://www.gdseng.com/services_process.asp

Scale-up

- Important: dimensional analysis and geometric similarity
  $Re_{labscale} = Re_{fullscale}$,
  height / diameter$_{labscale}$ = height / diameter$_{fullscale}$
  $\Delta p/(\tfrac{1}{2}\rho v^2)_{labscale} = \Delta p/(\tfrac{1}{2}\rho v^2)_{fullscale}$
  $Nu_{labscale} = Nu_{fullscale}$ etc. etc.
- Keep residence time constant !
- Constant power/volume, similar tip speed for mixers and impellers, ...
- Often scale-up involves non-geometric similarity !

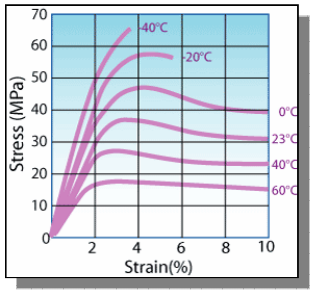




Picture: http://www.modular-process.com/pressrelease02.htm
Picture: http://www.chemicalprocessing.com/articles/2005/519.html

Materials and construction

- Temperature, pressure, material properties, weight, resistance to chemicals, durability, safety and cost requirements determine the choice of material:
  – iron, steel, alloys, ceramics, glass, plastics/polymers, wood
- Apparatus construction should resist and endure **static load and dynamic load:**
  – pull *(sv: drag)*, pressure *(sv: tryck)*, shear *(sv: skjuvning)*, turning *(sv: vridning)*, bending *(sv: böjning)*, breaking *(sv: knäckning)*

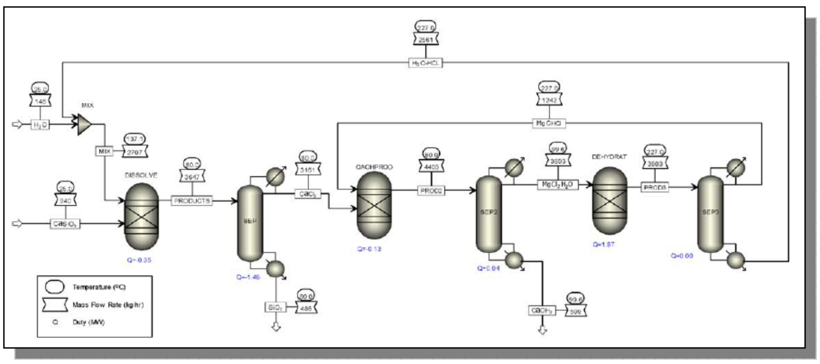


- Note: chemical engineer ≠ mechanical engineer !!
- *See courses Equipment Design I+II ("Apparatteknik I+II")*

Picture: http://www.omnexus.com/tc/mabs/index.aspx?id=mechanical

Process simulation

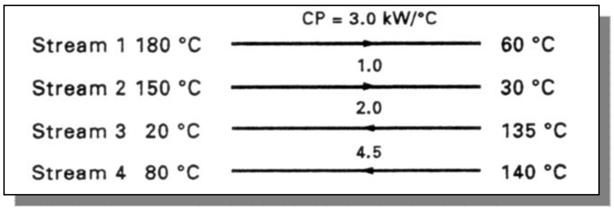
- Softwares such as *Aspen Plus, Process, GateCycle* (for power plants) and many others can be used to simulate complete chemical processing systems
- Based on simultaneously solving mass balances and energy balances, using stoichiometry data or Gibbs' energy minimisation to calculate reactor product composition
- Non-stationary and transient behaviour gives information on process dynamics



Aspen Plus model for $Ca(OH)_2$ production from $CaSiO_3$
(from S. Teir, TkL thesis TKK 2006)

Process integration, pinch /1

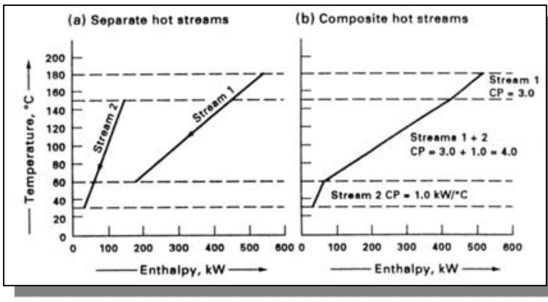
- Process integration deals primarily with **process energy** and **efficient design of heat exchanger networks (HENs)**
- Important for the system is the so-called **pinch point**; heat should not be ”transferred across the pinch”
- Combining the hot streams and cold streams of a system into two composite curves (temperature versus enthalpy) shows the minimum temperature: **the pinch**
- The pinch divides the system in two ”regions”



Example process with two hot streams to be cooled and two cold streams to be heated up.
CP = stream heat capacity = $\dot{m} \cdot c_p$ (W/°C) with c_p averaged between T_{in} and T_{out}

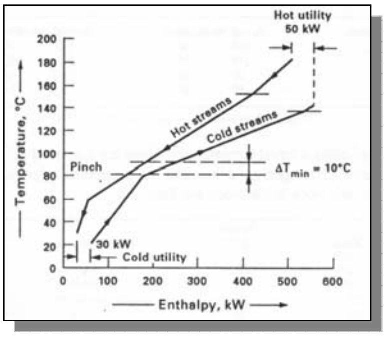
Picture: CR93

Process integration, pinch /2

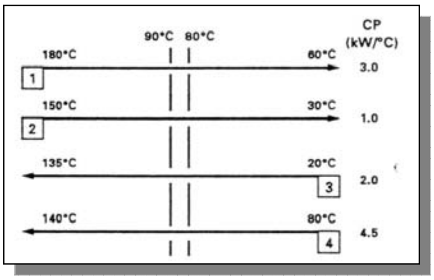


↑ Hot stream temperatures versus enthalphy

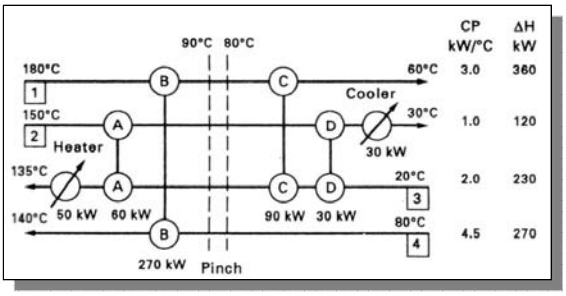
For the example on previous slide



Hot and cold stream **composite curves** ↑



↑ Grid for the four-stream network



Proposed heat exchanger network for ΔT_{min} = 10 K ↑

Pictures: CR93

Process optimisation

- Process optimisation mainly involves
  - Parameter/variable optimisation → optimal process conditions
  - Structural optimisation → the optimal process design for a given objective, usually max \$, €, ¥, £, … *i.e.* profit)
- A process design can be optimised by giving the possible process units a digit (existing = 1, non-existing = 0), besides the balance equations for mass and energy, using concentrations, volumes, temperature, pressure, ... (and time, if necessary)
- This gives a mixed integer non-linear programming (MINLP) problem that can be solved using (for example) an alternating procedure based on mixed integer linear programming (MILP) and non-linear programming (NLP)

See also W98 chapter 7 & TkF VT course 424500 "Optimization"

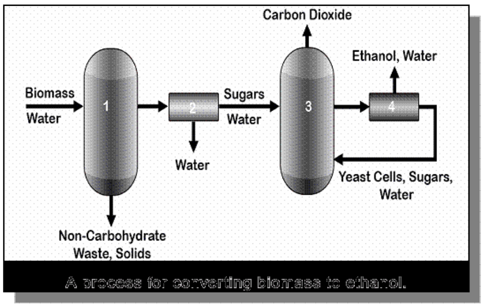
8.2 Biotechnology

See also courses offered by

Laboratory for Process Design *("Anläggningsteknik")*
and the
Laboratory for Heat Engineering *("Varmeteknik")*

Biotechnology: products

- Typical products from biotechnology
  - Cell biomass: yeast, single-cell protein, ...
  - Products of cell metabolism:
    - *Anaerobic: alcohols, organic acids, H_2, CO_2, ...*
    - *Aerobic: citrate, glutamate, lactate, antibiotics, hydrocarbons, polysaccharides, ...*
  - Products of reactions catalysed by enzymes: can be virtually anything ...



Picture:http://www.esd.ornl.gov/research/earth_sciences/water_treatment.shtml

Source: MMD01

Biotechnology – some issues

- Important applications: beer and wine production, more recently (waste) water treatment and production of medicine and drugs
- For its growth, a micro-organism needs energy, a **substrate** based on (organic) carbon, plus nitrogen, minerals, trace elements, vitamins, ...
- The micro-organism itself should be looked at as a reactor, with **enzymes** as the catalysts
- **Bio-reactors are usually batch or semi-batch (”fed-batch”) processes,** sometimes continuous
- (Semi-)batch processes have drawbacks (dead time, loading, unloading, sterilizing, ...) but allow for better process control
- Continuous processes have the risks of contaminations, mutations, and usually production volumes are too small. Also, continuous processing up-stream and down-stream may be difficult
- **Membrane technology** may make bio-processes more continuous in the future

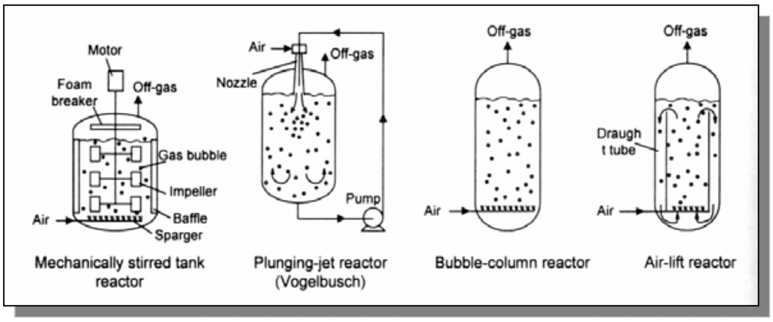
Picture: http://www.nationalaglawcenter.org/graphics/contentphoto_biotechnology.jpg

Source: MMD01

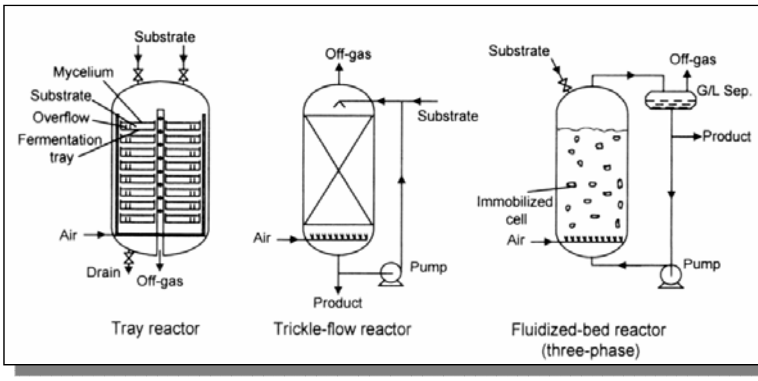
Bioreactors

pictures: MMD01

- Most bioreactors are multi-phase reactors
- The main distinction is how **contacting** between micro-organisms, substrate and (if aerobic) air is done
- In **submerged reactors** the micro-organisms are dispersed; in **surface reactors** they adhere to a solid surface or float on the substrate



↑ Submerged reactors ↓ Surface reactors



8.3 Process dynamics and control

See courses offered by
Laboratory for Process Control *("Reglerteknik")*
and by the
Department of Information Technologies
("Datateknik" avdelningen)

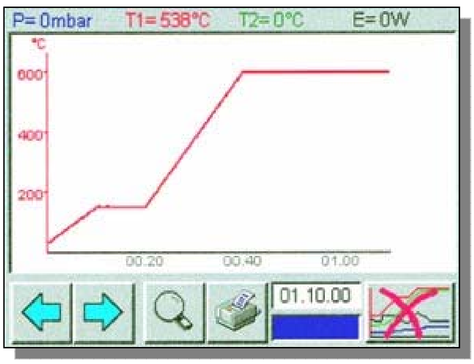
The role of process control

- Operation of (chemical) processing units should
  - Be **safe**, without risk to people's health, the environment or process equipment
  - Produce **product amounts** according to (market) requirements
  - Produce products according to **quality** specifications
- These three objectives are correlated: changing one results in changes for the other two
- Many processes, especially chemical processes, are **dynamic**: their variables change with time
- In order to maintain safe operation according to the objectives:
  - **selected variables are monitored**, and
  - based on the monitoring data, **changes can be made** to process operation
- This is referred to as **process control**

Picture: http://www.hsl.gov.uk/images/process.jpg

Process dynamics and control

- Process dynamics and control can be defined as: *"that aspect of chemical engineering concerned with the analysis, design and implementation of control systems that facilitate the achievement of specified objectives of safety, production rates and product quality" (OR94)*

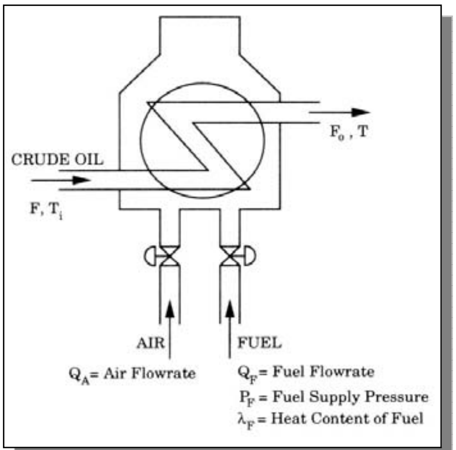


Picture: http://www.milestonesci.com/images/EasyControl2.jpg
Picture: http://www.ascoffanscuff.com/iocc/process/process01.html

Example 1: crude oil preheater furnace /1

- A furnace is used to **preheat crude oil** for fractionation in a refinery
- In: oil temperature T_i, flow F
- In: fuel flow Q_F, pressure P_F, heat content λ_F, air flow Q_A
- Out: temperature T, flow F_0
- Goal: temperature out T* and flow F_0
- Constraint: furnace tube temperature should be < T_{max}
- Problem: the heating fuel comes from the refinery downstream, therefore supply pressure and heat content vary

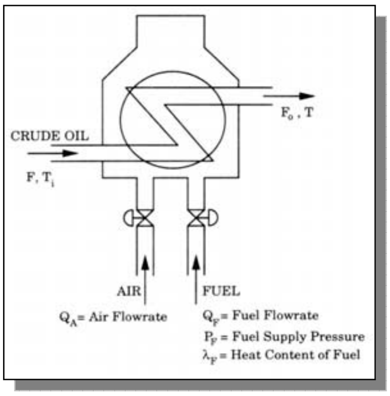
Set-point, changes from time to time

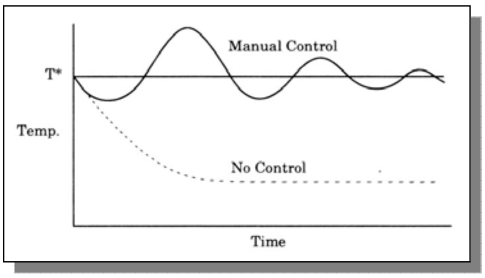


Picture: OR94

Example 1: crude oil preheater furnace /2

- Instrumentation:
  Thermocouples for T_i and T,
  + flow meters for F and Q_F,
  + control valves for fuel & air,
  + measurement of furnace tube temperature
- Manual control by the operator gives results that are not good enough, the Figure → shows the response to a step increase in the feedrate F
- **A (better) process control system is needed.**





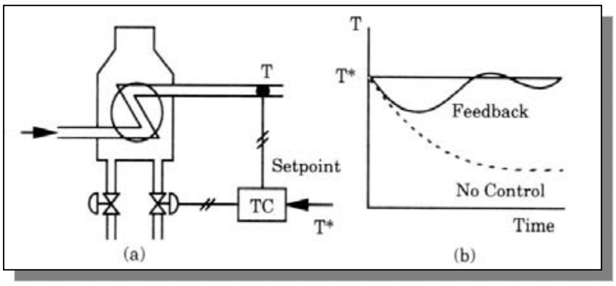
Pictures: OR94

Example 1: crude oil preheater furnace /3

- **Control system 1:**

  A feedback system based on a temperature controller (TC) at the crude oil outlet

  Result: sometimes too much of low temperature crude oil output for a long time



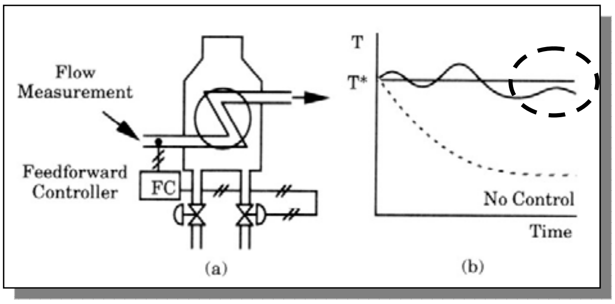
Picture: OR94

Example 1: crude oil preheater furnace /4

- **Control system 2:**

  A feedforward system based on a flow controller (FC) at the crude oil inlet

  Result: a different steady-state than the set-point T*, = ”offset”

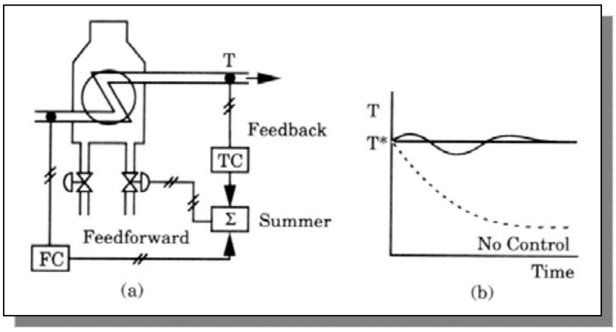


Pictures: OR94

Example 1: crude oil preheater furnace /5

- **Control system 3:**
  A feedforward system based on a flow controller (FC) at the crude oil inlet
  + feedback system based on a temperature controller (TC) at crude oil outlet

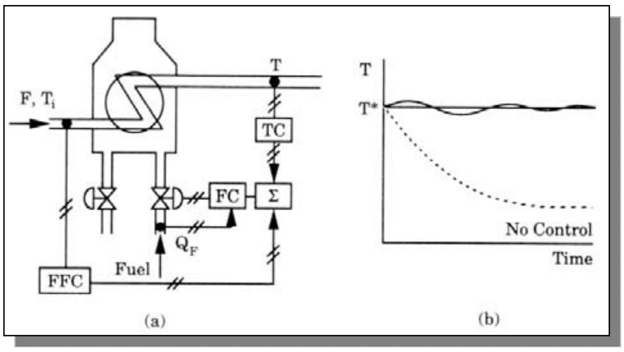
  Result: still sometimes unacceptable fluctuations in T
  (due to fuel pressure and quality variations)



Picture: OR94

Example 1: crude oil preheater furnace /6

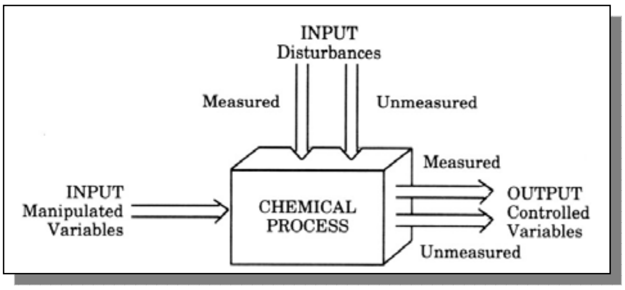
- **Control system 4:**
  Feedforward system based on FC at crude oil inlet
  + feedback system based on TC at crude oil outlet
  + flow controller between temperature controller and flow control valve for fuel flow Q_F : ”inner loop”



Picture: OR94

Process variables

- **Input variables** can independently change the internal state of the process:
  - Those that can be manipulated freely are **control variables**
  - Those that cannot be manipulated freely are **disturbance variables**
- **Output variables** give information about the internal state of the process
- Some input / output variables can be measured on-line, others cannot

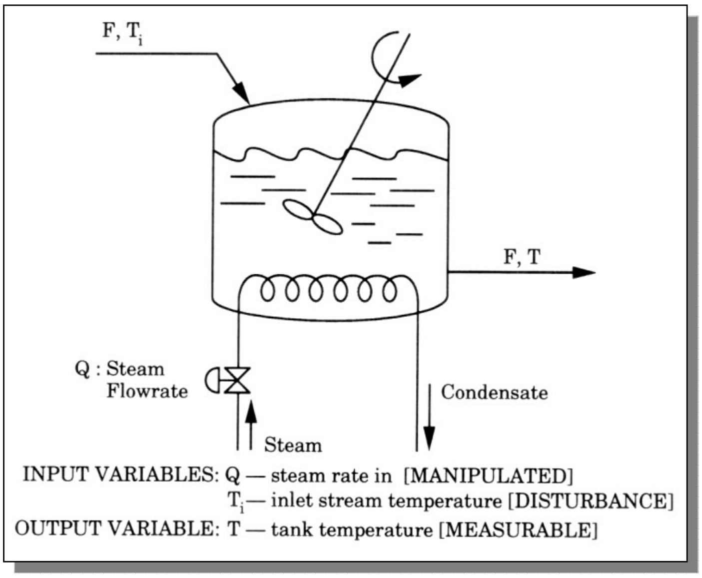


- **State variables** are the minimum set of variables that completely describe the internal state of the process

Picture: OR94

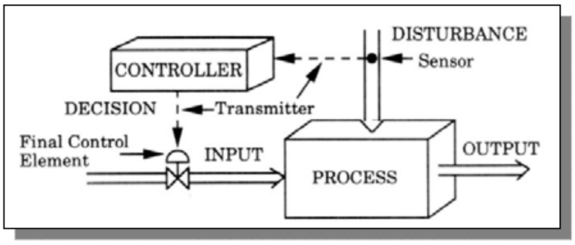
Example 2: stirred heating tank process

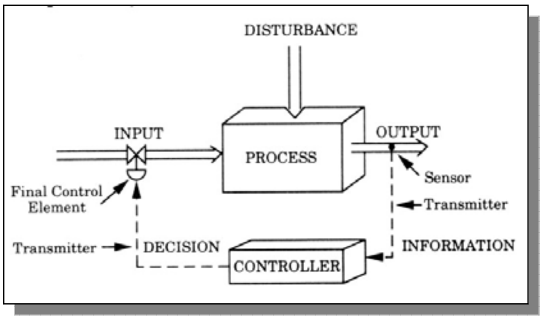
- The temperature T of the liquid in the tank must be regulated
- Incoming liquid temperature T_i fluctuates
- Steam flowrate Q can be manipulated

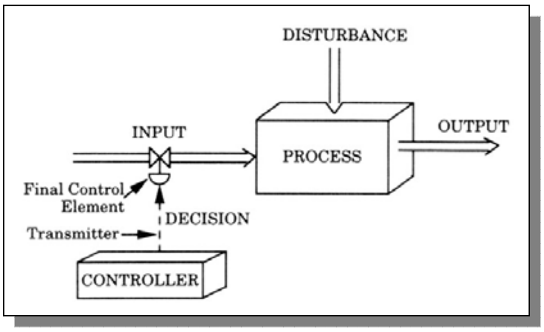


Picture: OR94

Control systems







Showing also sensors, controllers, transmitters and other control elements

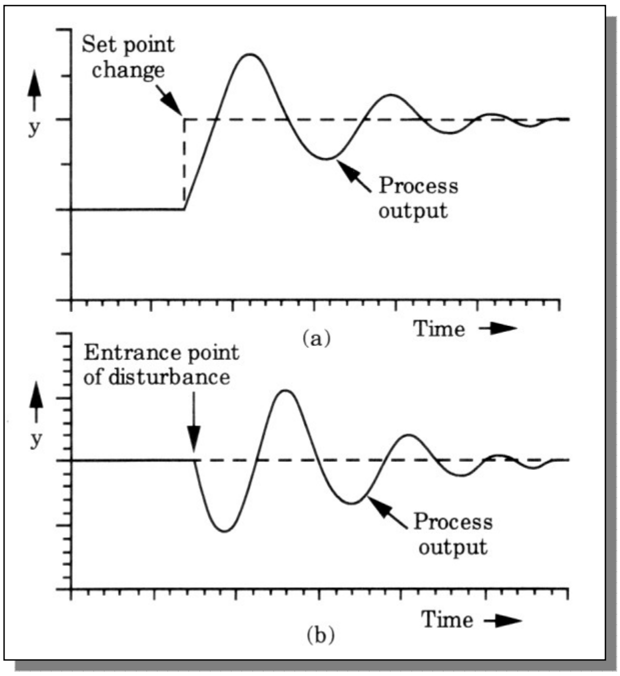
- Feedback control ↗
- Feedforward control ↑
- Open loop control → *(not based on measurement data from the process !)*

Pictures: OR94

Regulatory or servo control

For control systems that must maintain a set-point:

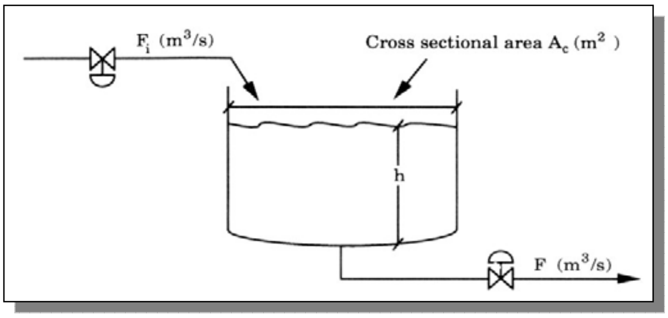
- In servo control systems the output is used to track a changing set-point → Figure (a)
- Regulatory control systems counteract the effect of disturbances → Figure (b)



Picture: OR94

Example 3: A liquid receiver tank /1

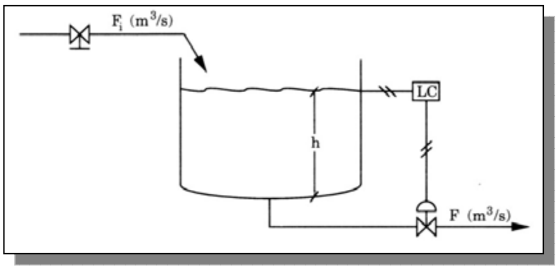
- Liquid inflow F_i, (different) outflow F
- Constant cross-sectional area A_c
- Control valves at inlet and outlet
- Measurement devices for liquid level + for in- and outflow
- <u>Objective</u>: a constant liquid level



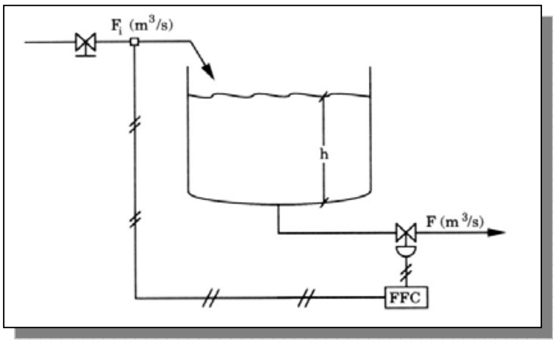
Picture: OR94

Example 3: A liquid receiver tank /2

- **Configuration 1**
  Feedback: outflow regulates the liquid level



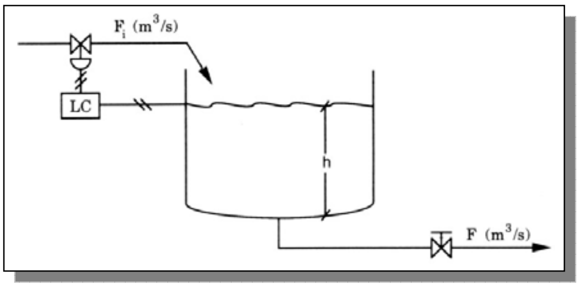
- **Configuration 2**
  Feedforward: outflow, controlled by the inflow, regulates the liquid level



Picture: OR94

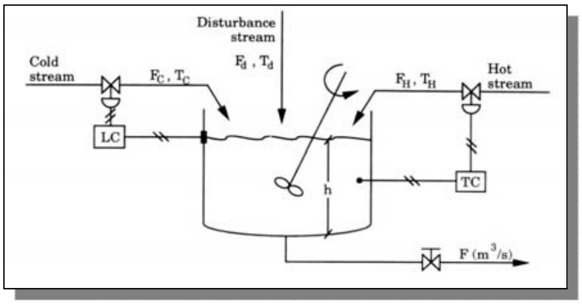
Example 3: A liquid receiver tank /3

- **Configuration 3**
  Liquid flows out by gravity, valve for F in fixed position (i.e. rate F is controlled by liquid level !) and inlet flow regulates the liquid level



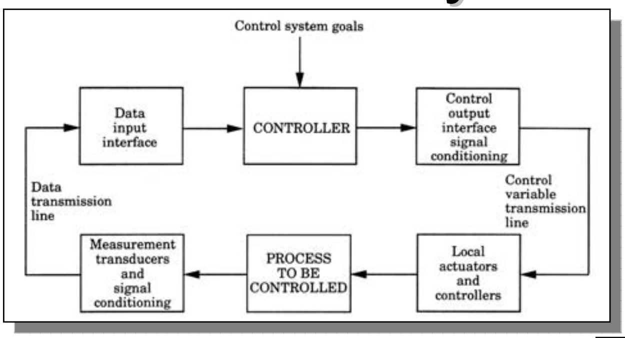
- **Configuration 4**
  Dual control system for liquid level +temperature

  The liquid level controller will always interfere with liquid temperature and its controller

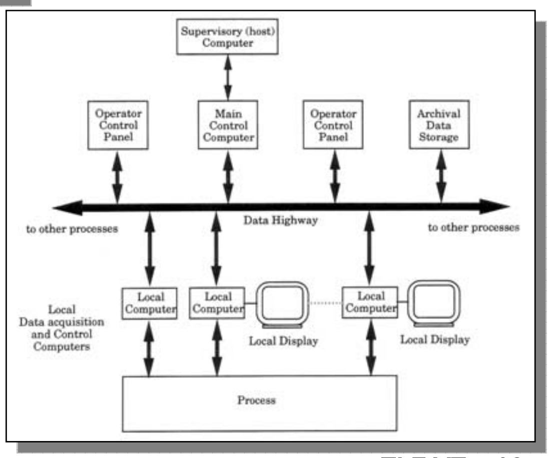


Picture: OR94

Control system structure

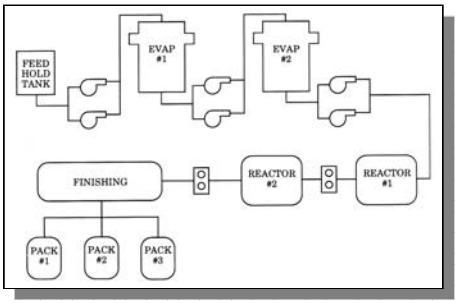


Pictures: OR94



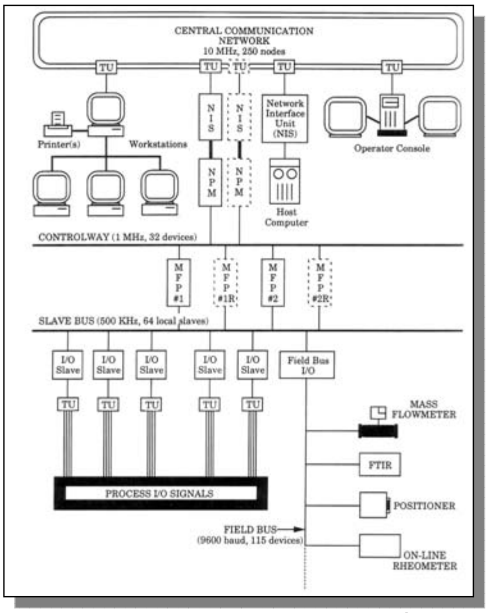
Typical elements of a commercial distributed control system (DCS) network

Distributed control system example

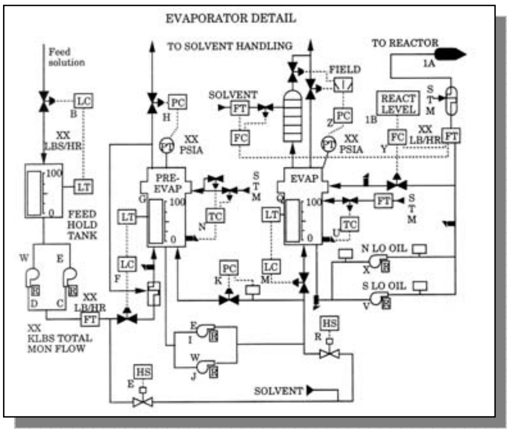


DCS for the evaporation section of a plastics manufacturing process

Commercial DCS network

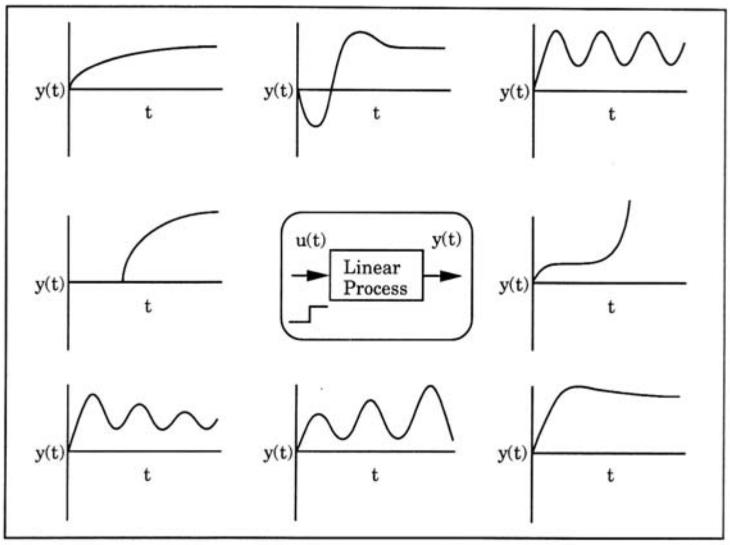


Graphic display



Pictures: OR94

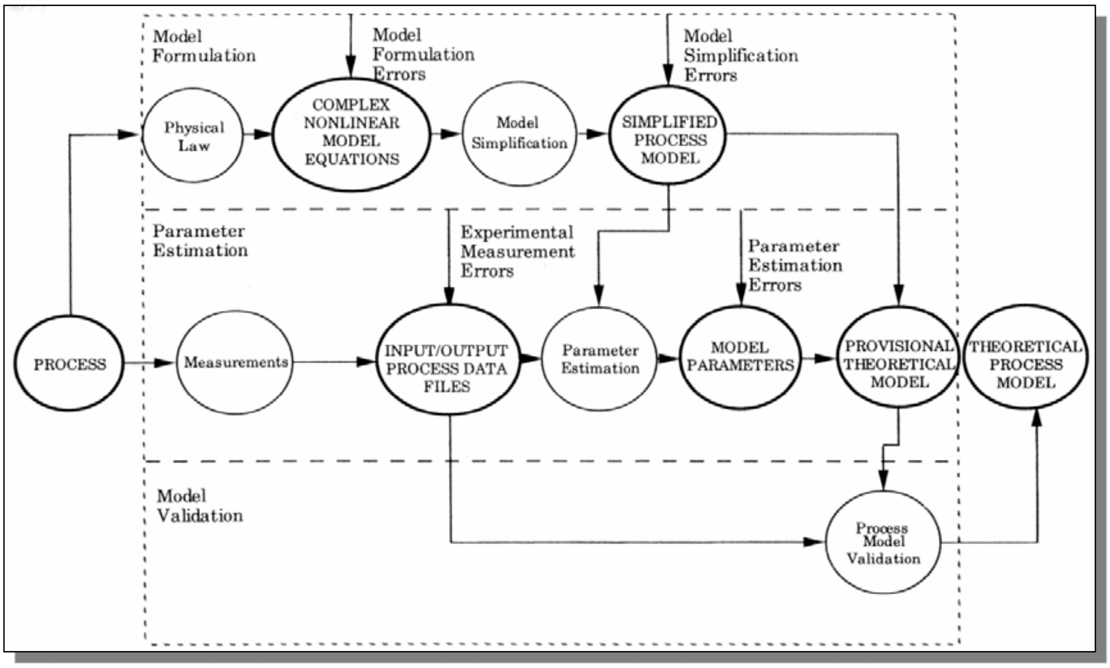
Process dynamics



Dynamics responses of a linear system to a step change in the input

Picture: OR94

Theoretical process modelling



Picture: OR94

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- W98: Westerlund, T. ”Anläggnings- och apparatteknik” Åbo Akademi Univesity (1998)

Picture: http://www.chemeng.ed.ac.uk/~jwp/headstart/