

Continuous Optimization

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Lesson 6 of "Process Systems Engineering" – Master Degree in Chemical Engineering – Politecnico di Milano



Optimization

- There are at least three distinct fields that characterize the optimization of industrial processes
 - **Management**
 - Project assessment
 - Selecting the optimal product
 - Deciding whether to invest in research or in production
 - Investment in new plants
 - Supervision of multiple production sites
 - **Design**
 - Process design and Equipment design
 - Equipment specifications
 - Nominal operating conditions
 - **Operation**
 - Plant operation
 - Process control
 - Use of raw materials
 - Minimizing energy consumption
 - Logistics (storage, shipping, transport) → Supply Chain Management



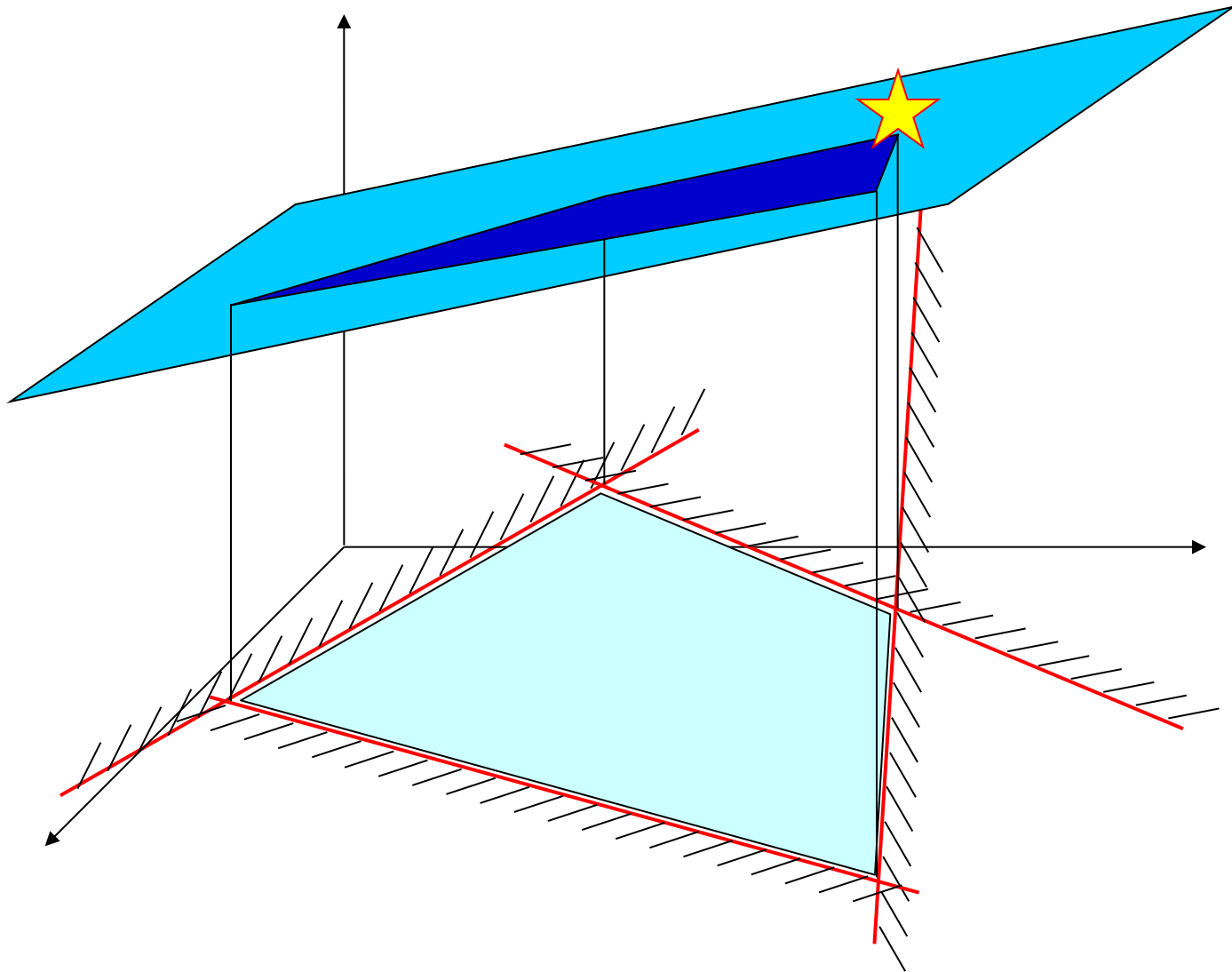
Definition

- The optimization problem is characterized by:
 - Objective function
 - Equality constraints (optional)
 - Inequality constraints (optional)
- The constraints may be:
 - Linear
 - Nonlinear
 - Violable
 - Not violable
 - Real constraints
 - Lower and upper bounds of the degrees of freedom
- The optimization variables are defined as: degrees of freedom (dof)

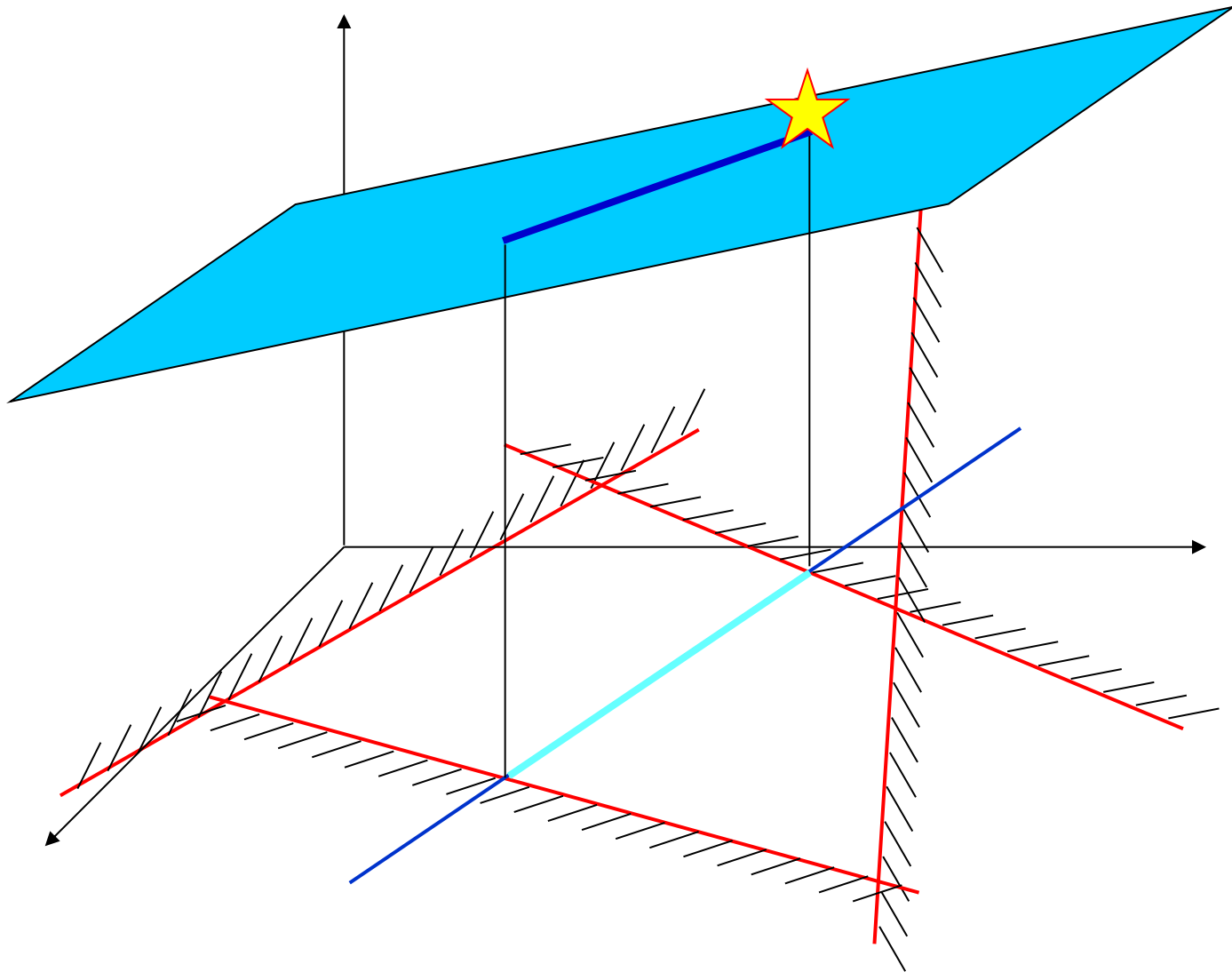


- Mathematically we have:
- $$\begin{cases} \text{Min}_{\mathbf{x}} & f(\mathbf{x}) \\ \text{s.t.} & \mathbf{h}(\mathbf{x}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{x}) \leq \mathbf{0} \end{cases}$$

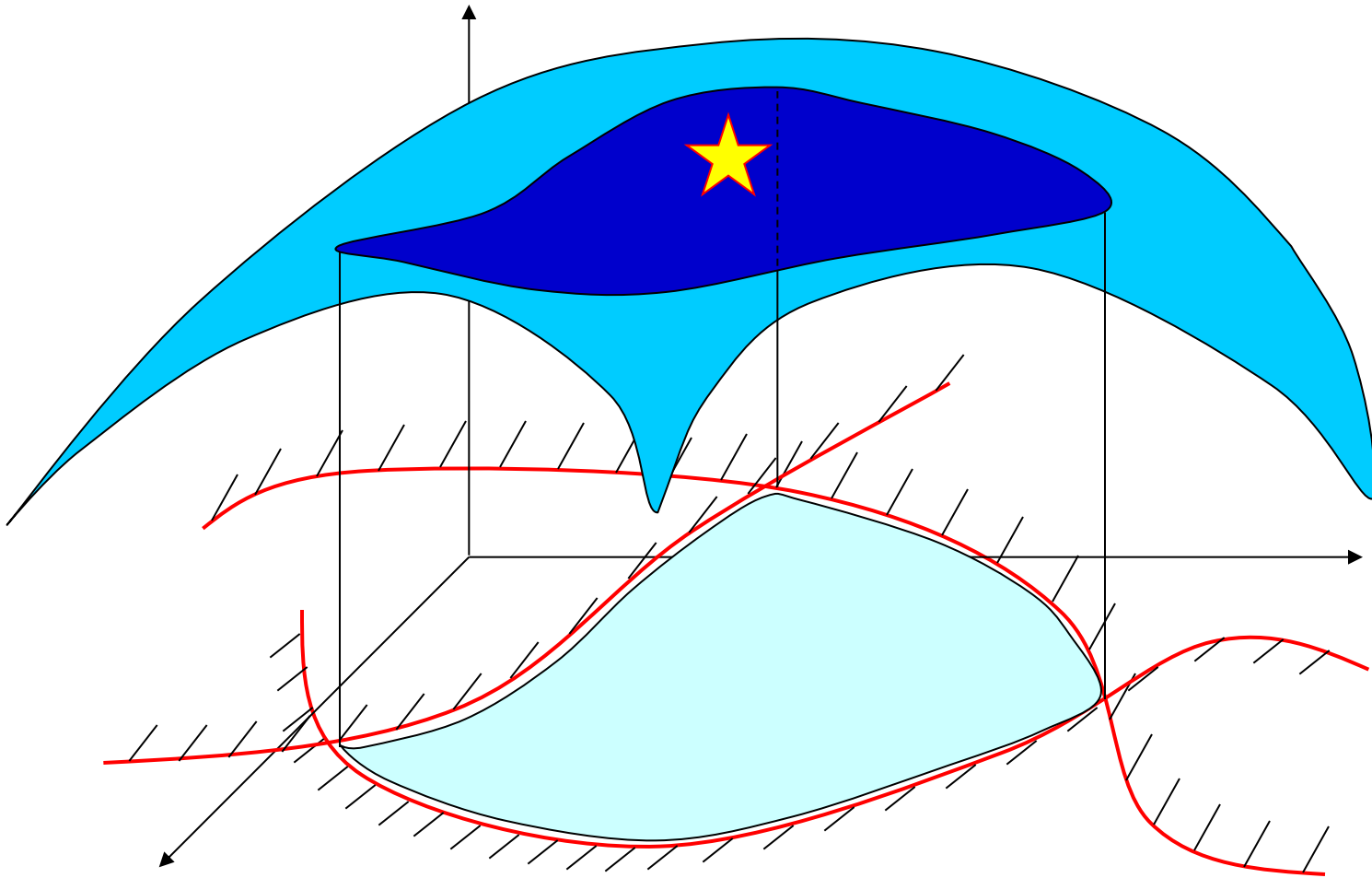
Linear function and constraints



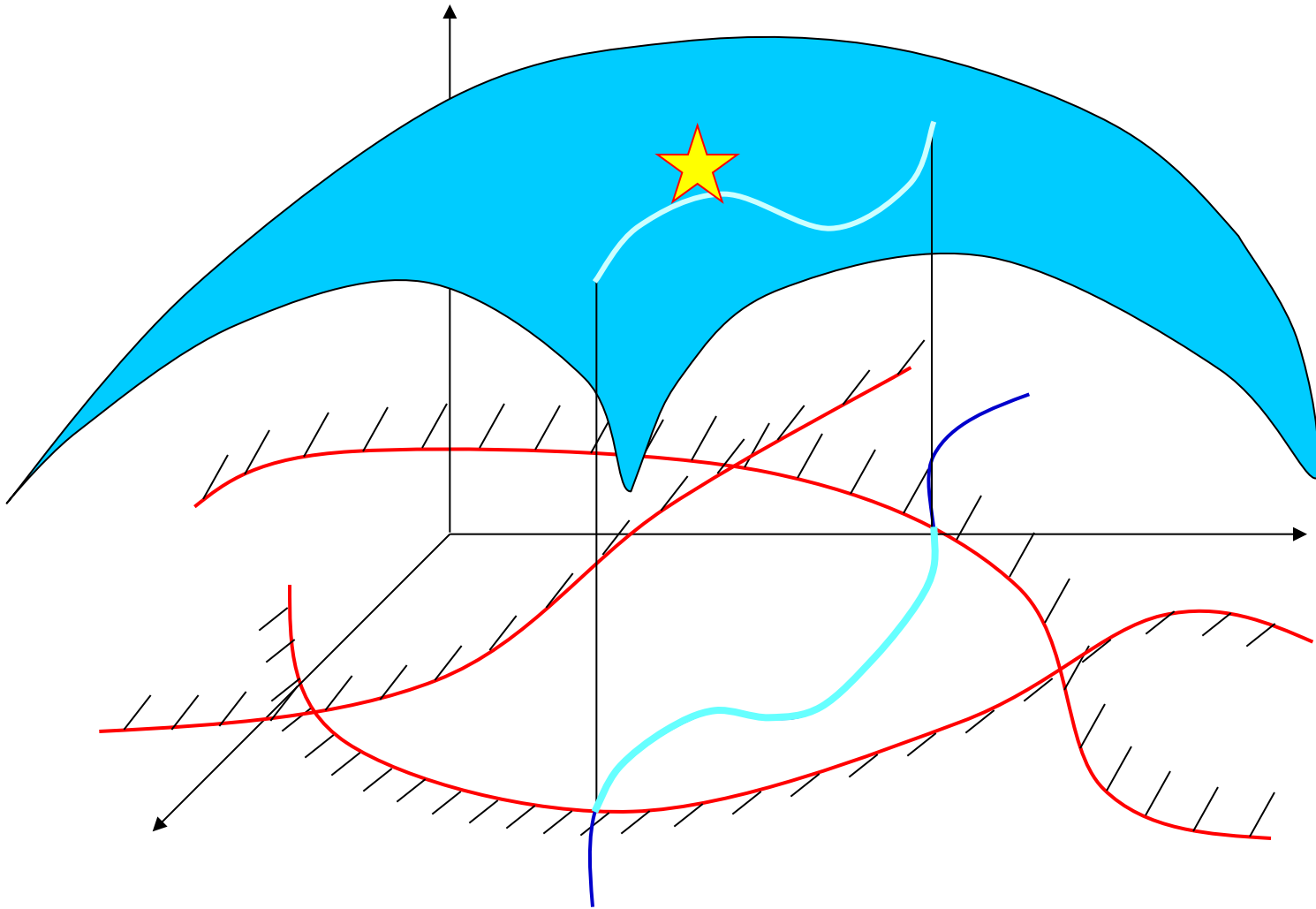
Linear function and constraints



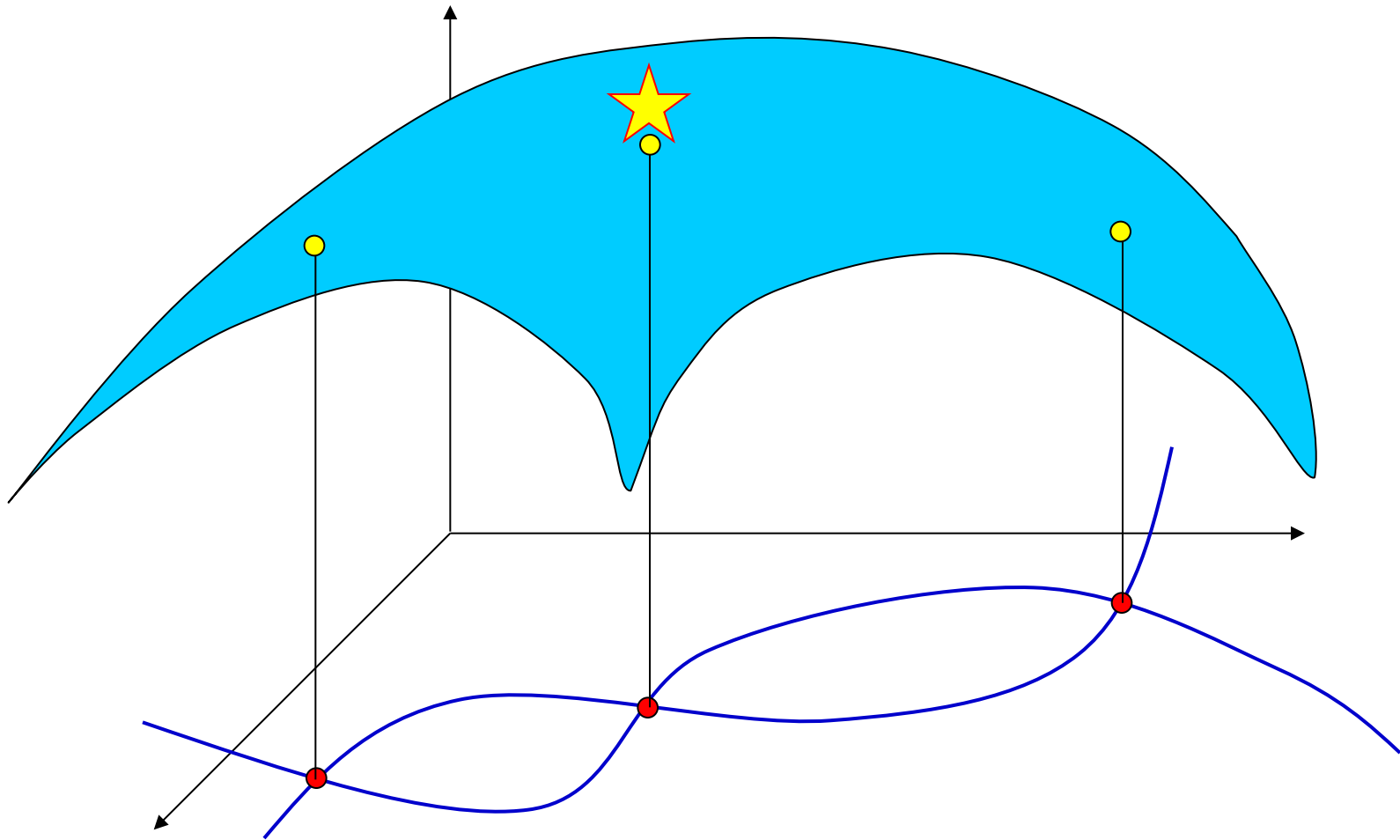
Nonlinear function and constraints



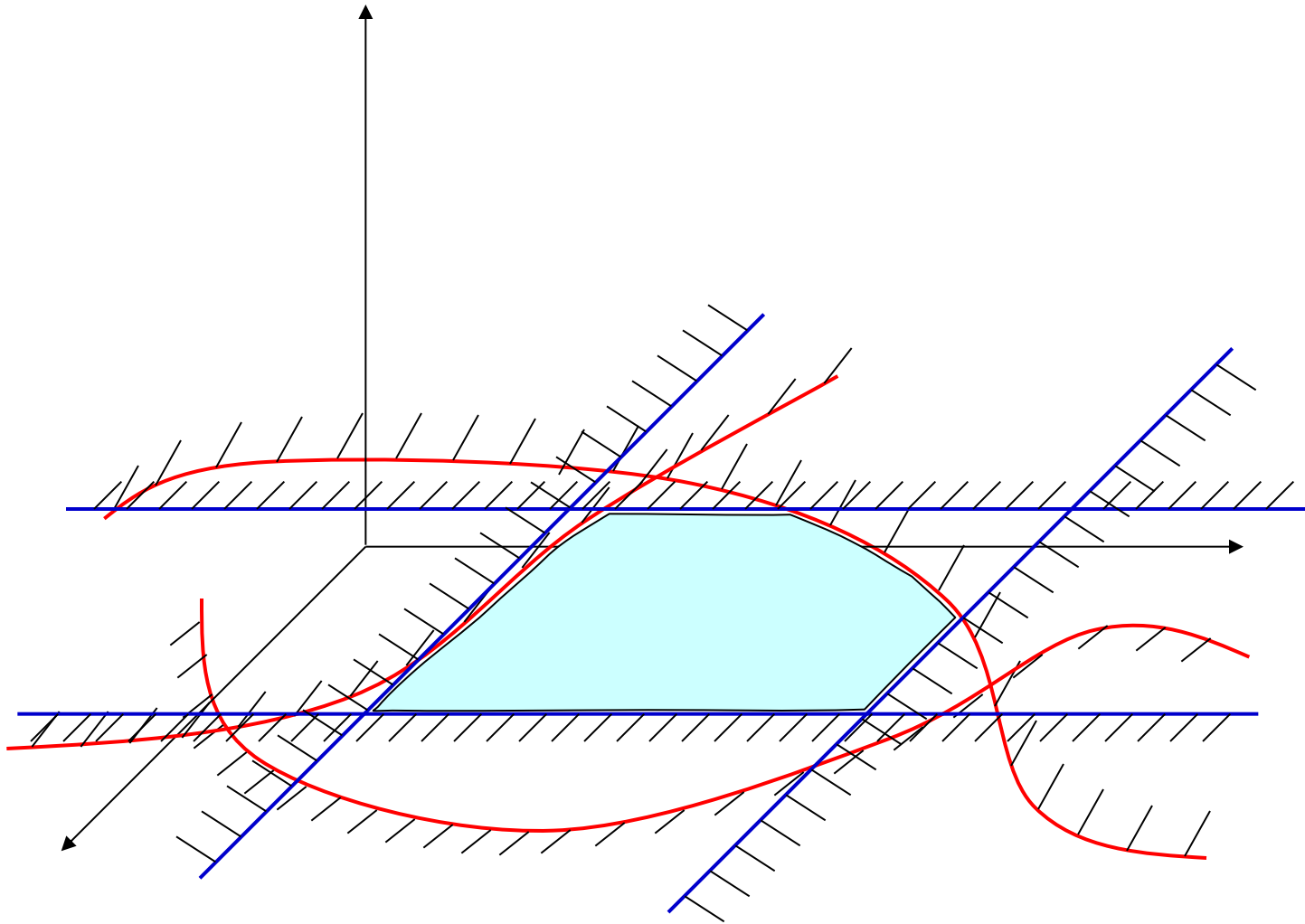
Nonlinear function and constraints



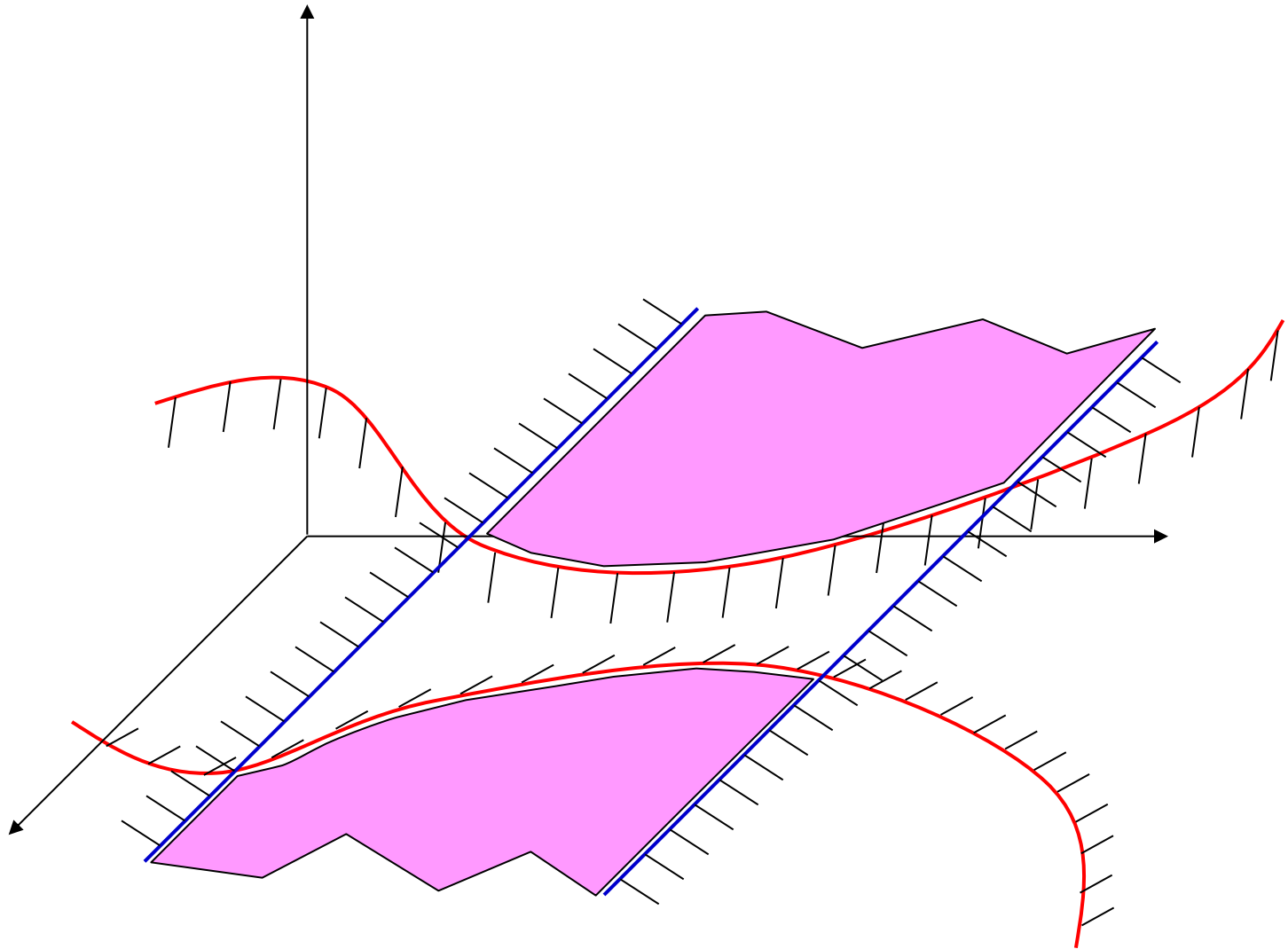
Nonlinear function and constraints



Nonlinear constraints + lower/upper bounds



Infeasible region



Constraints

- The equality and inequality constraints may also include the model of the process to be optimized and the law limits, process specifications and degrees of freedom.
- The constraints identify a “feasibility” area where the degrees of freedom can be modified to look for the optimum.
- The constraints have to be consistent in order to define a “feasible” searching area.
- There is no theoretical limit to the number of inequality constraints.
- If the number of equality constraints is equal to the number of degrees of freedom the only solution is with the optimal point. If there are multiple solutions of the nonlinear system, in order to obtain the absolute optimum, we will need to identify all the solutions and evaluate the objective function at each point, and eventually selecting the point that produces the best result.

Constraints

- If there are **more variables than equality constraints** then the problem is **UNDERDETERMINED** and we must proceed to the **effective search** of the **optimum point** of the objective function.
- If there are **more equality constraints than degrees of freedom** then the problem is **OVERDETERMINED** and there is NOT a solution that satisfies all the constraints. This is a typical example of **data reconciliation**.

Features

- If both the objective function and constraints are linear, the problem is called LINEAR PROGRAMMING (LP)
- If the objective function and/or the constraints are NOT linear with respect to the degrees of freedom, the problem is called NOT linear (NLP)
- A NLP is more complicated than a LP
- A LP has a unique solution only if it is feasible
- A NLP may have multiple local minima
- The research for the absolute optimum can be quite complicated
- Often we are NOT interested in the absolute optimum, especially if we are performing an online process optimization
- The research of the optimum point is influenced by the possible discontinuities of the objective function and/or constraints
- If there is a functional dependency among the *dof*, the optimization is strongly affected and the numerical method can fail. For example:

$$f_{obj}(x_1, x_2) = 3x_1^3 \sqrt{x_2}$$

Structure of the objective function

- Usually the objective function is based on an **economic assessment** of the involved problem. For instance:

$$\Sigma(\text{revenues} - \text{costs}),$$

- Also, the objective function may be based on **other criteria** such as:
 - pollutant minimization,
 - conversion maximization,
 - yield, reliability, response time, efficiency,
 - energy production
 - environmental impact
- With reference to the process, if we consider only the operating costs and the investment costs are neglected, then we have to solve the so called SUPERVISION problems (also CONTROL in SUPERVISION)

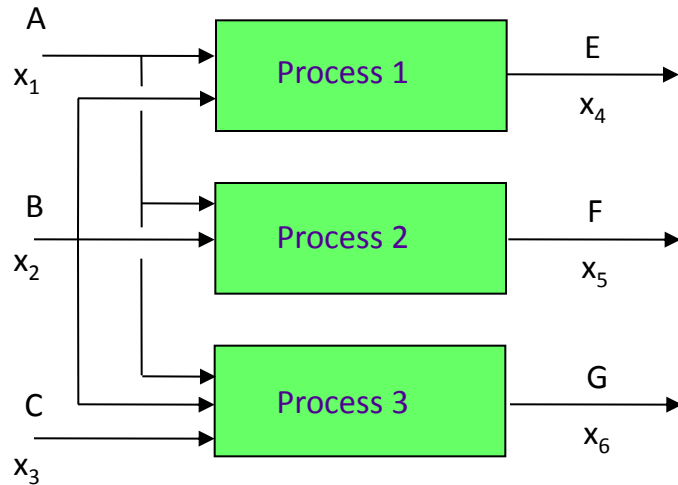
Structure of the objective function

- If we consider both operating and investment costs then we fall in the field of *“Conceptual Design”* and *“Dynamic Conceptual Design”*.
- Since in CD and DCD the CAPEX terms [€] and OPEX terms [€/y] are not directly comparable (due to the different units of measure) a suitable comparison basis must be found. This can be the discounted back approach together with the annualized approach to CAPEX assessment where the depreciation period allows transforming the CAPEX contribution from [€] into [€/y].

Introductory examples



Example #1: Operating profit



- PROCESS DATA**
- 1) $A + B \rightarrow E$
 - 2) $A + B \rightarrow F$
 - 3) $3A + 2B + C \rightarrow G$

RAW MATERIALS		
Component	Availability kg/d	Cost €/kg
A	40,000	1.5
B	30,000	2.0
C	25,000	2.5

PRODUCTS				
Process	Product	Reactant required for [kg] of product	Processing costs	Selling price
1	E	2/3 A, 1/3 B	1.5 €/kg E	4.0 €/kg E
2	F	2/3 A, 1/3 B	0.5 €/kg F	3.3 €/kg F
3	G	1/2 A, 1/6 B, 1/3 C	1.0 €/kg G	3.8 €/kg G

Example #1: Operating profit

Statement: We want to find the maximum daily profit.

The *dof* are the flowrates of the single components [kg/d]

- Profit from selling the products [€/d]

$$4x_4 + 3.3x_5 + 3.8x_6$$

- Cost of raw materials [€/d]

$$1.5x_1 + 2.0x_2 + 2.5x_3$$

- Operating costs [€/d]

$$1.5x_4 + 0.5x_5 + 1.0x_6$$

- Objective function

$$\begin{aligned} f(x) &= 4x_4 + 3.3x_5 + 3.8x_6 - 1.5x_1 - 2.0x_2 - 2.5x_3 - 1.5x_4 - 0.5x_5 + \\ &\quad - 1.0x_6 = 2.5x_4 - 2.8x_5 + 2.8x_6 - 1.5x_1 - 2x_2 - 2.5x_3 \end{aligned}$$

- Constraints on material balances

$$x_1 = 2/3 x_4 + 2/3 x_5 + 1/2 x_6$$

$$x_2 = 1/3 x_4 + 1/3 x_5 + 1/6 x_6$$

$$x_3 = 1/3 x_6$$

Example #1: Operating profit

- Upper & lower limits on the *dof*

$$0 \leq x_1 \leq 40,000$$

$$0 \leq x_2 \leq 30,000$$

$$0 \leq x_3 \leq 25,000$$

- The problem is LINEAR in the objective function and constraints.
- We use LINEAR PROGRAMMING techniques (*e.g.*, the simplex method) to solve the optimization problem. Since the objective function is a hyperplane with a research area bounded by hyper-lines (*i.e.* equality and inequality linear constraints) the optimal solution is on the intersection of constraints and more specifically of equality constraints.

Example #2: Investment costs

Statement:

We want to determine the optimal ratio, L/D , for a given cylindrical pressurized vessel with a given volume, V .

Hypotheses:

The extremities are closed and flat.

Constant wall thickness t .

The thickness t does not depend on the pressure.

The density ρ of the metal does not depend on the pressure.

Manufacturing costs M [€/kg] are equal for both the side walls and the bottoms.

There are not any production scraps

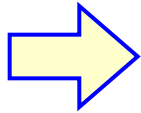
Unrolling:
$$S_{tot} = 2\left(\frac{\pi D^2}{4}\right) + \pi DL = \frac{\pi D^2}{2} + \pi DL$$

We can write three equivalent objective functions:

$$\begin{cases} f_1 = \frac{\pi D^2}{2} + \pi DL \\ f_2 = \rho \left(\frac{\pi D^2}{2} + \pi DL \right) t \\ f_3 = M \rho \left(\frac{\pi D^2}{2} + \pi DL \right) t \end{cases}$$

Example #2: Investment costs

By using the specification on the volume V : $f_1 = \frac{\pi D^2}{2} + \pi D \frac{4V}{\pi D^2} = \frac{\pi D^2}{2} + \frac{4V}{D}$

By differentiating we obtain: $\frac{df_1}{dD} = \pi D - \frac{4V}{D^2} = 0$  $D_{opt} = \sqrt[3]{\frac{4V}{\pi}}$ $L_{opt} = \sqrt[3]{\frac{4V}{\pi}}$

Then: $\left(\frac{L}{D}\right)_{opt} = 1$

N.B.: by modifying the assumptions and considering the bottoms characterized by an ellipsoidal shape with higher manufacturing cost, the thickness being also a function of the diameter D , the pressure and the corrosiveness of the liquid, we get a different optimal L/D : $\left(\frac{L}{D}\right)_{opt} \cong 2 \div 4$

Example #3: CAPEX + OPEX

Statement: we want to determine the optimal thickness s of the insulator for a large diameter pipe and a high internal heat exchange coefficient. We need to find a compromise between the energy savings and the investment cost for the installation of the refractory material.

- Heat exchanged with the environment in presence of the refractory:

$$Q = U A \Delta T = A \Delta T / (1/h_e + s/k)$$

- Cost of installation of the refractory material [€/m²]

$$F_0 + F_1 s$$

- The insulator has a five-year life. The capital for the purchase and installation is borrowed. r is the percentage of the capital + interests to be repaid each year. It follows that $r > 0.2$
- H_t is the cost of the energy losses [€/kcal]
- Y are the working hours in a year [h/y]
- Each year we must return to the bank which provided the loan:

$$(F_0 + F_1 s) A r [\text{€/y}]$$

Example #3: CAPEX + OPEX

- Heat exchanged with the environment without the refractory material:

$$Q = U A \Delta T = h_e A \Delta T$$

- Annual energy savings due to the refractory:

$$[h_e A \Delta T - A \Delta T / (1/h_e + s/k)] H_t Y \text{ [€/y]}$$

- The objective function in the *dof*s becomes:

$$f_{\text{obj}} = [h_e A \Delta T - A \Delta T / (1/h_e + s/k)] H_t Y - (F_0 + F_1 s) A r$$

- The problem is solved analytically by calculating:

$$d f_{\text{obj}} / ds = 0$$

- We obtain:

$$s_{\text{opt}} = k [((\Delta T H_t Y)/(k F_1 r))^{\frac{1}{2}} - 1/h_e]$$

- Note that s_{opt} depends neither on A nor on F_0



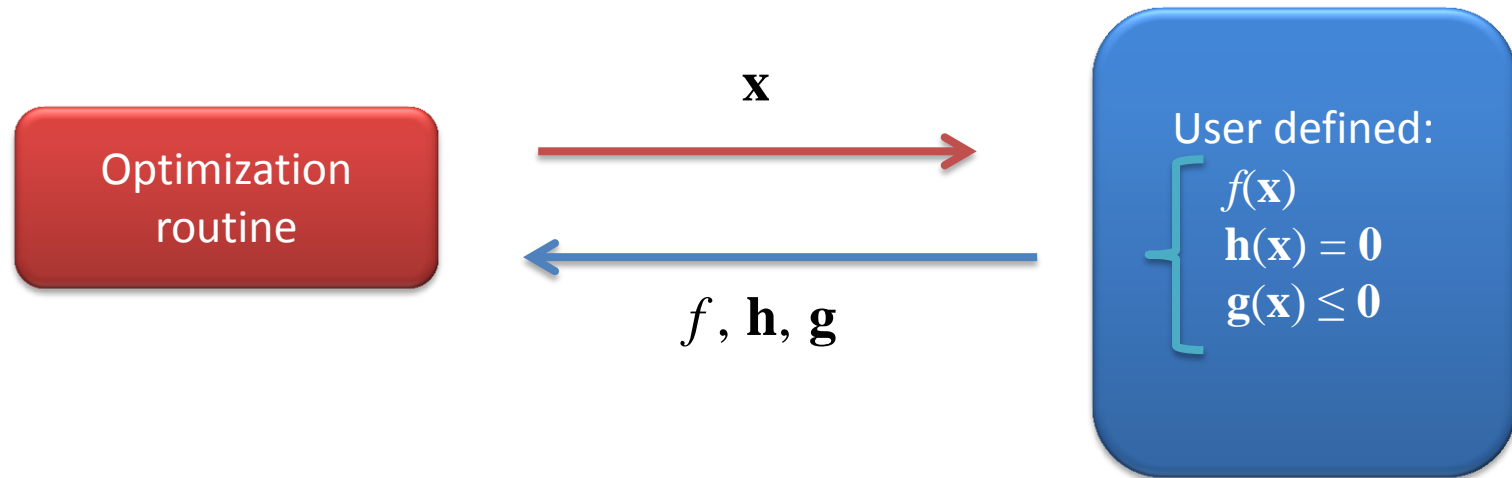
Solution methods



Solution methods

- The problem: $Max\ f(\mathbf{x})$ can always be turned into: $Min\ f(\mathbf{x})$ by changing the sign of the objective function
- The optimization problem can deal with two distinct approaches:
 - **Equation oriented**: based on an overall approach model that describes the process with a single system of equations (in general differential-algebraic) that solves the problem by considering it as a set of constraints
 - **Black-box** or Sequential modular: the process model is called by the optimization routine and returns the data required to evaluate the objective function
 - The simulation model can then work in terms of either **FEASIBLE PATH** or **INFEASIBLE PATH**, depending on whether the equations related to the recycle streams are solved for each call or if the consistency of the recycles is introduced as a linear constraint in the structure of the optimization problem

Equation-oriented formulation

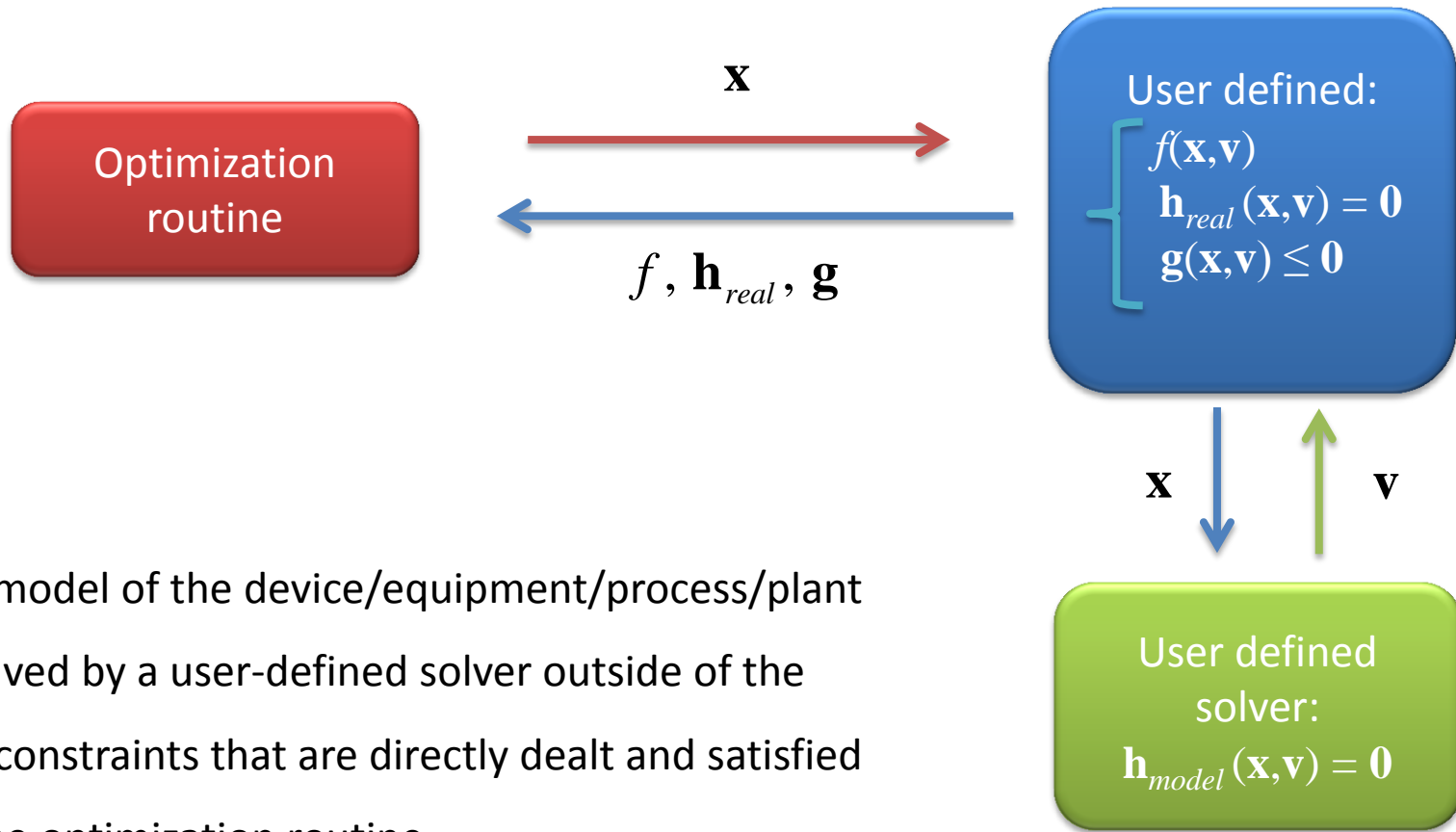


The equality constraints \mathbf{h} contain all the equations describing the model of the device/equipment/process/plant to be optimized.

In general \mathbf{h} can be a system of differential-algebraic equations, DAE, in the form:

$$\mathbf{h}(\mathbf{x}', \mathbf{x}, \mathbf{p}, t) = \mathbf{0}$$

Black-box formulation



The model of the device/equipment/process/plant is solved by a user-defined solver outside of the *real* constraints that are directly dealt and satisfied by the optimization routine.

Also in this case, \mathbf{h}_{model} can be a DAE system: $\mathbf{h}_{model}(\mathbf{x}', \mathbf{x}, \mathbf{v}', \mathbf{v}, t) = \mathbf{0}$

Methods for multidimensional unconstrained optimization

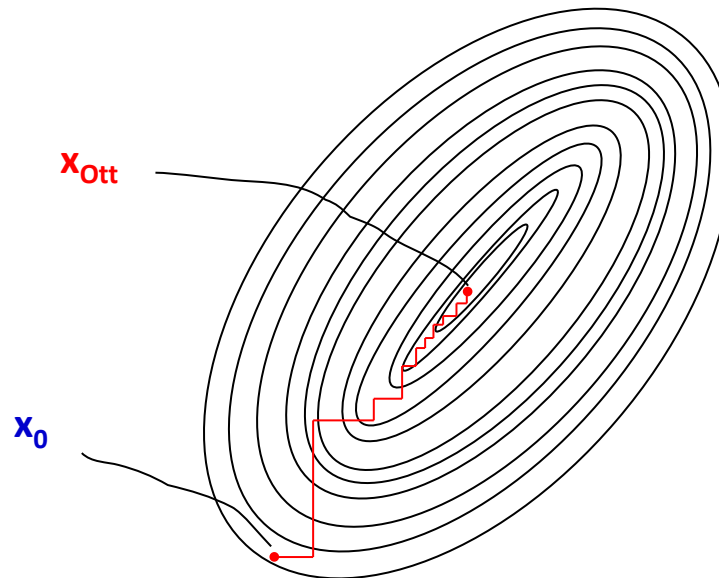


Multidimensional unconstrained optimization

- There is a **necessary condition** to be fulfilled for the optimal point: $\nabla f(\mathbf{x}^*) = 0$ that is the gradient of $f(\mathbf{x})$ must be zero (this is not true for cusp points and more in general for discontinuous functions)
- **Sufficient condition** for the minimum is that: $\nabla^2 f(\mathbf{x}^*) > 0$ the Hessian matrix of $f(\mathbf{x})$ must be positive definite.
- There are three distinct classes of methods that differ in the use of the derivatives of the objective function during the search for the minimum:
 - **HEURISTIC methods** do not use the derivatives of $f(\mathbf{x})$. They are more robust because they are slightly if not affected by the discontinuities of the problem to be solved.
 - **FIRST ORDER methods** work with the first order partial derivatives of $f(\mathbf{x})$ *i.e.* the GRADIENT of the objective function.
 - **SECOND ORDER methods** use also the second order partial derivatives of $f(\mathbf{x})$ *i.e.* the HESSIAN of the objective function.

Multidimensional unconstrained optimization

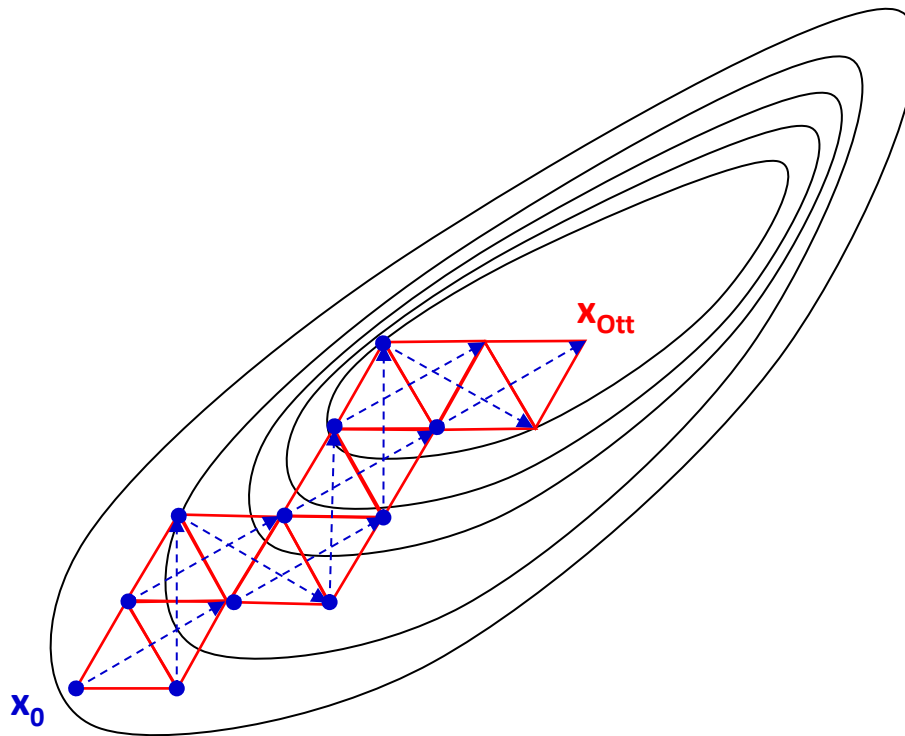
- The numerical algorithms are intrinsically iterative and usually perform a series of direction-searches. At the k -th iteration we have the k -th direction s_k and the method minimizes $f(\mathbf{x})$ along s_k .
- **DIRECT or HEURISTIC methods:**
 - **Random search** (Montecarlo)
 - **Grid search** (heavy but exhaustive)
 - **Univariate research** we identify n directions (where n is the number of *dof*) with respect to which perform iteratively the optimization.



Multidimensional unconstrained optimization

Simplex method (Nelder & Mead, 1965)

- The simplex is a geometric figure having $n+1$ vertices for n *dof*. We identify the worst vertex (*i.e.* having the highest value for $f(\mathbf{x})$) and we reverse it symmetrically with respect to the center of gravity of the remaining $n-1$ vertices. We identify a new simplex respect to which continue the search. The overturning of the simplex may be subject to expansion or contraction according to the actual situation.



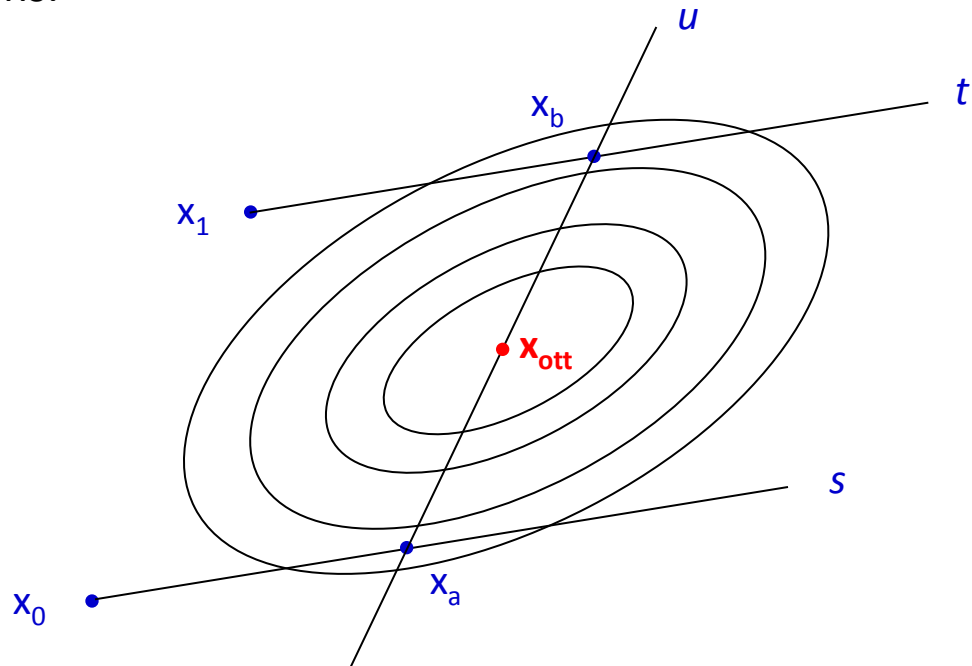
Multidimensional unconstrained optimization

Conjugate directions method

Considering a quadratic approximation of the objective function it is possible to identify its conjugate directions.

Hp.: $f(\mathbf{x})$ is quadratic

1. x_0 generic
2. s generic
3. x_a minimum on s
4. x_1 generic
5. t parallel to s
6. x_b minimum on t
7. u from joining x_a and x_b

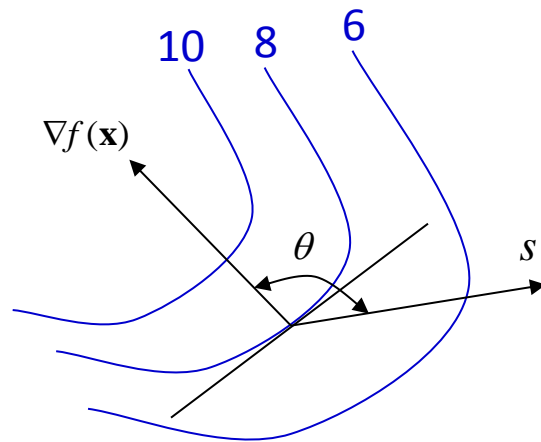


u is the conjugated direction with respect to s and t and by minimizing it we identify the optimal point x_{ott} of $f(\mathbf{x})$ (for that quadratic approximation).

Multidimensional unconstrained optimization

First order indirect methods

A possible candidate search direction s must decrease the function $f(\mathbf{x})$. It must satisfy the condition: $\nabla^T f(\mathbf{x})s < 0$



In fact:

$$\nabla^T f(\mathbf{x})s = \|\nabla f(\mathbf{x})\| \|s\| \cos \theta < 0$$

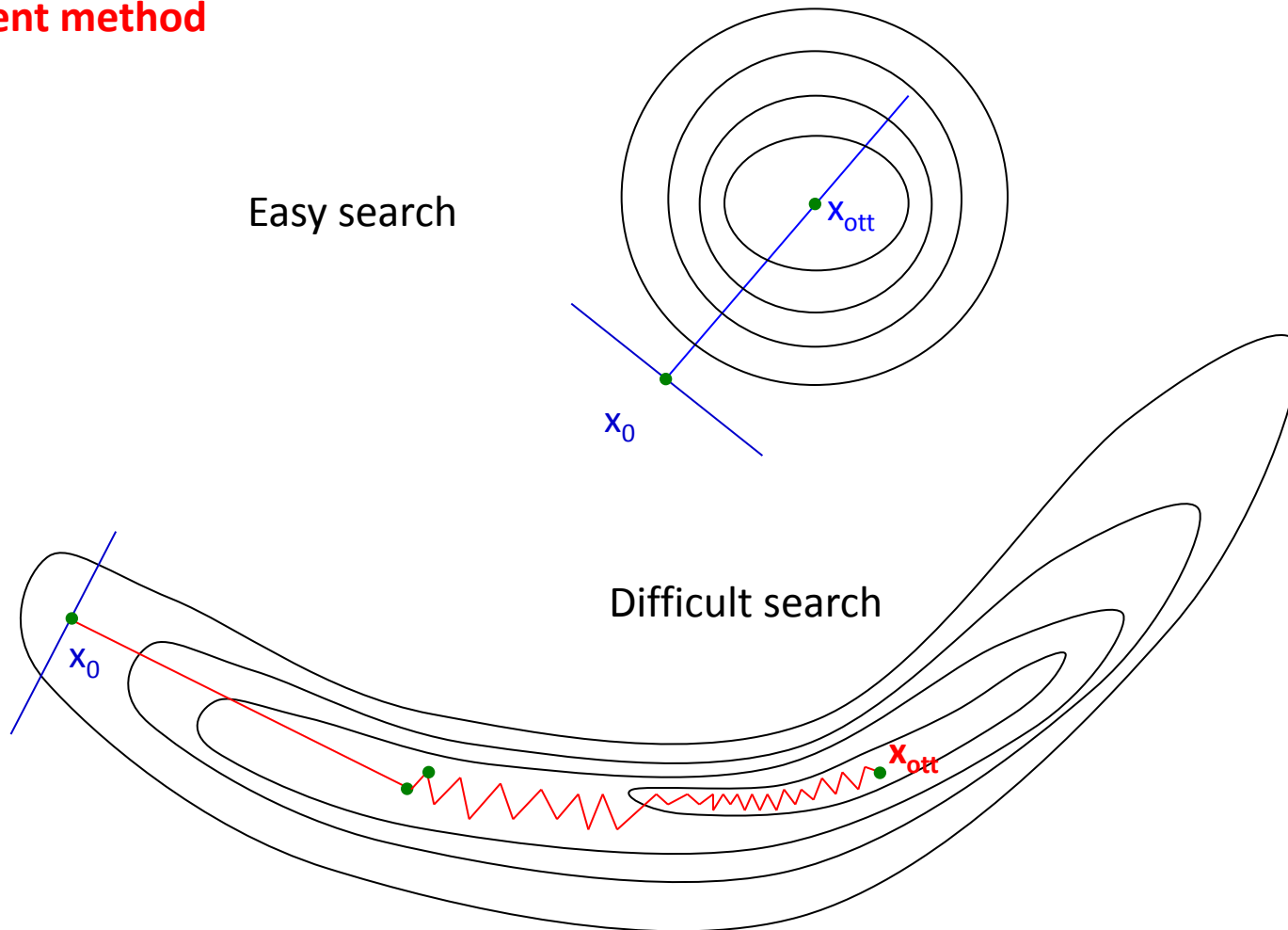
only if: $\cos \theta < 0 \Rightarrow \theta > 90^\circ$

The **gradient method** selects the gradient of the objective function (in the opposite direction) as the search direction .

The idea of moving in the direction of the maximum slope (*i.e.* “*Steepest Descent*”) may be not *optimal*.

Multidimensional unconstrained optimization

Gradient method



Multidimensional unconstrained optimization

Second order indirect methods

They exploit the second order partial derivatives of the objective function.

Implementing the Taylor series truncated at the second term and equating the gradient to zero we get: $\nabla f(\mathbf{x}_k) + \mathbf{H}(\mathbf{x}_k)\Delta\mathbf{x}_k = 0$

Consequently, it must be: $\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{H}^{-1}(\mathbf{x}_k)\nabla f(\mathbf{x}_k)$

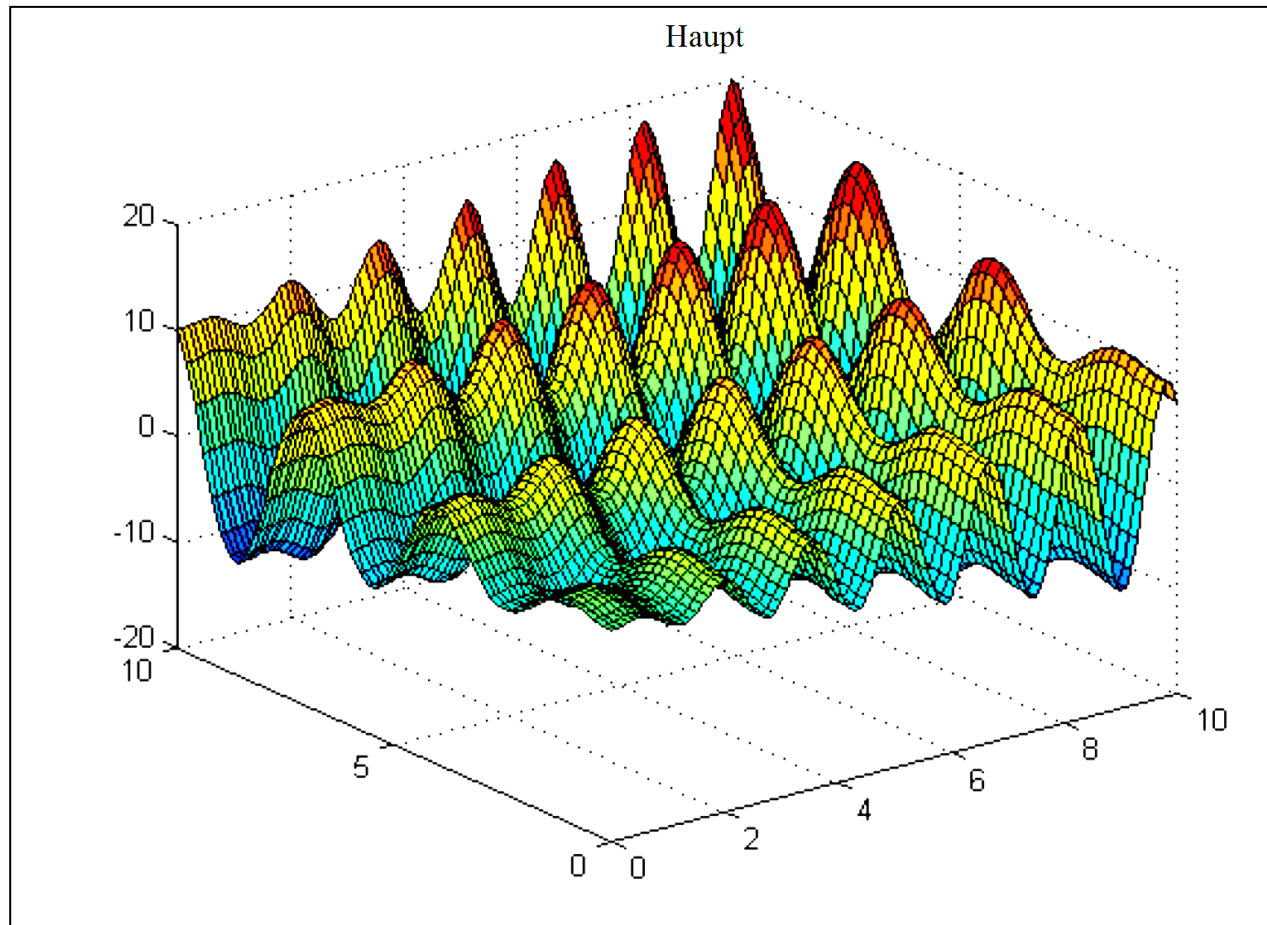
N.B.: the Hessian matrix is not inverted, we solve the resulting linear system via the LU factorization.

In addition, the Hessian matrix is NOT calculated directly as it would be very expensive in terms of CPU computing time. On the contrary, the **BFGS formulas** (Broyden, Fletcher, Goldfarb, Shanno) allow starting from an initial estimation of H (often the identity matrix) and with the gradient of $f(\mathbf{x})$ they evaluate iteratively $\mathbf{H}(\mathbf{x})$.

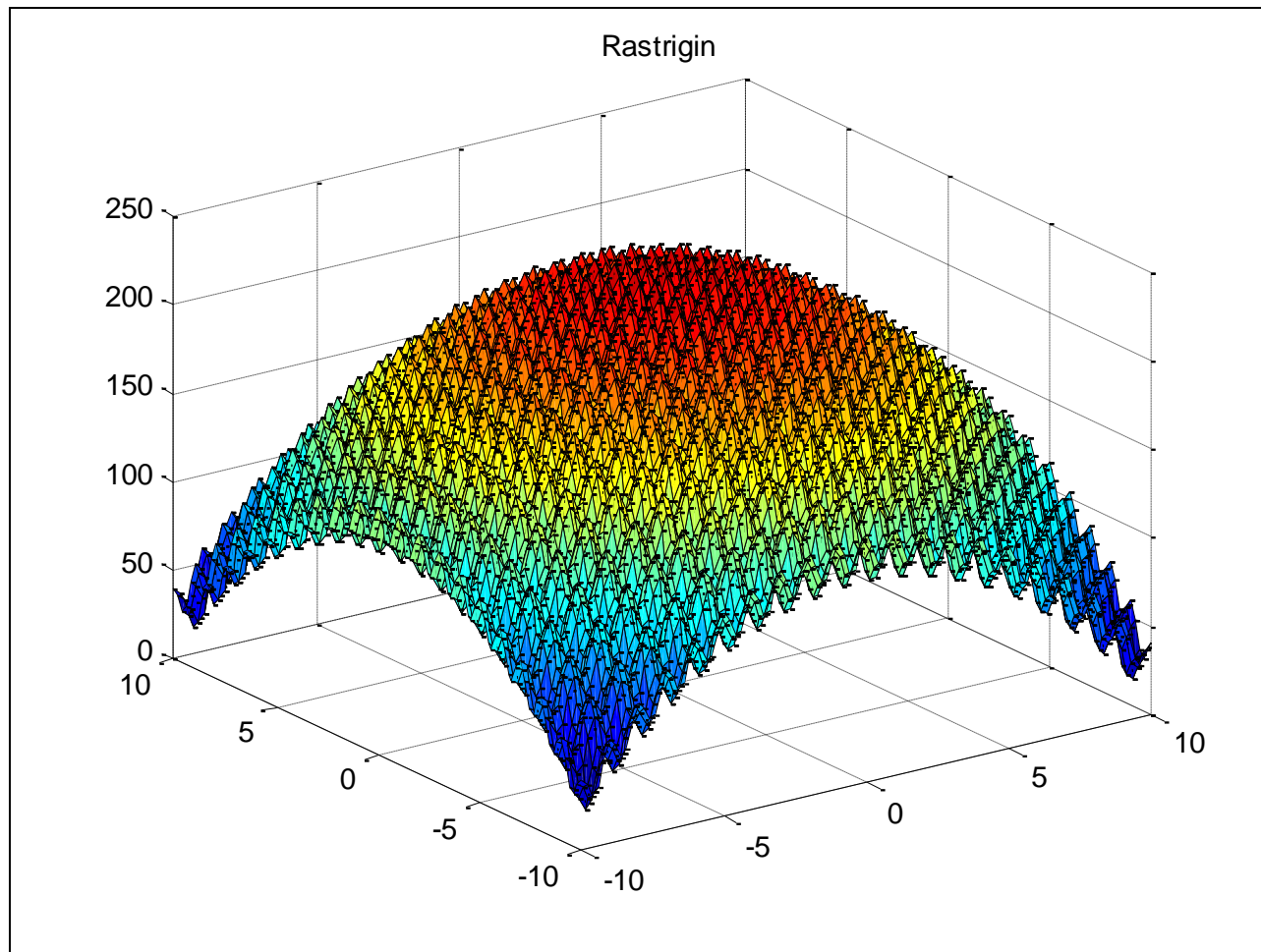
The solving numerical methods are:

Newton, Newton modified: Levemberg-Marquardt, Gill-Murray.

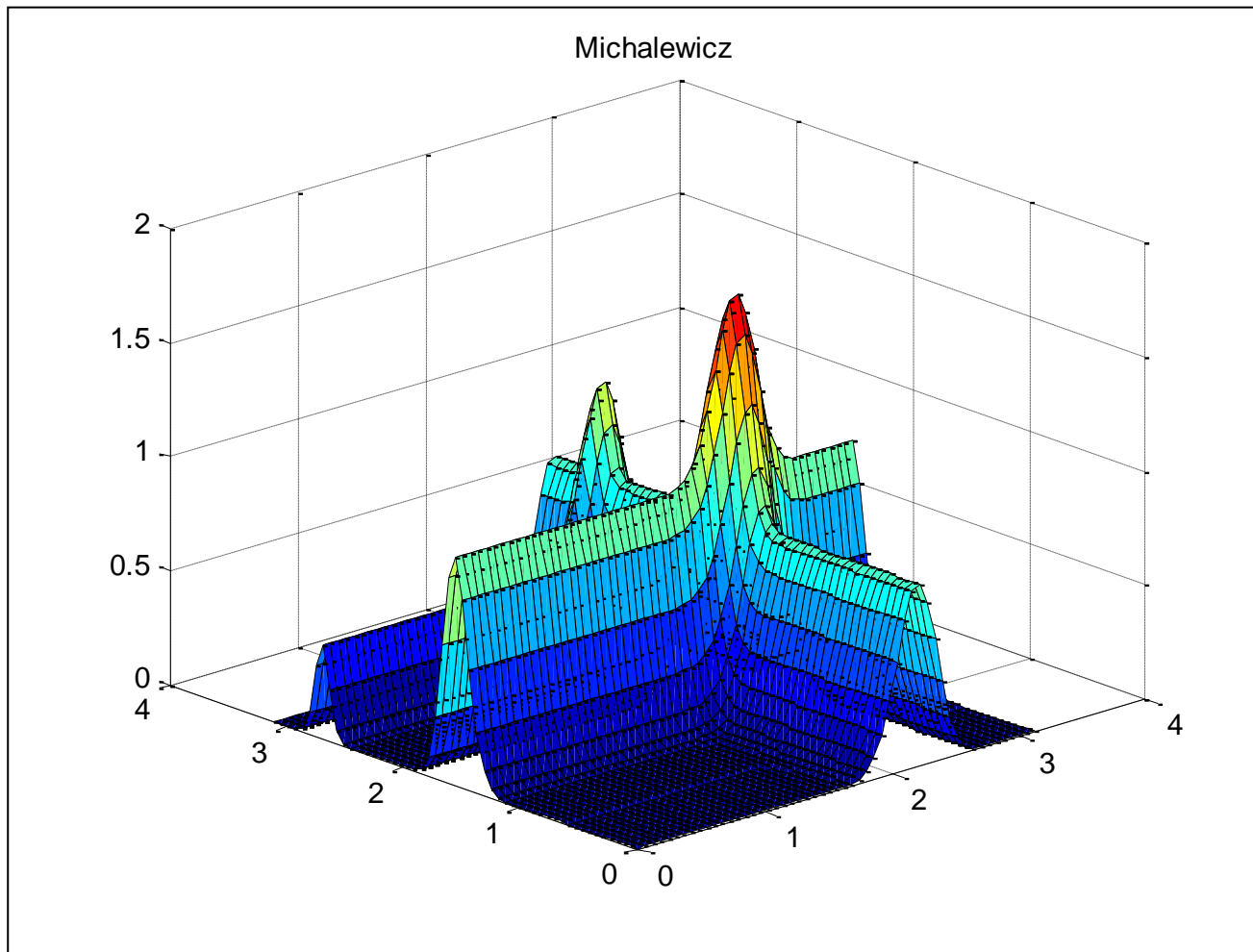
Some peculiar objective functions



Some peculiar objective functions



Some peculiar objective functions



Methods for multidimensional constrained optimization



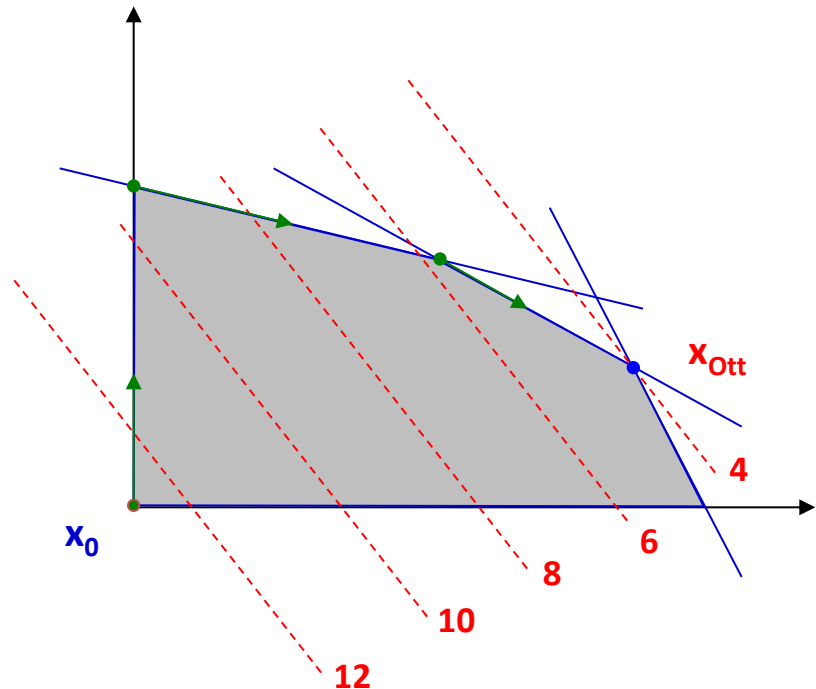
Linear Programming

- The objective function and the equality and inequality constraints are all LINEAR. Thus, the objective function is neither concave nor convex. Actually, it is either a plane (2D) or a hyperplane (with n *dof*).
If the region identified by the constraints is consistent we have to solve a problem (“feasible”) that will take us on the way to the constraints and more specifically towards their intersection.
- Simplex Method LP**

It is first necessary to identify a starting point that belongs to the “feasible” region.

Then we move along the sequence of constraints until we reach the optimal point.

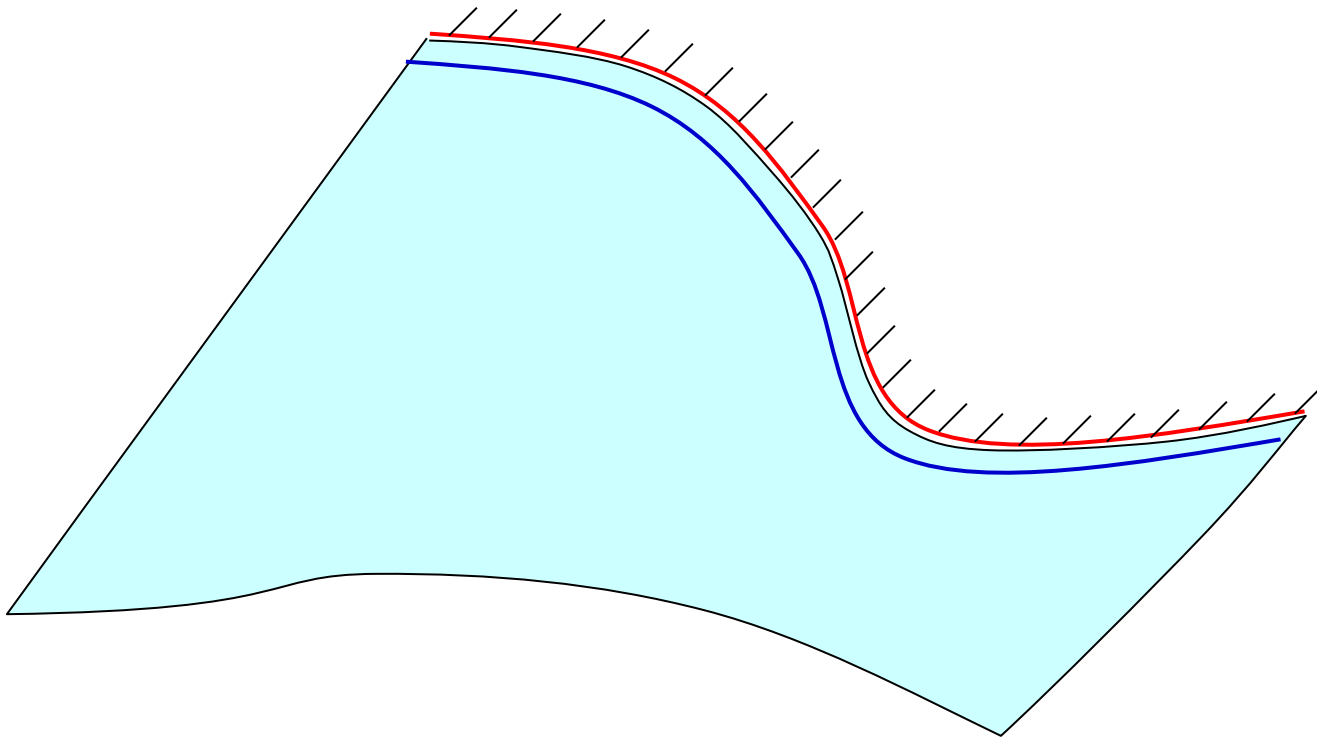
The problem may also NOT have a “feasible” region of research.



Nonlinear Programming

Method of the Lagrange multipliers

The inequality constraints, $g(\mathbf{x}) \geq 0$, if violated, are rewritten as equality constraints by introducing the *slack variables*: $g(\mathbf{x}) - \sigma^2 = 0$



Nonlinear Programming

Method of the Lagrange multipliers

The objective function is reformulated to contain both the equality and inequality constraints:

$$L(\mathbf{x}, \boldsymbol{\omega}, \boldsymbol{\sigma}) = f(\mathbf{x}) + \sum_{i=1}^{NEC} \omega_i h_i(\mathbf{x}) + \sum_{i=NEC+1}^{NCTOT} \omega_i \left[g_i(\mathbf{x}) - \sigma_i^2 \right]$$

There are necessary and sufficient conditions to identify the optimal point that simultaneously satisfies the imposed constraints.

It is easy to see how the problem dimensionality increases.

Nonlinear Programming

Penalty Function method

We change the objective function by summing some penalty terms that quantify the violation of inequality and equality constraints:

$$\text{Min} \left(f(\mathbf{x}) + \mu h^2(\mathbf{x}) + \eta |\min\{0, g(\mathbf{x})\}| \right)$$

More generally:

$$\text{Min} \left(f(\mathbf{x}) + \sum_{i=1}^{NEC} \phi(h_i(\mathbf{x})) + \sum_{i=NEC+1}^{NCTOT} \varphi(g_i(\mathbf{x})) \right)$$

$$\phi(y) = y^{2n} \quad \varphi(y) = (\min(0, y))^{2n}$$

Nonlinear Programming

SQP method (Successive Quadratic Programming)

The objective function $f(\mathbf{x})$ is approximated iteratively with a quadratic function, while the constraints are linearized and added to the objective function:

$$\begin{cases} \text{Min} & f(\mathbf{x}) = \text{Min} \quad \mathbf{c}^T \mathbf{x} + \frac{1}{2} \mathbf{x}^T \mathbf{B} \mathbf{x} \\ \text{s.t.} & \mathbf{A} \mathbf{x} = \mathbf{b} \end{cases}$$

the search for the optimal point is made along a direction s (identified by the vector \mathbf{x}) over which the objective function and constraints have been formulated.

Matrix \mathbf{B} is an approximation of the Hessian matrix \mathbf{H} and is calculated with the **BFGS formulas** (Broyden, Fletcher, Goldfarb, Shanno).

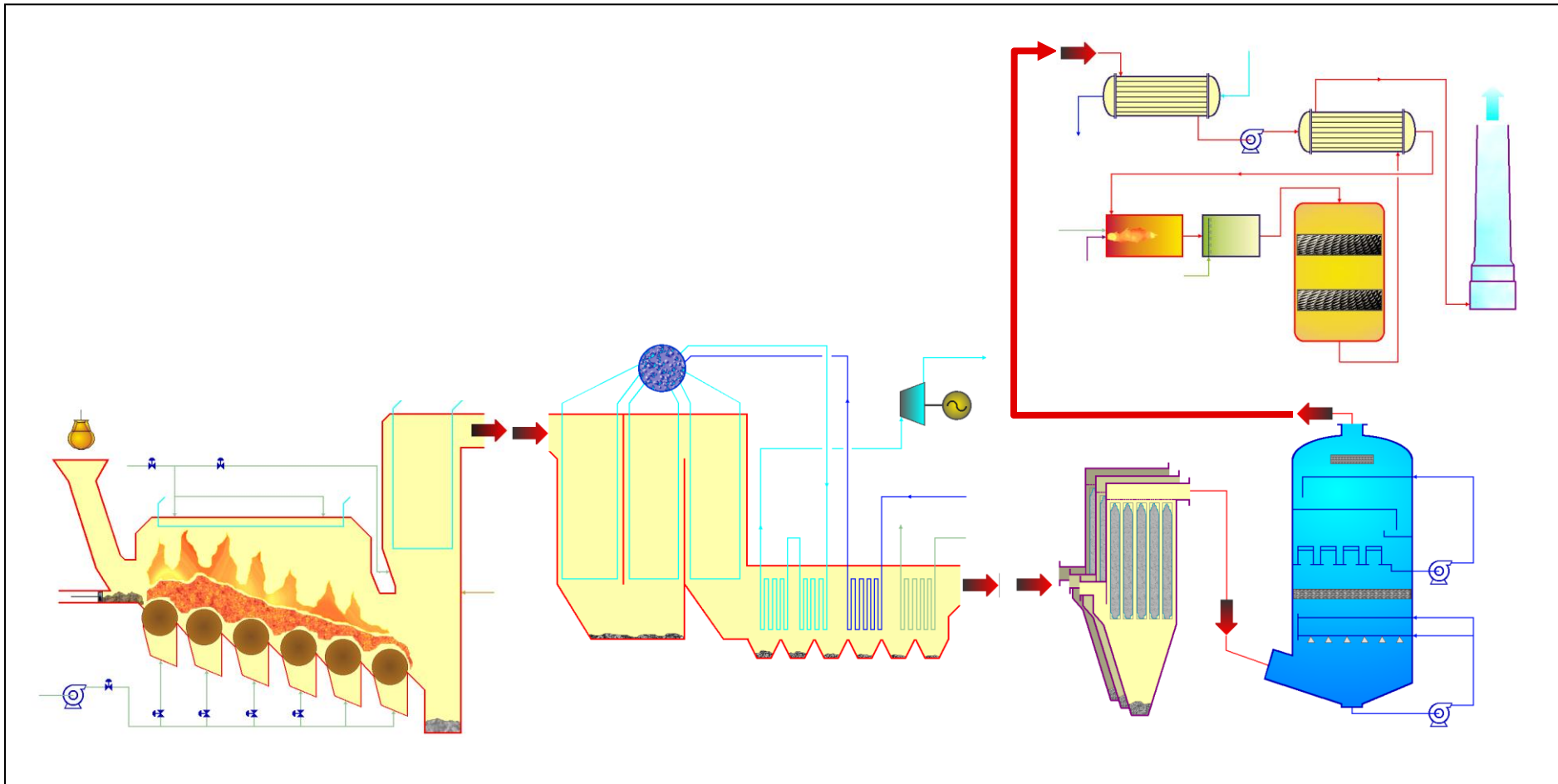
Case-study #1

On-line optimization of continuous processes



On-line optimization of continuous processes

Waste to energy plant with DeNOx catalytic section



D. Manca, M. Rovaglio, G. Pazzaglia, G. Serafini. Comp. & Chem. Eng., 22(12), 1879-1896, (1998)

On-line optimization of continuous processes

- **Requirements of the optimization procedure**
 - Economic optimization of the process:
 - maximize the steam production and then electrical energy.
 - Minimize the operating costs
 - Respect the process constraints for a correct plant operation
 - Respect the law constraints
- ***Alternatively***
 - Minimize the production of micropollutants
 - Reduce environmental impact
 - Optimal mixing of wastes having different nature

On-line optimization of continuous processes

Objective function to be maximized

$$F_{obj} = W_{rif} c_{rif} + W_{vap} c_{vap} - \left(W_{CH_4, PC} + W_{CH_4, DeNOx} \right) c_{CH_4} - W_{NH_3} c_{NH_3}$$

Degrees of freedom

Waste flowrate	Total air flowrate to the furnace	Air flow first drum
Air flow rate second drum	Air flow third drum	Air flow fourth drum
Secondary air flow to furn.	Air flow afterburner	CH4 flow rate afterburner
First drum speed	Second drum speed	Third drum speed
Fourth drum speed	NaOH flow	CH4 DeNOx flow
NH3 DeNOx flowrate		

Law constraints

% vol. min. O2 afterburner
T out min. afterburner
HCl max to the stack
SO2 max to the stack
NOx max to the stack
NH3 max to the stack

Process constraints

Delta P max on every drum
T in max. and min. DeNOx reactor
% max. unburnt in ashes
Max. and min. steam produced
% vol. max. O2 afterburner
Delta max. combustion on the first 3 drums
T out max. and min. primary combustion chamber

Higher and lower constraints on the degrees of freedom

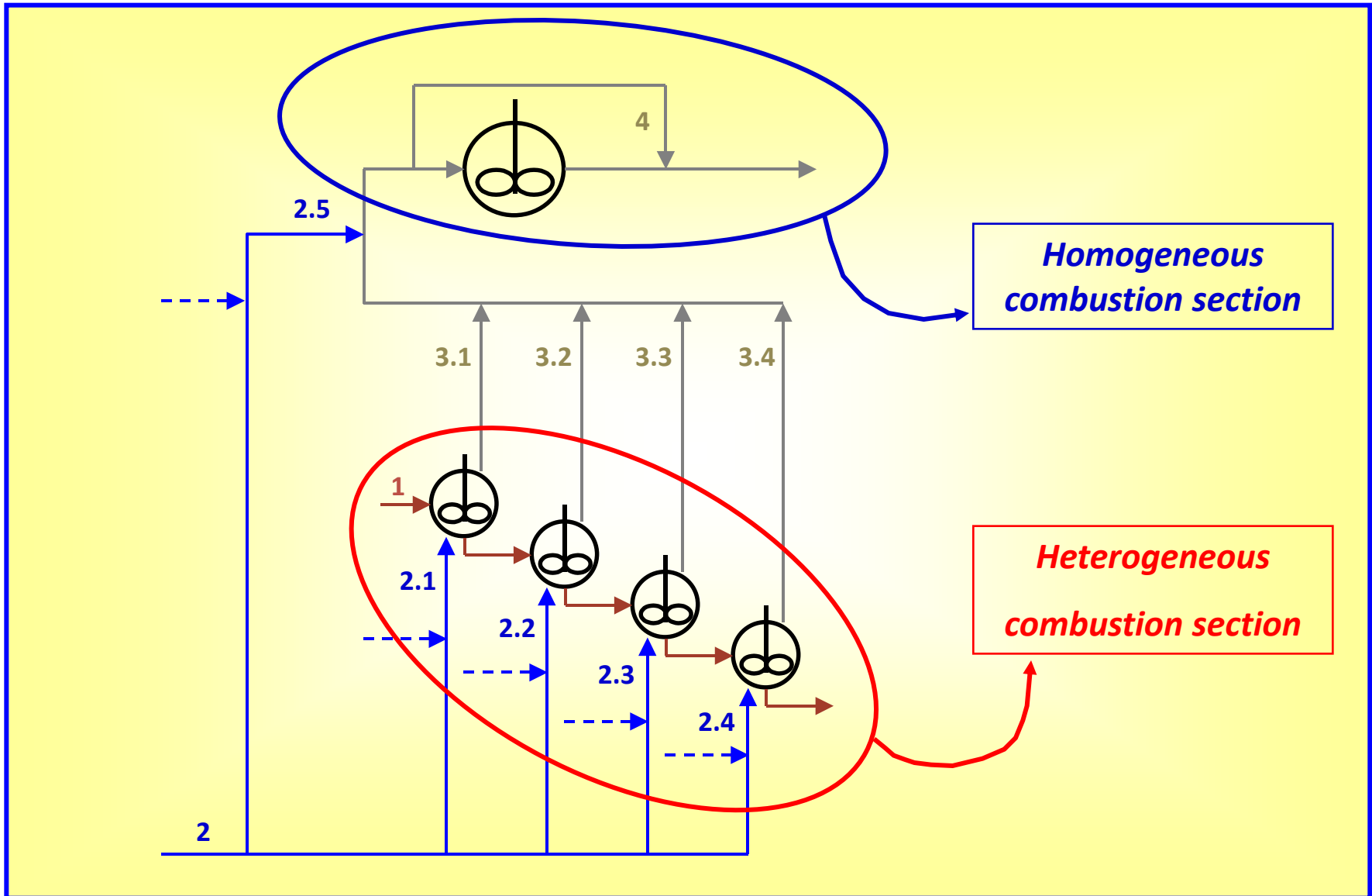


On-line optimization of continuous processes

Problem solution

- We must adopt a nonlinear constrained multivariable optimization routine which is efficient (in terms of CPU time) and robust (able to identify the solution).
- We must implement a detailed model of the process able to simulate the response of the system whenever the optimization routine proposes a new degrees of freedom vector.
- The process optimizer has as its main task to bring the system to operate in the “feasible” region, where the constraints are respected. In some cases, it may happen that the objective function worsens compared to the initial conditions since the process is brought to operate within the feasibility region. Then, within this region, the optimizer maximizes the objective function.
- Note that the explicit computation of the objective function is almost instantaneous. This does not occur for the evaluation of each single term which composes the objective function as they come from the simulation procedure of the process.

Process Model – Primary kiln



Material balances on each drum

Solid phase

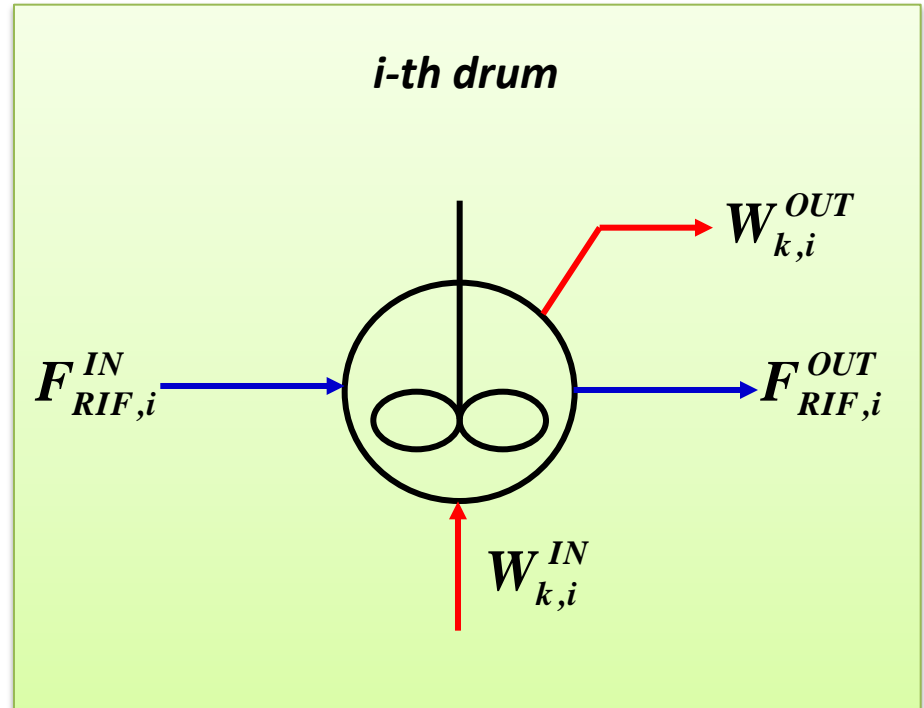
$$\frac{dM_{RIF,i}}{dt} = F_{RIF,i}^{IN} - F_{RIF,i}^{OUT} - R_{RIF,i}$$

$$i = 1, NG$$

Gaseous phase

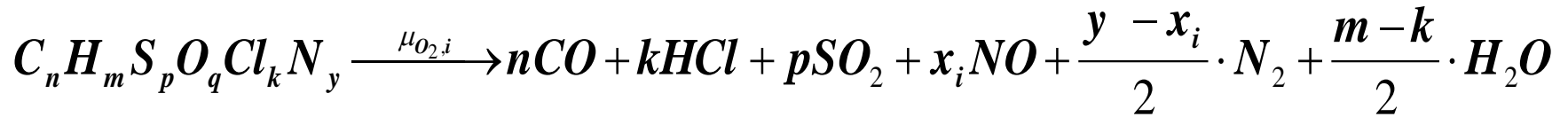
$$W_{k,i}^{OUT} + \frac{R_{RIF,i}}{PM_{rif}} \cdot x_k - W_{k,i}^{OUT} = 0$$

$$k = 1, NC \quad i = 1, NG$$



Chemical reactions

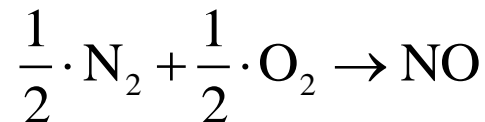
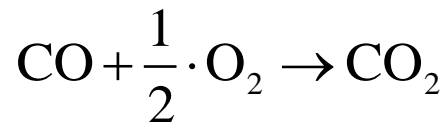
Combustion reactions in the solid phase



$$x_i = \psi_{NO,i} \cdot y$$

$$\psi_{NO,i} = \frac{2}{\frac{1}{\psi_{NO,i}} - \frac{2500 \cdot W_{G\ NO,i}^{100\%}}{T \cdot \exp(-3150/T) \cdot W_{G\ O_2,i}^{out}}} - 1 \quad (\text{Bowman, 1975})$$

Combustion reactions in the homogeneous phase



Primary kiln – combustion kinetics

Kinetic determining step: O_2 diffusion

$$R_{RIF,i} = \frac{k_{x,i} \cdot x_{O_2,i}}{\mu_{O_2,i}} \cdot A_{sc,i}^* \cdot PM_{rif}$$

$$\begin{cases} A_{sc,i} = f(d_{p,i}, \varepsilon_i, M_{rif,i}, M_{inerti,i}) \\ k_{x,i} = f(d_{p,i}, \varepsilon_i, W_{aria,i}, x_{k,i}, T) \end{cases} \quad \Rightarrow \quad \text{Granular solid bed}$$

$$\begin{cases} A_{sc,i}^* = \Gamma_i \cdot A_{sc,i} \\ \Gamma_i = 1 + \delta \cdot \left(1 - \exp\left(-\frac{N_{CG,i}}{\lambda}\right) \right) \end{cases} \quad \text{Corrective factors: } \delta, \lambda \text{ (adaptive parameters)}$$

Process model – the equations

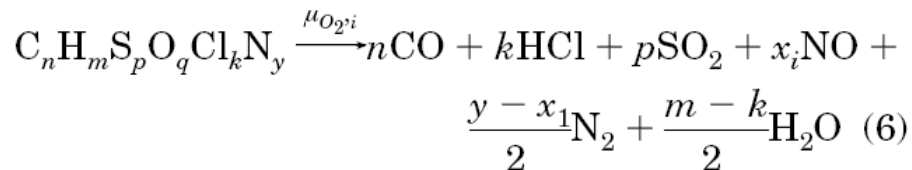
$$\frac{dM_{W,i}}{dt} = F_{W,i}^{in} - F_{W,i}^{out} - R_{W,i} \quad i = 1, \dots, NG \quad (1)$$

$$\frac{dM_{I,i}}{dt} = F_{I,i}^{in} - F_{I,i}^{out} \quad i = 1, \dots, NG \quad (2)$$

$$F_{W,i}^{in} = F_{W,i-1}^{out}, F_{I,i}^{in} = F_{I,i-1}^{out} \quad i = 2, \dots, NG \quad (3)$$

$$F_{W,1}^{in} = F_W(1 - \omega_{I,0} - \omega_{M,0}) \quad (4)$$

$$F_{I,1}^{in} = F_W \omega_{I,0} \quad (5)$$



$$R_{W,i} = \frac{k_{x,i} x_{O_2,i}}{\mu_{O_2,i}} \quad (7)$$

$$\mu_{O_2,i} = \frac{1}{2} \left(n + 2p + x_i + \frac{m - k}{2} - q \right) \quad (8)$$

$$k_{x,i} = Sh_i \mathcal{D}_{O_2,i}^{mix} a_i c_{tot,i} \quad (9)$$

$$a_i = \frac{6(1 - \epsilon_i)}{d_{p,i}} \quad (10)$$

$$Sh_i = j_{D,i} Re_i Sc_i^{1/3} \quad (11)$$

$$\begin{cases} Re_i = \frac{\rho_A v_{A,i}}{\mu_A a_i} \\ Sc_i = \frac{\mu_A}{\rho_A \mathcal{D}_{O_2,i}^{mix}} \end{cases} \quad (12)$$

$$A_{E,i} = \Gamma_i \frac{a_i}{(1 - \epsilon_i)} f_{W,i} \frac{M_{W,i} + M_{I,i}}{\rho_W} \quad (13)$$

$$\Gamma_i = 1 + \delta(1 - e^{-N_{GS,i}/\lambda}) \quad (14)$$



Process model – the equations

$$\frac{\Delta P_i}{s_{B,i}} = \frac{150\mu_A v_{A,i}(1 - \epsilon_i)^2}{d_{p,i}^2 \epsilon_i^3} + \frac{1.75\rho_A v_{A,i}^2(1 - \epsilon_i)}{d_{p,i} \epsilon_i^3} \quad (15)$$

$$s_{B,i} = \frac{M_{W,i} + M_{L,i}}{\rho_W l_G w_G} \quad (16)$$

$$\left\{ \begin{array}{l} (W_{A,G,i} + W_{A,L,G,i})x_{O_2,A} - \frac{R_{W,i}\mu_{O_2}}{MW_W} - W_{O_2,G,i}^{out} = 0 \\ (W_{A,G,i} + W_{A,L,G,i})x_{N_2,A} - \frac{R_{W,i}}{MW_W} \frac{x_{N,W}}{2}(1 - \Psi_{NO,i}) - \\ \quad W_{N_2,G,i}^{out} = 0 \\ \frac{R_{W,i}}{MW_W} x_{C,W} - W_{CO,G,i}^{out} = 0 \\ \frac{R_{W,i}}{MW_W} x_{S,W} - W_{SO_2,G,i}^{out} = 0 \\ \frac{R_{W,i}}{MW_W} x_{Cl,W} - W_{HCl,G,i}^{out} = 0 \\ \frac{R_{W,i}}{MW_W} x_{N,W} \Psi_{NO,i} - W_{NO,G,i}^{out} = 0 \\ \left\{ \begin{array}{l} \frac{R_{W,1}}{MW_W} \frac{x_{H,W} - x_{Cl,W}}{2} - W_{H_2O,G,1}^{out} + \frac{F_W \omega_{H_2O,0}}{MW_{H_2O}} = 0 \\ \frac{R_{W,i}}{MW_W} \frac{x_{H,W} - x_{Cl,W}}{2} - W_{H_2O,G,i}^{out} = 0 \quad i = 2, \dots, NG \end{array} \right. \end{array} \right. \quad (17)$$



Process model – the equations

$$M_{W,F,i} = \rho_W \Delta x_G w_{GSB,i} \quad (18)$$

$$F_{W,i}^{out} = M_{W,F,i} f_{W,i} N_{GS,i} \quad (19)$$

$$\frac{\int_0^{3600} M_{W,F,0} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{[t - (t_{0,k} + \theta)]^2}{2\sigma^2}\right) dt}{3600} \cong$$

$$F_{I,i}^{out} = M_{W,F,i} (1 - f_{W,i}) N_{GS,i} \quad (20)$$

$$\bar{F}_W \quad t_{0,k} < t < t_{0,k} + \frac{1}{N_{GS,0}} \quad (25)$$

$$f(z) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(z - z_0)^2}{2\sigma^2}\right) \quad (21)$$

$$\theta = k\sqrt{\sigma^2} \quad (26)$$

$$F_{W,i}^{out} = M_{W,F,i} f_{W,i} \frac{1}{\sqrt{2\pi}\sigma^2} \exp\left(-\frac{[t - (t_{0,i} + \theta_i)]^2}{2\sigma^2}\right) \quad (22)$$

$$Z = -\frac{t_0 - (t_0 + \theta)}{\sqrt{\sigma^2}}$$

$$F_{I,i}^{out} = M_{W,F,i} (1 - f_{W,i}) \frac{1}{\sqrt{2\pi}\sigma^2} \exp\left(-\frac{[t - (t_{0,i} + \theta_i)]^2}{2\sigma^2}\right) \quad (23)$$

$$\theta = \bar{Z}\sqrt{\sigma^2} \Rightarrow k = \bar{Z} = -\frac{t_0 - (t_0 + \theta)}{\sqrt{\sigma^2}} \quad (27)$$

$$h_i \cong \frac{0.5}{N_{GS,i}} \quad (24)$$

Manca D., M. Rovaglio, Ind. Eng. Chem. Res. 2005, 44, 3159-3177



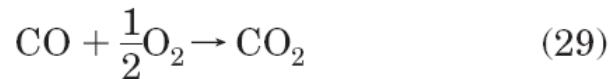
Process model – the equations

$$W_{Hom,j}^{in} = \sum_{i=1}^{NG} W_{G,j,i}^{out} \quad j = \text{CO}, \text{SO}_2, \text{HCl}, \text{NO}, \text{H}_2\text{O}$$

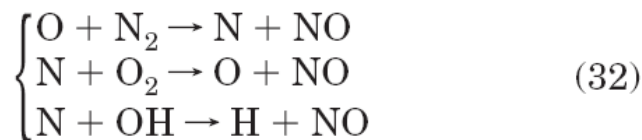
$$W_{Hom,O_2}^{in} = \sum_{i=1}^{NG} W_{G,O_2,i}^{out} + (W_{A,S} + W_{A,LS})x_{O_2,A}$$

$$W_{Hom,N_2} = \sum_{i=1}^{NG} W_{G,N_2,i}^{out} + (W_{A,S} + W_{A,LS})x_{N_2,A}$$
(28)

$$x_{Hom,j}^{in} = \frac{W_{Hom,j}^{in}}{\sum_{j=1}^{NC} W_{Hom,j}^{in}} \quad j = \text{O}_2, \text{N}_2, \text{CO}, \text{SO}_2, \text{HCl}, \text{NO}, \text{H}_2\text{O}$$



$$\frac{dc_{CO}}{dt} = 1.8 \times 10^{10} c_{CO} \sqrt{c_{O_2}} \exp\left(-\frac{25000}{RT}\right) \quad (31)$$



$$\frac{dn_{Hom,CO_2}}{dt} = -(W_{Hom}^{out} + W_L^{out})x_{Hom,CO_2}^{out} + R_{Hom,CO_2}V_{Hom} + W_{Hom,CO_2}^{in}$$

$$\frac{dn_{Hom,j}}{dt} = -(W_{Hom}^{out} + W_L^{out})x_{Hom,j}^{out} + W_{Hom,j}^{in} \quad j = \text{SO}_2, \text{H}_2\text{O}, \text{HCl}$$

$$\frac{dn_{Hom,N_2}}{dt} = -(W_{Hom}^{out} + W_L^{out})x_{Hom,N_2}^{out} - \frac{1}{2}R_{Hom,NO}V_{Hom} + W_{Hom,N_2}^{in} \quad (33)$$

$$\frac{dn_{Hom,O_2}}{dt} = -(W_{Hom}^{out} + W_L^{out})x_{Hom,O_2}^{out} - \frac{1}{2}R_{Hom,NO}V_{Hom} - \frac{1}{2}R_{Hom,CO_2}V_{Hom} + W_{Hom,O_2}^{in}$$

$$\frac{dn_{Hom,CO^*}}{dt} = -(W_{Hom}^{out} + W_L^{out})x_{Hom,CO^*}^{out} - R_{Hom,CO_2}V_{Hom} + W_{Hom,CO}^{in}(1 - f_{bypass})$$

$$\frac{dn_{Hom,CO^{**}}}{dt} = -(W_{Hom}^{out} + W_L^{out})x_{Hom,CO^{**}}^{out} + W_{Hom,CO}^{in}f_{bypass}$$

$$x_{Hom,CO}^{out} = \frac{n_{Hom,CO^*} + n_{Hom,CO^{**}}}{\sum_{j=1}^{NC+1} n_{Hom,j}}$$



Process model – the equations

$$P_1 - P_2 = \gamma \rho_1 \frac{v_1^2}{2} \quad (34)$$

$$W_L^{in} = \bar{k} \sqrt{\Delta P} \quad (35)$$

$$W_L^{out} = \bar{k} \frac{c_{tot,g}}{c_{tot,amb}} \sqrt{\frac{\rho_{amb}}{\rho_g}} \sqrt{\Delta P} \quad (36)$$

$$W_{Hom}^{out} = \sqrt{\frac{2P_{PK}}{\gamma} \cdot \frac{|P_{PK} - P_{PC}|}{MW_g RT}} A^{out} \quad (37)$$

$$\frac{dU}{dt} = \dot{H}_{in} - \dot{H}_{out} - \dot{Q}_{disp} - \dot{Q}_{V,PK} \quad (38)$$

$$U = \sum_{i=1}^{NC} n_i U_{g,i} + M_S U_S$$

$$\dot{H} = \sum_{i=1}^{NC} W_i H_{g,i} + \dot{M}_S H_S \quad (39)$$

$$\tilde{c}_p = \tilde{c}_v + R$$

$$H_{g,i} = U_{g,i} + P\tilde{V} = U_{g,i} + RT \quad (40)$$

$$\hat{c}_{v,S} \approx \hat{c}_{p,S} \Rightarrow U_S \approx H_S \quad (41)$$

$$(M_S \hat{c}_{p,S} + \sum_{i=1}^{NC} n_i \tilde{c}_{v,i}) \frac{dT}{dt} = - \sum_{i=1}^{NC} (W_{Hom,i}^{in} \int_{T^{in}}^T \tilde{c}_{p,i} dT) -$$

$$\dot{M}_S^{in} \int_{T^{in}}^T \hat{c}_{p,s} dT - \sum_{j=1}^{NR} \Delta H_j^R(T) R_j(T) + R_W WLHC +$$

$$RT \frac{d}{dt} (\sum_{i=1}^{NC} n_i) - \dot{Q}_{disp,PK} - \dot{Q}_{V,PK} \quad (42)$$



Process model – the equations

$$\sum_{i=1}^{NC} (W_{Hom,i}^{in} \int_{T^{in}}^T \tilde{c}_{p,i} dT) = (W_{A,PK} + W_{A,L}) \int_{T_{amb}}^T \tilde{c}_{p,A} dT \quad (43)$$

$$\dot{M}_S^{in} \int_{T^{in}}^T \hat{c}_{p,S} dT = F_W^{in} (1 - \omega_{H_2O}) \hat{c}_{p,S} (T - T^{in}) + \frac{F_W^{in} \omega_{H_2O}}{MW_{H_2O}} \int_{T_{eb}}^T \tilde{c}_{p,H_2O}^v dT \quad (44)$$

$$\sum_{j=1}^{NR} \Delta H_j^R(T) R_j(T) = \Delta H_{CO \rightarrow CO_2}^R R_{CO_2} + \Delta H_{N_2 \rightarrow NO}^R R_{NO} \quad (45)$$

$$R_W WLHC^* = \sum_{i=1}^{NG} \frac{R_{W,i}}{1 - \omega_I - \omega_{H_2O}} \left(WLHC + \Delta H_{CO \rightarrow CO_2}^R \frac{\omega_C}{MW_C} + \Delta H_{N_2 \rightarrow NO}^R \frac{\omega_N}{MW_N} (1 - \varphi_{NO,i}) \right) \quad (46)$$

$$RT \frac{d}{dt} \sum_{i=1}^{NC} n_i \quad (47)$$

$$\dot{Q}_{rad} = \sigma (A_{G \rightarrow W} T_g^4 - A_{W \rightarrow G} T_W^4) \quad (48)$$

$$A_{G \rightarrow W} T_g \cong A_{W \rightarrow G} T_W \quad (49)$$

$$\dot{Q}_{rad} = \sigma A_{G \rightarrow W} (T_g^4 - T_W^4) \frac{1 - k^3}{1 - k^4} \quad k = \frac{T_W}{T_g} \quad (50)$$

$$A_{G \rightarrow W} = \frac{A_{GW}}{\frac{1}{\epsilon_g} + \frac{1}{\epsilon_R} - 1} \quad (51)$$

$$\dot{Q}_{conv} = \sigma A_{G \rightarrow W} (T_g^4 - T_W^4) A_{GW} \frac{h_{int}}{4 \sigma T_{G \rightarrow W}^3} \quad T_{G \rightarrow W} = \frac{T_g + T_W}{2} \quad (52)$$

Process model – the equations

$$\dot{Q}_{V,PK} = \beta_{PK} \dot{Q}_{disp,PK} \quad (53)$$

$$\frac{\partial T}{\partial t} = k_W \frac{\partial^2 T}{\partial z^2} \quad (54)$$

$$\rho_i \hat{c}_{p,i}^W V_i \frac{dT_i}{dt} = \dot{q}_i^{in} A_i^{int} - \dot{q}_i^{out} A_i^{out} \quad i = 1, \dots, NL \quad (55)$$

$$\begin{aligned} T(z_i) &= T_i \\ T(z_{i+1}) &= T_{i+1} \end{aligned} \quad (56)$$

$$\dot{q}_i^{out} = -k_W \left. \frac{dT}{dz} \right|_{i+1/2} = k_W \frac{T_i - T_{i+1}}{z_{i+1} - z_i} \quad (57)$$

$$\dot{q}_{RI} = \frac{T_{NRL}^R - T_1^I}{\frac{s_R}{2k_R} + \frac{s_I}{2k_I}} \quad (58)$$

$$h_{int}(T_{g,PK} - T_W^{int}) = \frac{2k_R}{s_R}(T_W^{int} - T_1^R) \quad (59)$$

$$h_{ext}(T_S^{ext} - T_{amb}) = \frac{2k_I}{s_I}(T_{NIL}^I - T_S^{ext}) \quad (60)$$

$$\begin{aligned} h_{ext} &= \frac{Nuk_A}{L} + 4\sigma\epsilon_{met}T_{met}^3 \\ T_{met} &= \frac{T_{amb} + T_S^{ext}}{2} \end{aligned} \quad (61)$$

$$\frac{dn_{CO_2}}{dt} = -W_{PC}^{out} x_{CO_2,PC}^{out} + R_{CO_2} V_{PC} + W_{PC}^{in} x_{CO_2,PC}^{in} \quad (62)$$

$$\frac{dn_{SO_2}}{dt} = -W_{PC}^{out} x_{SO_2,PC}^{out} + W_{PC}^{in} x_{SO_2,PC}^{in} \quad (63)$$

Process model – the equations

$$\frac{dn_{H_2O}}{dt} = -W_{PC}^{out}x_{H_2O,PC}^{out} + W_{PC}^{in}x_{H_2O,PC}^{in} \quad (64)$$

$$P_{PC} - P_{PK} = \Delta P_{dis} + \Delta P_{loc} \quad (70)$$

$$\frac{dn_{HCl}}{dt} = -W_{PC}^{out}x_{HCl,PC}^{out} + W_{PC}^{in}x_{HCl,PC}^{in} \quad (65)$$

$$\Delta P_{dis} = \frac{2f_D \rho_g v_g^2 L_{PC}}{D_{h,PC}} \quad (71)$$

$$\frac{dn_{N_2}}{dt} = -W_{PC}^{out}x_{N_2,PC}^{out} - \frac{1}{2}R_{NO}V_{PC} + W_{PC}^{in}x_{N_2,PC}^{in} \quad (66)$$

$$f_D = \frac{1}{\left[4 \log\left(0.27 \frac{\epsilon}{D_h} + \left(\frac{7}{Re}\right)^{0.9}\right)\right]^2} \quad (72)$$

$$\frac{dn_{O_2}}{dt} = -W_{PC}^{out}x_{O_2,PC}^{out} - \frac{1}{2}R_{NO}V_{PC} - \frac{1}{2}R_{CO_2}V_{PC} + W_{PC}^{in}x_{O_2,PC}^{in} \quad (67)$$

$$\Delta P_{loc} = \gamma \frac{\rho_g v_g^2}{2} \quad (73)$$

$$\frac{dn_{CO}}{dt} = -W_{PC}^{out}x_{CO,PC}^{out} - R_{CO_2}V_{PC} + W_{PC}^{in}x_{CO,PC}^{in} \quad (68)$$

$$\frac{dn_{NO}}{dt} = -W_{PC}^{out}x_{NO,PC}^{out} + R_{NO}V_{PC} + W_{PC}^{in}x_{NO,PC}^{in} \quad (69)$$

$$\frac{dU}{dt} = \dot{H}_{in} - \dot{H}_{out} - \dot{Q}_{disp,PC} - \dot{Q}_{V,PC} \quad (74)$$

Process model – the equations

$$\left(\sum_{i=1}^{NC} n_i \tilde{c}_{v,i}\right) \frac{dT}{dt} = - \sum_{i=1}^{NC} (W_{i,PC}^{in} \int_{T^{in}}^T \tilde{c}_{p,i} dT) - \sum_{j=1}^{NR} \Delta H_j^R(T) R_j(T) + RT \frac{d}{dt} \left(\sum_{i=1}^{NC} n_i\right) - \dot{Q}_{disp,PC} - \dot{Q}_{V,PC} \quad (75)$$

$$\frac{dM_L}{dt} = \dot{G}_{H_2O}^{in} - \dot{G}_{L \rightarrow V} \quad (76)$$

$$\frac{dM_V}{dt} = \dot{G}_{L \rightarrow V} - \dot{G}_V \quad (77)$$

$$\Delta P_{SH} = 2f_D \rho_V v_V^2 \frac{L_{SH}}{D_{h,SH}} \quad (78)$$

$$\dot{G}_V = \rho_V A_V v_V \quad (79)$$

$$\dot{G}_V = A_V \sqrt{\frac{\rho_V D_{h,SH} \Delta P_{SH}}{2f_D L_{SH}}} \quad (80)$$

$$P = \exp\left(73.649 - \frac{7258.2}{T} - 7.3037 \log(T) + 4.1653 \times 10^{-6} \cdot T^2\right) \quad (81)$$

$$\dot{G}_{L \rightarrow V} = \frac{\dot{G}_{abs}^B - \dot{G}_{H_2O}^{in} \hat{c}_{p,L}(T_{eq} - T_{H_2O}^{in})}{\Delta H_{ev}(T_{eq})} \quad (82)$$

$$\Delta H_{ev}(T) = \Delta H_{ev}(T_{ref}) \left(\frac{1 - T_R}{1 - T_{R,ref}} \right) \quad T_R = \frac{T}{T_C} \quad (83)$$

$$\dot{G}_{H_2O}^{in} = \dot{G}_{H_2O}^{in,0} + k_p \left(\epsilon_c + \frac{1}{\tau_I} \int_0^t \epsilon_c dt \right) \quad (84)$$

Process model – the equations

$$\frac{dn_{g,B}}{dt} = W_{g,B}^{in} - W_{g,B}^{out} \quad (85)$$

$$W_{g,B}^{out} = \frac{\rho_g A_B v_g}{MW_{g,B}^{mix}} \quad (86)$$

$$\dot{H}_B^{in} - \dot{H}_B^{out} - \dot{Q}_{V,B} = 0 \quad (87)$$

$$m = \frac{1}{1 + \frac{155.3\sqrt{q}}{h_g}} \quad (88)$$

$$q = \frac{\dot{H}_B^{in}}{A_B^{exc}} \quad h_g = \int_{T_{ref}}^{T_{g,B}^{in}} \hat{c}_{p,g}^{mix} dT$$

$$\dot{Q}_{V,B} = m\dot{H}_{in} = m\dot{W}_{g,B} \int_{T_{ref}}^{T_{g,B}^{in}} \hat{c}_{p,g}^{mix} dT \quad (89)$$

$$\left(\frac{T_{g,B}^{rad,out}}{100}\right)^4 + 239 \cdot q \cdot \left(\frac{T_{g,B}^{rad,out}}{T_{ref} + \frac{h_g}{\hat{c}_{p,g}^{mix}}} - 1\right) = 0 \quad (90)$$

$$\dot{Q}_{V,B} = m\dot{H}_{in} = \frac{1}{\frac{461.9}{h_g^{0.15}}\sqrt{q}} W_{g,B}^{in} \int_{T_{ref}}^{T_{g,B}^{in}} \hat{c}_{p,g}^{mix} dT \quad (91)$$

$$1 + \frac{h_g}{h_g}$$

$$T_{g,B}^{rad,out} = T_{ref} + \frac{1000}{\frac{2.52}{\sqrt{q}} h_g^{0.15} + \frac{\hat{c}_{p,g}^{mix}}{h_g}} \quad (92)$$

$$W_{g,SH}^{in} = W_{g,B}^{out} + W_{L,SH} \quad (93)$$

$$W_{g,SH}^{in} \int_{T_{ref}}^{T_{g,SH}^{in}} \hat{c}_{p,g}^{mix} dT = W_{g,B}^{out} \int_{T_{ref}}^{T_{g,B}^{out}} \hat{c}_{p,g}^{mix} dT + W_{L,SH} \int_{T_{ref}}^{T_{L,SH}} \hat{c}_{p,A} dT \quad (94)$$

Process model – the equations

$$u_m = \frac{u_{in}s_t}{s_t - d_t} \text{ if } 2(s_d - d_t) \geq (s_t - d_t)$$

$$u_m = \frac{u_{in}s_t}{2(s_d - d_t)} \text{ if } 2(s_d - d_t) < (s_t - d_t)$$
(95)

$$h_{rad} = \sigma A_{G \rightarrow T} \left(\frac{\bar{T}_H + \bar{T}_C}{2} \right)^3$$
(96)

$$U = \frac{1}{\frac{1}{h_{int}} + \frac{1}{h_{conv} + h_{rad}} + f_{fou}}$$
(97)

$$\begin{cases} \eta = \frac{1 - \exp(-NTU(1-r))}{1 - r \cdot \exp(-NTU(1-r))} & \text{if } r \leq 0.98 \\ \eta = \frac{NTU}{1 + NTU} & \text{if } 0.98 < r \leq 1 \end{cases}$$

$$r = \frac{c_{MIN}}{c_{MAX}}$$
(98)

$$\begin{cases} c_{MIN} = \text{Min}\{F_H \hat{c}_{p,H}, F_C \hat{c}_{p,C}\} \\ c_{MAX} = \text{Max}\{F_H \hat{c}_{p,H}, F_C \hat{c}_{p,C}\} \end{cases}$$

$$NTU = \frac{UA_{GT}}{c_{MIN}}$$

$$T_C^{out} = T_C^{in} + \eta(T_{H,eff}^{in} - T_C^{in})$$
(99)

$$T_H^{out} = T_{H,eff}^{in} - \eta r(T_{H,eff}^{in} - T_C^{in})$$

$$T_C^{out} = T_C^{in} + \eta r(T_{H,eff}^{in} - T_C^{in})$$
(100)

$$T_H^{out} = T_{H,eff}^{in} - \eta(T_{H,eff}^{in} - T_C^{in})$$

$$\Delta P_{exc} = f_D \rho_g v_{g,MAX}^2 n_T$$
(101)

On-line optimization of continuous processes

Results:

Results.opt - Blocco note	
File Modifica Cerca ?	

DEMO CYCOM Plus : PROCEDURA DI OTTIMIZZAZIONE - RIEPILOGO	

Impianto Rifiuti Solidi Urbani	18-May-01

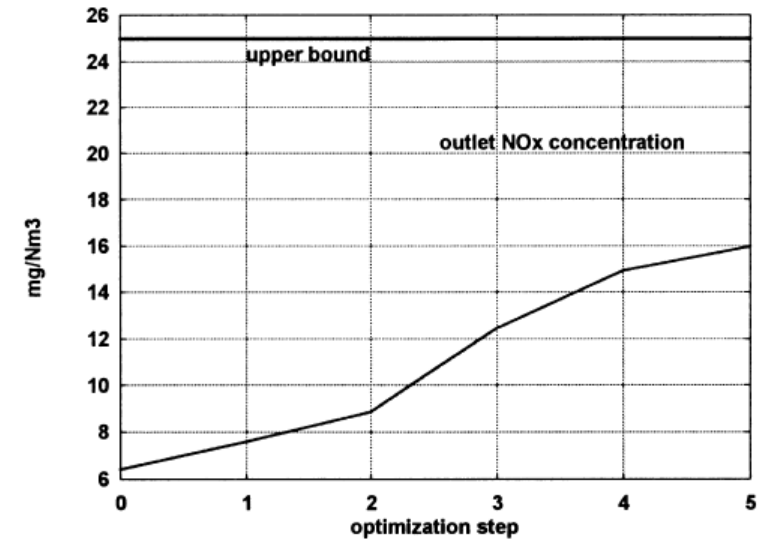
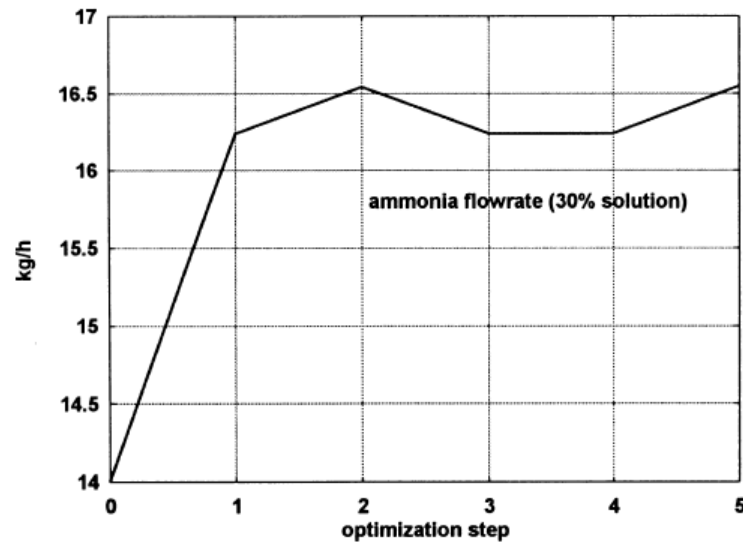
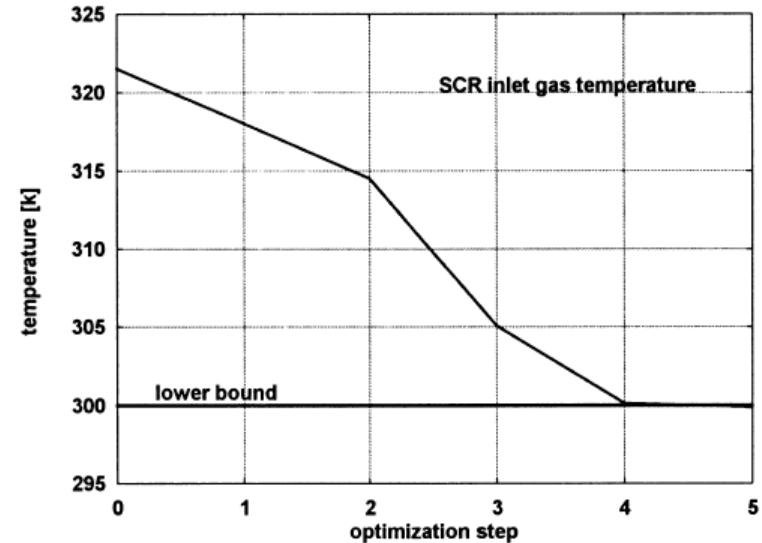
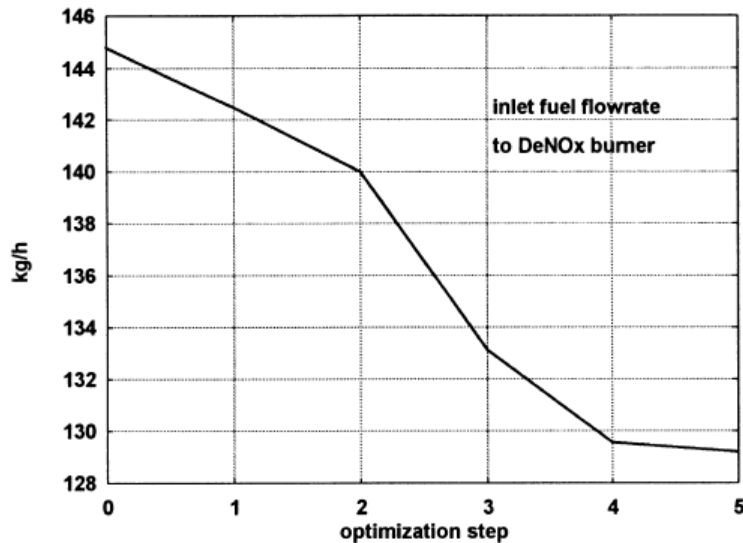
VALORE INIZIALE DEI GRADI DI LIBERTA':	
Portata di rifiuto (kg/h).....	5307.524000
Velocità di rotazione 1° rullo (rpm).....	5.465818E-02
Velocità di rotazione 2° rullo (rpm).....	7.363241E-02
Velocità di rotazione 3° rullo (rpm).....	7.366168E-02
Velocità di rotazione 4° rullo (rpm).....	6.911036E-02
Portata di CH4 al bruciatore DENOX (kg/h).....	164.789700
VINCOLI OPERATIVI:	
Massimo delta P primo rullo (mmH2O).....	75.000
Minimo delta P primo rullo (mmH2O).....	55.000
Massimo delta P secondo rullo (mmH2O).....	65.000
Minimo delta P secondo rullo (mmH2O).....	45.000
Massimo delta P terzo rullo (mmH2O).....	45.000
Minimo delta P terzo rullo (mmH2O).....	25.000
Massimo delta P quarto rullo (mmH2O).....	25.000
Minimo delta P quarto rullo (mmH2O).....	10.000
Ossigeno massimo in uscita dalla postcomb. (% vol).....	10.000
Ossigeno minimo in uscita dalla postcombust. (%vol).....	7.0000
Temperatura minima ingresso DENOX (^C).....	295.00
Temperatura massima ingresso DENOX (^C).....	310.00
Massima Portata Vapore (ton/h).....	21.000
Minima Portata Vapore (ton/h).....	15.000
Massimo contenuto di incomb. nelle ceneri (% mas).....	15.000
Massimo HCl al camino (mg/Nm3).....	10.000
Massimo SO2 al camino (mg/Nm3).....	50.000
Massimo NOx al camino (mg/Nm3).....	25.000

On-line optimization of continuous processes

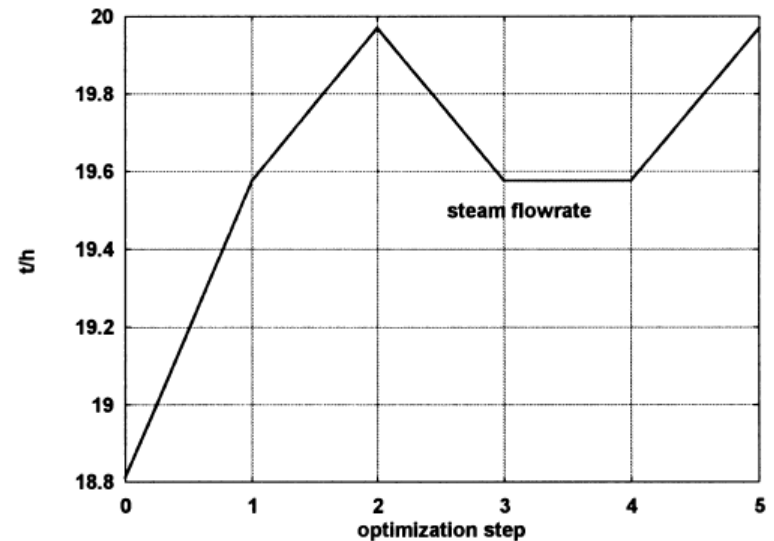
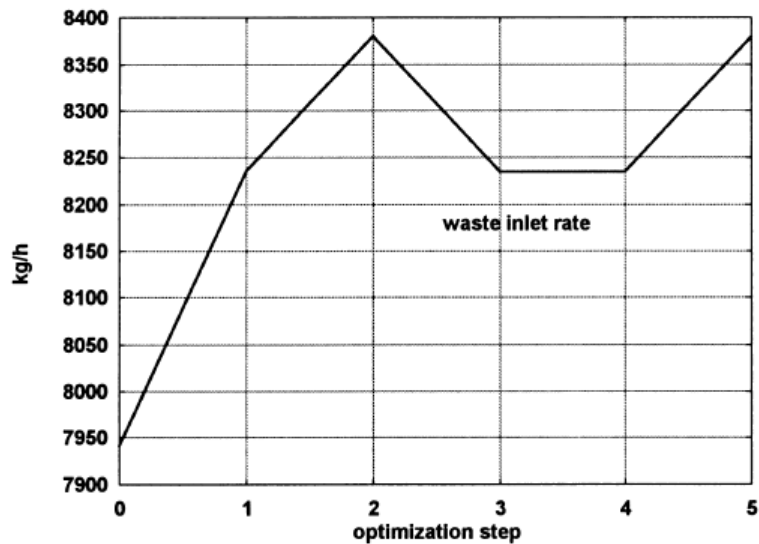
Results:

Results.opt - Blocco note	
File Modifica Cerca ?	
VALORE INIZIALE VARIABILI VINCOLATE:	
Massimo delta P primo rullo (mmH2O).....	78.102
Massimo delta P secondo rullo (mmH2O).....	50.640
Massimo delta P terzo rullo (mmH2O).....	30.424
Massimo delta P quarto rullo (mmH2O).....	15.295
Ossigeno massimo in uscita dalla postcomb. (% vol).....	10.765
Temperatura minima ingresso DENOX (^C).....	291.64
Massima Portata Vapore (ton/h).....	18.150
Massimo contenuto di incomb. nelle ceneri (% mas).....	1.4154
Massimo HCl al camino (mg/Nm3).....	.95055
Massimo SO2 al camino (mg/Nm3).....	4.7685
Massimo NOx al camino (mg/Nm3).....	24.756
VALORE FINALE GRADI DI LIBERTA':	
Portata di rifiuto (kg/h).....	6031.404000
Velocità di rotazione 1° rullo (rpm).....	7.811134E-02
Velocità di rotazione 2° rullo (rpm).....	7.541323E-02
Velocità di rotazione 3° rullo (rpm).....	7.092959E-02
Velocità di rotazione 4° rullo (rpm).....	6.601541E-02
Portata di CH4 al bruciatore DENOX (kg/h).....	168.642900
VALORE FINALE VARIABILI VINCOLATE:	
Massimo delta P primo rullo (mmH2O).....	61.455
Massimo delta P secondo rullo (mmH2O).....	56.641
Massimo delta P terzo rullo (mmH2O).....	36.934
Massimo delta P quarto rullo (mmH2O).....	18.612
Ossigeno massimo in uscita dalla postcom. (% vol).....	9.5163
Temperatura minima ingresso DENOX (^C).....	294.90
Massimo diff. di rif. bruciato 1-3 rulli (kg/h).....	294.90
Temperatura massima postcombustione (^C).....	20.989
Massimo HCl al camino (mg/Nm3).....	2.2035
Massimo SO2 al camino (mg/Nm3).....	1.0763
Massimo NOx in ingresso al DENOX (mg/Nm3).....	5.3944
Massimo NH3 al camino (mg/Nm3).....	24.901
VALORE INIZIALE FUNZIONE OBIETTIVO:	1,207,303 Lit/h
VALORE FINALE FUNZIONE OBIETTIVO:	1,319,730 Lit/h
FUNZIONE OBIETTIVO INCREMENTATA DEL	9.31 %

On-line optimization of continuous processes



On-line optimization of continuous processes



Rovaglio, M., Manca, D., Rusconi, F. Waste Management 18, 525-538, (1998)

Case-study #2

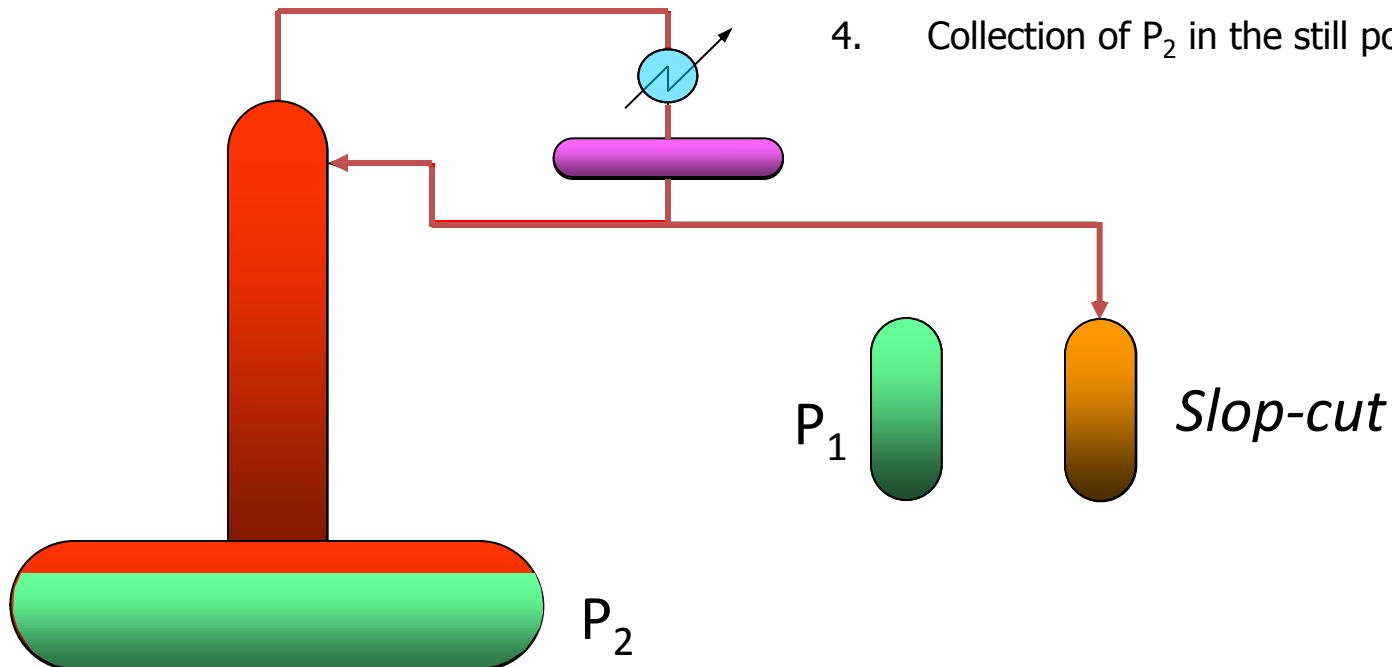
On-line optimization of discontinuous processes



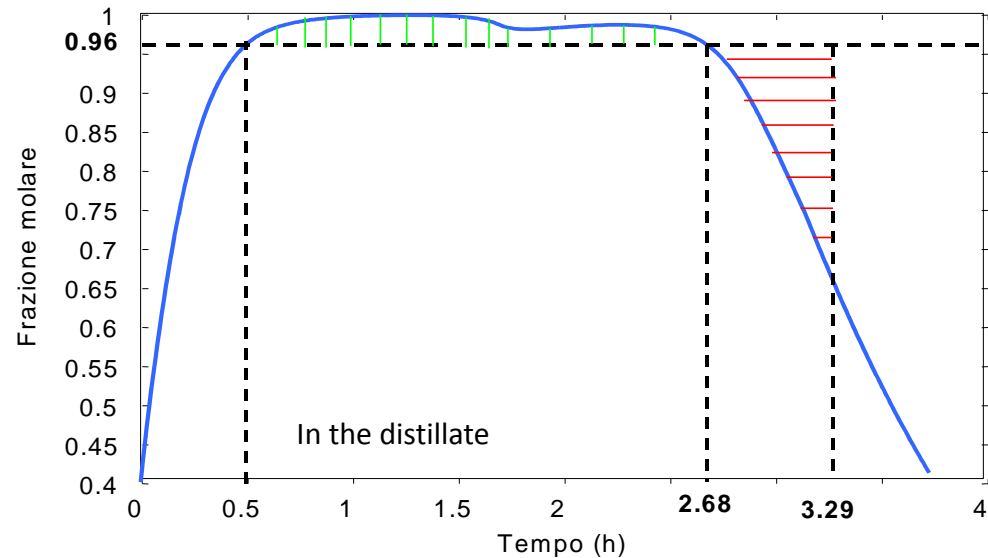
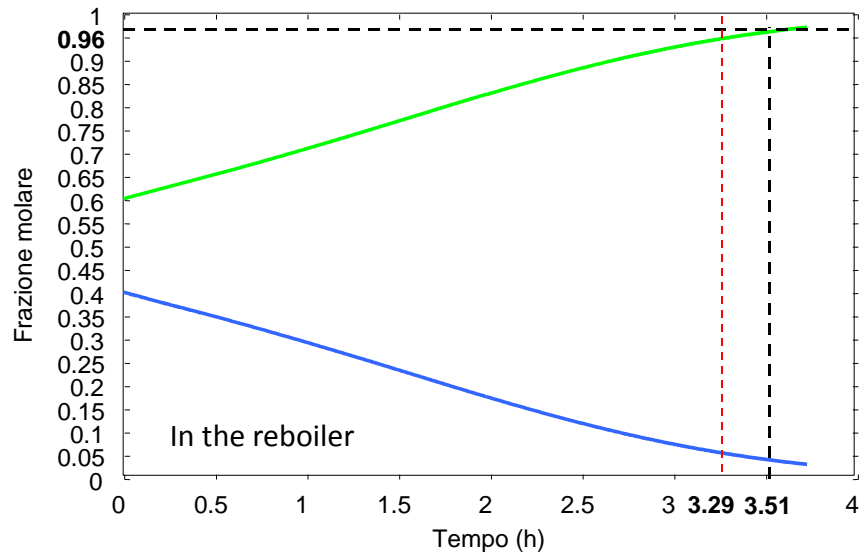
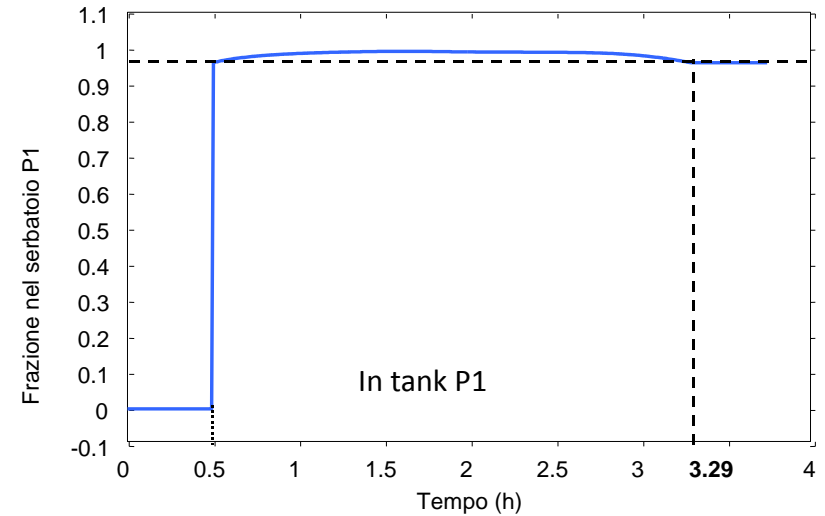
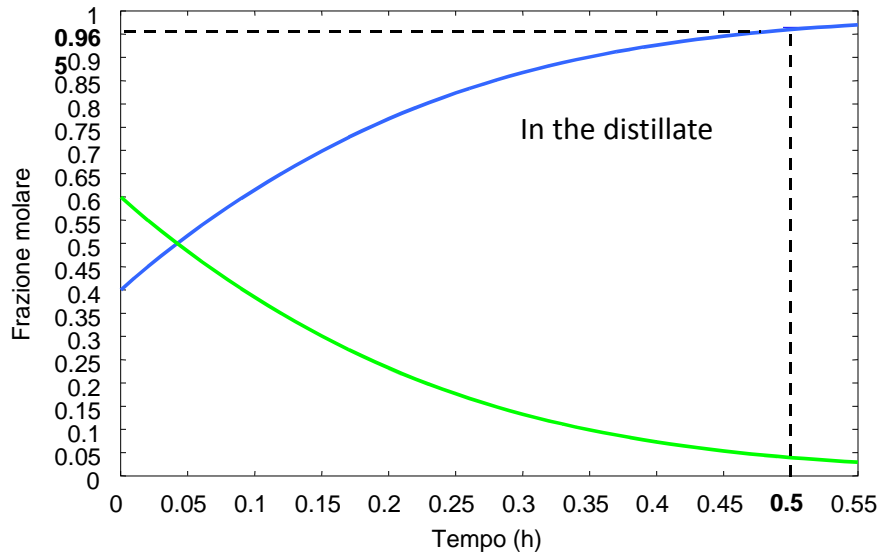
On-line optimization of discontinuous processes

Two-components batch distillation

1. Total reflux
2. Collection of P_1 in the dedicated tank
3. Out-of-spec collection in the "slop-cut"
4. Collection of P_2 in the still pot



Optimal trajectory



Light component
 Heavy component

D. Manca. Chemical Product and Process Modeling, 2,12 (2007)



Optimal trajectory

- There are three distinct approaches to the selection of the **objective function** when distillation batch processes are involved:

1. Maximizing the product quantity

Converse and Gross (1963) were the first researchers to face the optimization problem for a batch distillation column. Logsdon *et al.* (1990) solved the NLP.

2. Minimization of the distillation time

The reflux profile is divided into a number of intervals with the target of reducing the total distillation time (Coward, 1967). Mujtaba and Macchietto (1988) solved the problem adopting the SQP algorithm.

3. Profit maximization

The method is based on a profit function, for instance the *capacity factor*, that takes into account both the quantity/quality of the product and the total distillation time. Kerkhof and Vissers (1978), Logsdon *et al.* (1990), Diwekar (1992).

Optimal trajectory

- There are three distinct approaches to the selection of the **degrees of freedom** when distillation batch processes are involved:

1. Constant reflux distillation

The degrees of freedom are: pressure, vapor flowrate inside the column, distillate flowrate.

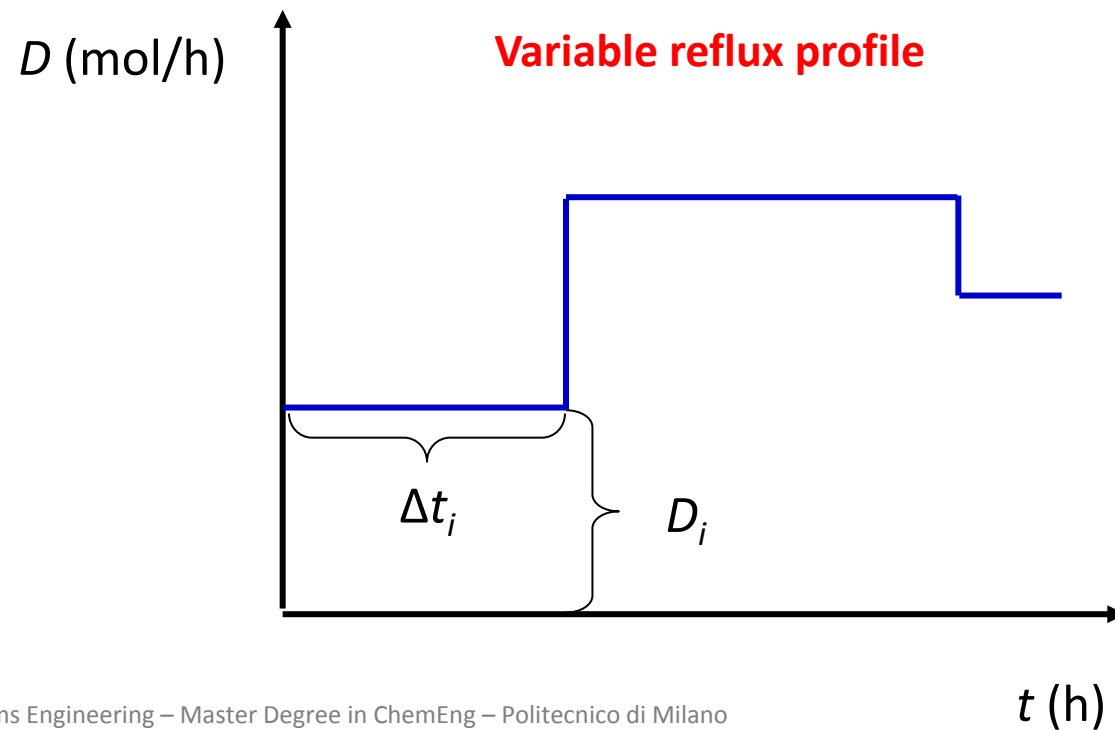
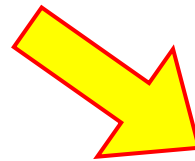
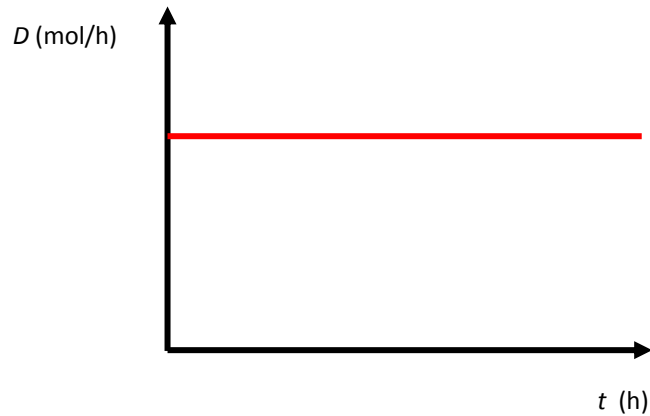
2. Constant composition

The degrees of freedom are: pressure, vapor flowrate, and the purity of the key component that remains constant throughout the batch.

3. Variable reflux profile

The degrees of freedom are: pressure and reflux ratio (or equivalently the distillate flowrate) at every time of the batch → **Optimal trajectory**.

Optimal trajectory



Optimal trajectory

$$\underset{\Delta t_i, D_i}{Max} \left\{ \frac{P_1 + P_2}{0.5 + t_{tot}} \right\}$$

Capacity Factor
Luyben (1978)

s.t.

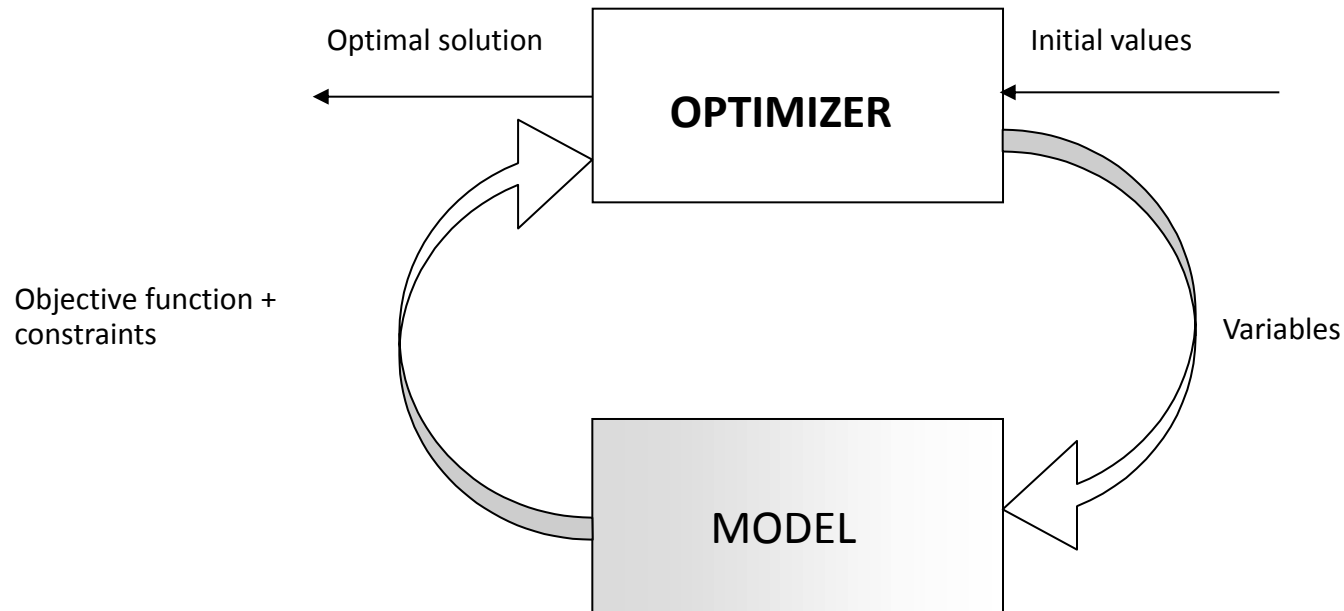
$$\left\{ \begin{array}{l} g(x, x', u, \eta, t) = 0 \\ \bar{x}_{Pi} = x_{Di}^{spec} \\ 0 \leq D_i \leq D_{max} \\ 0 \leq \Delta t_i \leq t_{max} \end{array} \right.$$

The **DAE** system comprises

(NS+2)(NC-1)+1	ODE (mass + energy balances)
(NS+1) NC	AE (thermodynamic equilibria)
(NS+2)	AE (stoichiometric equations)

D. Manca. Chemical Product and Process Modeling, 2,12 (2007)

Optimal trajectory



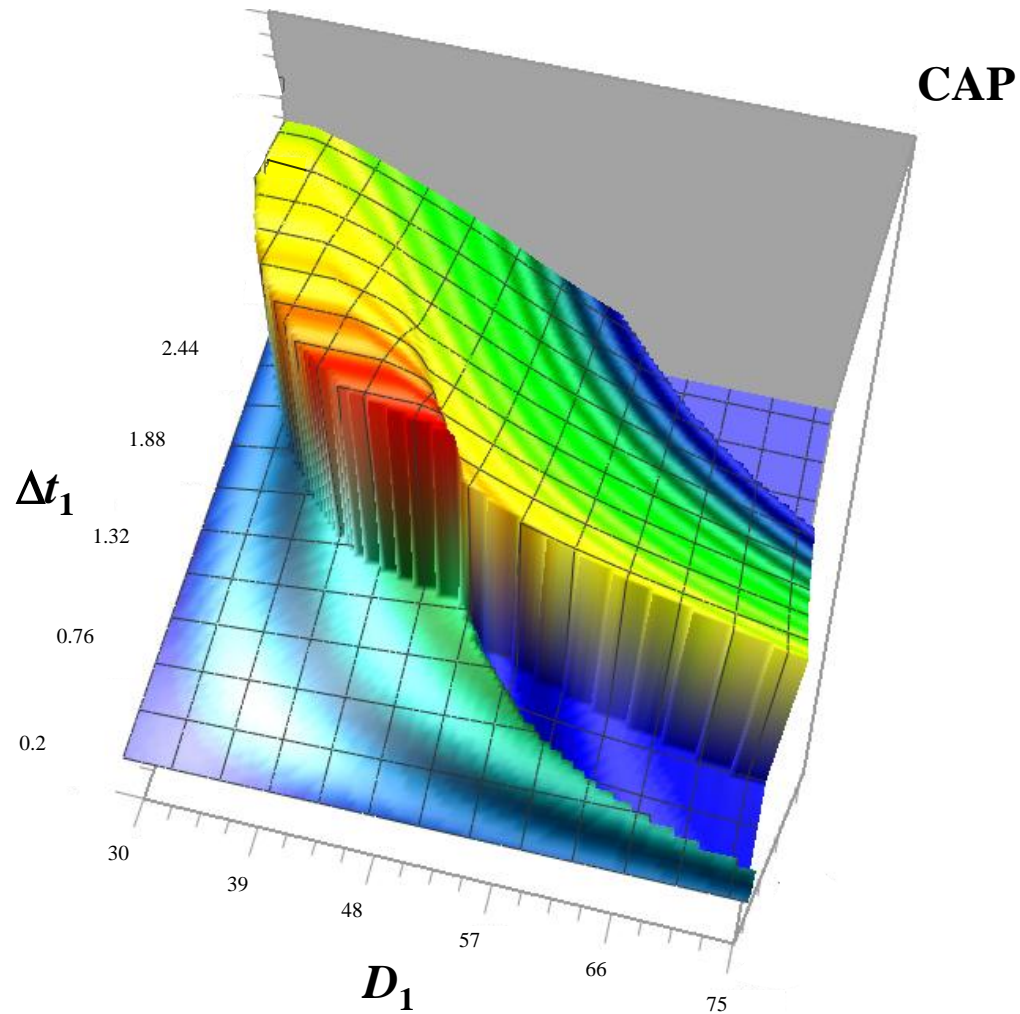
OPTIMIZATION METHODS

SQP

Simplex

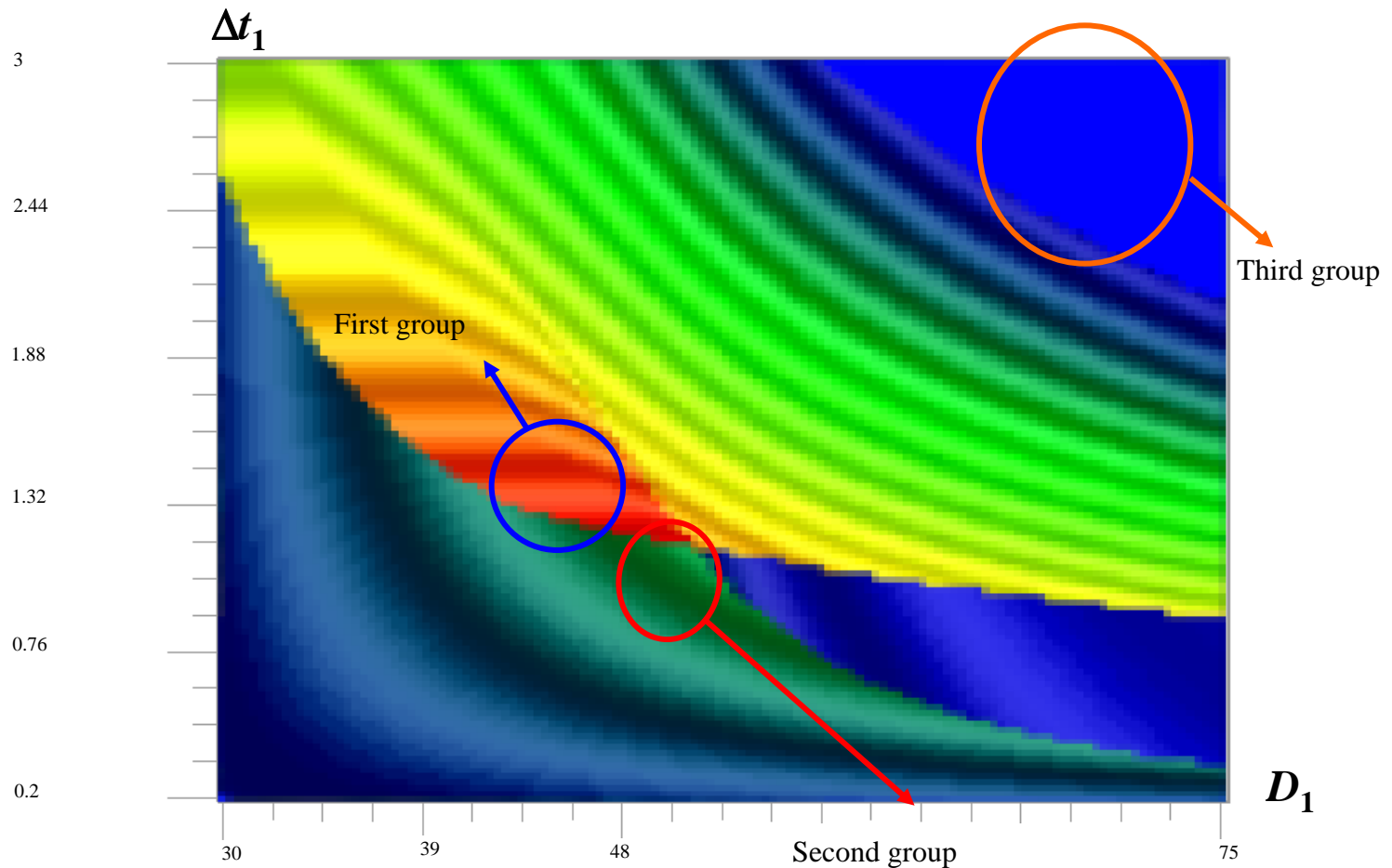
Robust method searching the solution within the entire domain of the *dof*

Optimal trajectory



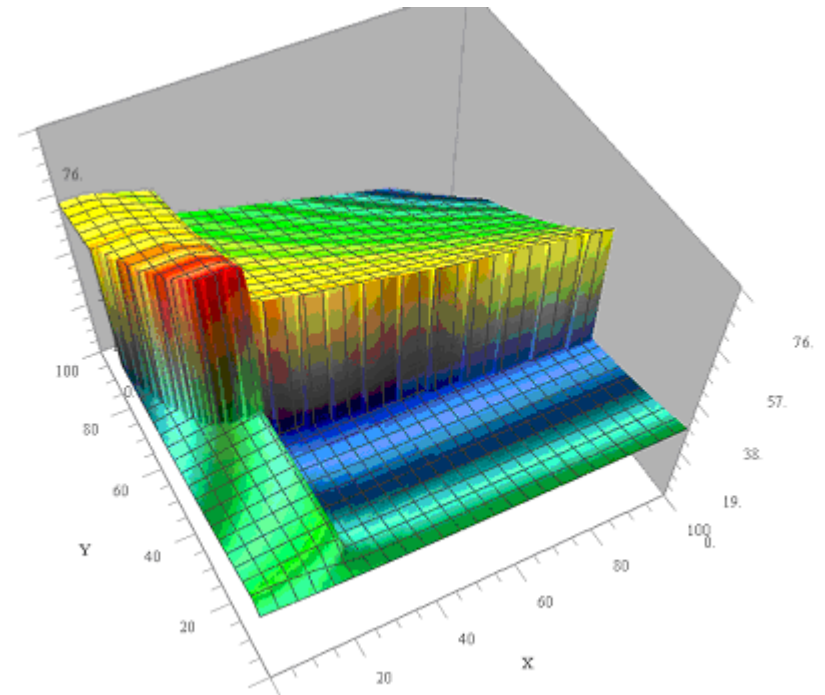
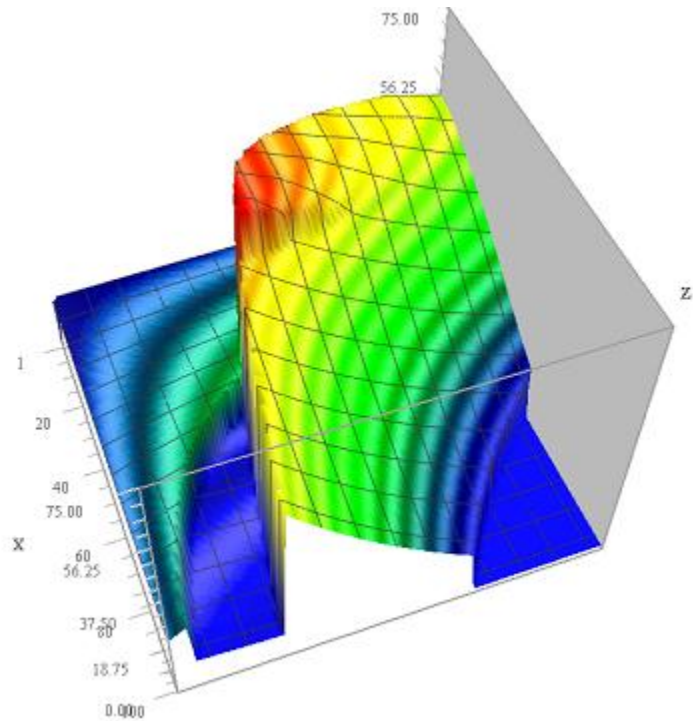
D. Manca. Chemical Product and Process Modeling, 2,12 (2007)

Optimal trajectory



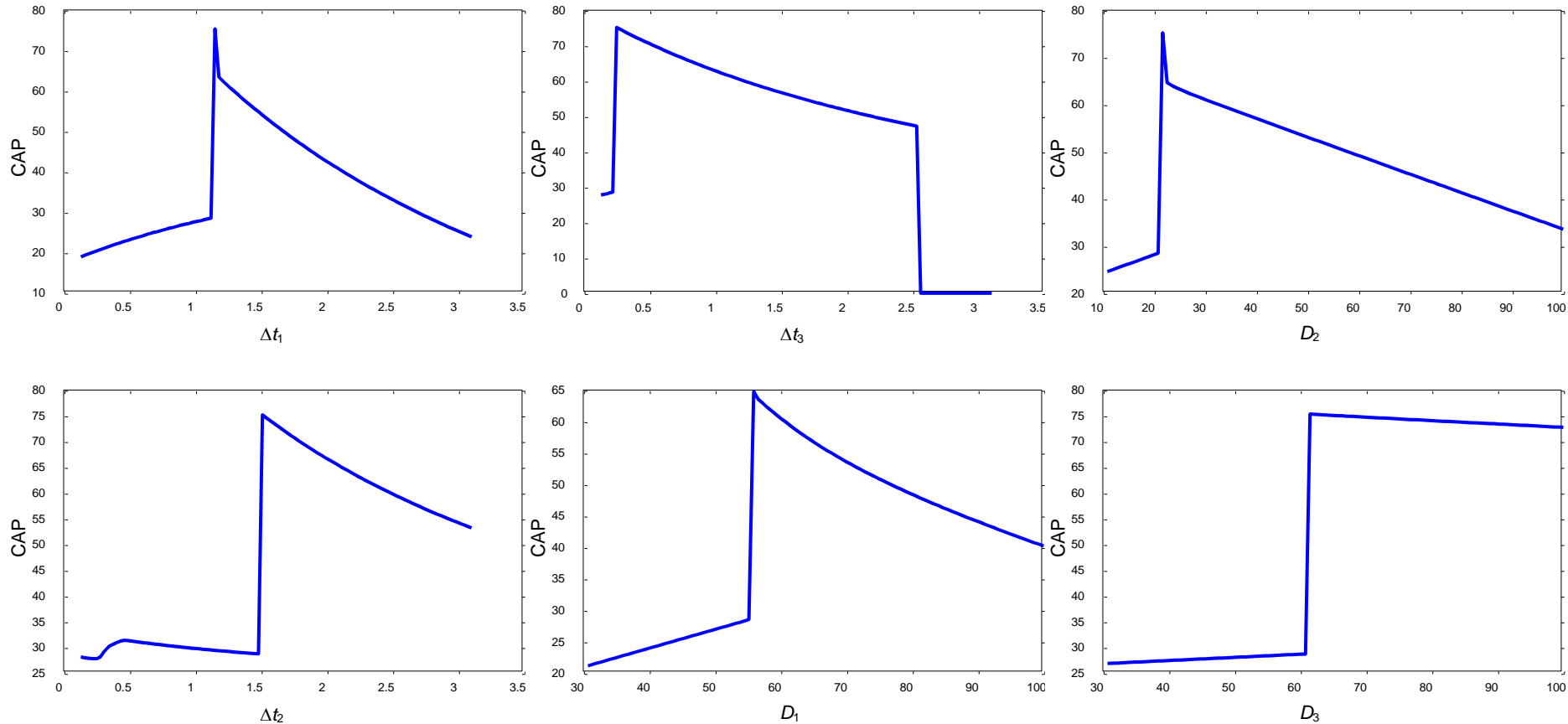
D. Manca. Chemical Product and Process Modeling, 2,12 (2007)

Optimal trajectory



D. Manca. Chemical Product and Process Modeling, 2,12 (2007)

Optimal trajectory



The objective function, CAP, as a function of the six *dof* respect to the absolute optimum value.

Case-study #3

Model based control of industrial processes



Introduction

- Industrial processes are characterized by the following control problems:
 1. The **process** is almost usually **multivariate**
 - several controlled variables: y_1, y_2, \dots, y_n
 - several manipulated variables: u_1, u_2, \dots, u_m
 - several disturbance variables: d_1, d_2, \dots, d_k
 2. **Complex dynamic** behaviour:
 - *time delays* due to the inertia of the system (either material or energetic), mass flow in the pipes, long measuring times
 - Inverse response
 - possible instability at open-loop

Introduction

3. Intrinsic **nonlinearity** of the system

4. **Operative constraints** that are quite dissimilar and complex

- constraints on the input and output variables
- constraints on the changing rate of the input variables
- Constraints on the optimal value of the input variables (*e.g.*, economic value)
- process and law constraints
- soft and hard constraints



Model based control

An **ideal control system** should be:

- Multivariable and capable of managing:
 - time delays,
 - inverse response,
 - process and law constraints,
 - measurable and non-measurable disturbances
- Minimize the control effort
- Able of inferring the unmeasured/unmeasurable variables from the measured ones
- Robust respect to the modeling errors/simplifications and the noise of the measured variables
- Able to manage both the startups and shutdowns (either programmed or emergency) as well as the steady-state conditions

Model based control

- The availability of **dynamic numerical models** of:
 - chemical/industrial processes,
 - unit operations
 - process units,
 - plant subsections
 - ...

allows **forecasting the response** of the simulated plant/process to possible **disturbances** and **manipulated variables**.

- The availability of such **dynamic numerical models** paves the way to the so-called: **model based control**.
- The model of the process can be *used* to forecast the system response to a set of control actions originated by modifying a suitable set of manipulated variables.

Model based control

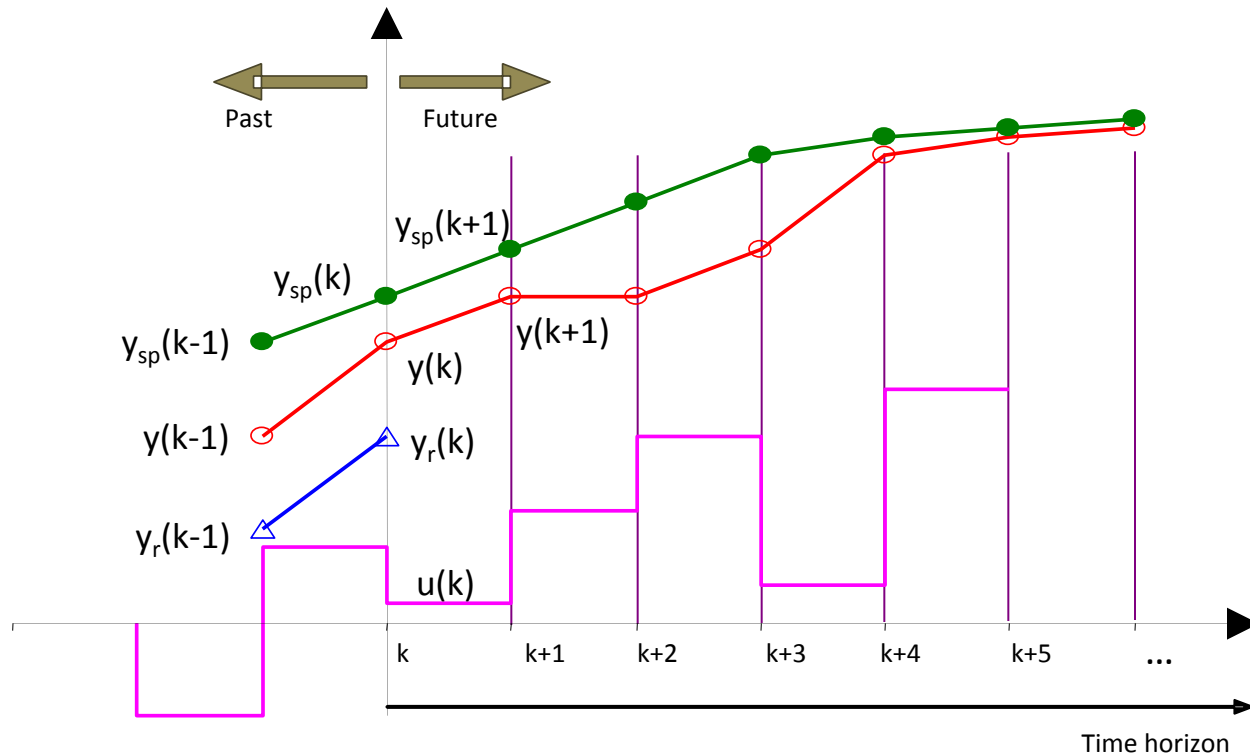
- We are going to answer the following question:

What is the response of the system to a modification of the manipulated variables?

- More specifically, we can imagine to deploy an optimizing procedure that looks for the best response of the system subject to the manipulation of the process variables.
- According to the most simplified approach, we have:
 - the control specifications, *i.e.* the setpoint
 - the objective function that measures the distance of the controlled variable from the setpoint
 - the dynamic model of the system usually described by a DAE system, which plays the role of the equality constraints
 - the manipulated variables that are the degrees of freedom of optimization problem



Model predictive control



y_{sp} = y set point (setpoint **trajectory**)

y = y model response

y_r = y real, measured response

u = manipulated variable

MPC features

- The system follows a specified trajectory \rightarrow optimal setpoint trajectory, y_{sp}
- The model is called to produce a prediction, y , of the real response of the system.
- We have:
 - response in the future: $y(k+1)$, $y(k+2)$, $y(k+3)$, ...
 - respect to past real inputs: $u(k)$, $u(k-1)$, $u(k-2)$, ...
 - respect to future manipulated inputs: $u(k+1)$, $u(k+2)$, ...
- The numerical model of the process to be controlled is *used* to evaluate a sequence of control actions that optimize an objective function to:
 - Minimize the system response y respect to the optimal set-point trajectory, y_{sp}
 - Minimize the control effort

MPC features

- Since the model is a simplified representation of the real system, it is intrinsically not perfect. This means that there is a discrepancy between the real system and the modeled one.
- The present error ε_k between the real system and the model is:

$$\varepsilon_k = y_r(k) - y(k)$$

- This error is kept constant and it is used for future forecasts.

MPC mathematical formulation

$$\min_{\mathbf{u}(k), \mathbf{u}(k+1), \dots, \mathbf{u}(k+h_c-1)} \left\{ \sum_{j=k+1}^{k+h_p} [\omega_y \mathbf{e}_y^2(j) + \mathbf{P}\mathbf{F}_y(j)] + \sum_{i=k}^{k+h_p-1} [\omega_u \Delta \mathbf{u}^2(i) + \mathbf{P}\mathbf{F}_u(i)] + \sum_{l=k}^{k+h_p-1} \omega_T \delta \mathbf{u}_T^2(l) \right\}$$

$$\mathbf{e}_y(j) = \frac{[\mathbf{y}(j) + \delta_y(k)] - \mathbf{y}_{sp}(j)}{\mathbf{y}_{sp}(j)} \quad \delta_y(k) = \mathbf{y}_r(k) - \mathbf{y}(k) = \mathbf{y}_{real}(k) - \mathbf{y}_{model}(k)$$

$$\mathbf{P}\mathbf{F}_y(j) = \left\{ \text{Max} \left[\mathbf{0}, \frac{\mathbf{y}(j) - \mathbf{y}_{MAX}}{\mathbf{y}_{MAX}} \right] \right\}^2 + \left\{ \text{Min} \left[\mathbf{0}, \frac{\mathbf{y}(j) - \mathbf{y}_{MIN}}{\mathbf{y}_{MIN}} \right] \right\}^2$$

$$\Delta \mathbf{u}(i) = \frac{\mathbf{u}(i) - \mathbf{u}(i-1)}{\mathbf{u}(i-1)} \quad \Delta \mathbf{u}_{MIN} \leq \Delta \mathbf{u}(i) \leq \Delta \mathbf{u}_{MAX}$$

$$\mathbf{P}\mathbf{F}_u(i) = \left\{ \text{Max} \left[\mathbf{0}, \frac{\mathbf{u}(i) - \mathbf{u}_{MAX}}{\mathbf{u}_{MAX}} \right] \right\}^2 + \left\{ \text{Min} \left[\mathbf{0}, \frac{\mathbf{u}(i) - \mathbf{u}_{MIN}}{\mathbf{u}_{MIN}} \right] \right\}^2$$

$$\delta \mathbf{u}_T(l) = \mathbf{u}(l) - \mathbf{u}_T(l)$$

$$s.t. \begin{cases} \mathbf{h}(\mathbf{y}, \mathbf{u}, \mathbf{d}, t) = \mathbf{0} \\ \mathbf{f}(\mathbf{y}', \mathbf{y}, \mathbf{u}, \mathbf{d}, t) = \mathbf{0} \end{cases}$$

MPC mathematical formulation

$$\min_{\mathbf{u}(k), \mathbf{u}(k+1), \dots, \mathbf{u}(k+h_c-1)} \{ \dots \}$$

MPC mathematical formulation

$$\min_{\mathbf{u}(k), \mathbf{u}(k+1), \dots, \mathbf{u}(k+h_c-1)} \left\{ \sum_{j=k+1}^{k+h_p} \left[\boldsymbol{\omega}_y \mathbf{e}_y^2(j) + \mathbf{PF}_y(j) \right] + \dots \right\}$$

$$\mathbf{e}_y(j) = \frac{[\mathbf{y}(j) + \boldsymbol{\delta}_y(k)] - \mathbf{y}_{sp}(j)}{\mathbf{y}_{sp}(j)} \quad \boldsymbol{\delta}_y(k) = \mathbf{y}_r(k) - \mathbf{y}(k) = \mathbf{y}_{real}(k) - \mathbf{y}_{model}(k)$$

$$\mathbf{PF}_y(j) = \left\{ \text{Max} \left[\mathbf{0}, \frac{\mathbf{y}(j) - \mathbf{y}_{MAX}}{\mathbf{y}_{MAX}} \right] \right\}^2 + \left\{ \text{Min} \left[\mathbf{0}, \frac{\mathbf{y}(j) - \mathbf{y}_{MIN}}{\mathbf{y}_{MIN}} \right] \right\}^2$$

MPC mathematical formulation

$$\min_{\mathbf{u}(k), \mathbf{u}(k+1), \dots, \mathbf{u}(k+h_c-1)} \left\{ \dots + \sum_{i=k}^{k+h_p-1} \left[\boldsymbol{\omega}_u \Delta \mathbf{u}^2(i) + \mathbf{PF}_u(i) \right] + \dots \right\}$$

$$\Delta \mathbf{u}(i) = \frac{\mathbf{u}(i) - \mathbf{u}(i-1)}{\mathbf{u}(i-1)} \quad \Delta \mathbf{u}_{MIN} \leq \Delta \mathbf{u}(i) \leq \Delta \mathbf{u}_{MAX}$$

$$\mathbf{PF}_u(i) = \left\{ \text{Max} \left[\mathbf{0}, \frac{\mathbf{u}(i) - \mathbf{u}_{MAX}}{\mathbf{u}_{MAX}} \right] \right\}^2 + \left\{ \text{Min} \left[\mathbf{0}, \frac{\mathbf{u}(i) - \mathbf{u}_{MIN}}{\mathbf{u}_{MIN}} \right] \right\}^2$$

In general, $\Delta \mathbf{u}_{MIN}$ is negative

MPC mathematical formulation

$$\min_{\mathbf{u}(k), \mathbf{u}(k+1), \dots, \mathbf{u}(k+h_c-1)} \left\{ \dots + \dots + \sum_{l=k}^{k+h_p-1} \omega_T \delta \mathbf{u}_T^2(l) \right\}$$
$$\delta \mathbf{u}_T(l) = \mathbf{u}(l) - \mathbf{u}_T(l)$$

$T =$ target.

It can be the same optimal value of the steady state conditions for the manipulated variables (*e.g.*, nominal operating conditions).

MPC mathematical formulation

$$\min_{\mathbf{u}(k), \mathbf{u}(k+1), \dots, \mathbf{u}(k+h_c-1)} \left\{ \sum_{j=k+1}^{k+h_p} [\omega_y \mathbf{e}_y^2(j) + \mathbf{PF}_y(j)] + \sum_{i=k}^{k+h_p-1} [\omega_u \Delta \mathbf{u}^2(i) + \mathbf{PF}_u(i)] + \sum_{l=k}^{k+h_p-1} \omega_T \delta \mathbf{u}_T^2(l) \right\}$$

$$\mathbf{e}_y(j) = \frac{[\mathbf{y}(j) + \delta_y(k)] - \mathbf{y}_{sp}(j)}{\mathbf{y}_{sp}(j)} \quad \delta_y(k) = \mathbf{y}_r(k) - \mathbf{y}(k) = \mathbf{y}_{real}(k) - \mathbf{y}_{model}(k)$$

$$\mathbf{PF}_y(j) = \left\{ \text{Max} \left[\mathbf{0}, \frac{\mathbf{y}(j) - \mathbf{y}_{MAX}}{\mathbf{y}_{MAX}} \right] \right\}^2 + \left\{ \text{Min} \left[\mathbf{0}, \frac{\mathbf{y}(j) - \mathbf{y}_{MIN}}{\mathbf{y}_{MIN}} \right] \right\}^2$$

$$\Delta \mathbf{u}(i) = \frac{\mathbf{u}(i) - \mathbf{u}(i-1)}{\mathbf{u}(i-1)} \quad \Delta \mathbf{u}_{MIN} \leq \Delta \mathbf{u}(i) \leq \Delta \mathbf{u}_{MAX}$$

$$\mathbf{PF}_u(i) = \left\{ \text{Max} \left[\mathbf{0}, \frac{\mathbf{u}(i) - \mathbf{u}_{MAX}}{\mathbf{u}_{MAX}} \right] \right\}^2 + \left\{ \text{Min} \left[\mathbf{0}, \frac{\mathbf{u}(i) - \mathbf{u}_{MIN}}{\mathbf{u}_{MIN}} \right] \right\}^2$$

$$\delta \mathbf{u}_T(l) = \mathbf{u}(l) - \mathbf{u}_T(l)$$

$$s.t. \begin{cases} \mathbf{h}(\mathbf{y}, \mathbf{u}, \mathbf{d}, t) = \mathbf{0} \\ \mathbf{f}(\mathbf{y}', \mathbf{y}, \mathbf{u}, \mathbf{d}, t) = \mathbf{0} \end{cases}$$

Critical elements of the MPC

$$h_c$$

$$h_p$$

$$\omega_y$$

$$\omega_u$$

$$\omega_T$$

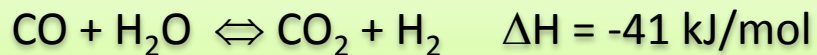
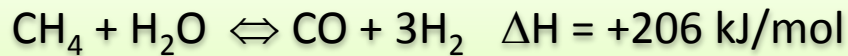
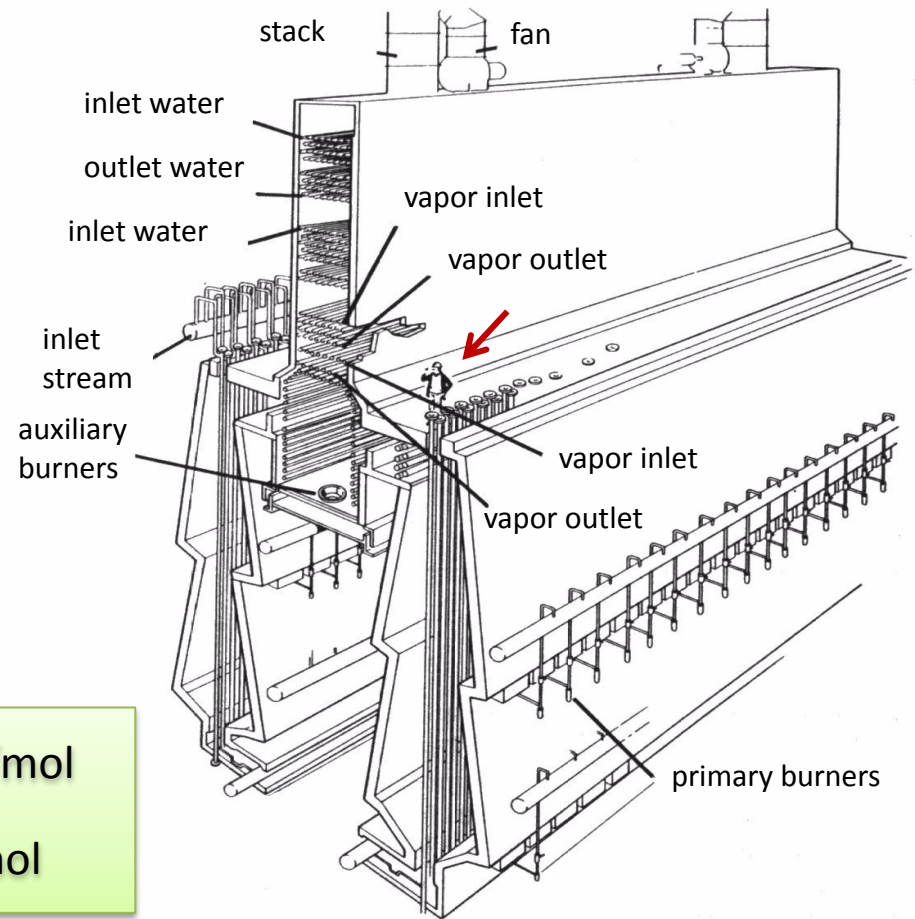
$$\delta_y(k)$$

$$y = y_{model}$$

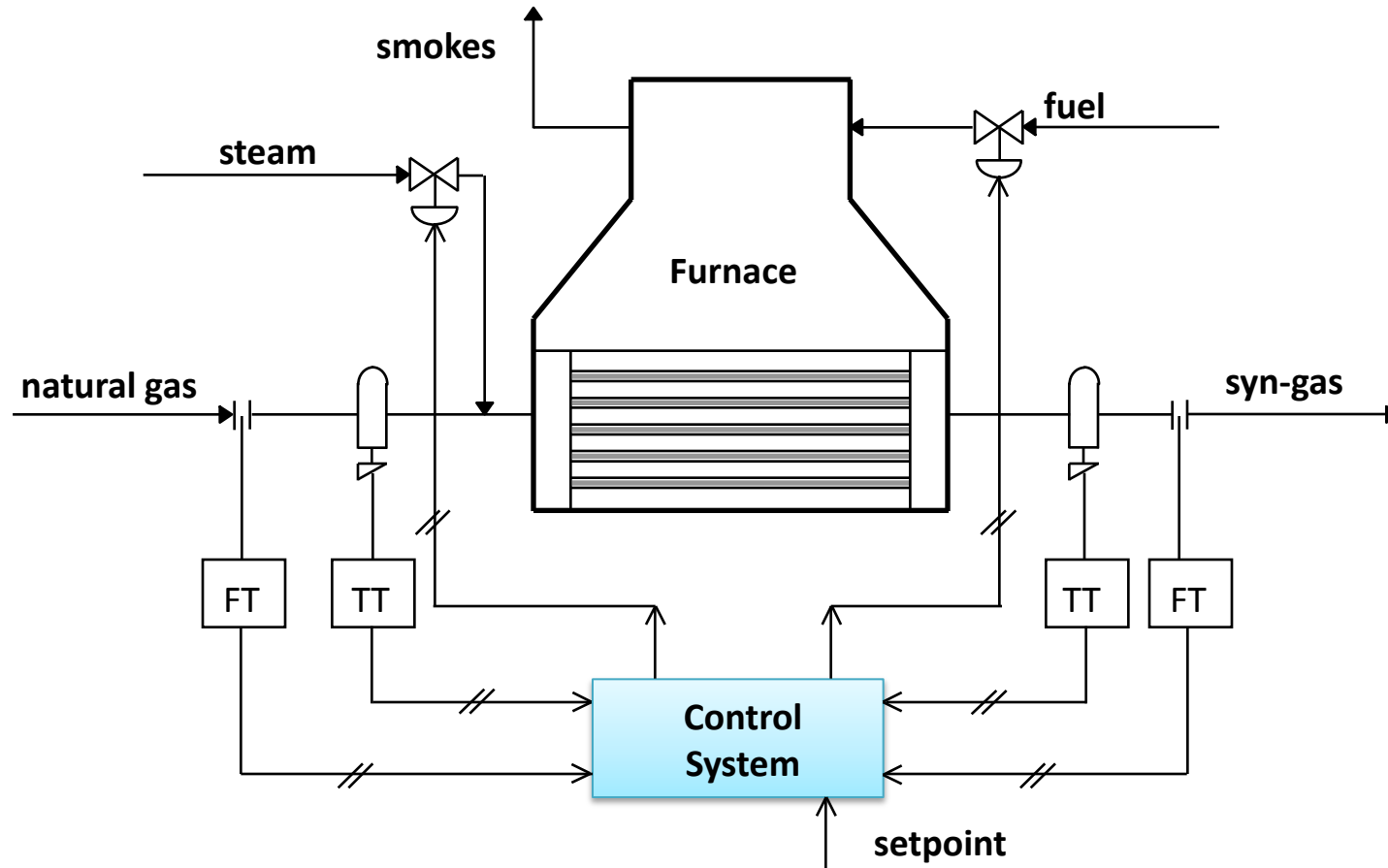
$$\Delta u$$

$$u_T$$

MPC of the steam reforming process



Control layout of the steam reforming section



Process model

We start from the steady-state model of Singh and Saraf (1979)

Main assumptions:

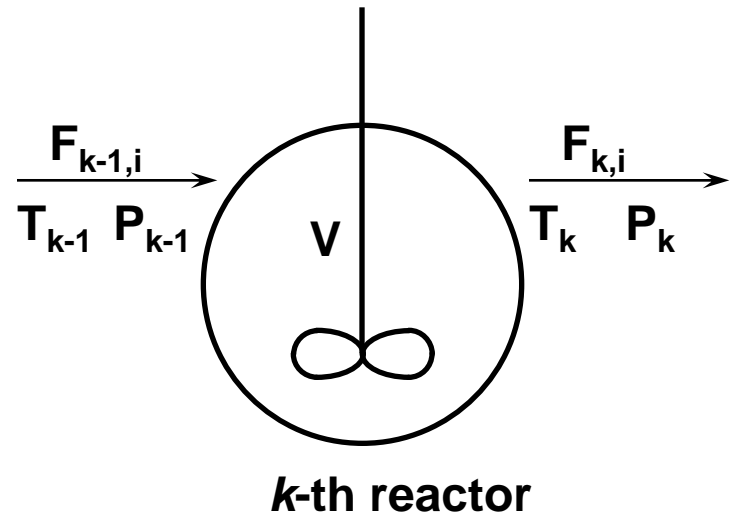
- pseudo-homogeneous
- monodimensional model: neither axial nor radial dispersions
- discretization into a series of CSTR
- subdivision into layers of the pipe thickness

Process model: inside the reforming pipes

Material balance

$$\frac{dW_{i,k}}{dt} = F_{i,k-1} - F_{i,k} + \sum_{j=1}^{NR} \nu_{i,j} \cdot R_{j,k} \cdot V$$

$$k = 1, \dots, NCSTR \quad i = 1, \dots, NC$$



Energy balance on the gas-catalyst system

$$\begin{aligned} & \left(c_{p,mix,k} \cdot W_{tot,k} + c_{p,cat} \cdot \rho_{cat} \cdot V \right) \cdot \frac{dT_k}{dt} = (T_{k-1} - T_k) \cdot c_{p,mix,k-1} \cdot F_{tot,k-1} + \\ & + \pi \cdot D_{in} \cdot h_{in,k} \cdot (T_{p,in,k} - T_k) \cdot dz + \sum_{j=1}^{NR} R_{j,k} \cdot (-\Delta H_{j,k}) \cdot V \end{aligned}$$

Process model: pipes

Balance on the i -th discretized layer

$$\rho_{met} \cdot V_{met} \cdot c_{p,met} \cdot \frac{dT_i}{dt} = \frac{k_{met}}{\frac{\Delta x}{2}} \cdot (T_{i+1/2} - T_i) \cdot \pi \cdot dz \cdot \frac{D_{i+1/2} - D_i}{\ln\left(\frac{D_{i+1/2}}{D_i}\right)} +$$

$$- \frac{k_{met}}{\frac{\Delta x}{2}} (T_i - T_{i-1/2}) \cdot \pi \cdot dz \cdot \frac{D_i - D_{i-1/2}}{\ln\left(\frac{D_i}{D_{i-1/2}}\right)}$$

Flux continuity

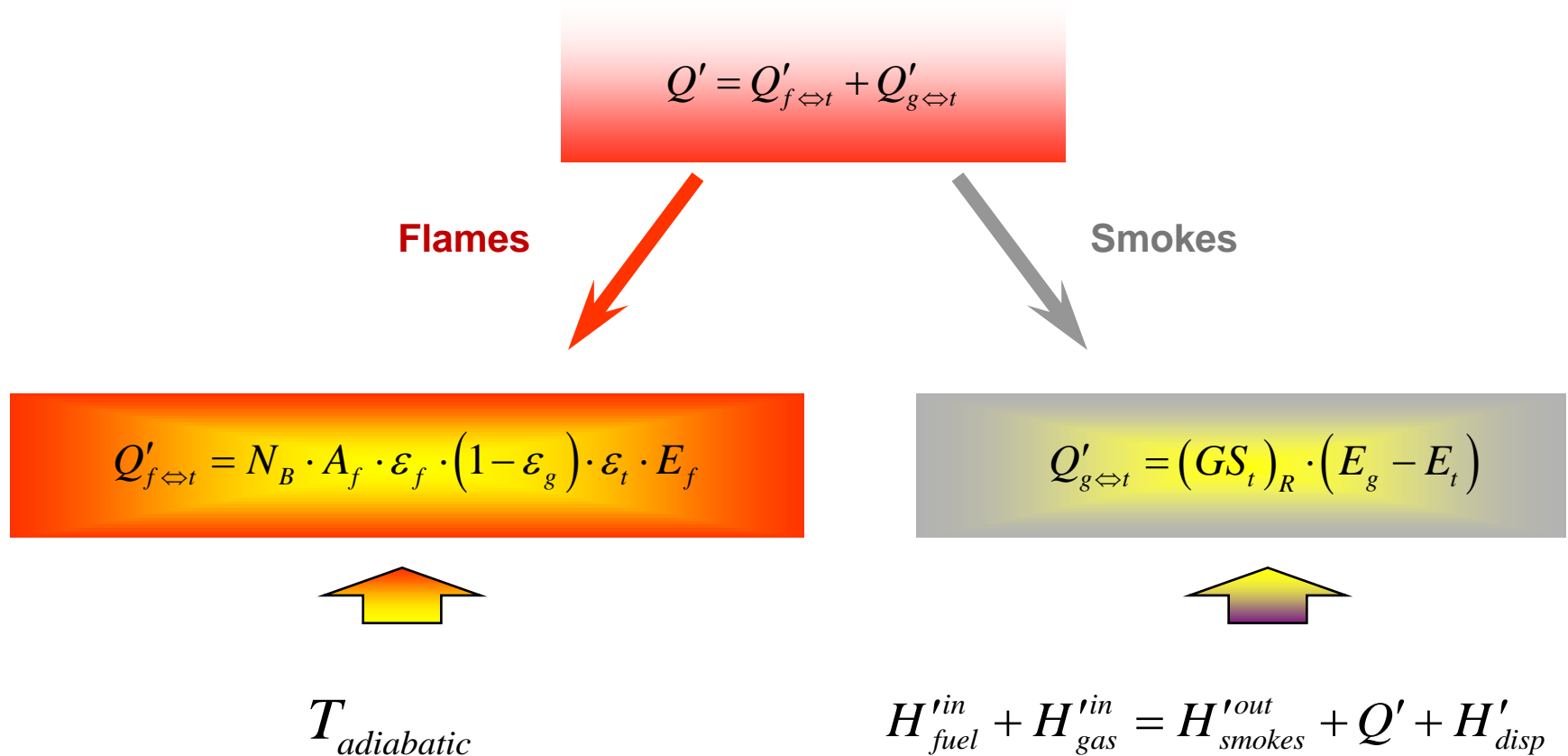
Internal surface

$$h_{in} \cdot (T_{p,in} - T) = \frac{2 \cdot k_{met} \cdot (T_1 - T_{p,in})}{D_{in} \cdot \ln\left(\frac{D_1}{D_{in}}\right)}$$

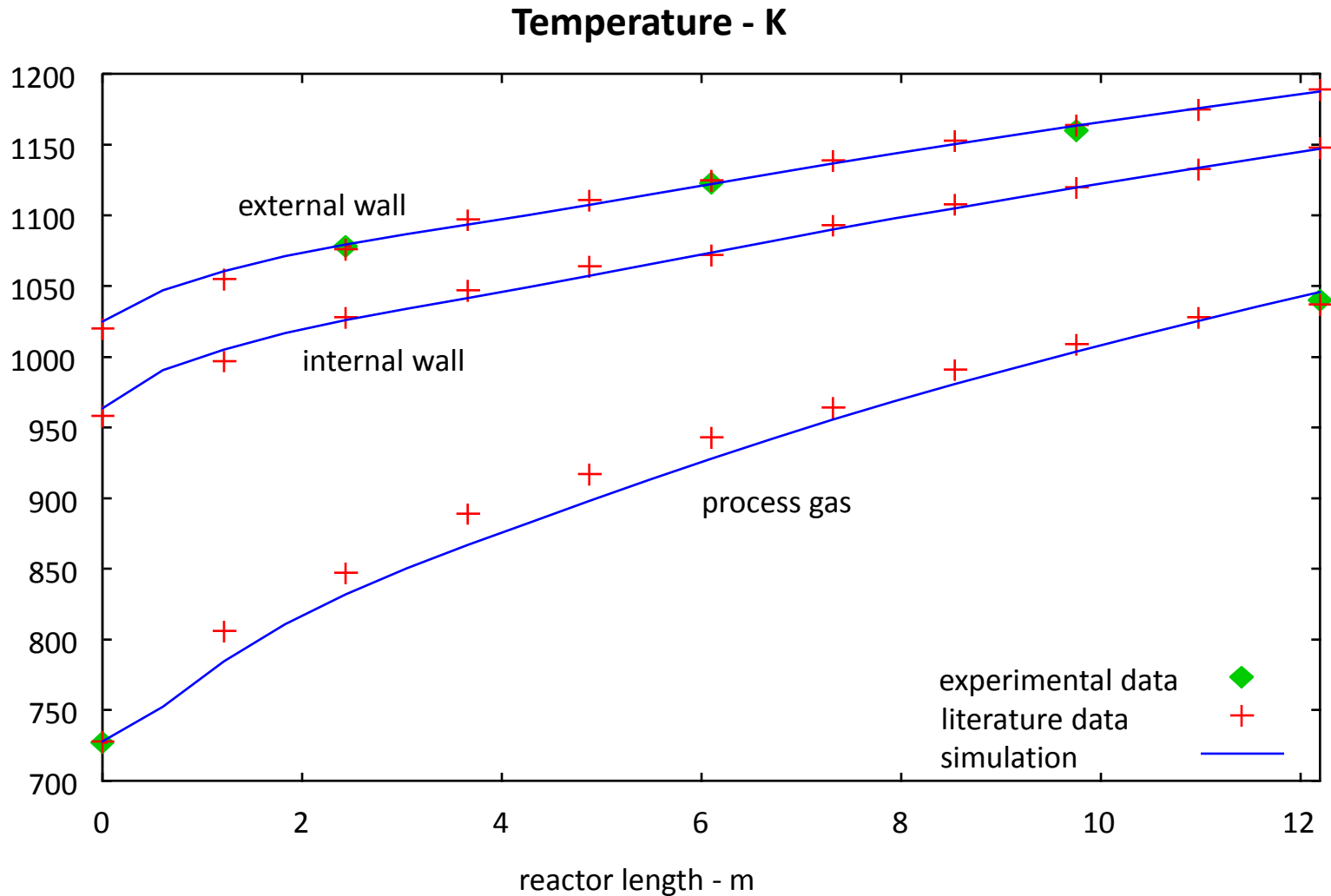
External surface

$$\frac{(GS_t)_R \cdot \sigma \cdot (T_{gas}^4 - T_{p,out}^4)}{A_t \cdot N_t} = \frac{2 \cdot k_{met} \cdot (T_{p,out} - T_N)}{D_{out} \cdot \ln\left(\frac{D_{out}}{D_N}\right)}$$

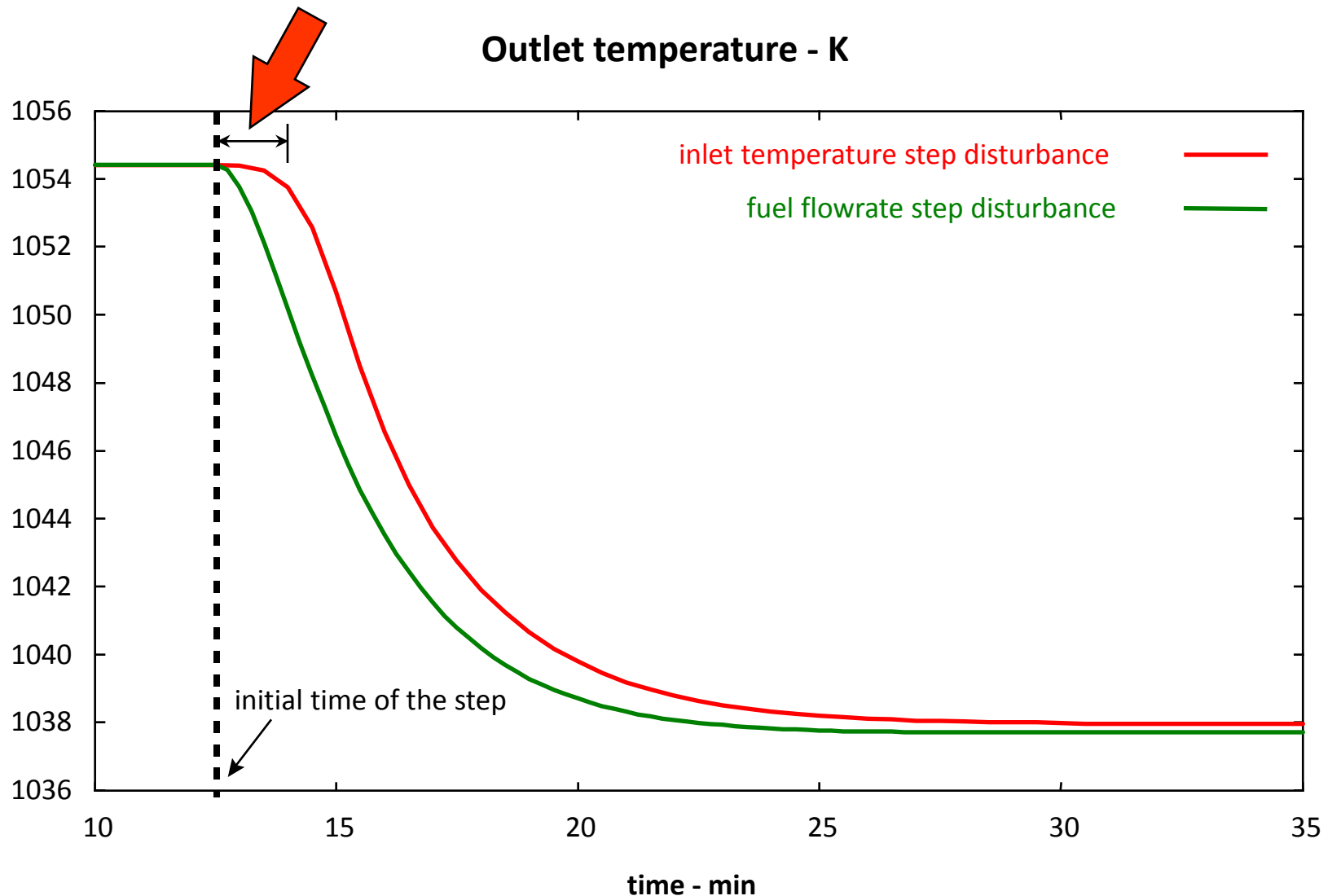
Process model: firebox (radiative chamber)



Validation of the numerical model

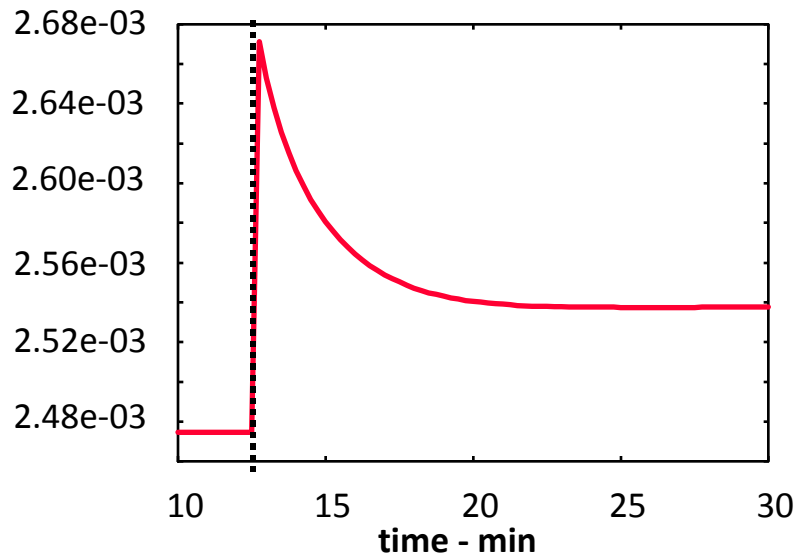


System dynamics at open loop

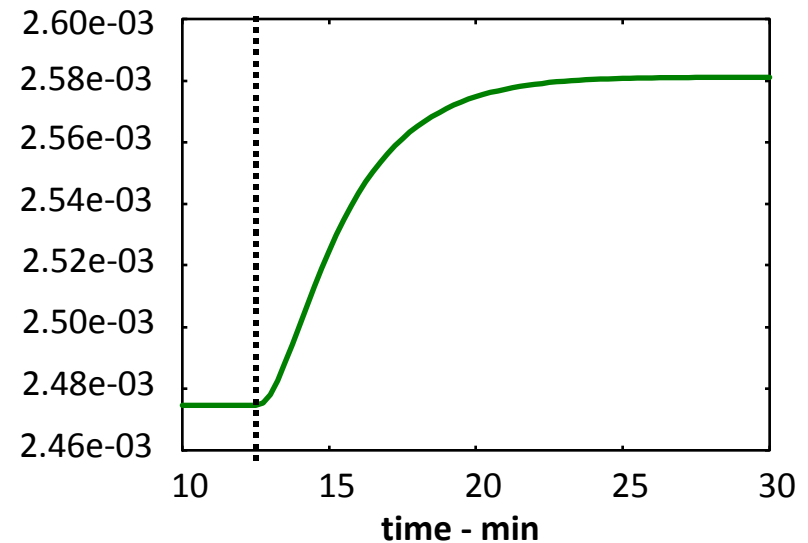


System dynamics at open loop

Hydrogen flowrate - kmol/s



Dry flowrate step



Fuel flowrate step

Over-response: slow dynamics + fast dynamics

Definition of the main variables

Input

Manipulated variables:

- fuel flowrate
- steam flowrate

Measurable disturbances:

- dry flowrate
- inlet gas temperature

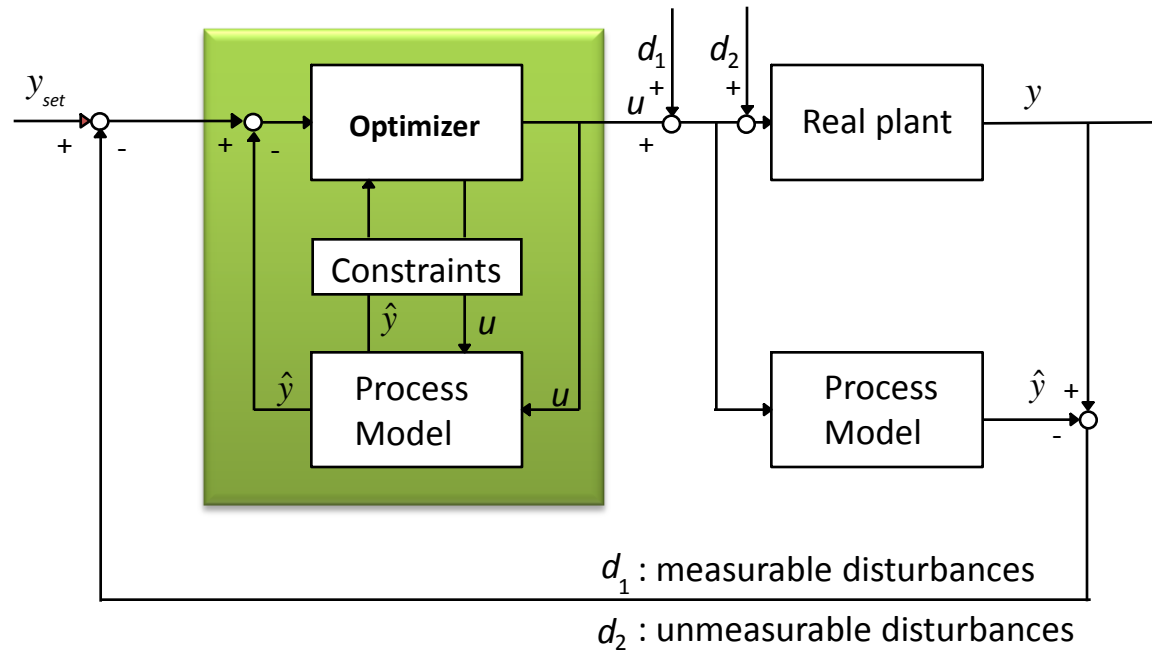


Output

Controlled variables:

- outlet gas temperature
- hydrogen flowrate

Model Predictive Control scheme



$$\min_{\hat{u}} \left(\sum_{i=1}^{h_p} (y(i) - y_{set}(i))^2 \right)$$



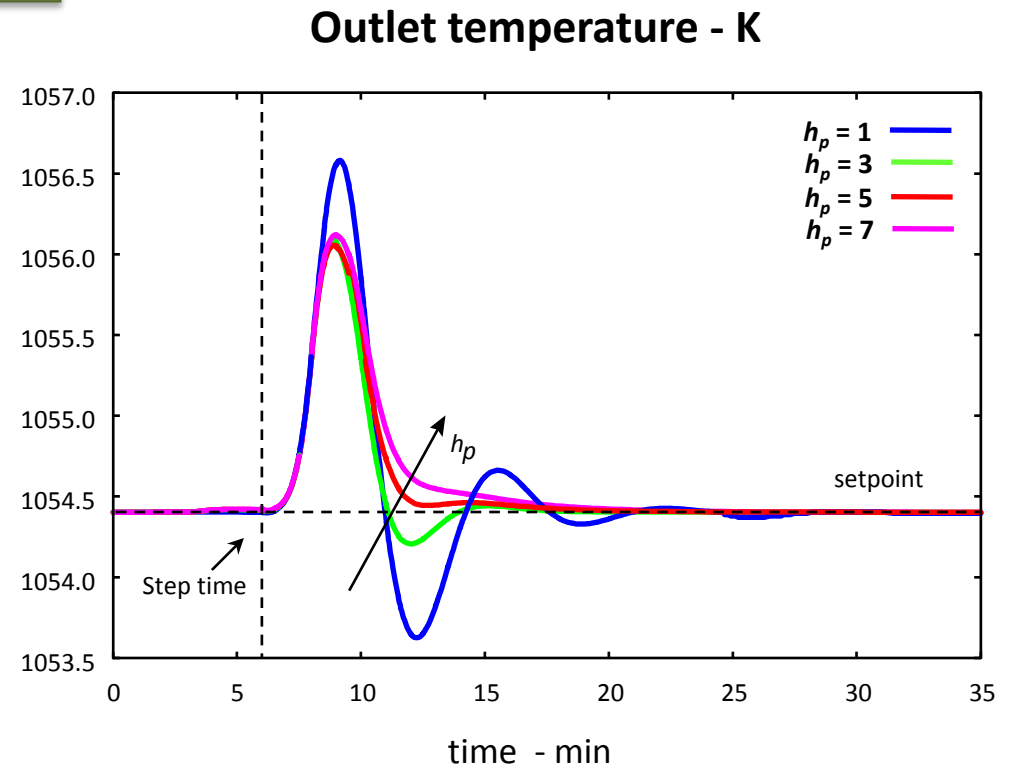
$$\min_{\hat{u}(k) \dots \hat{u}(k+h_c-1)} \left\{ \sum_{j=k+1}^{k+h_p} \omega_y (\hat{e}_y(j))^2 + \sum_{i=k}^{k+h_p-1} \omega_u (\Delta \hat{u}(i))^2 \right\}$$

Control horizon and prediction horizon

h_p : prediction horizon

High values of h_p produce:

- increased predictive capability
- less vigorous control actions
- higher distances from setpoints



Control horizon and prediction horizon

h_c : control horizon

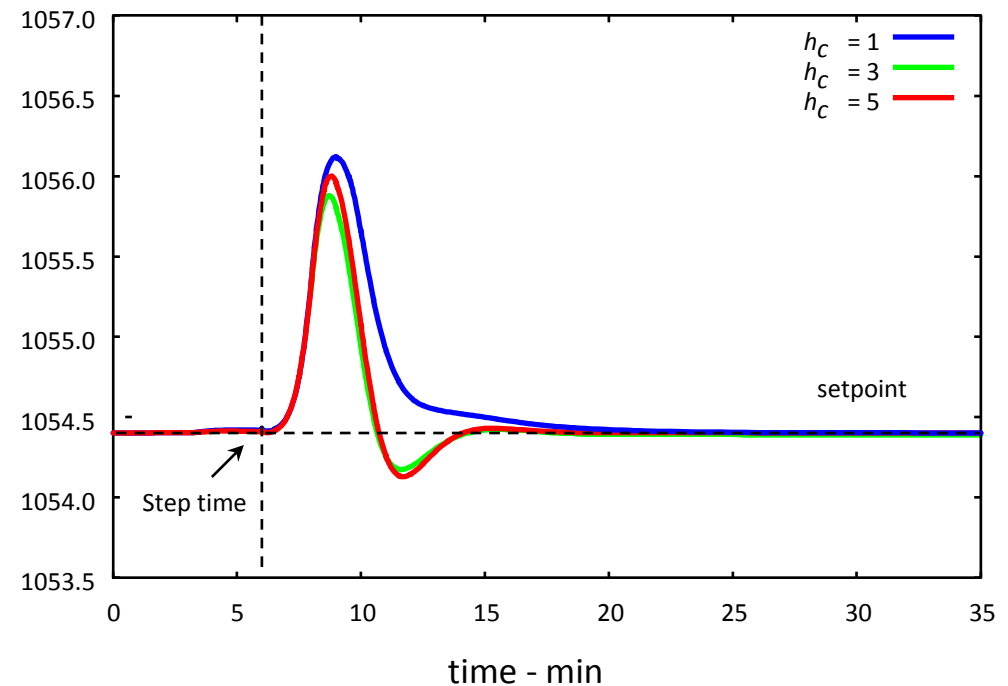
N.B.

$$n_{dof} = h_c \cdot n_c$$

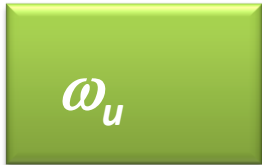
High values of h_c produce:

- better controllability
- more vigorous control actions
- higher number of *dof*

Outlet temperature - K

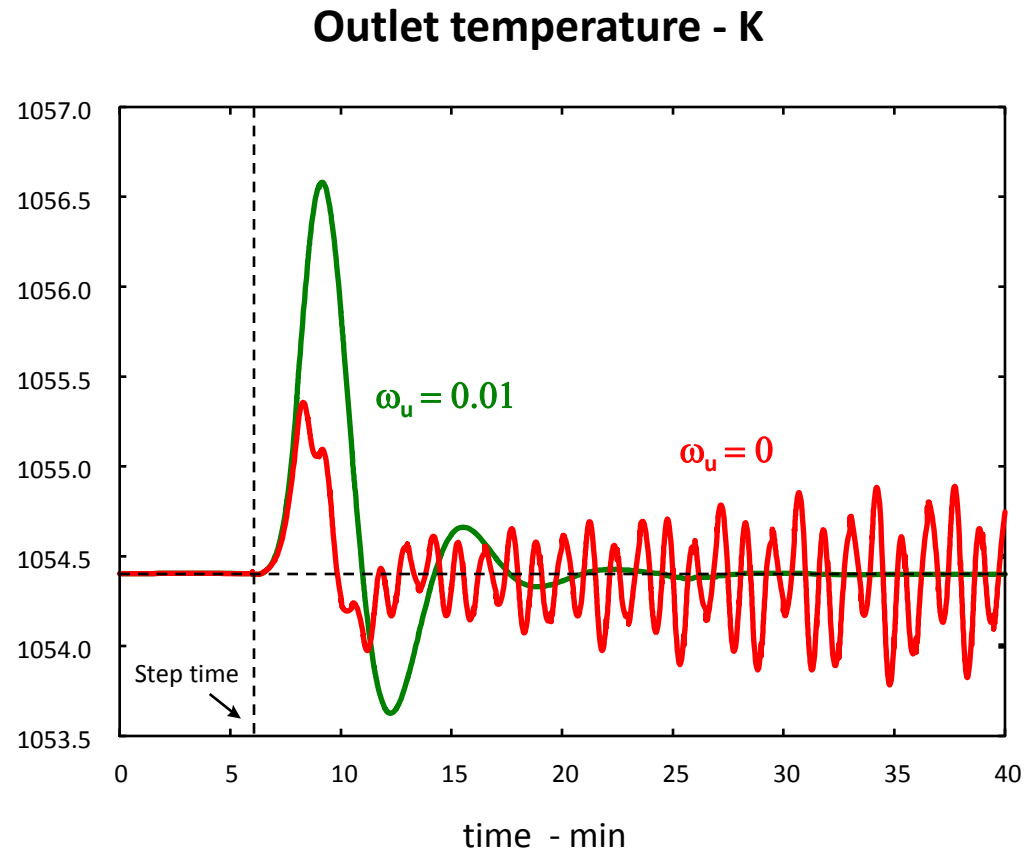


The parameter ω_u



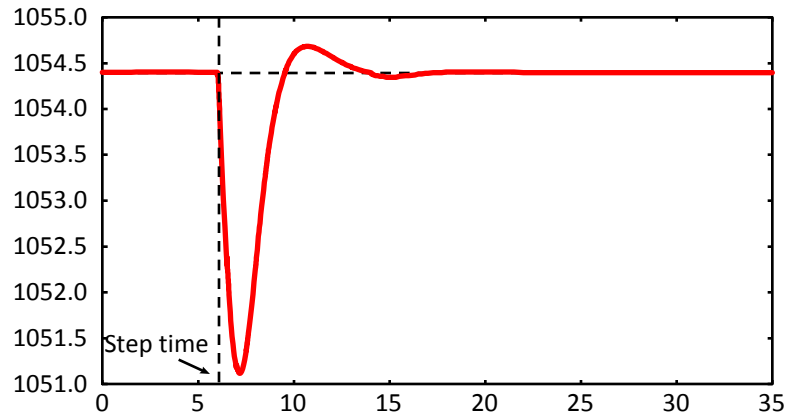
High values of ω_u produce:

- small variations of the manipulated variables
- more sluggish controllers
- more stable controllers

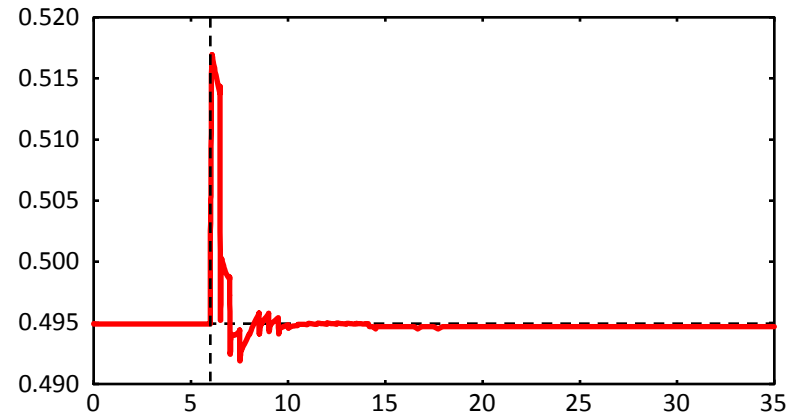


MPC: closed loop response

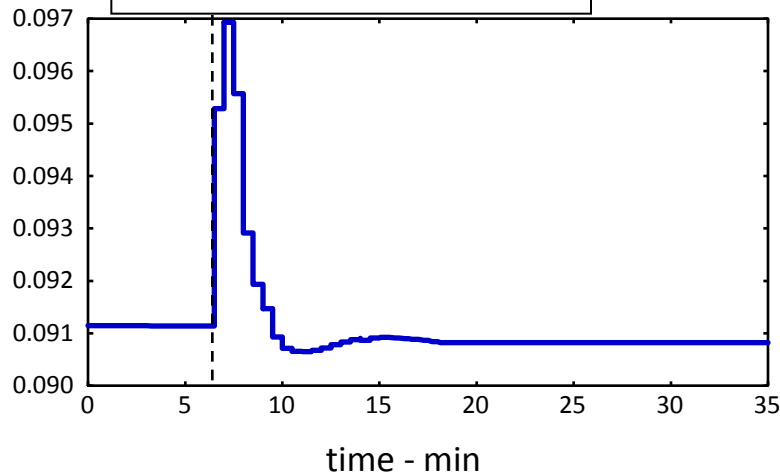
Outlet temperature - K



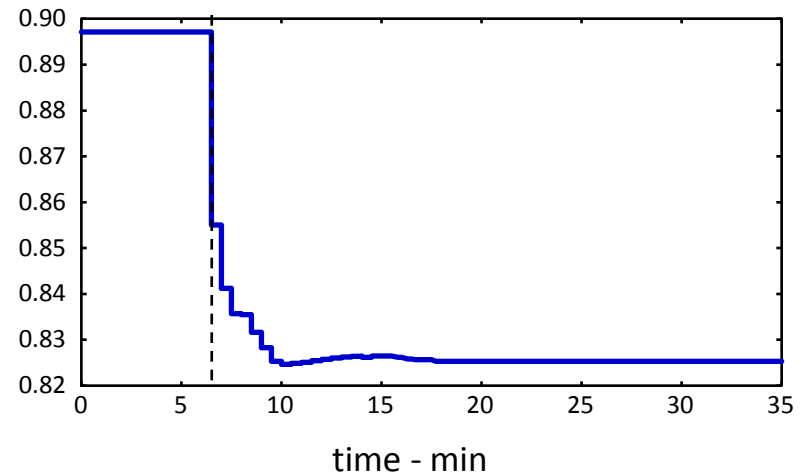
Hydrogen flowrate - kmol/s



Fuel flowrate - kmol/s

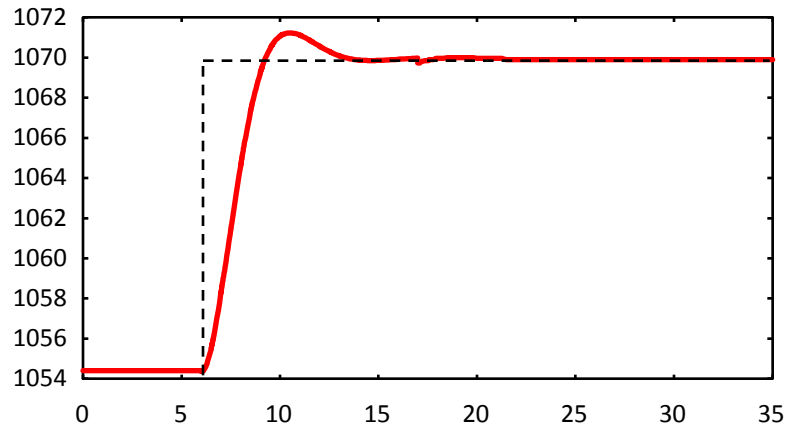


Steam flowrate - kmol/s

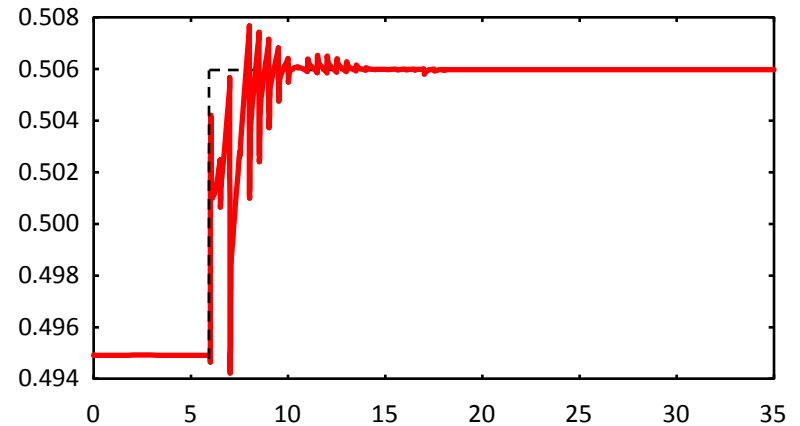


MPC: closed loop response

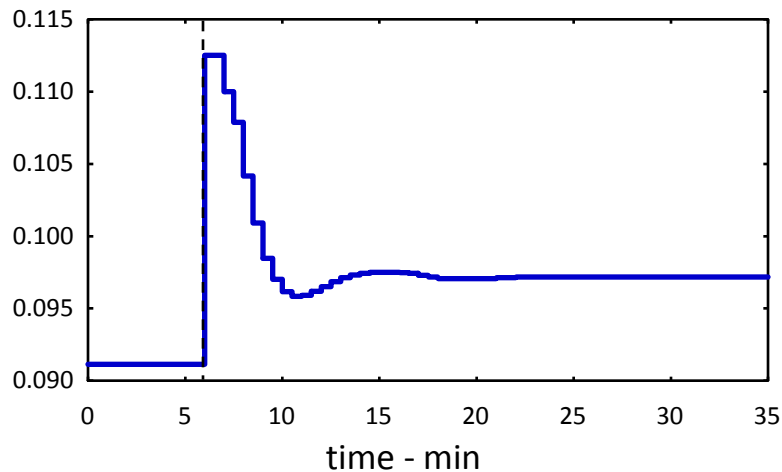
Outlet temperature - K



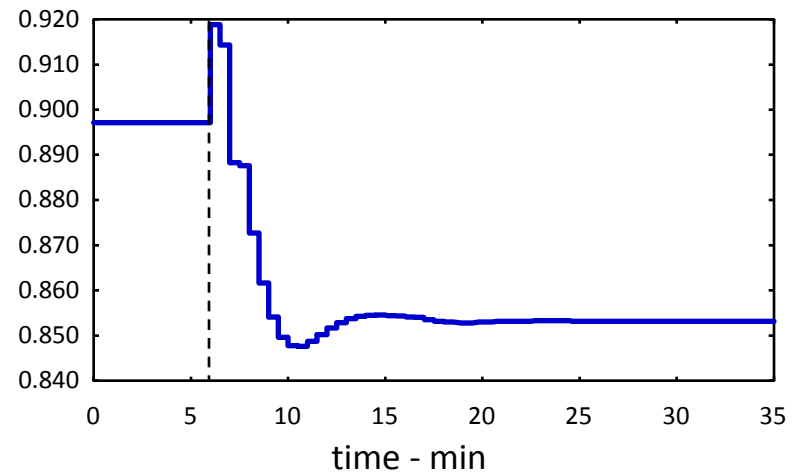
Hydrogen flowrate - kmol/s



Fuel flowrate - kmol/s

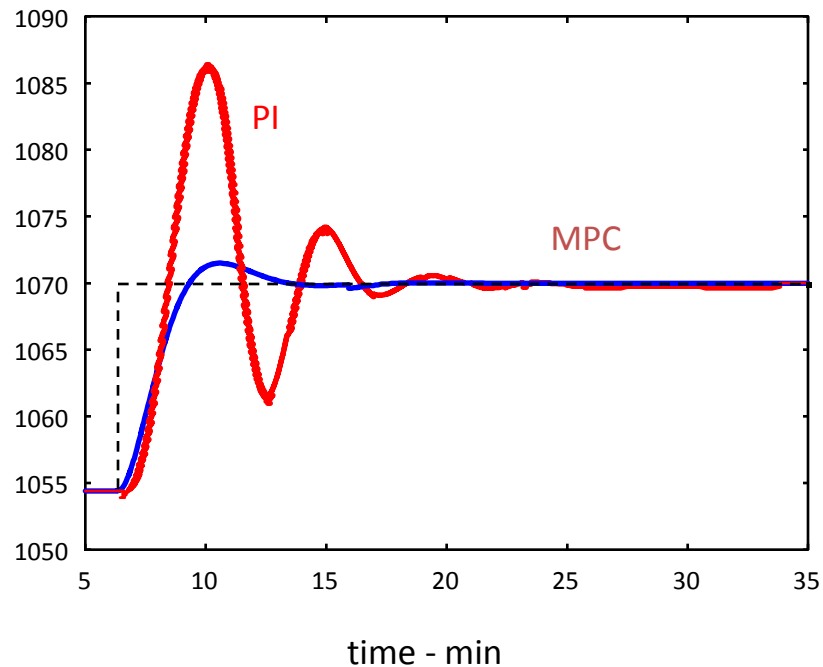


Steam flowrate - kmol/s

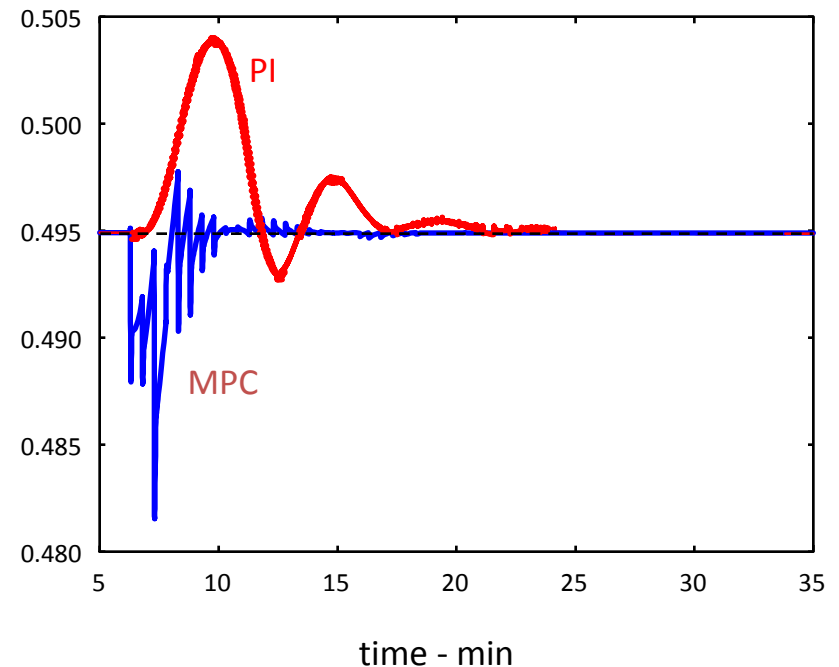


Comparison between MPC and PI control

Outlet temperature - K



Hydrogen flowrate - kmol/s



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