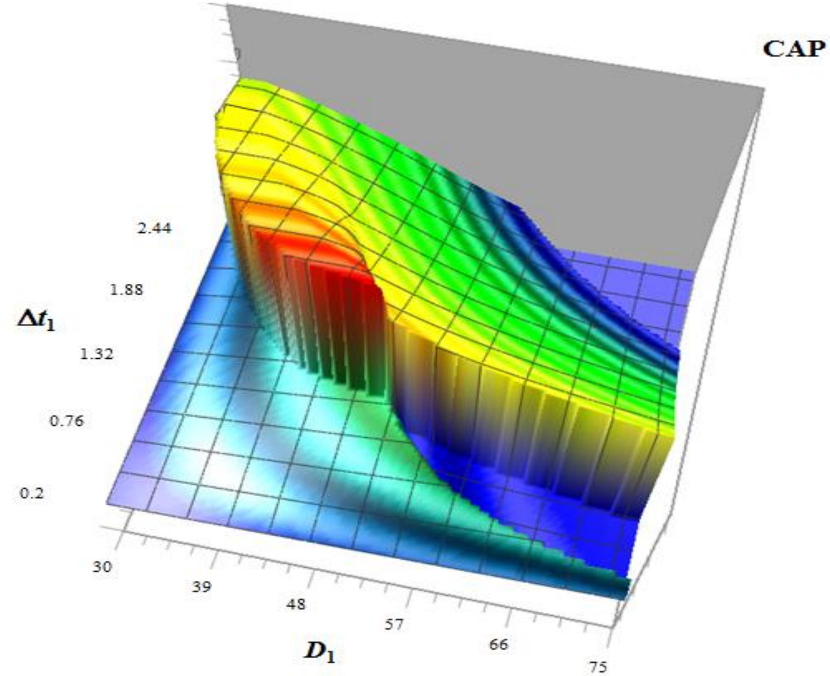



# Continuous Optimization

**Davide Manca**

Lesson 5 of "Process Systems Engineering A" – 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)

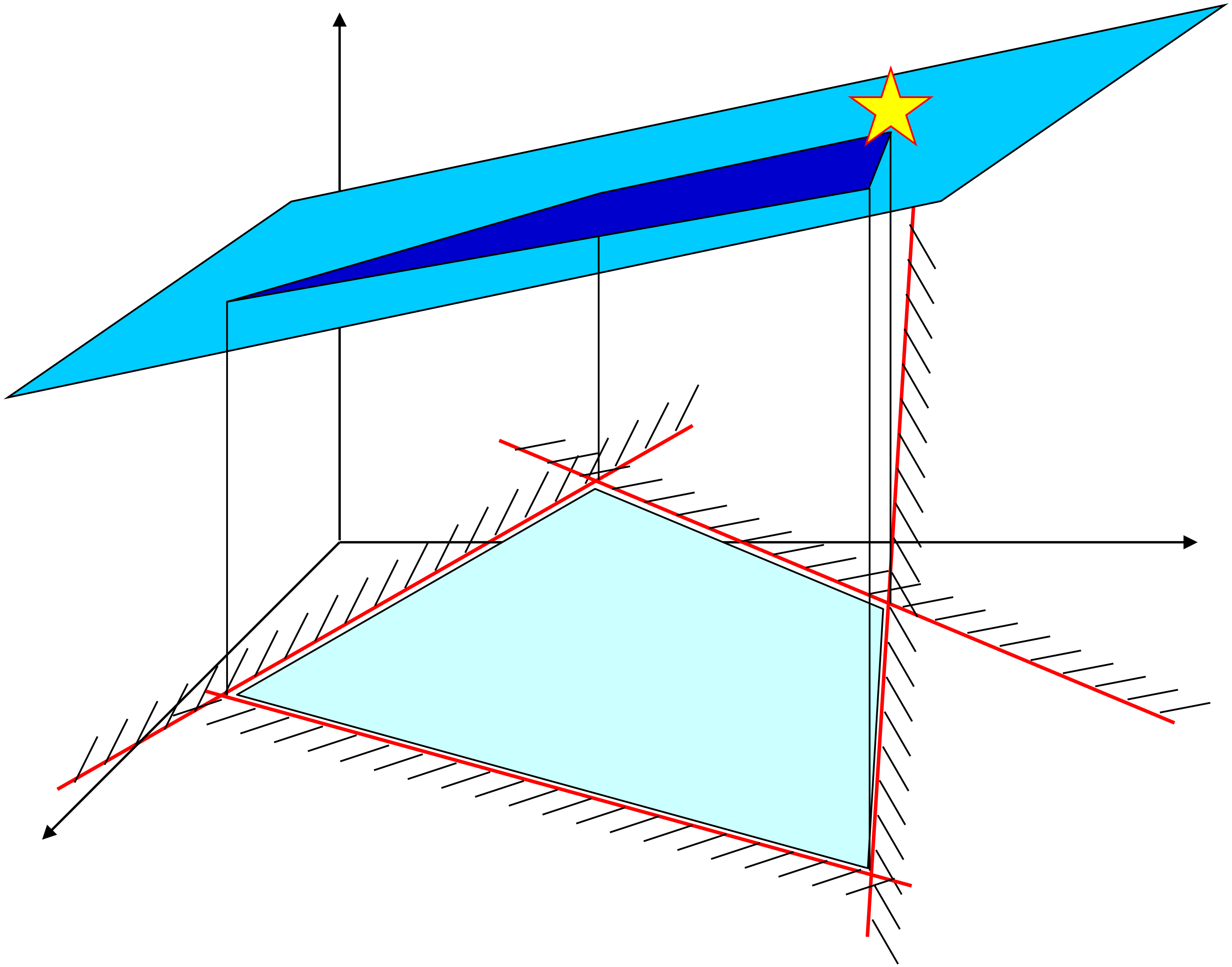
- The constraints may be:
  - Linear
  - Nonlinear

  - Violable
  - Not violable

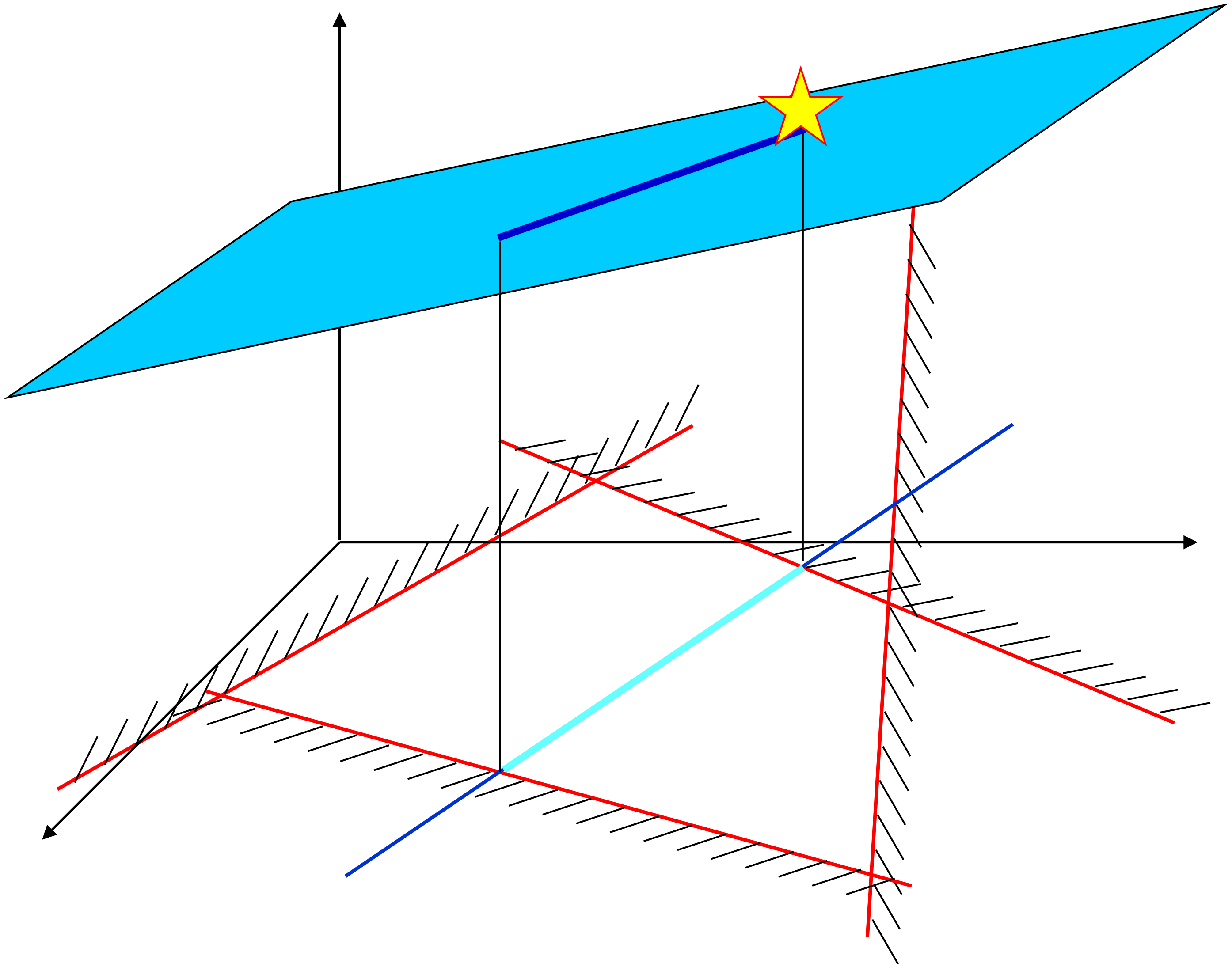
  - Real constraints
  - Lower and upper bounds of the degrees of freedom
- The optimization variables are defined as: *degrees of freedom* (*dof*)
- Mathematically we have:

$$\begin{cases} \underset{\mathbf{x}}{\text{Min}} \quad f(\mathbf{x}) \\ s.t. \quad \mathbf{h}(\mathbf{x}) = \mathbf{0} \\ \qquad \mathbf{g}(\mathbf{x}) \le \mathbf{0} \end{cases}$$

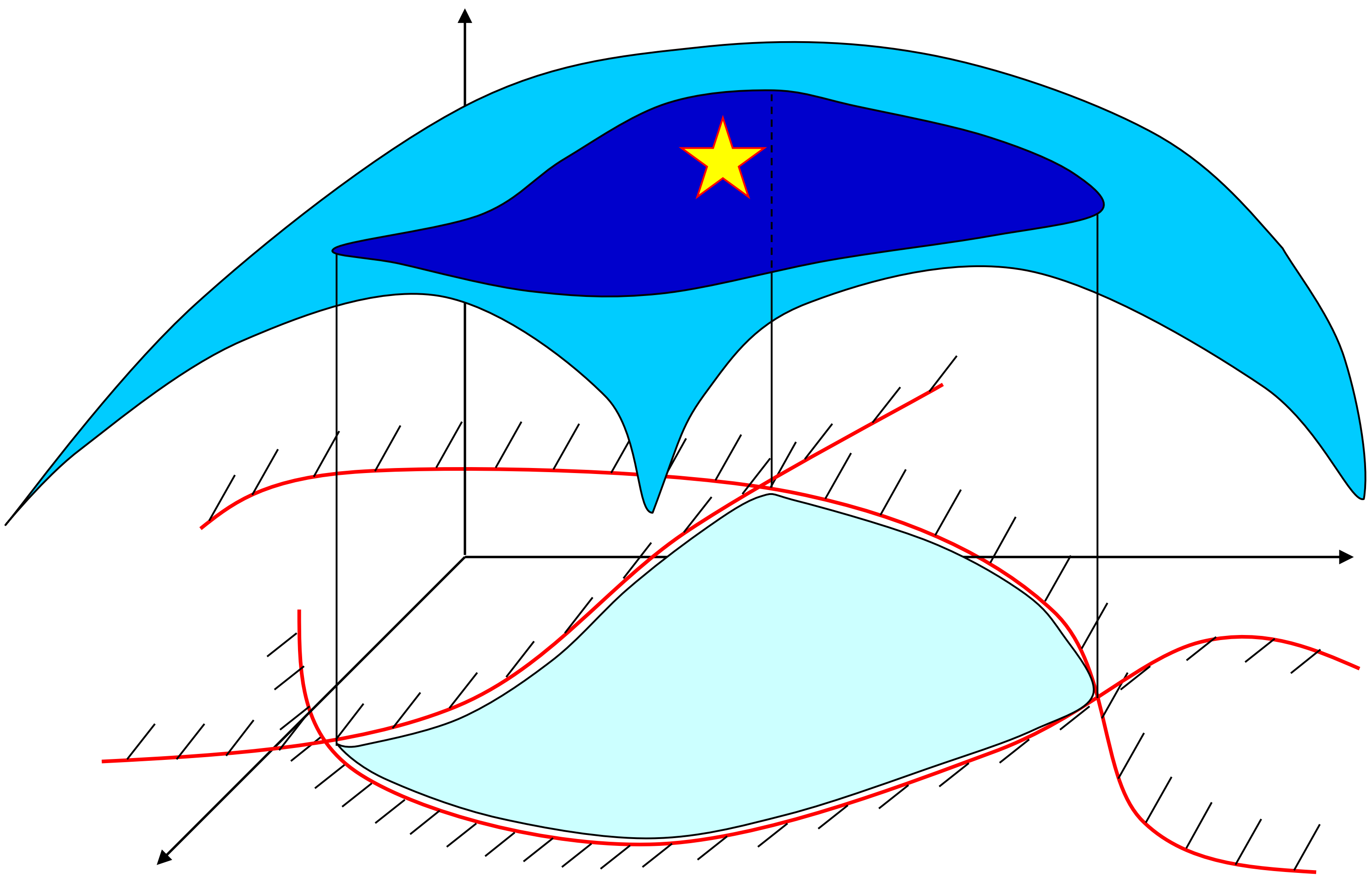
# Linear function and constraints



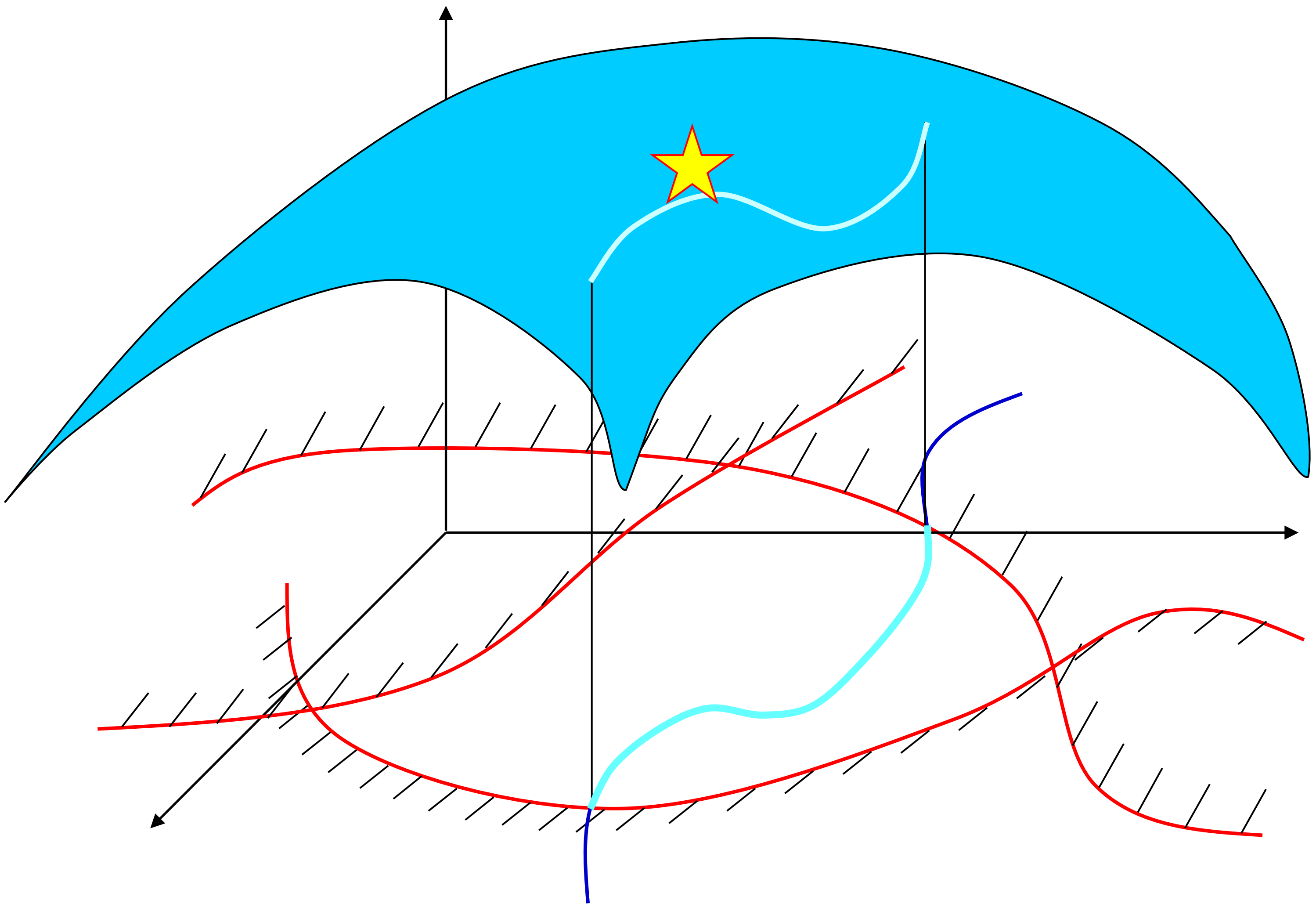
# Linear function and constraints



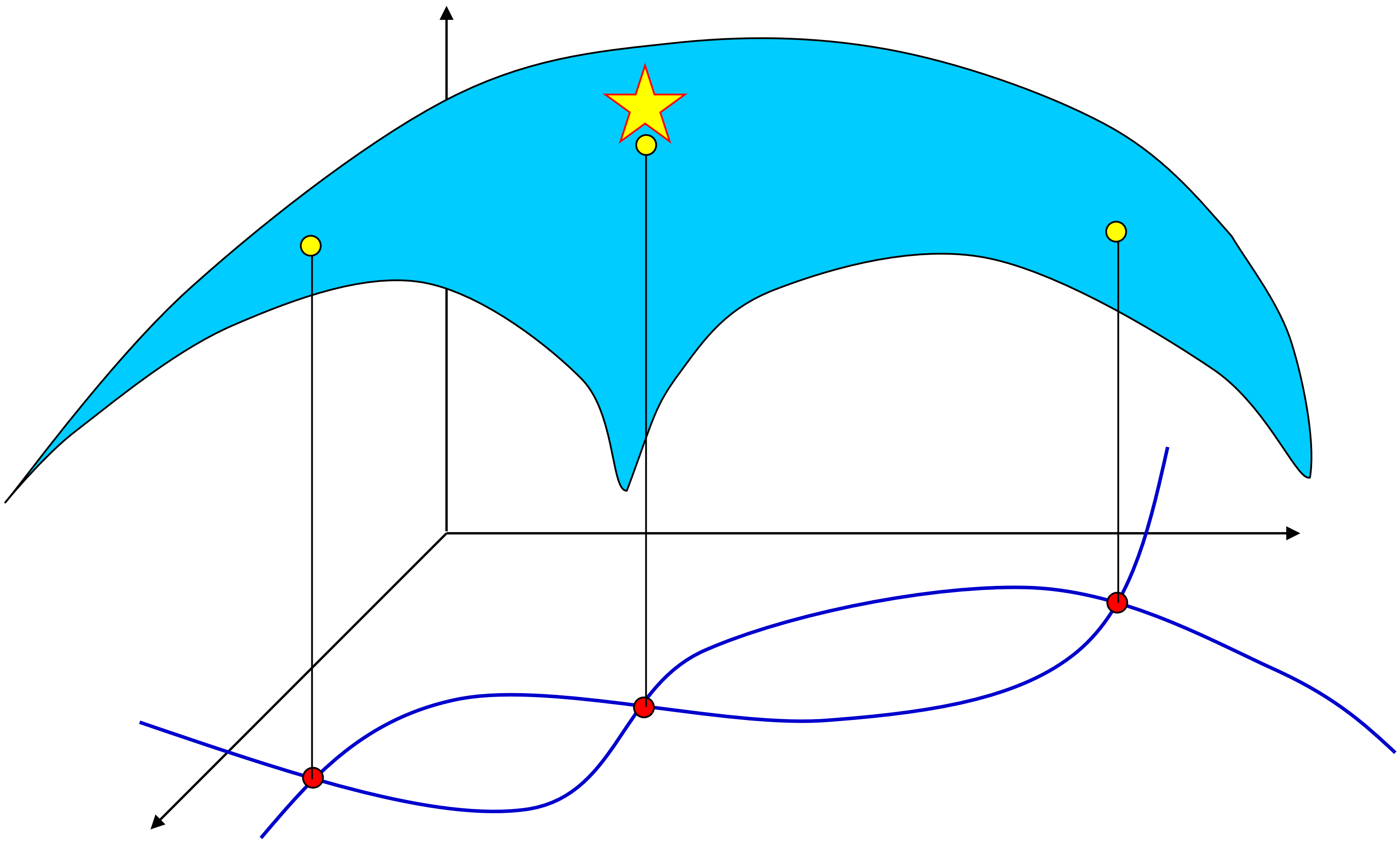
# Nonlinear function and constraints



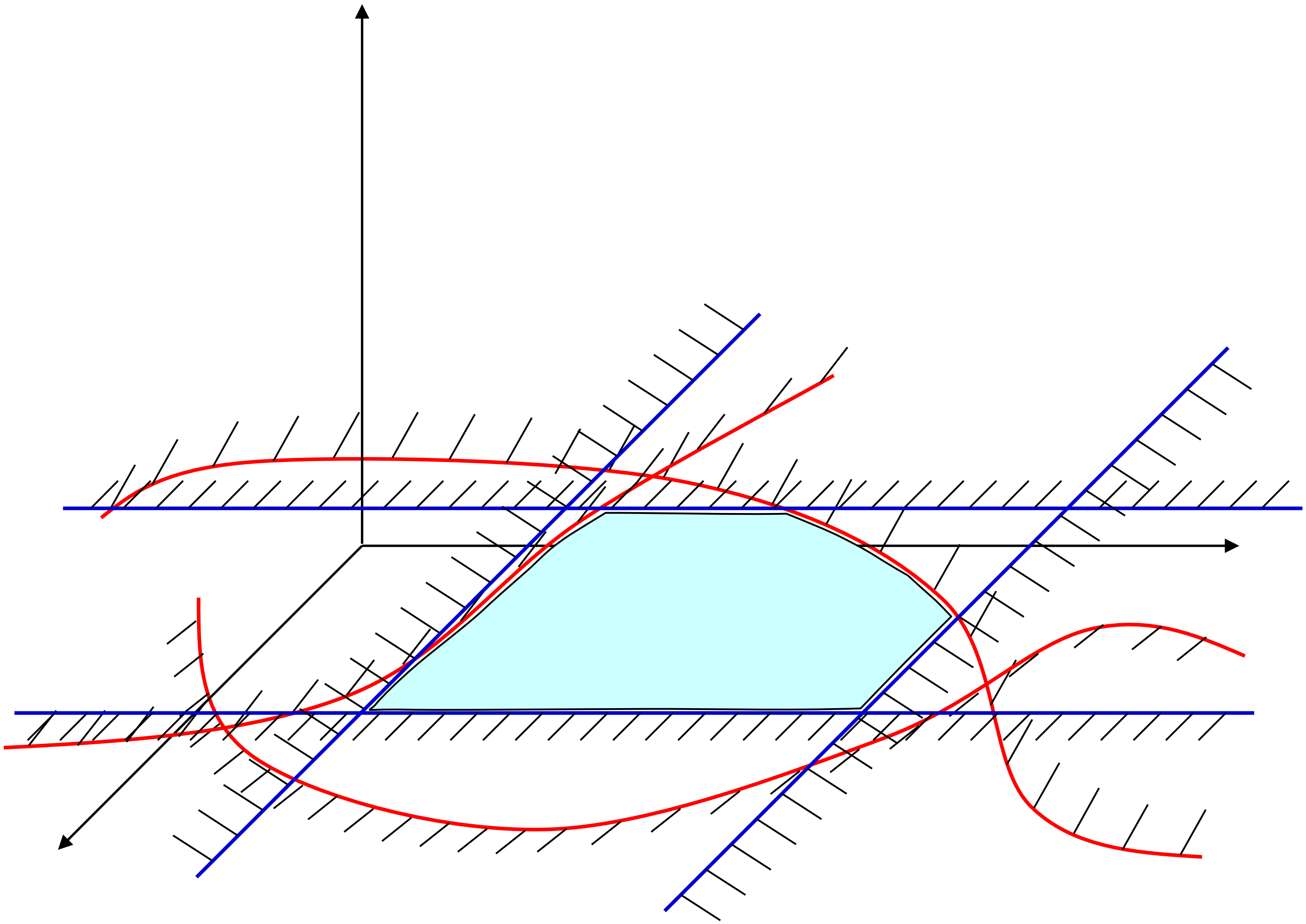
# Nonlinear function and constraints



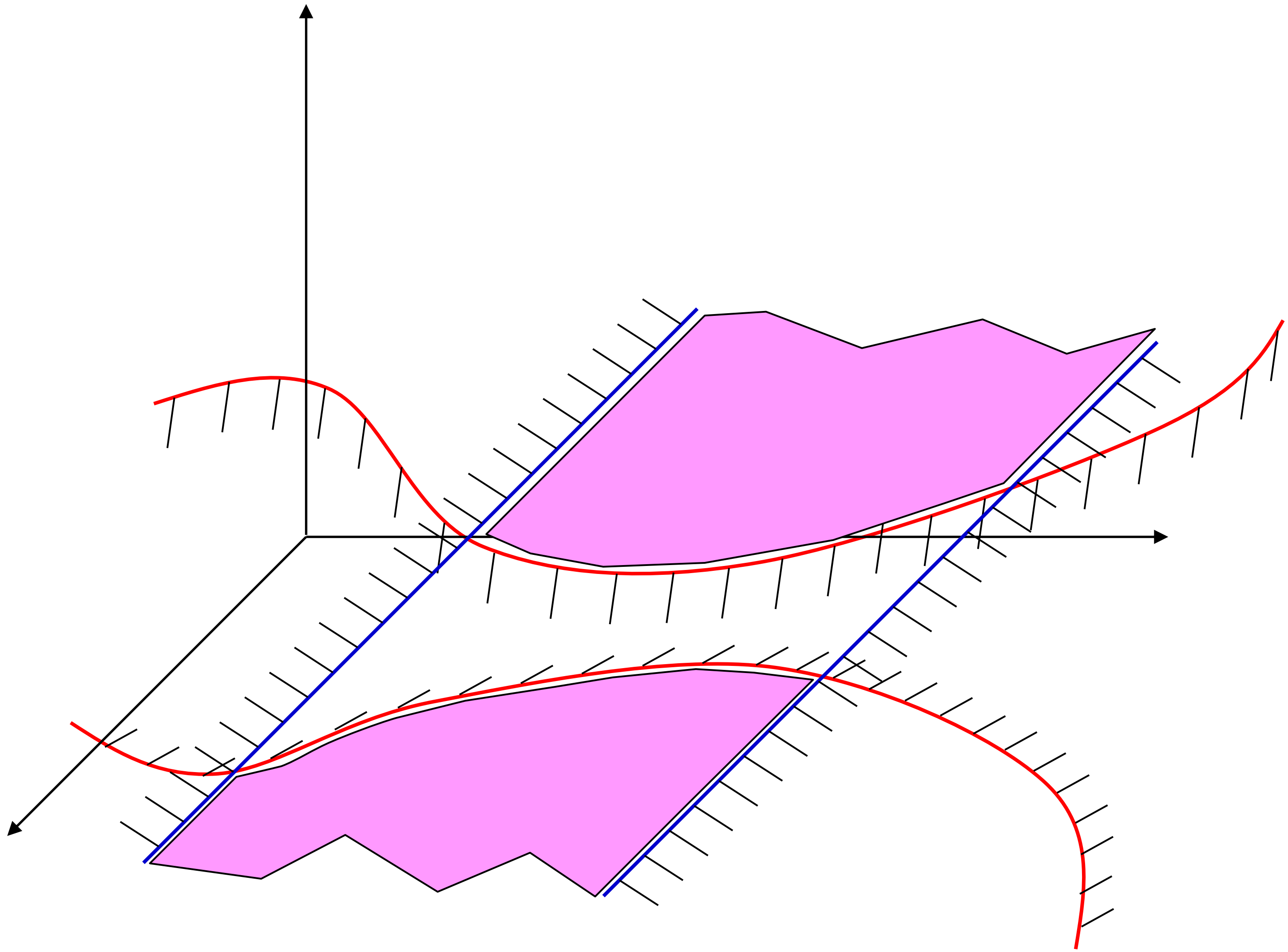
# Nonlinear function and constraints



# 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” region 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 isn’t any 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 possible solution coincides 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 select 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:

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

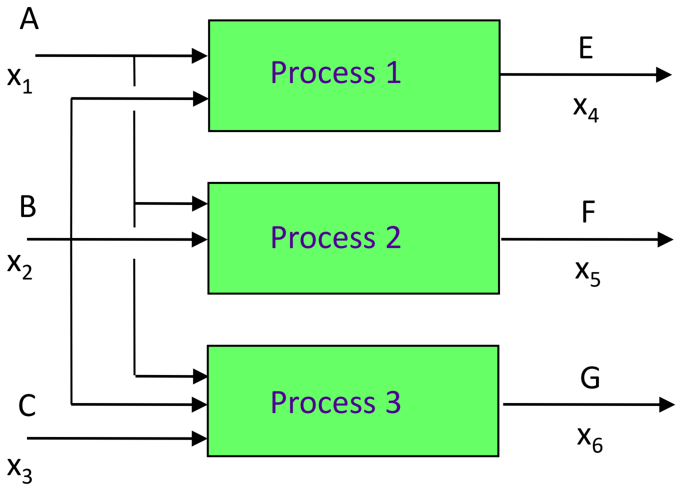
- Also, the objective function may be based on **other criteria** such as:
  - pollutant minimization
  - conversion maximization
  - yield, reliability, response time, efficiency
  - energy production
  - environmental impact
- With reference to the process, if we consider only the operating costs and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

  $$f(x) = 4x_4 + 3.3x_5 + 3.8x_6 - 1.5x_1 - 2.0x_2 - 2.5x_3 - 1.5x_4 - 0.5x_5 + \\ - 1.0x_6 = 2.5x_4 - 2.8\,x_5 + 2.8\,x_6 - 1.5\,x_1 - 2x_2 - 2.5x_3$$

- 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*

  $0 \le x_1 \le 40{,}000$

  $0 \le x_2 \le 30{,}000$

  $0 \le x_3 \le 25{,}000$

- 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 $\rho$ 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:

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

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

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 corrosivity 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 [€/m$^2$]

  $F_0 + F_1\,s$
- 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:

  $(F_0 + F_1\,s)\,A\,r$ [€/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:

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

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

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

- The problem is solved analytically by calculating:

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

- We obtain:

  $s_{opt} = k\,[((\Delta T\,H_t\,Y)/(k\,F_1\,r))^{½} - 1/h_e]$

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

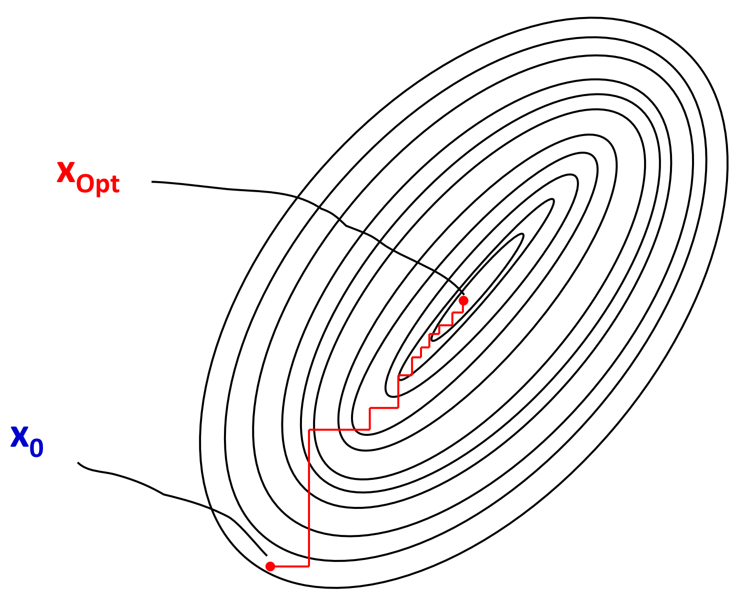
# Methods for multidimensional unconstrained optimization

# 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(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(**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(**x**). They are more robust because they are slightly if not at all affected by the discontinuities of the problem to be solved.
    - **FIRST ORDER methods** work with the first order partial derivatives of f(**x**) *i.e.* the GRADIENT of the objective function.
    - **SECOND ORDER methods** use also the second order partial derivatives of f(**x**) *i.e.* the HESSIAN of the objective function.

# Multidimensional unconstrained optimization

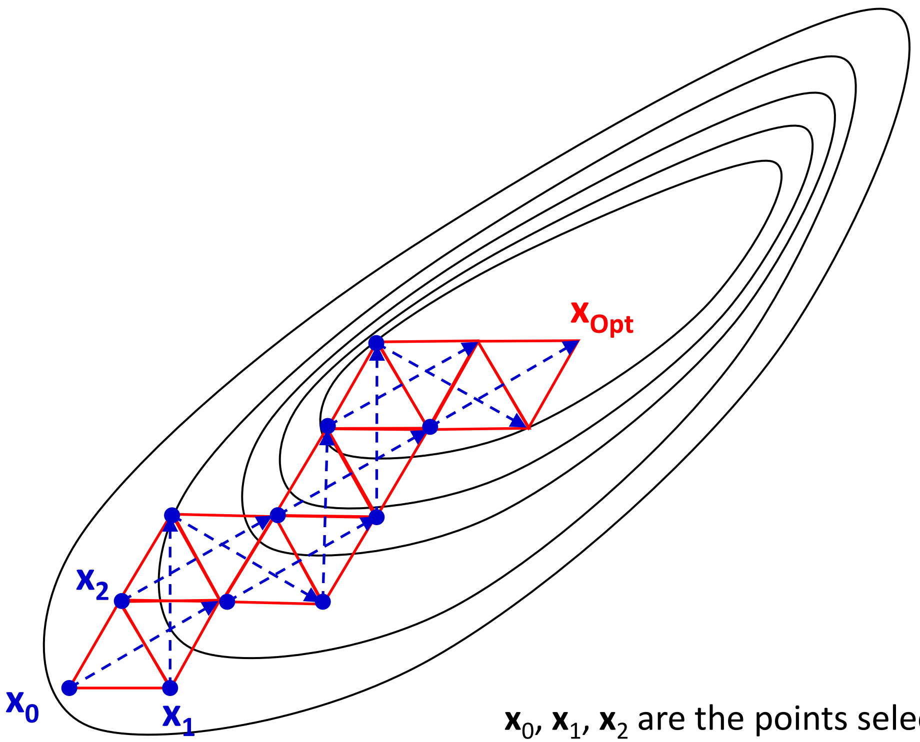
- The numerical algorithms are intrinsically iterative and usually perform a series of direction searches. At the *k*-th iteration we have the *k*-th direction $s_k$ and the method minimizes f(**x**) along $s_k$.
- **DIRECT or HEURISTIC methods**:
  - **Random search** (Monte Carlo)
  - **Grid search**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



# 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(**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.




$\mathbf{x}_0$, $\mathbf{x}_1$, $\mathbf{x}_2$ are the points selected to initialize the simplex sequence

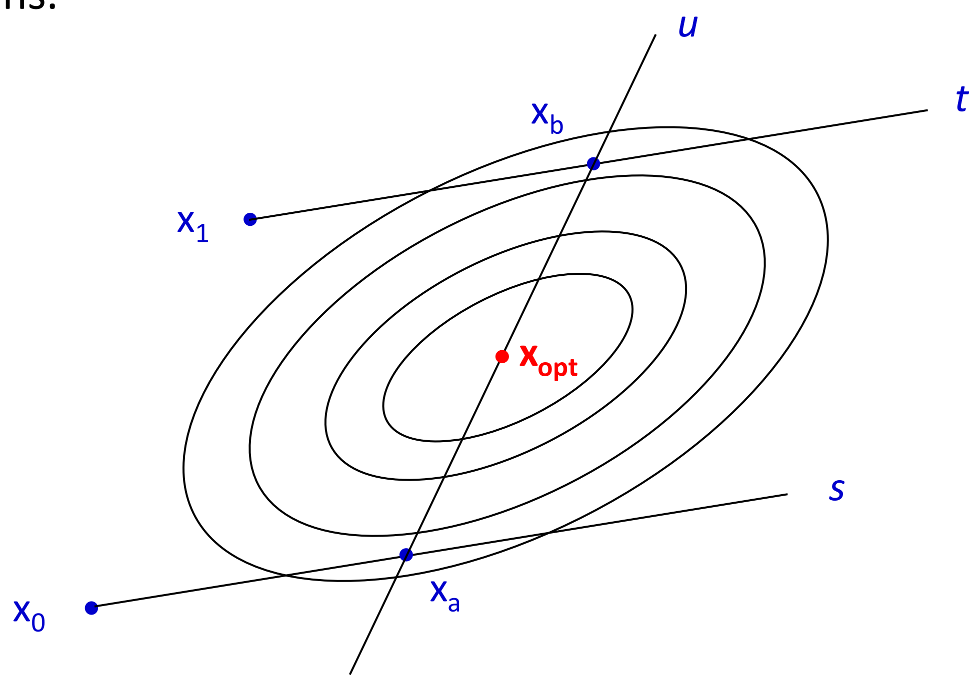
# Multidimensional unconstrained optimization

## Conjugate directions method

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

Hp.: f(**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 *s*
7. *u* from joining $x_a$ and $x_b$

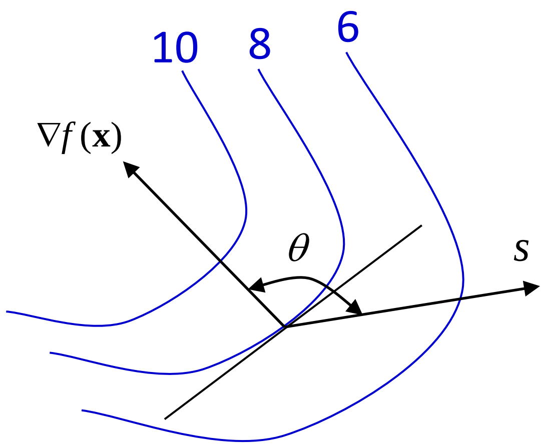



*u* is the conjugated direction with respect to *s* and *t* and by minimizing it we identify the optimal point $x_{opt}$ of f(**x**) (for that quadratic approximation).

# Multidimensional unconstrained optimization

## First order indirect methods

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




In fact:

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

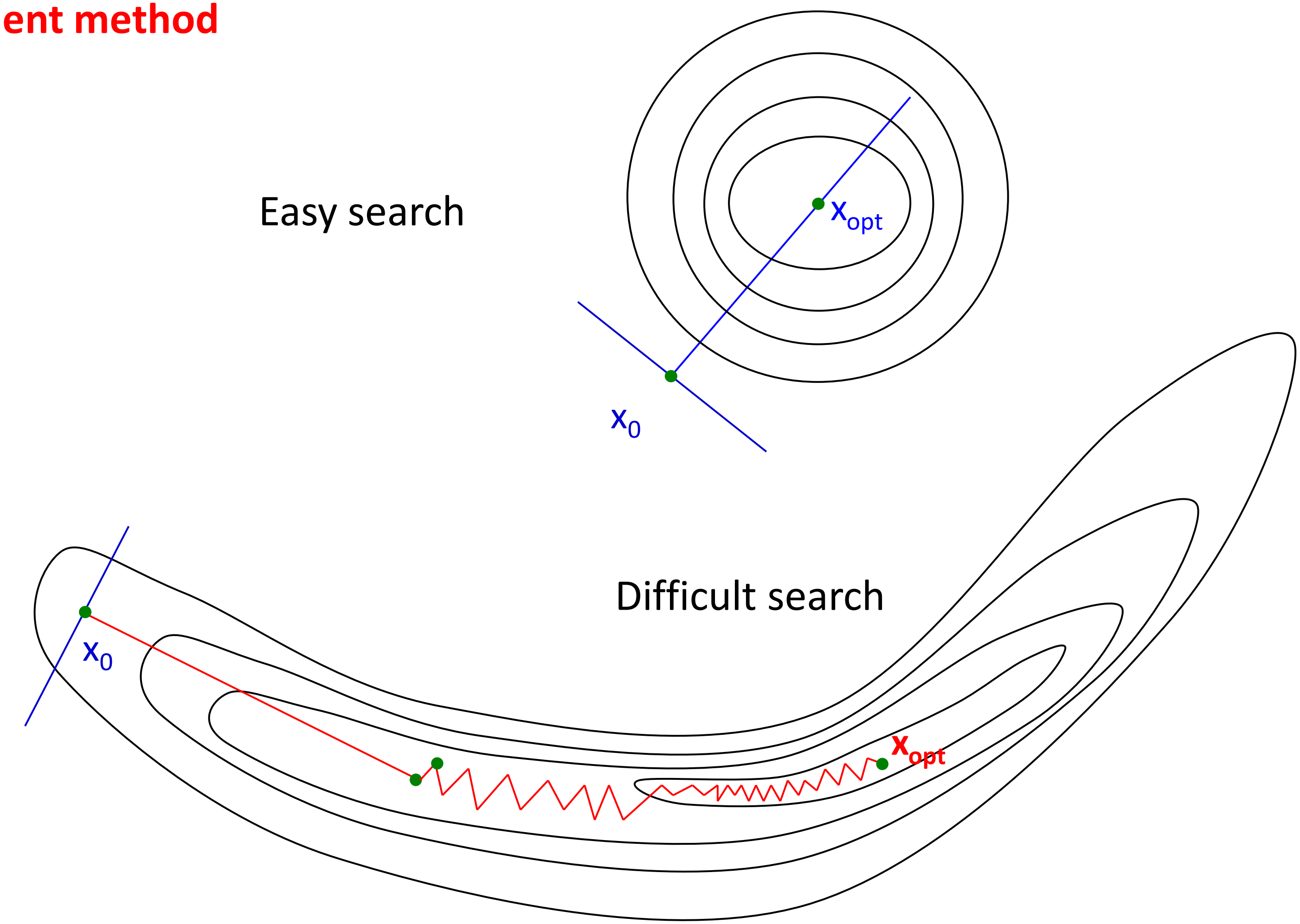
only if: $\cos\theta < 0 \quad \Rightarrow \quad \theta > 90^\circ$

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.

By 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: $\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{H}^{-1}(\mathbf{x}_k)\nabla f(\mathbf{x}_k)$

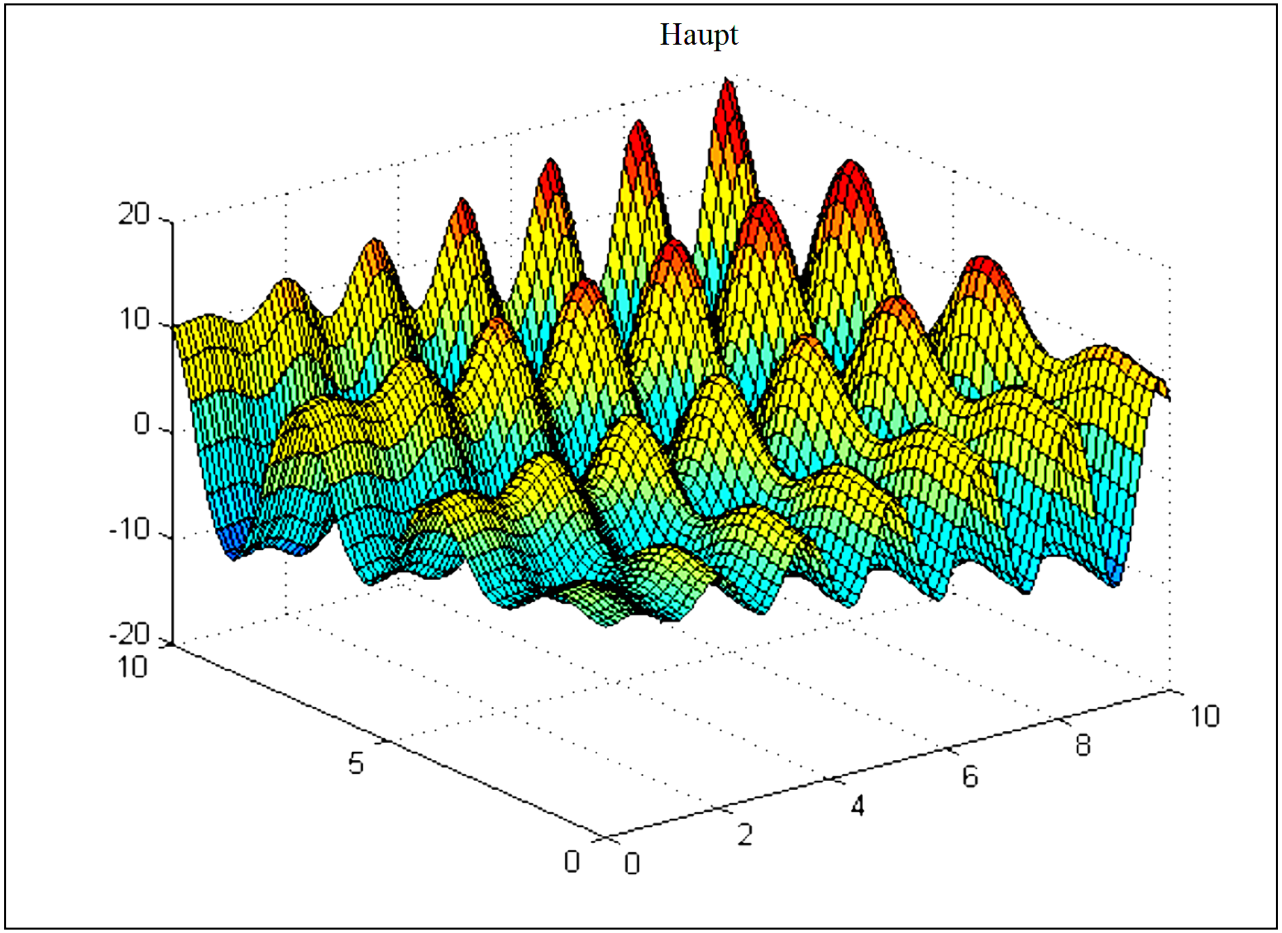
**N.B.**: the Hessian matrix is not inverted, we solve the resulting linear system via the LU factorization.

In addition, the Hessian matrix is NOT calculated directly as it would be costly regarding CPU time.

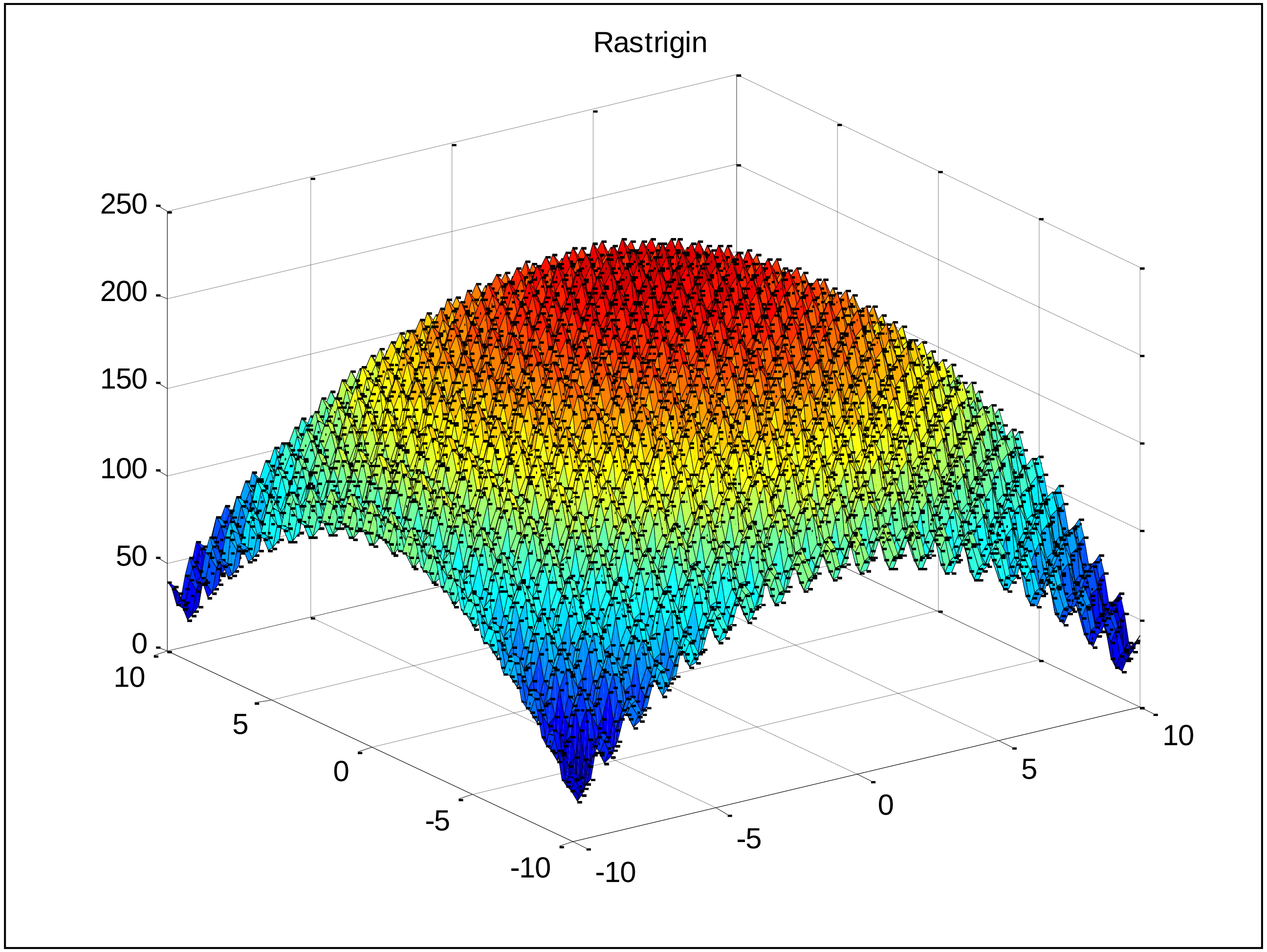
On the contrary, the **BFGS formulas** (Broyden, Fletcher, Goldfarb, Shanno) allow starting from an initial estimation of **H** (often the identity matrix) and with the gradient of f(**x**) they evaluate iteratively **H**(**x**).

The corresponding numerical methods are:
Newton, Newton modified: Levemberg-Marquardt, Gill-Murray.

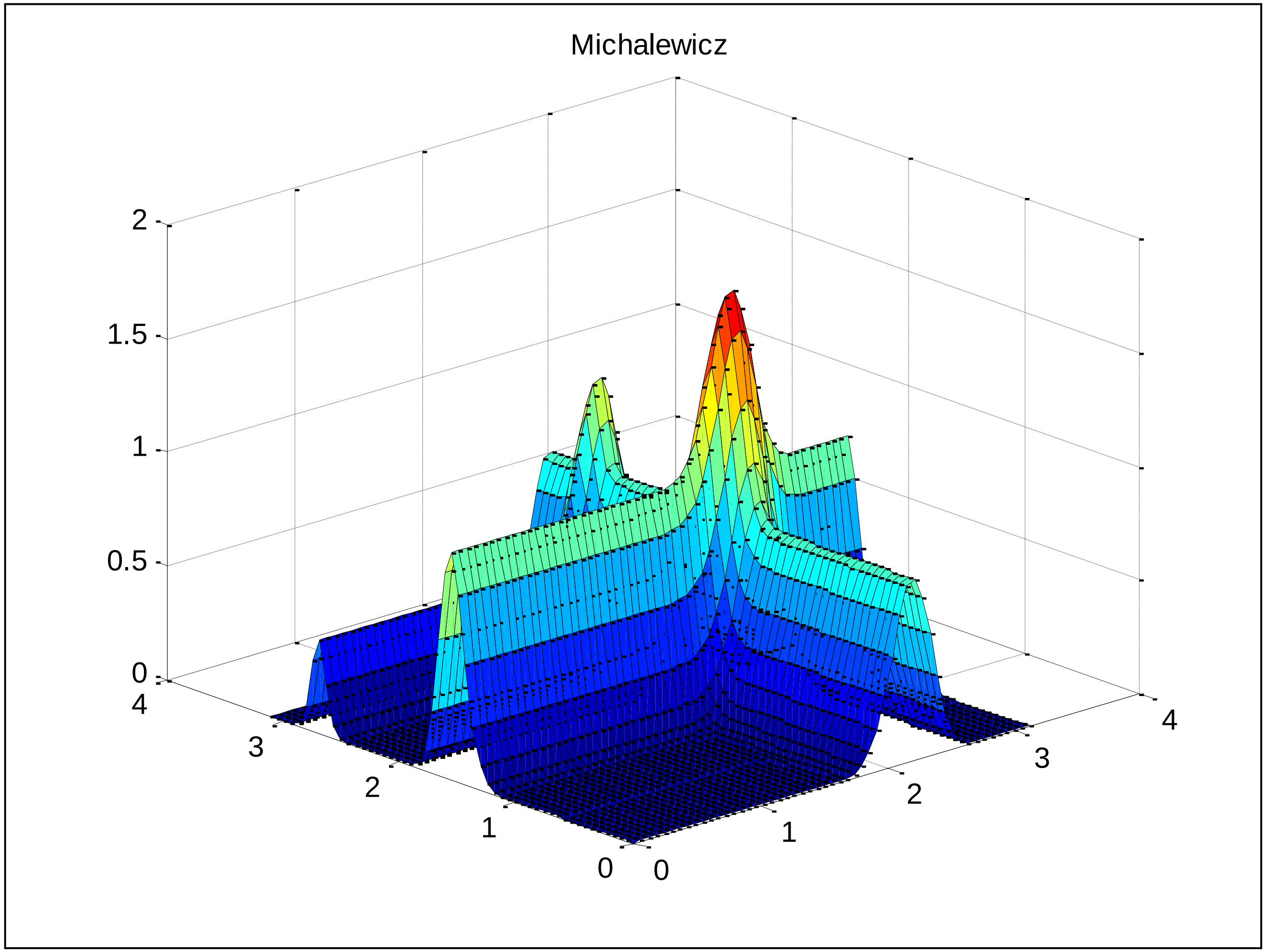
# Some peculiar objective functions



# Some peculiar objective functions



# Some peculiar objective functions



# Methods for multidimensional constrained optimization

# Linear Programming

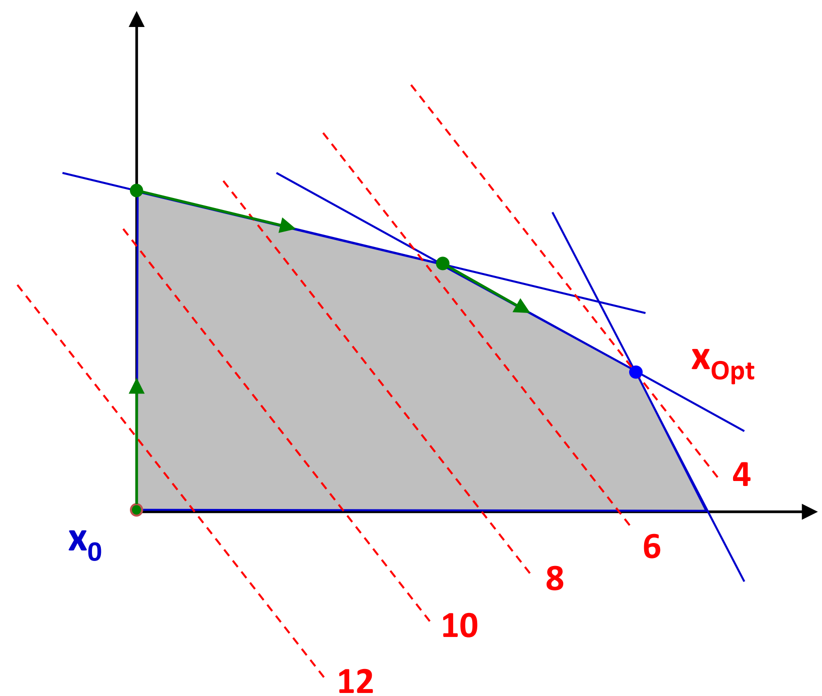
- The objective function and the equality and inequality constraints are all LINEAR. Thus, the objective function is neither concave nor convex. Actually, it is either a plane (2D) or a hyperplane (with *n dof*).
  If the region identified by the constraints is consistent we have to solve a problem (“feasible”) 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.

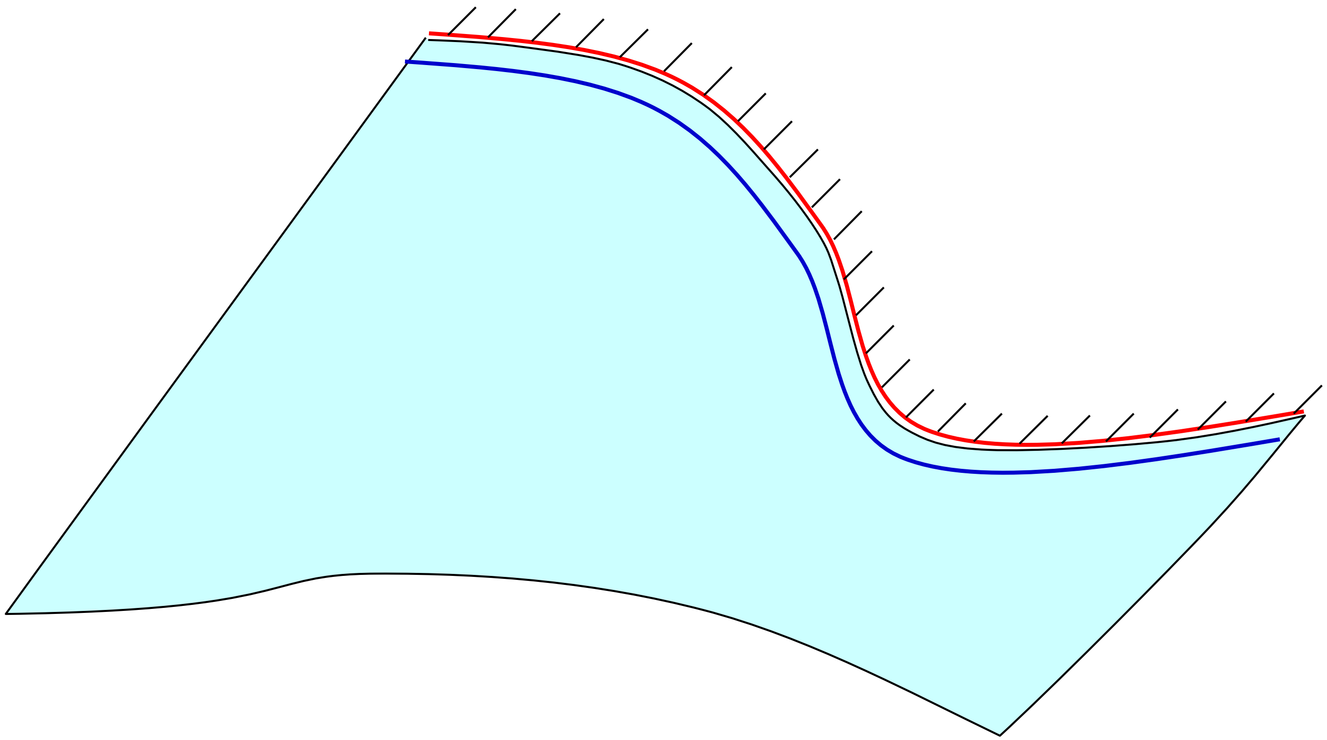
  The problem may also NOT have a “feasible” region of research.



# 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:

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

More generally:

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

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

# Nonlinear Programming

**SQP method (Successive Quadratic Programming)**

The objective function f(**x**) is approximated iteratively with a quadratic function, while the constraints are linearized and added to the objective function:

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

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

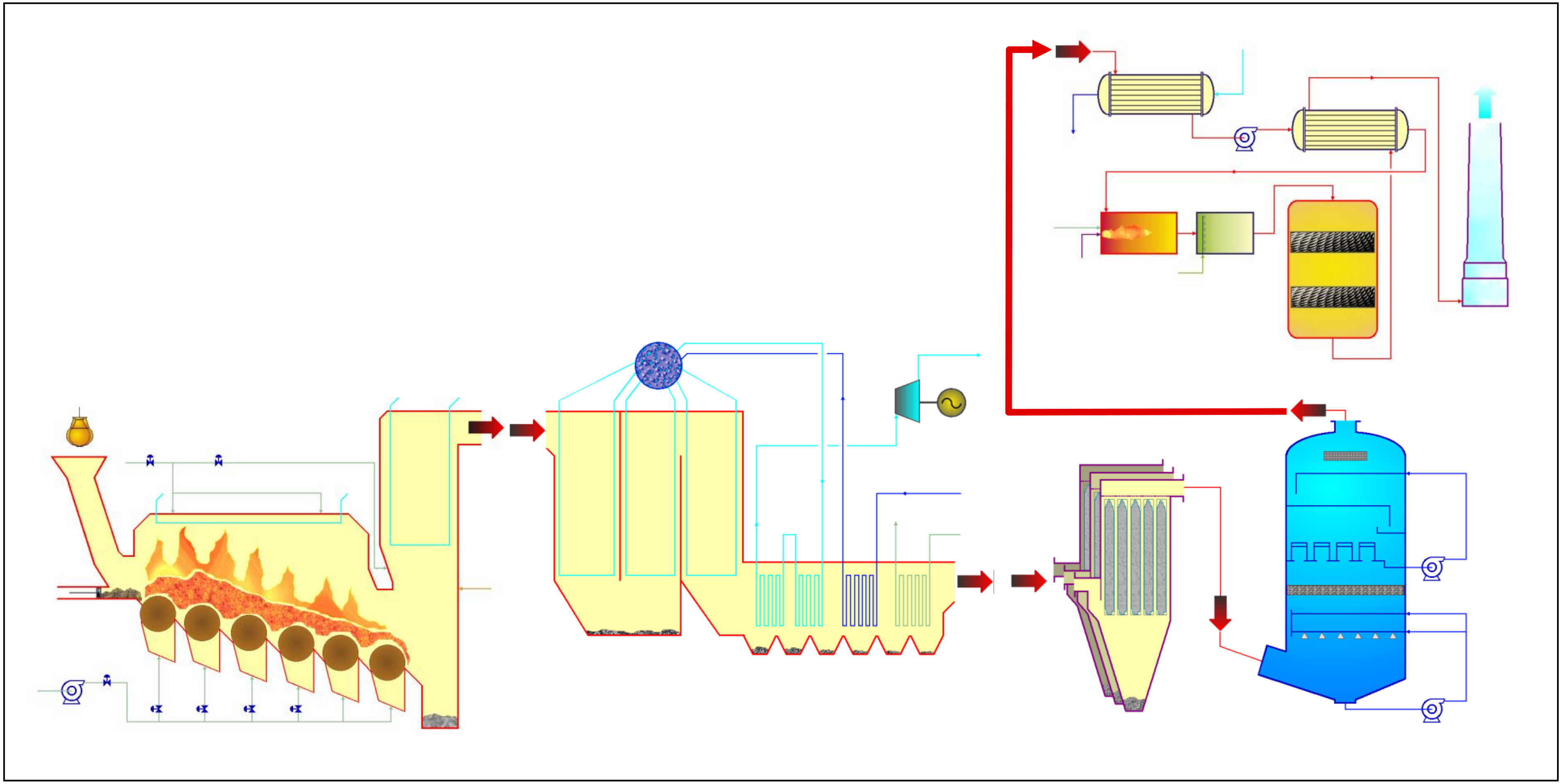
Matrix **B** is an approximation of the Hessian matrix **H** and is calculated with the **BFGS formulas** (Broyden, Fletcher, Goldfarb, Shanno).

# 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 therefore the 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
Air flow rate second drum
Secondary air flow to furn.
First drum speed
Fourth drum speed
NH3 DeNOx flowrate

Total air flowrate to the furnace
Air flow third drum
Air flow afterburner
Second drum speed
NaOH flow

Air flow first drum
Air flow fourth drum
CH4 flow rate afterburner
Third drum speed
CH4 DeNOx flow

## 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

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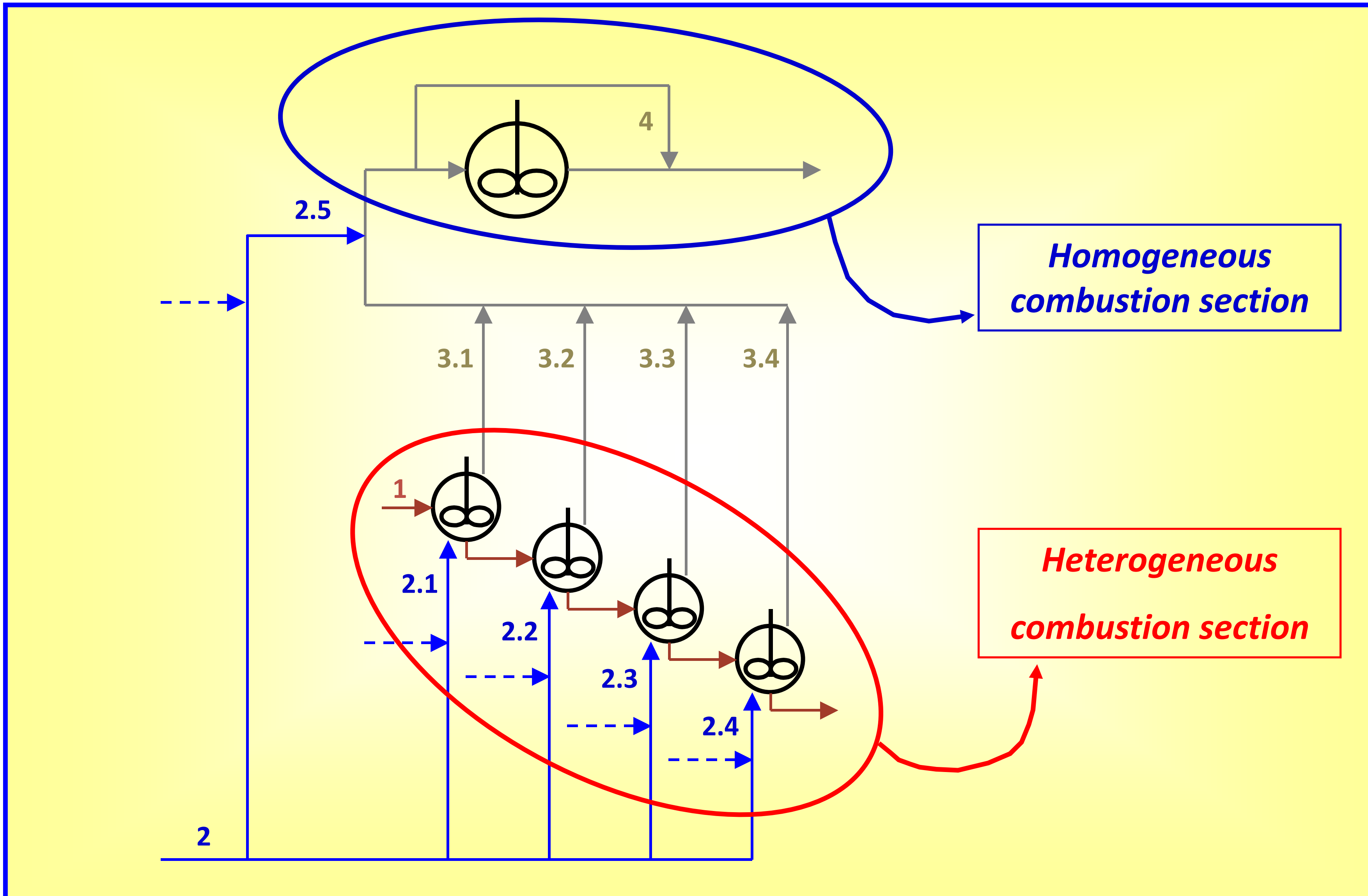
# On-line optimization of continuous processes

**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 provides a new vector of degrees of freedom.
- The main task of the process optimizer is 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***

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

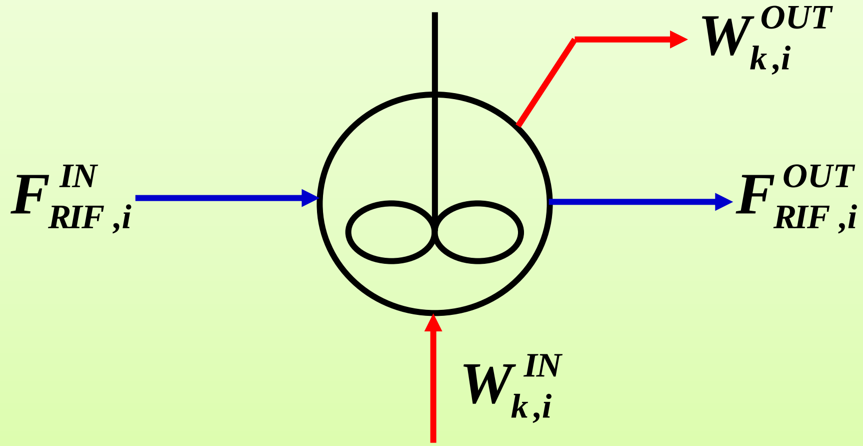
$$i = 1, NG$$

***Gaseous phase***

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

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

***i-th drum***



# Chemical reactions

***Combustion reactions in the solid phase***

$$C_nH_mS_pO_qCl_kN_y \xrightarrow{\mu_{O_2,i}} nCO + kHCl + pSO_2 + x_iNO + \frac{y - x_i}{2} \cdot N_2 + \frac{m-k}{2} \cdot H_2O$$

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

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

***(Bowman, 1975)***

***Combustion reactions in the homogeneous phase***

$$CO + \frac{1}{2} \cdot O_2 \rightarrow CO_2 \qquad \frac{1}{2} \cdot N_2 + \frac{1}{2} \cdot O_2 \rightarrow NO$$

# Primary kiln – combustion kinetics

*Kinetic determining step: $O_2$ diffusion*

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

$$\begin{cases} A_{sc,i} = f\left(d_{p,i}, \varepsilon_i, M_{rif,i}, M_{inerti,i}\right) \\ k_{x,i} = f\left(d_{p,i}, \varepsilon_i, W_{aria,i}, x_{k,i}, T\right) \end{cases}$$

$\Rightarrow$ *Granular solid bed*

$$\begin{cases} A^*_{sc,i} = \Gamma_i \cdot A_{sc,i} \\ \Gamma_i = 1 + \delta \cdot \left(1 - \exp\left(-\frac{N_{CG,i}}{\lambda}\right)\right) \end{cases}$$

*Corrective factors:* $\delta, \lambda$
*(adaptive parameters)*

# Process model – the equations

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

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

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

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

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

$$C_nH_mS_pO_qCl_kN_y \xrightarrow{\mu_{O_2,i}} nCO + kHCl + pSO_2 + x_iNO + \frac{y - x_1}{2}N_2 + \frac{m - k}{2}H_2O \qquad (6)$$

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

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

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

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

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

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

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

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

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# Process model – the equations

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

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

$$\begin{cases}
(W_{A,G,i} + W_{A,L,G,i})x_{O_2,A} - \dfrac{R_{W,i}\mu_{O_2}}{MW_W} - W^{out}_{O_2,G,i} = 0 \\
(W_{A,G,i} + W_{A,L,G,i})x_{N_2,A} - \dfrac{R_{W,i}}{MW_W}\dfrac{x_{N,W}}{2}(1-\Psi_{NO,i}) - \\
\qquad W^{out}_{N_2,G,i} = 0 \\
\dfrac{R_{W,i}}{MW_W}x_{C,W} - W^{out}_{CO,G,i} = 0 \\
\dfrac{R_{W,i}}{MW_W}x_{S,W} - W^{out}_{SO_2,G,i} = 0 \\
\dfrac{R_{W,i}}{MW_W}x_{Cl,W} - W^{out}_{HCl,G,i} = 0 \\
\dfrac{R_{W,i}}{MW_W}x_{N,W}\Psi_{NO,i} - W^{out}_{NO,G,i} = 0 \\
\begin{cases}
\dfrac{R_{W,1}}{MW_W}\dfrac{x_{H,W} - x_{Cl,W}}{2} - W^{\ out}_{,H_2OG,1} + \dfrac{F_W\omega_{H_2O,0}}{MW_{H_2O}} = 0 \\
\dfrac{R_{W,i}}{MW_W}\dfrac{x_{H,W} - x_{Cl,W}}{2} - W^{out}_{H_2O,G,i} = 0 \quad i = 2,\ldots,NG
\end{cases}
\end{cases} \qquad (17)$$

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# Process model – the equations

$$M_{W,F,i} = \rho_W \Delta x_G w_G s_{B,i} \qquad (18)$$

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

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

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

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

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

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

$$\frac{\int_0^{3600} M_{W,F,0} \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{[t - (t_{0,k} + \theta)]^2}{2\sigma^2}\right) dt}{3600} \cong \bar{F}_W \quad t_{0,k} < t < t_{0,k} + \frac{1}{N_{GS,0}} \qquad (25)$$

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

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

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

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# Process model – the equations

$$W^{in}_{Hom,j}=\sum_{i=1}^{NG}W^{out}_{G,j,i}\quad j=\mathrm{CO,SO_2,HCl,NO,H_2O}$$

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

$$W_{Hom,N_2}=\sum_{i=1}^{NG}W^{out}_{G,N_2i}+(W_{A,S}+W_{A,LS})x_{N_2,A} \tag{28}$$

$$x^{in}_{Hom,j}=\frac{W^{in}_{Hom,j}}{\sum_{j=1}^{NC}W^{in}_{Hom,j}}\quad j=\mathrm{O_2,N_2,CO,SO_2,HCl,NO,H_2O}$$

$$\mathrm{CO}+\frac{1}{2}\mathrm{O_2}\rightarrow\mathrm{CO_2} \tag{29}$$

$$\mathrm{N_2}+\mathrm{O_2}\rightarrow 2\mathrm{NO} \tag{30}$$

$$\frac{dc_{CO}}{dt}=1.8\times10^{10}c_{CO}\sqrt{c_{O_2}}\exp\left(-\frac{25000}{RT}\right) \tag{31}$$

$$\begin{cases}\mathrm{O+N_2\rightarrow N+NO}\\ \mathrm{N+O_2\rightarrow O+NO}\\ \mathrm{N+OH\rightarrow H+NO}\end{cases} \tag{32}$$

$$\frac{dn_{Hom,CO_2}}{dt}=-(W^{out}_{Hom}+W^{out}_{L})x^{out}_{Hom,CO_2}+R_{Hom,CO_2}V_{Hom}+W^{in}_{Hom,CO_2}$$

$$\frac{dn_{Hom,j}}{dt}=-(W^{out}_{Hom}+W^{out}_{L})x^{out}_{Hom,j}+W^{in}_{Hom,j}\qquad j=\mathrm{SO_2,H_2O,HCl}$$

$$\frac{dn_{Hom,N_2}}{dt}=-(W^{out}_{Hom}+W^{out}_{L})x^{out}_{Hom,N_2}-\frac{1}{2}R_{Hom,NO}V_{Hom}+W^{in}_{Hom,N_2} \tag{33}$$

$$\frac{dn_{Hom,O_2}}{dt}=-(W^{out}_{Hom}+W^{out}_{L})x^{out}_{Hom,O_2}-\frac{1}{2}R_{Hom,NO}V_{Hom}-\frac{1}{2}R_{Hom,CO_2}V_{Hom}+W^{in}_{Hom,O_2}$$

$$\frac{dn_{Hom,CO^*}}{dt}=-(W^{out}_{Hom}+W^{out}_{L})x^{out}_{Hom,CO^*}-R_{Hom,CO_2}V_{Hom}+W^{in}_{Hom,CO}(1-f_{bypass})$$

$$\frac{dn_{Hom,CO^{**}}}{dt}=-(W^{out}_{Hom}+W^{out}_{L})x^{out}_{Hom,CO^{**}}+W^{in}_{Hom,CO}f_{bypass}$$

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

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# Process model – the equations

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

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

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

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

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

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

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

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

$$(M_S\hat{c}_{p,S} + \sum_{i=1}^{NC} n_i \tilde{c}_{v,i})\frac{dT}{dt} = -\sum_{i=1}^{NC}(W_{Hom,i}^{in}\int_{T^{in}}^{T}\tilde{c}_{p,i}\,dT) - \dot{M}_S^{in}\int_{T^{in}}^{T}\hat{c}_{p,s}\,dT - \sum_{j=1}^{NR}\Delta H_j^R(T)R_j(T) + R_W WLHC + RT\frac{d}{dt}(\sum_{i=1}^{NC} n_i) - \dot{Q}_{disp,PK} - \dot{Q}_{V,PK} \quad (42)$$

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# Process model – the equations

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

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

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

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

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

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

$$A_{G\to W}T_g \cong A_{W\to G}T_W \tag{49}$$

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

$$A_{G\to W} = \frac{A_{GW}}{\dfrac{1}{\epsilon_g}+\dfrac{1}{\epsilon_R}-1} \tag{51}$$

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

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# Process model – the equations

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

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

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

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

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

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

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

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

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

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

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

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# Process model – the equations

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

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

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

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

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

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

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

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

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

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

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

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# Process model – the equations

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

$$\frac{dM_L}{dt} = \dot{G}_{H_2O}^{in} - \dot{G}_{L\to V} \tag{76}$$

$$\frac{dM_V}{dt} = \dot{G}_{L\to V} - \dot{G}_V \tag{77}$$

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

$$\dot{G}_V = \rho_V A_V v_V \tag{79}$$

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

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

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

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

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

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# Process model – the equations

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

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

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

$$m = \frac{1}{1 + \frac{155.3\sqrt{q}}{h_g}}$$

$$q = \frac{\dot{H}_B^{in}}{A_B^{exc}} \quad h_g = \int_{T_{ref}}^{T_g^{in}} \hat{c}_{p,g}^{mix}\, dT \quad (88)$$

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

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

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

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

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

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

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# Process model – the equations

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

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

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

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

$$r = \frac{c_{MIN}}{c_{MAX}}$$
$$\begin{cases} c_{MIN} = \text{Min}\{F_H \hat{c}_{p,H}, F_C \hat{c}_{p,C}\} \\ c_{MAX} = \text{Max}\{F_H \hat{c}_{p,H}, F_C \hat{c}_{p,C}\} \end{cases} \qquad (98)$$
$$NTU = \frac{UA_{GT}}{c_{MIN}}$$

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

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

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

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# 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

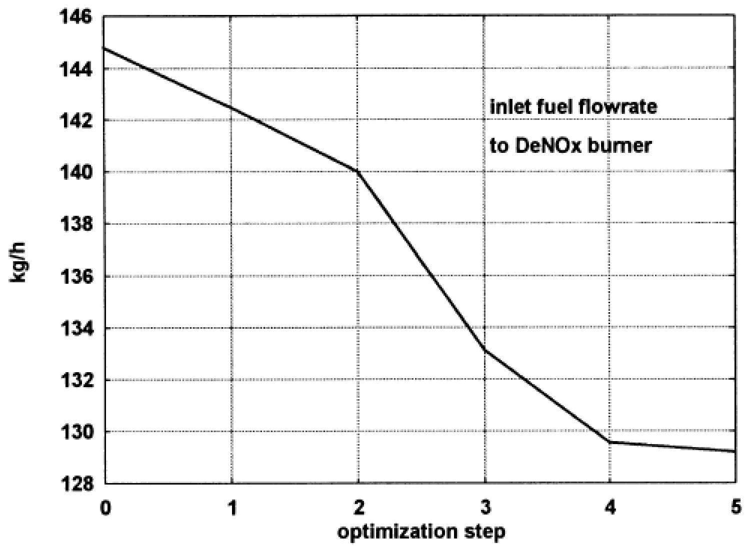
**Results:**

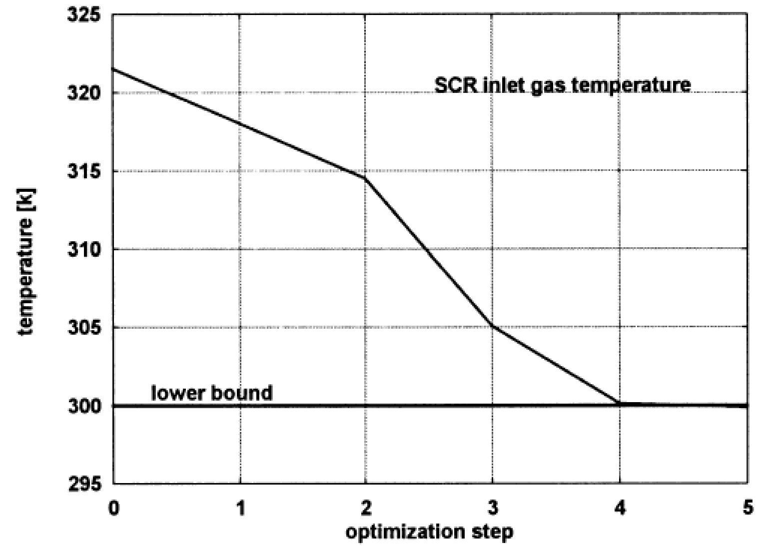
Results.opt - Blocco note

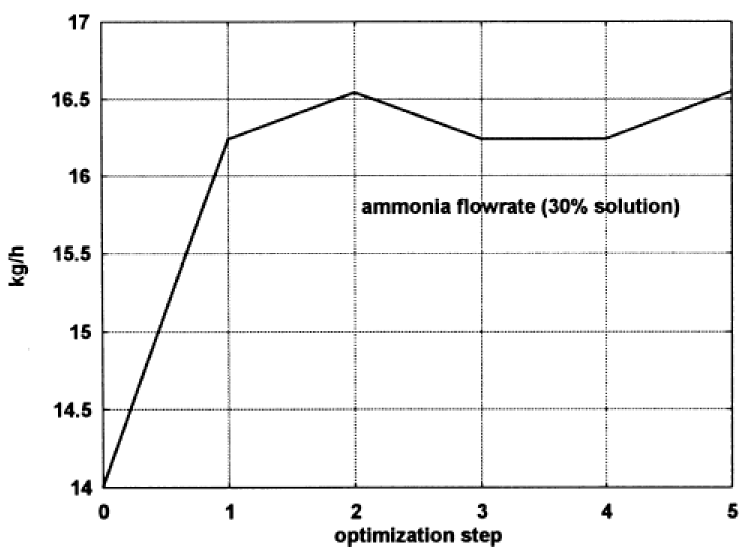
File Modifica Cerca ?

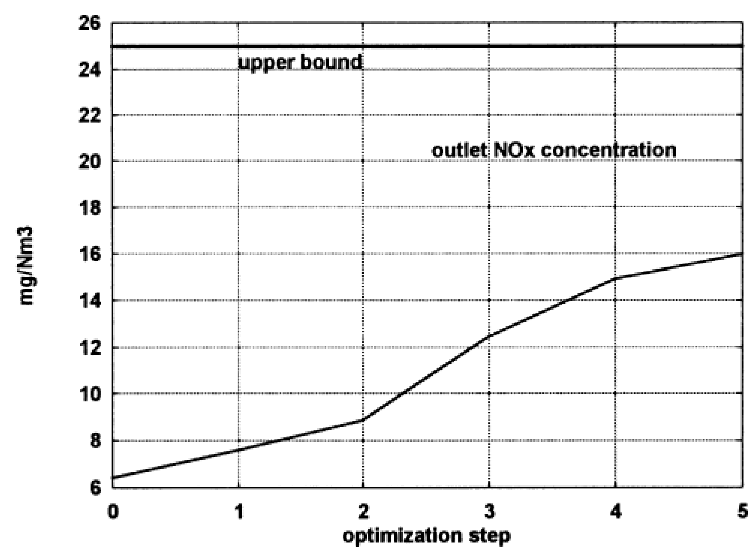
```
VALORE INIZIALE VARIABILI VINCOLATE:
Massimo delta P primo rullo (mmH2O)......................  78.102
Massimo delta P secondo rullo (mmH2O)....................  50.640
Massimo delta P terzo rullo (mmH2O)......................  30.424
Massimo delta P quarto rullo (mmH2O).....................  15.295
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



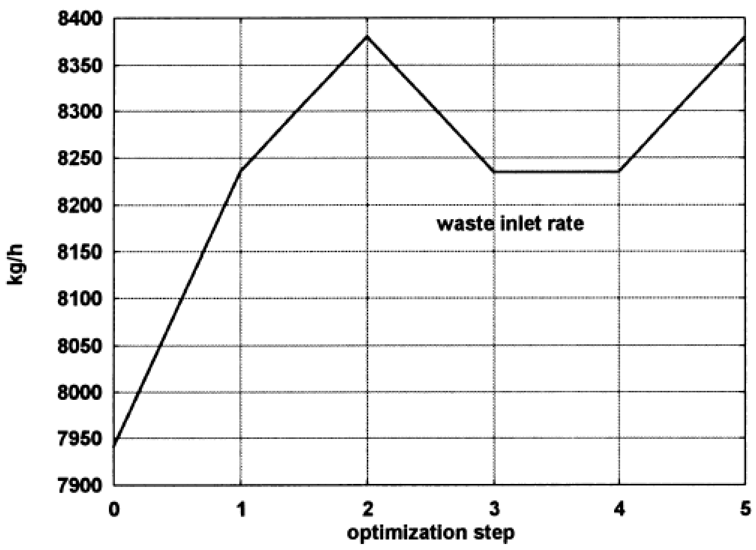



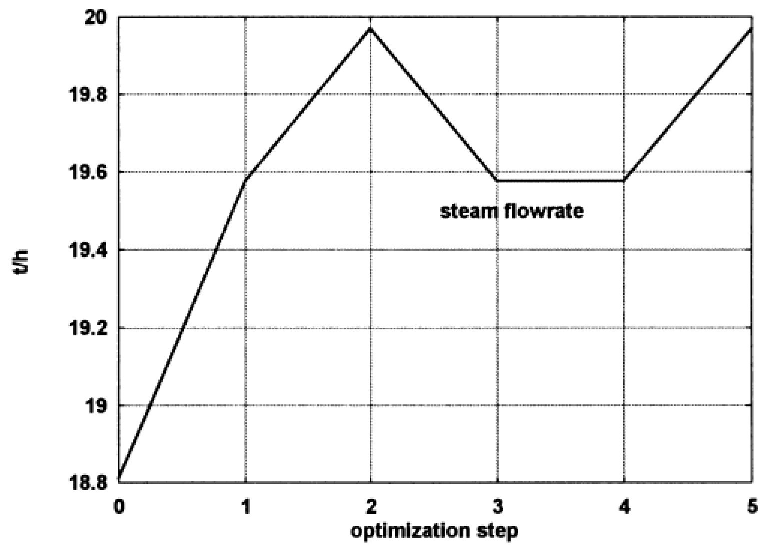




Rovaglio, M., Manca, D., Rusconi, F. Waste Management 18, 525-538, (1998)

# On-line optimization of continuous processes



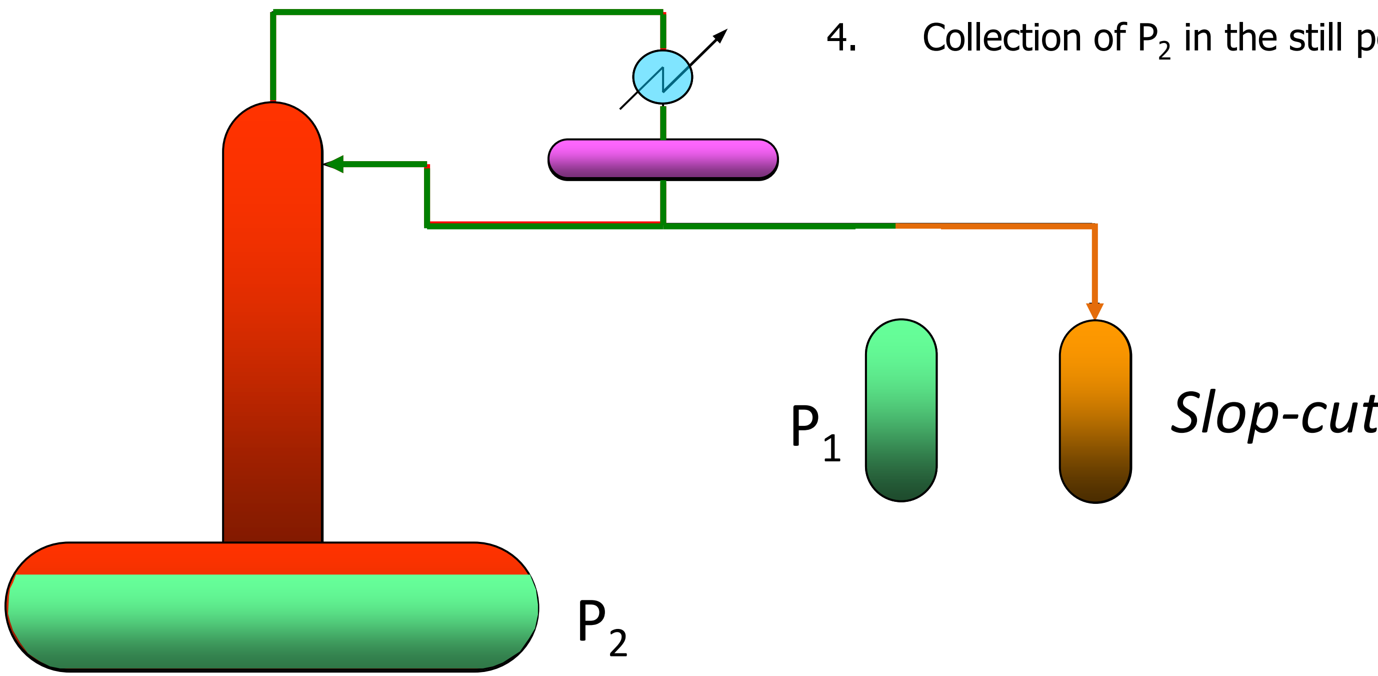




Rovaglio, M., Manca, D., Rusconi, F. Waste Management 18, 525-538, (1998)

# Case-study #2

## On-line optimization of discontinuous processes

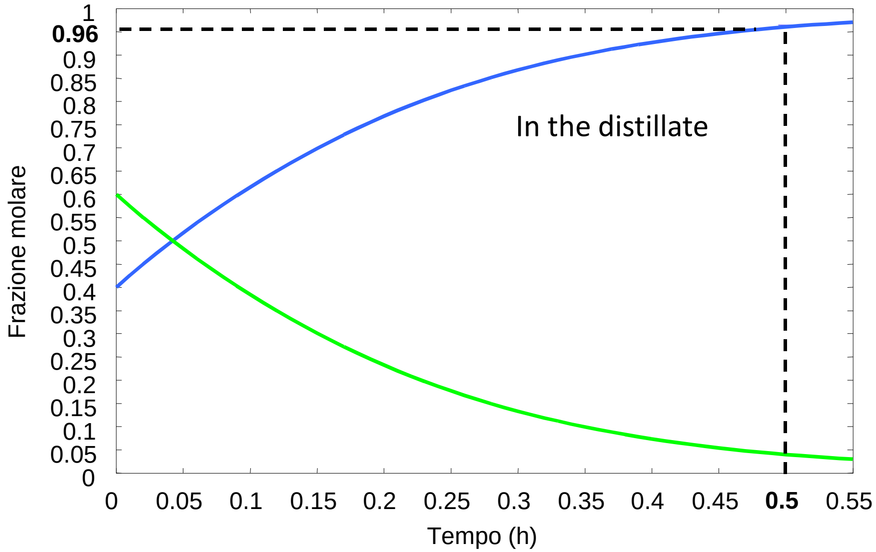
# On-line optimization of discontinuous processes

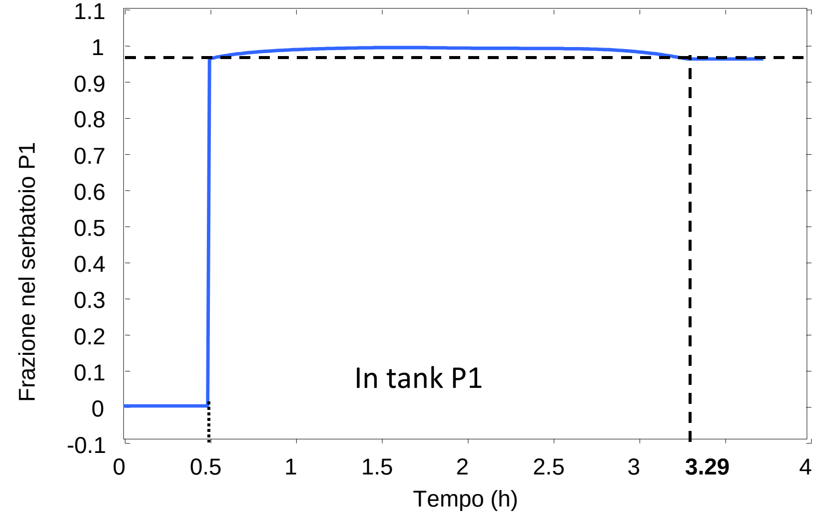


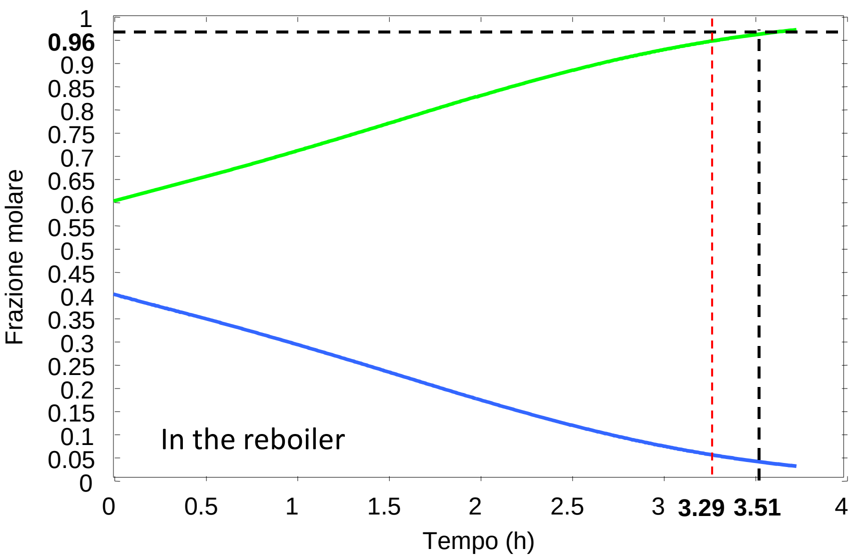

Two-components batch distillation

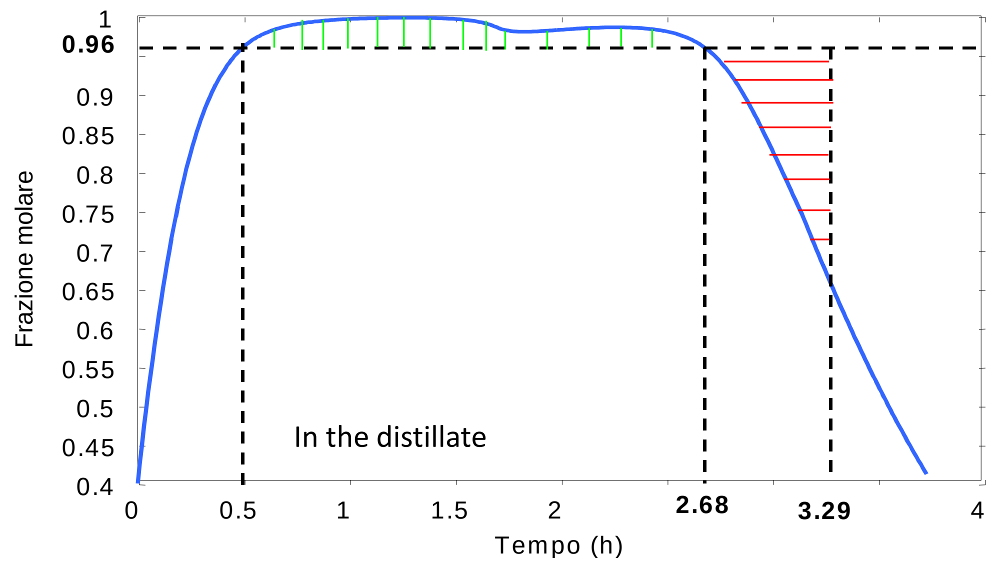
1. Total reflux
2. Collection of $P_1$ in the dedicated tank
3. Out-of-spec collection in the “slop-cut”
4. Collection of $P_2$ in the still pot

# 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. **Maximize 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. **Minimize 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 with an SQP algorithm.

3. **Maximize the profit**

   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.

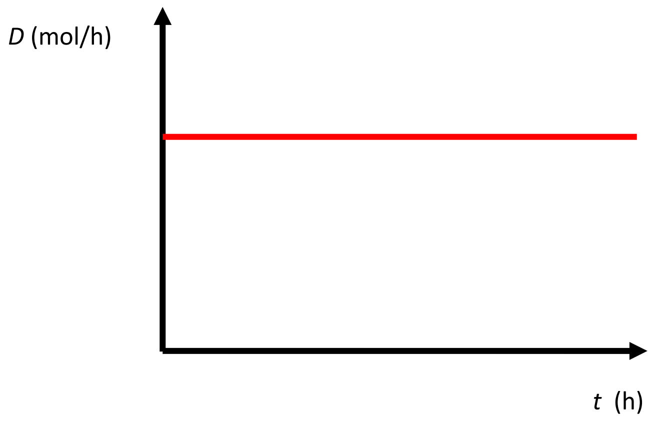
2. **Constant composition**

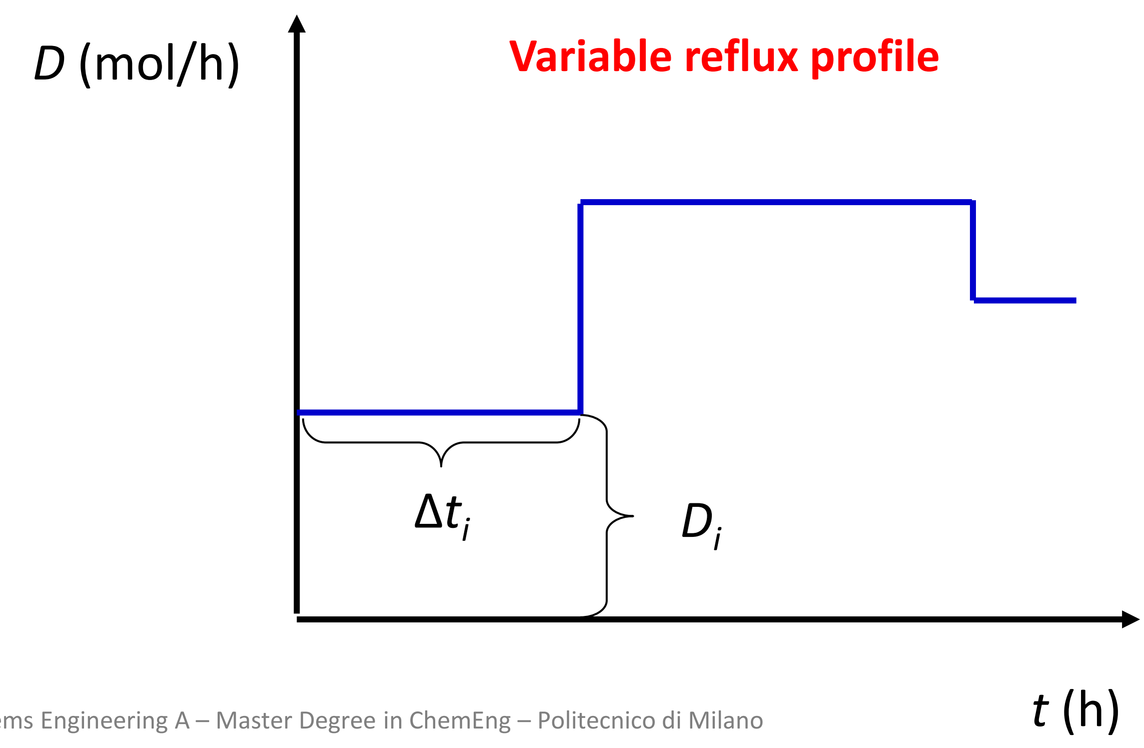
   The degrees of freedom are: pressure, vapor flowrate, and the purity of the key component that remains constant throughout the batch.

3. **Variable reflux profile**

   The degrees of freedom are: pressure and reflux ratio (or equivalently the distillate flowrate) at any 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)

$s.t.$

$$\begin{cases} g(x,x',u,\eta,t)=0 \\ \bar{x}_{Pi} = x_{Di}^{spec} \\ 0 \le D_i \le D_{\max} \\ 0 \le \Delta t_i \le t_{\max} \end{cases}$$

**The DAE system comprises**

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

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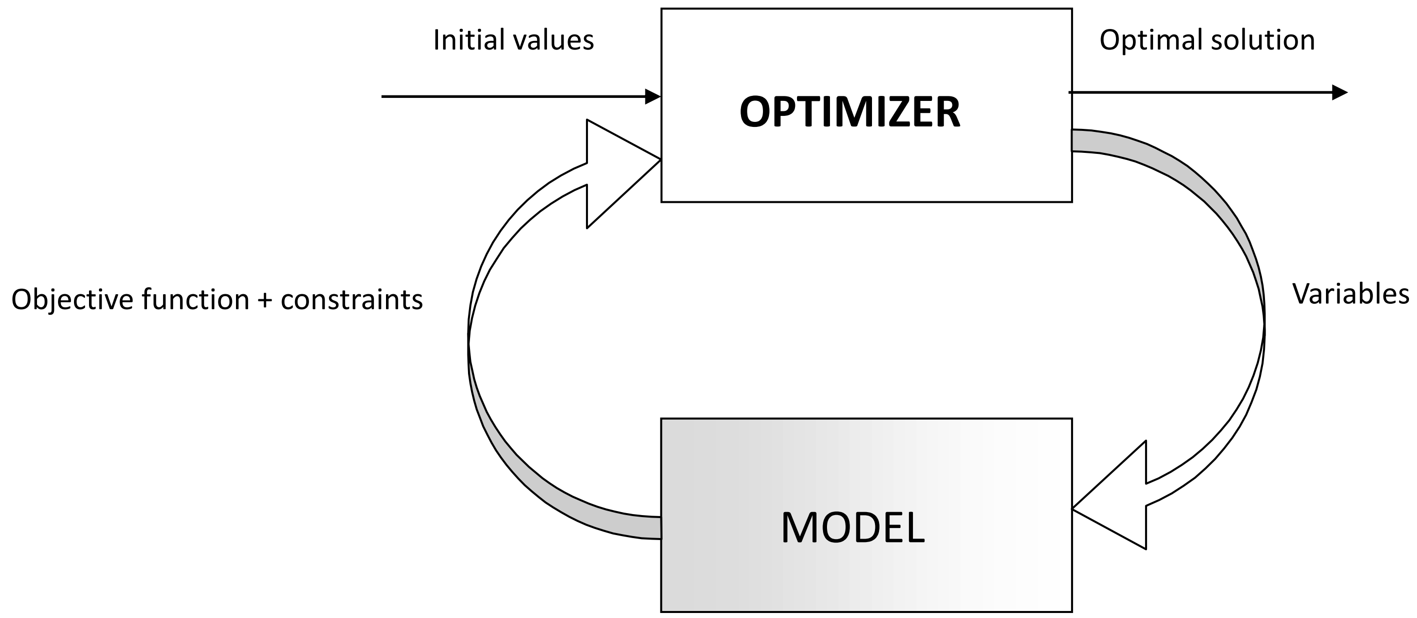
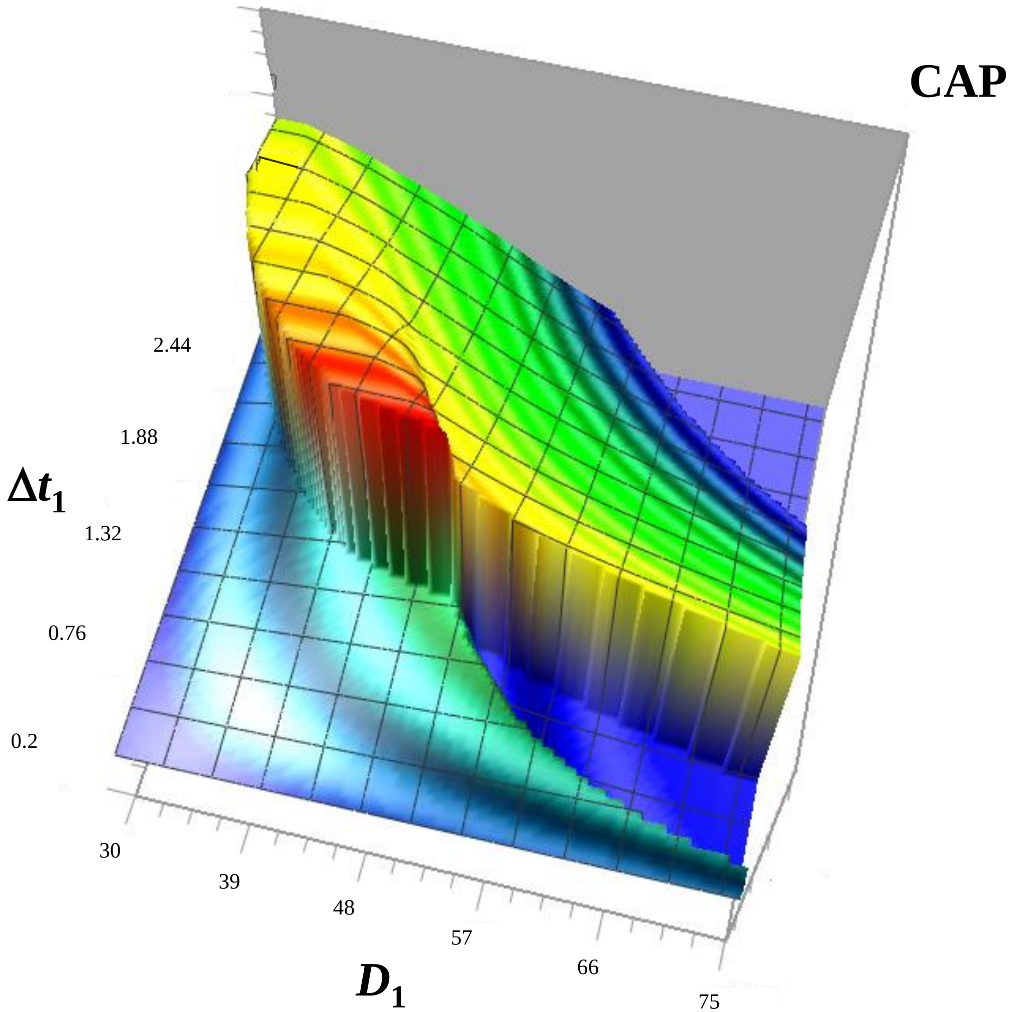
# Optimal trajectory




**OPTIMIZATION METHODS**

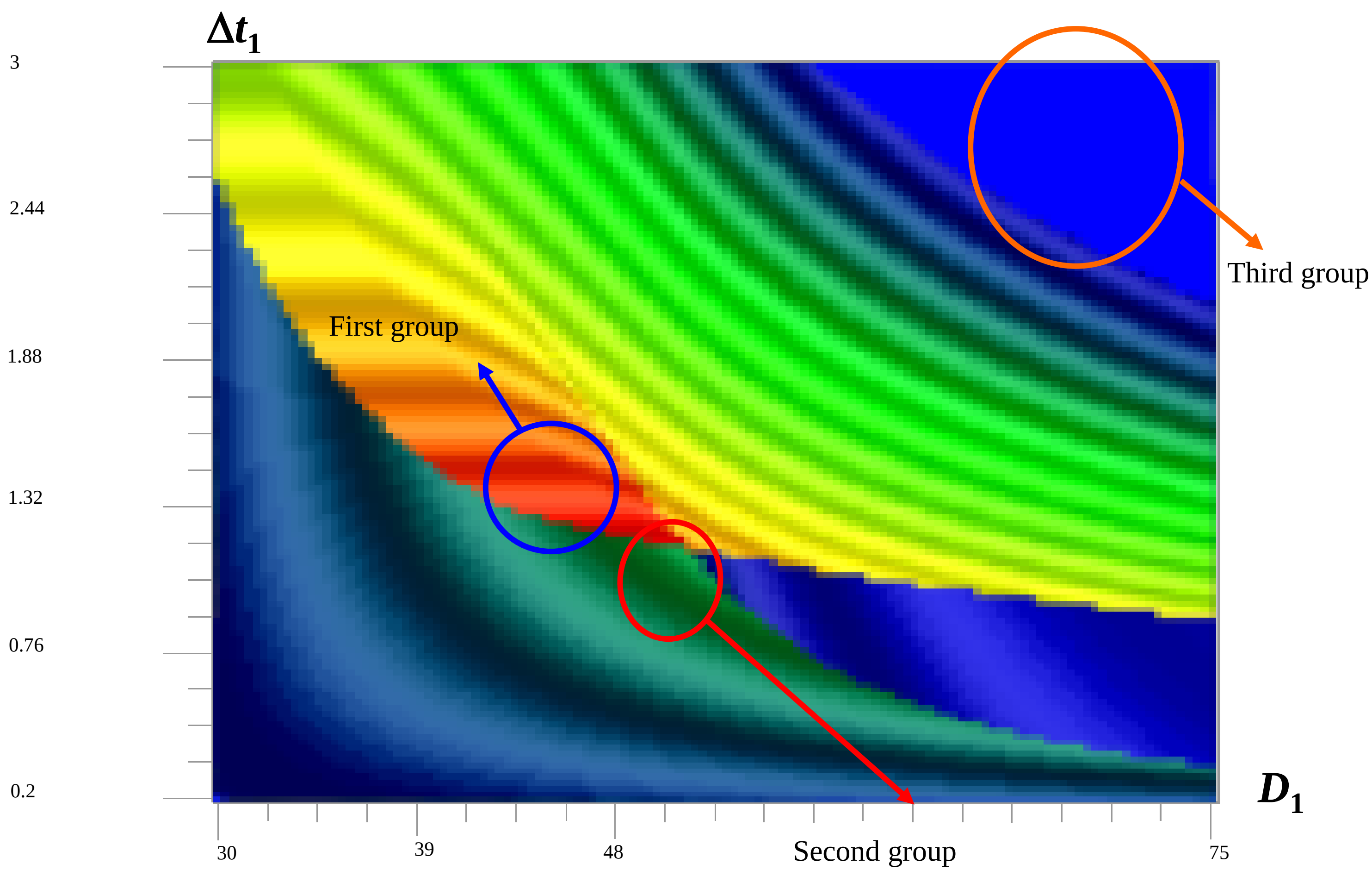
- SQP
- Simplex
- Robust method searching the solution within the entire domain of the *dof*

# Optimal trajectory



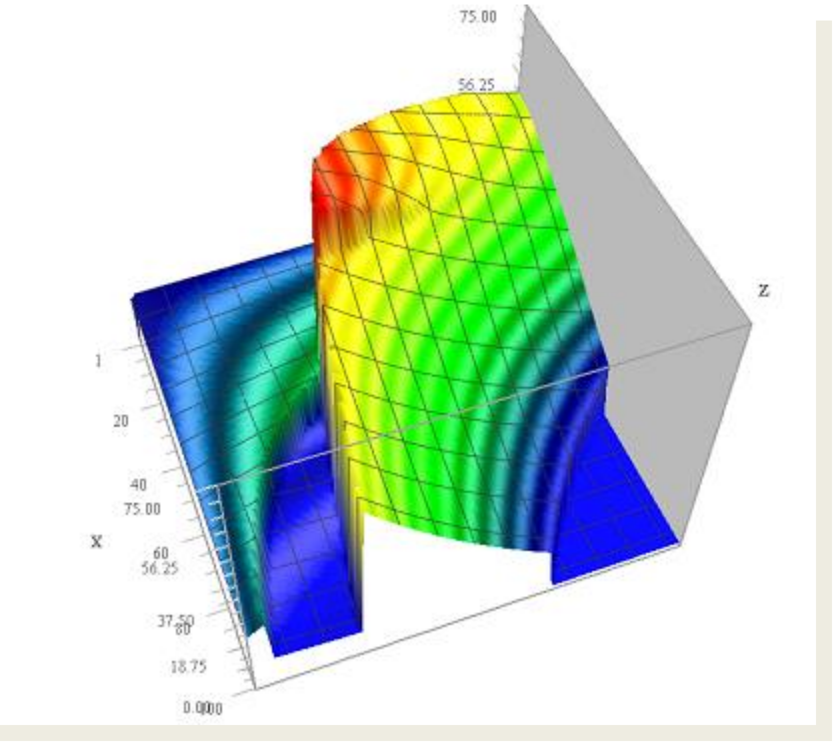

D. Manca. Chemical Product and Process Modeling, 2,12 *(2007)*

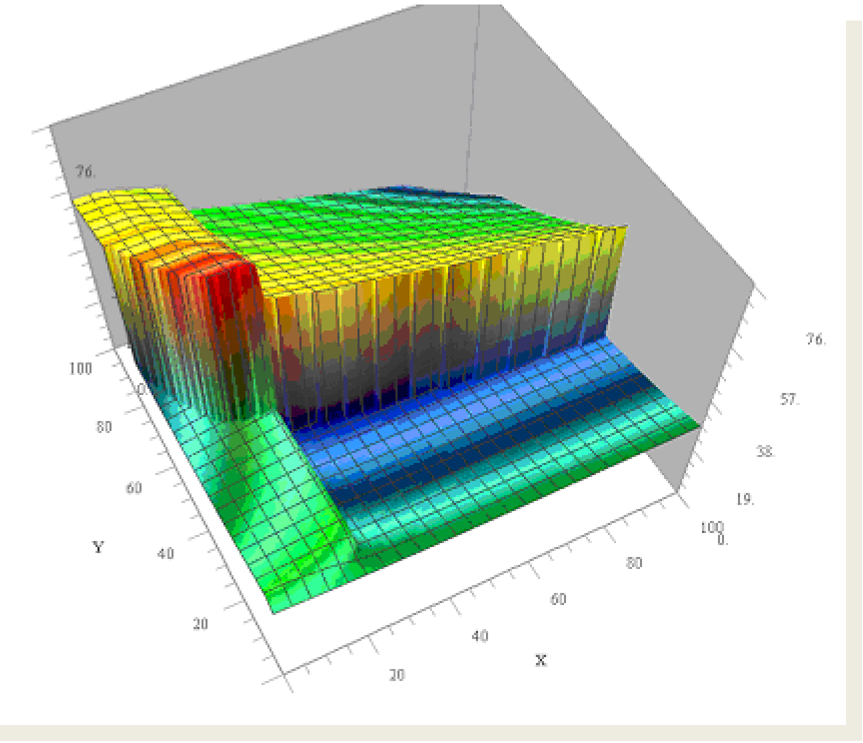
# Optimal trajectory




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

# Optimal trajectory

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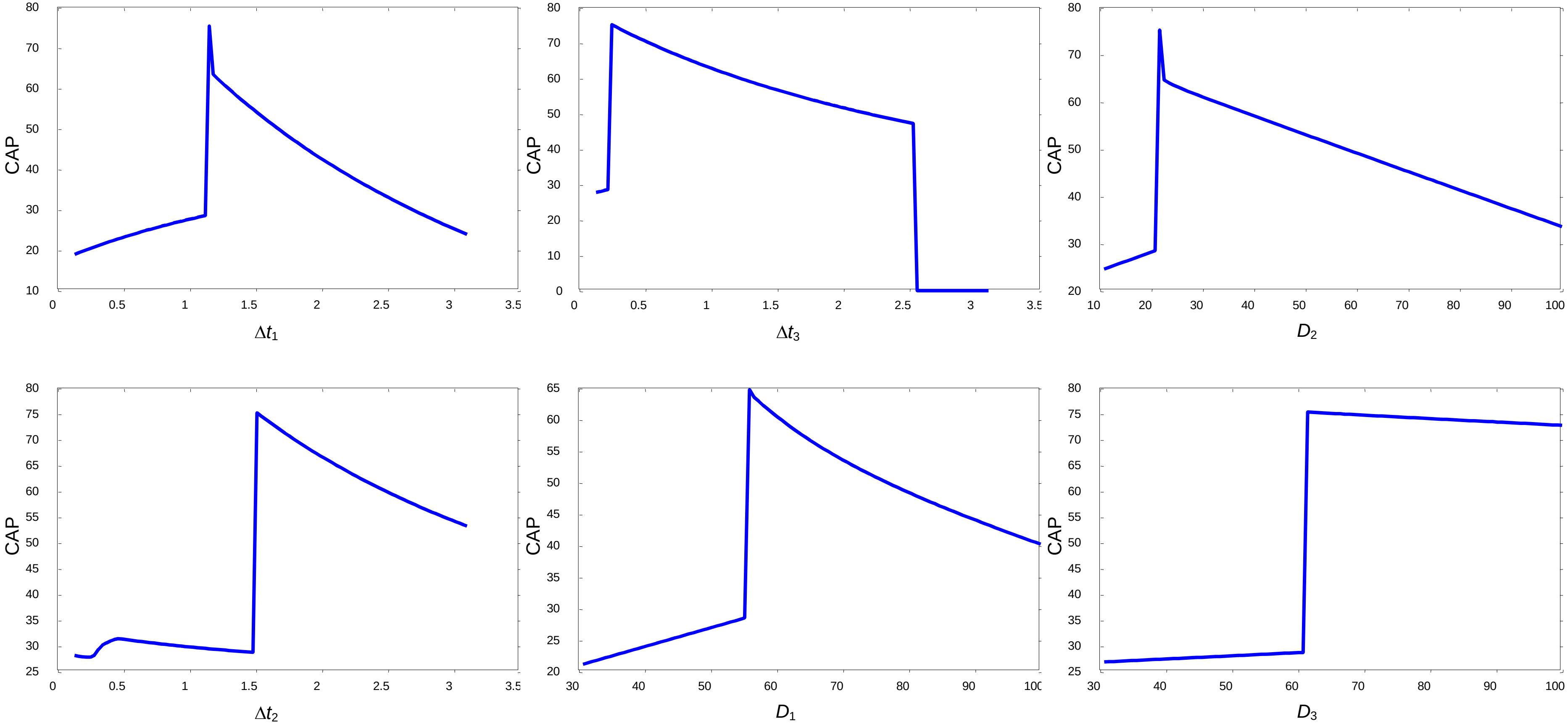
# Optimal trajectory




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

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

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