Chemical Processes Optimization

Prof. Cesar de Prada

Dpt. of Systems Engineering and Automatic Control (ISA)

UVA

prada@autom.uva.es

Chemical Processes Optimization

- Compulsory, 5th year Chemical Eng. Code 44337
- Background: Math / Processes
- 2nd semester 4.5 (3+1.5) credits
- 2 hours lecturing Monday, Tuesday, 11.00h
  1 hour lab Monday, 4-5 h / 5-6h
- Prof. Cesar de Prada / Gloria Gutierrez
- Web: www.isa.cie.uva.es/~prada/
- E-mail: prada@autom.uva.es
- Moodle: http://campusvirtual.uva.es

Process Optimization

- Introduction
- Aims
- Programme
- Laboratory
- Marks
- Visits / Conferences

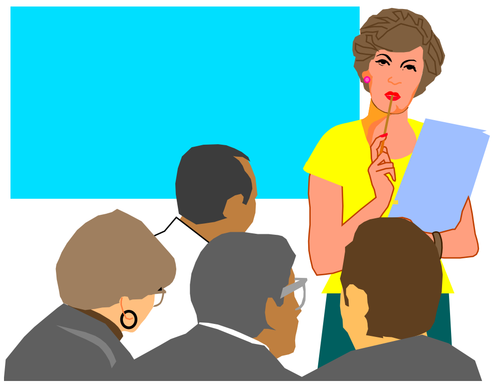
Optimization Problems

- How to choose the best option among several ones
- Problems of very wide nature
  - Design (p.e. equipment sizing with minimum cost)
  - Operation (p.e. more profitable operating point of a process)
  - Logistics (p.e. minimum time route for distributing a product)
  - Planning (p.e. best place to build a process plant)
  - Control (p.e. control action that minimize the variance of the error)
  - Etc.

Optimization problems

- They appear in a wide range of fields
  - Processes
  - Economy
  - Biology
  - Electronics,….
- Sharing some common features:
  - An aim or criterion to minimize (maximize)
  - A set of decision variables
  - A set of constraints on the decision variables

How to make (rational) optimal decisions?



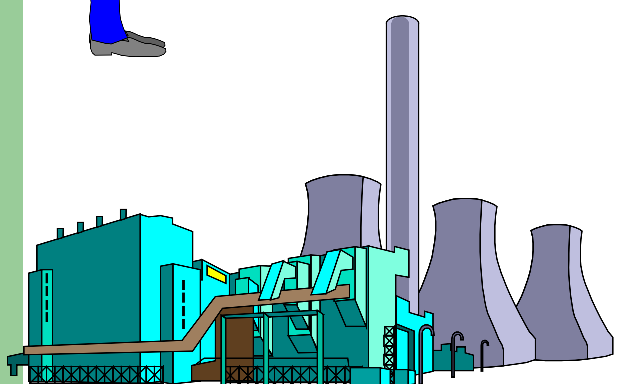
By experience?

Testing all possibilities?

Formulating the problem mathematically as an optimization one

Methodology

1 Analyse the problem



2 Formulate it in mathematical terms

$$\min_{x} J(x, y)$$

$$h(x, y) = 0$$

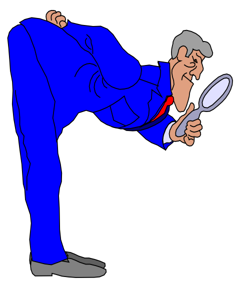
$$g(x, y) \leq 0$$

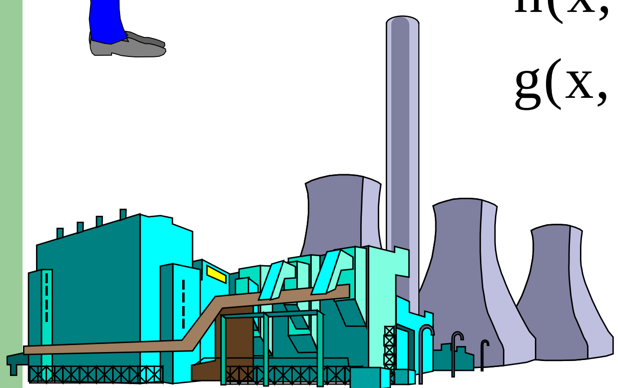
3 Solve it with the adequate algorithms and software

4 Interpreting the solution and apply it

Analysis / Formulation (Modelling)

1 Analyse the problem





2 Formulate it in mathematical terms

$$\min_{x} J(x, y)$$

$$h(x, y) = 0$$

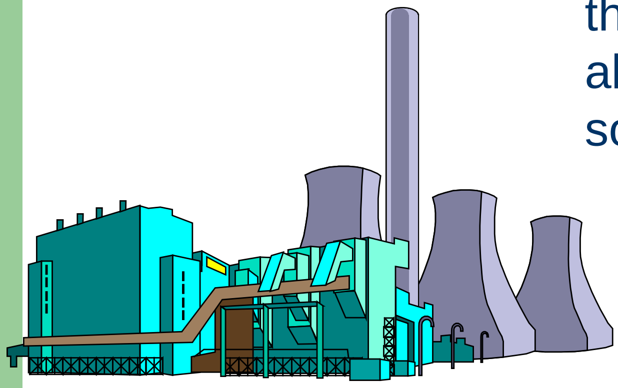
$$g(x, y) \leq 0$$

1. Study the process. List the variables of interest
2. Choose and optimization criterion and formulate it in terms of the variables of the problem
3. Specify the mathematical relations among the variables imposed by physical laws, balances, etc.
4. Choose the admissible range of the variables and other physical constraints
5. Decide if there are degrees of freedom for selecting the best option

Solving / Implementing (Optimization)

$$\min_{x} J(x, y)$$
$$h(x, y) = 0$$
$$g(x, y) \leq 0$$

3 Solve it with the adequate algorithms and software



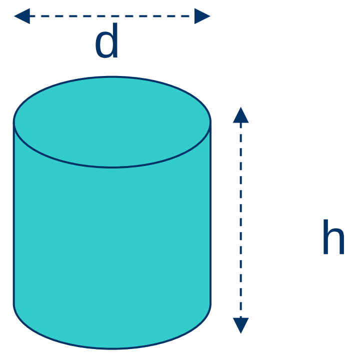
4 Interpreting the solution and apply it

6. Formulate the problem as one of optimization with a given structure (LP, NLP;..)
7. Study its mathematical structure and try to improve it
8. Select a solution method and a software tool and obtain a solution
9. Analyse the solution and study its sensibility to changes in the parameters of the problem.

PSE Process Systems Engineering

- The topic belong to the field of Process Systems Engineering (PSE)
- **Process systems engineering** is the body of knowledge in chemical engineering that deals with the systematic modelling and development of tools and solution methods for synthesis, analysis and evaluation of Process Design, Process Control and Process Operation
- PSE is a field where multiple disciplines cooperate in order to find useful solutions: from chemical, control, electrical, etc. engineering, to applied mathematics, basic sciences (biology, physics, etc.) and computer science.

An example



Variables:

V volume

d diameter

h height

A surface

Find the size of an open cylindrical tank of 6 m^3, so that its surface is minimal

Cost function to be minimized:

$A = \pi dh + \frac{1}{4}\pi d^2$

Relations among variables:

$V = \frac{1}{4}\pi d^2 h = 6$

Formulation:

$$\min_{d,h} \quad \pi dh + \frac{1}{4}\pi d^2$$

under :

$$\pi d^2 h = 4V$$

$$d \geq 0, h \geq 0$$

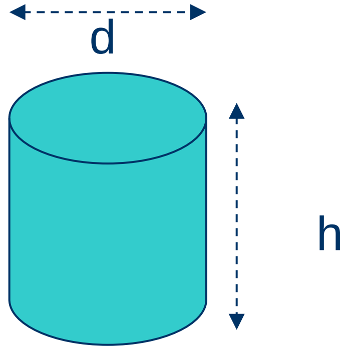
Degrees of freedom: number of variables – number of independent equations: 2-1=1

Constraints:

$d \geq 0 \quad , \quad h \geq 0$

Data : V

An example



1 degree of freedom

$$\min_{d,h} \quad \pi dh + \frac{1}{4}\pi d^2$$

$$\text{under:}$$

$$\pi d^2 h = 4V$$

$$d \geq 0,\ h \geq 0$$

Analytical solution (not possible most of the times)

$$h = \frac{4V}{\pi d^2}$$

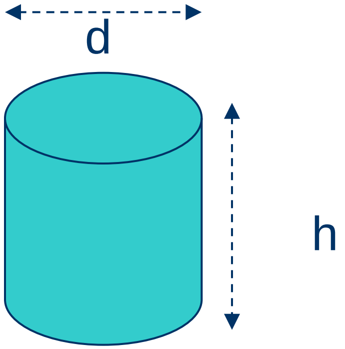
$$\text{area} = \pi d \frac{4V}{\pi d^2} + \frac{\pi d^2}{4} = \frac{4V}{d} + \frac{\pi d^2}{4}$$

$$\left.\frac{\partial \text{area}}{\partial d}\right|_{d^*} = 0 \quad \Rightarrow \frac{-4V}{d^{*2}} + \frac{\pi d^*}{2} = 0$$

$$\pi d^{*3} = 8V, \quad d^* = \left(\frac{8V}{\pi}\right)^{1/3} \quad h^* = \left(\frac{V}{\pi}\right)^{1/3}$$

Sensibility: How much change the solution if the volume changes 1%?

A more realistic example



Find the size of an open cylindrical tank of 6 m^3, so that its surface is minimal, assuming that the thickness ε (and the cost) depends on d according:
ε =0.0001d + 0.0004 m

$$\min_{d,h} \quad (\pi dh + \frac{1}{4}\pi d^2)10^{-4}(d+4)p\rho$$

under :

$$\pi d^2 h = 4V$$

$$d \geq 0, h \geq 0$$

Relations among variables:

$V = ¼ \pi d^2 h = 6$

Constraints:

$d \geq 0$, $h \geq 0$

Variables:

V volume

d diameter

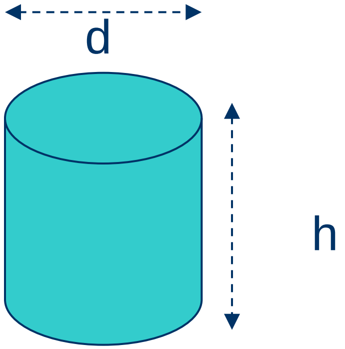
h height

A cross section

p is the price in € per kg of metal sheet spent

The factor $10^{-4}p\rho$ does not affect the result of the optimization and can be cancelled in the cost function

A more realistic example



$$\min_{d,h} \quad (\pi d h + \frac{1}{4}\pi d^2)(d+4)$$

$$h = \frac{4V}{\pi d^2}$$

under:

$$\pi d^2 h = 4V$$

$$d \geq 0,\ h \geq 0$$

$$\text{cost} = (\pi d \frac{4V}{\pi d^2} + \frac{\pi d^2}{4})(d+4) \qquad \left.\frac{\partial \text{area}}{\partial d}\right|_{d^*} = 0$$

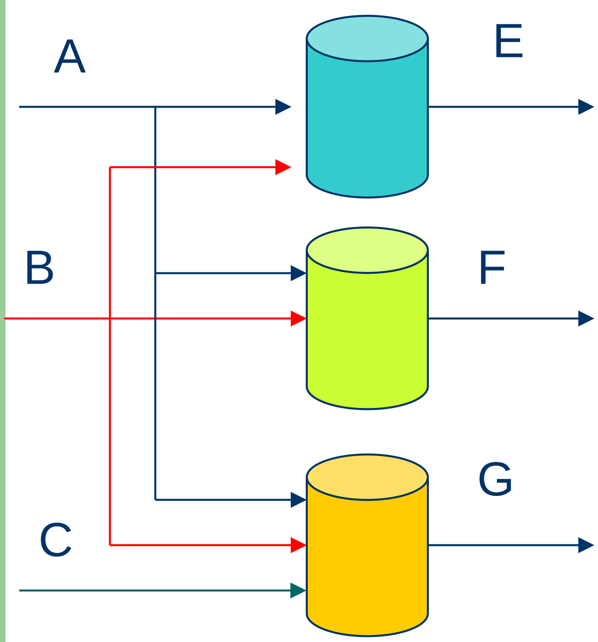
$$\frac{4V}{d^*} + \frac{\pi d^{*2}}{4} + (\frac{-4V}{d^{*2}} + \frac{\pi d^*}{2})(d^* + 4) = 0$$

$$3\pi d^{*4} + 8\pi d^{*3} - 64V = 0$$

A direct numerical solution can be a better alternative

This equation has no analytical solution and must be solved using numerical methods

Example: Production Planning

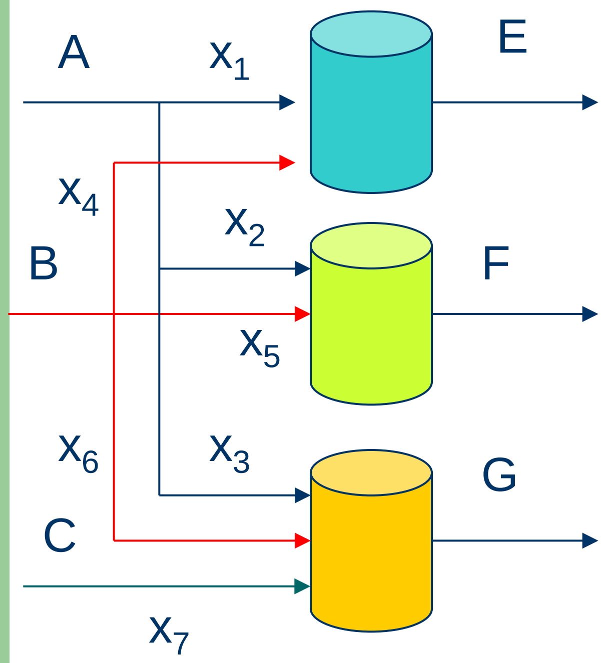


Product	Kg A / Kg	Kg B / Kg	Kg C / Kg	Man. Cost € / Kg	Price € /Kg
E	0.6	0.4	0	1.5	4
F	0.7	0.3	0	0.5	3
G	0.5	0.2	0.3	1	3.7

Material	Availability Kg /day	Cost € /Kg
A	40000	1.5
B	30000	2
C	25000	2.5

What amounts of E, F, G must be produced every day in order to maximize the benefits?

Example: Production Planning



Aim: Maximize the daily benefit

Variables: x_i Kg /day of each product processed in every process unit

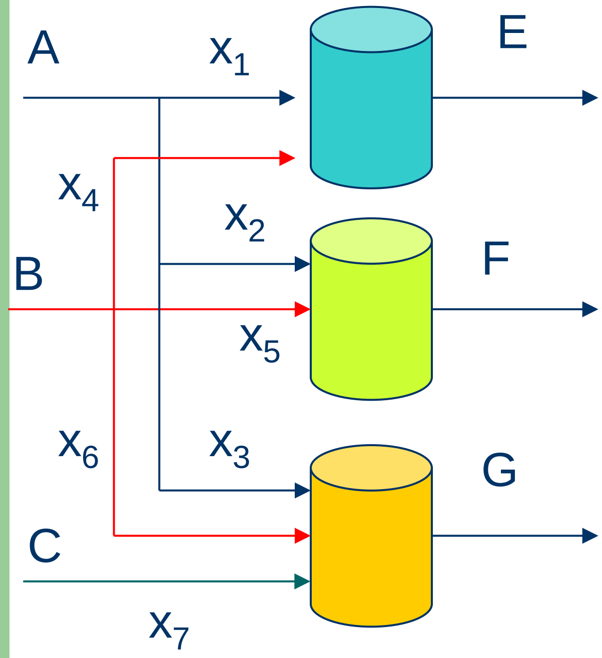
A, B, C Kg /day of row materials

E, F, G Kg/dia of finished products

Benefit /day = sells – processing costs – row material costs =

(4E+3F+3.7G) – (1.5E+0.5F+G) – (1.5A+2B+2.5C)

Example: Production Planning



Aim: Maximize the daily benefit

$$\max 2.5E + 3.5F + 2.7G - 1.5A - 2B - 2.5C$$

$$E = x_1 + x_4 \quad F = x_2 + x_5 \quad G = x_3 + x_6 + x_7$$

$$A = x_1 + x_2 + x_3 \quad B = x_4 + x_5 + x_6 \quad C = x_7$$

$$x_1 = 0.6E \quad x_2 = 0.7F \quad x_3 = 0.5G \quad x_6 = 0.2G$$

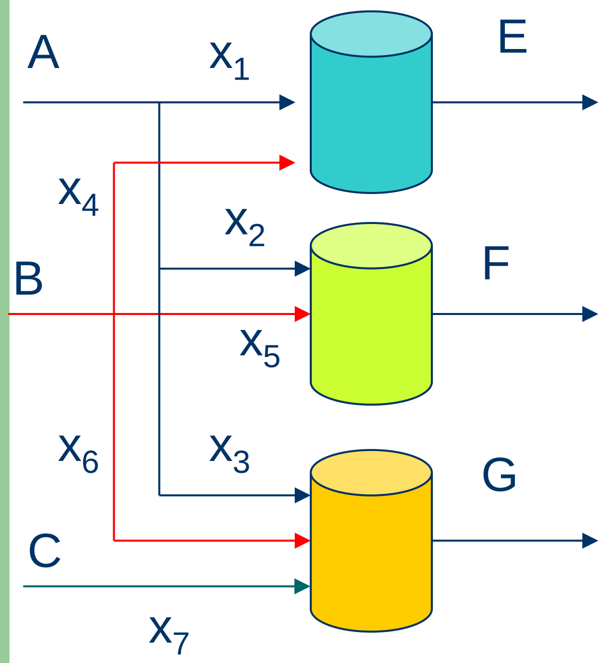
$$0 \le x_1 + x_2 + x_3 \le 40000$$

$$0 \le x_4 + x_5 + x_6 \le 30000$$

$$0 \le x_7 \le 25000$$

$$x_i \ge 0$$

Example: Production Planning



$$\max\ 2.5E + 3.5F + 2.7G - 1.5A - 2B - 2.5C$$

$$E = x_1 + x_4 \quad F = x_2 + x_5 \quad G = x_3 + x_6 + x_7$$

$$A = x_1 + x_2 + x_3 \quad B = x_4 + x_5 + x_6 \quad C = x_7$$

$$x_1 = 0.6E \quad x_2 = 0.7F \quad x_3 = 0.5G \quad x_6 = 0.2G$$

$$0 \le x_1 + x_2 + x_3 \le 40000$$

$$0 \le x_4 + x_5 + x_6 \le 30000$$

$$0 \le x_7 \le 25000$$

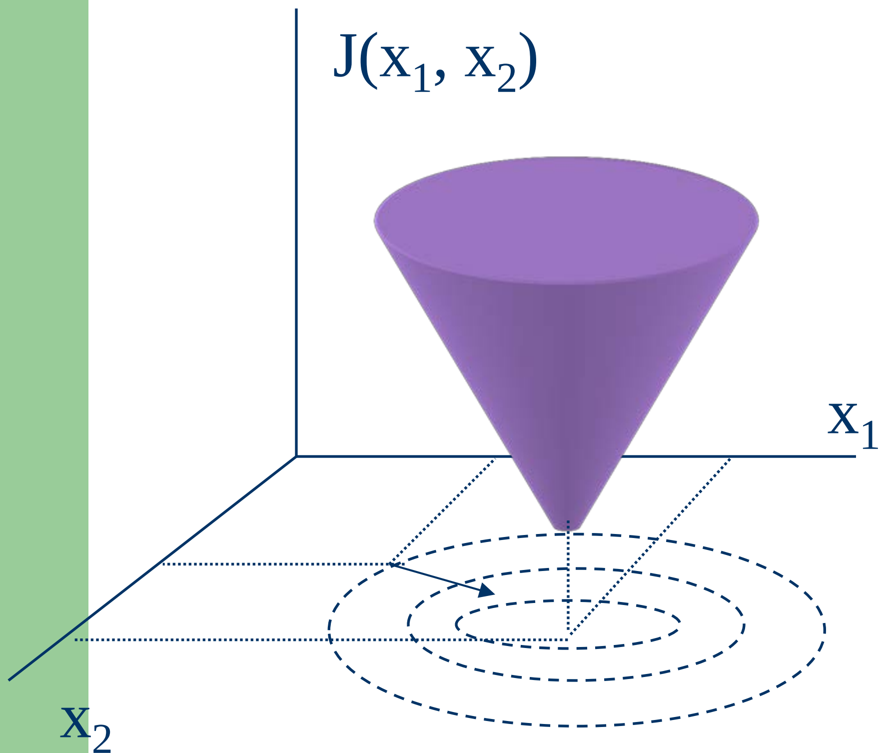
$$x_i \ge 0$$

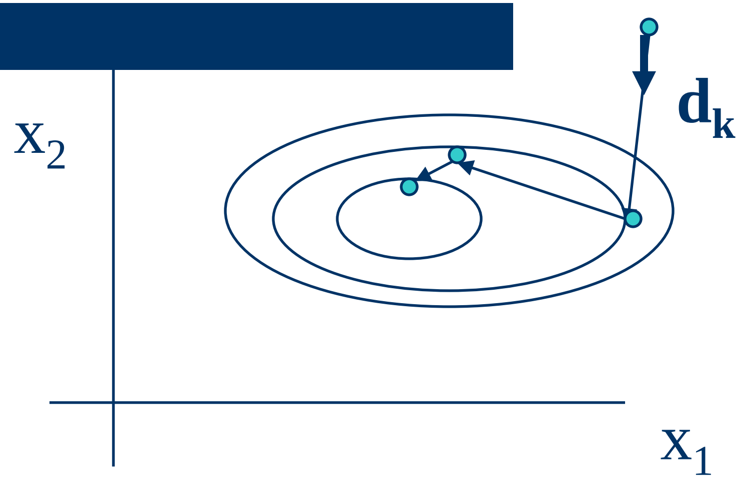
13 variables – 10 equations = 3 degrees of freedom

Aim: Maximize the daily benefit

An analytical solution is not feasible

Numerical optimization of a function





$$x_{k+1} = x_k + \alpha \mathbf{d}_k$$

Iterative methods

d search direction

α step length

Aims of the course

- Learn to model and formulate in mathematical terms optimization problems
- Be able to classify an optimization problem
- Understand the fundamentals of the optimization methods
- Learn to use optimization software and interpret the proposed solution
- Be able to apply the theory in the solution of practical decision making problems

Syllabus (30h theory, 15 h lab)

- Introduction, Basic mathematical concepts (3h)
- Unconstraint optimization (1+2h)
- Constraint optimization
  - LP (3h)
  - KKT, QP, Penalty (2h)
  - NLP, stochastic methods (4+1h)
- Mix-integer problems, MILP (2h)
- Scheduling of batch processes (1h)
- Dynamic optimization (1h)
- Software, GAMS (2h)
- Applications in the process industry (8h)

Laboratory / Practical work

- Aim:
  - Learn software tools
  - Learn to formulate and solve optimization problems
- Computer room
- 2 groups.
- Tools:
  - Matlab Optimization Toolbox (Excel)
  - GAMS
- Practical work: 3 compulsory reports
  - Matlab Optimization Toolbox
  - GAMS, LP, NLP problems
  - A design mini-project (GAMS) MILP, NLP
- Weight in the final mark: 30% (5, 10, 15%). A minimum of 4 is required in the exam. Oral presentation of selected groups.

Reports

- Matlab Optimization Toolbox, Unconstraint Optimization, report due: 3 March, with oral presentation of a selected group. (5%)
- GAMS, LP, NLP problems, report due: 7 April, with oral presentation of a selected group (10%)
- A design mini-project (GAMS) NLP, MILP, report due: 26 May, with oral presentation of three selected groups (15%)

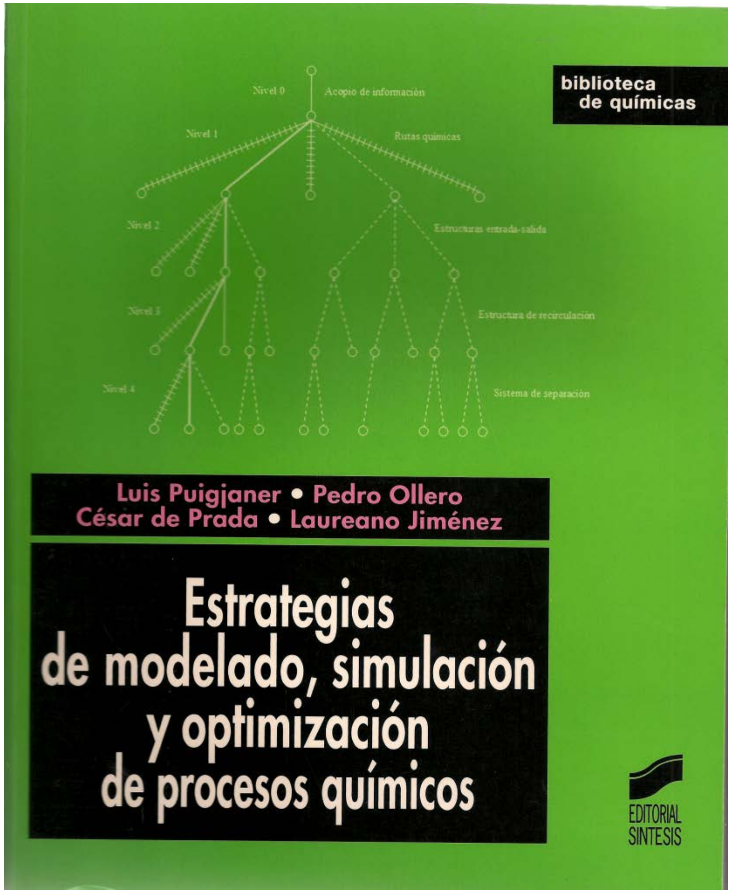
- Groups will be organized by the students' representatives

Bibliography

- Optimization of Chemical Processes, T.F. Edgar, D.M. Himmenblau, L.S. Lasdon, McGraw Hill, 2ª edición, 2001
- Systematic Methods of Chemical Process Design, L.T. Biegler, I.E. Grossmann, A.W. Westerberg, Prentice Hall 1997
- Engineering Optimization, G.V. Reklaitis, A. Ravindran, K.M. Ragsdell, J. Wiley 1983
- Practical Methods of Optimization, R. Fletcher, J. Wiley, 2ª edición, 1991
- Model Building in Mathematical Programming, H.P. Williams, J. Willey 4ª edic., 2002
- Non-linear and Mix-Integer Optimization, C. A. Floudas, Edt. Oxford Univ. Press, 1995
- Estrategias de Modelado, Simulación y Optimización de Procesos Químicos, L. Puigjaner, P. Ollero, C. de Prada, L. Jimenez, Edt. Síntesis, 2006

- Slides of the course in: http://www.isa.cie.uva.es/~prada/

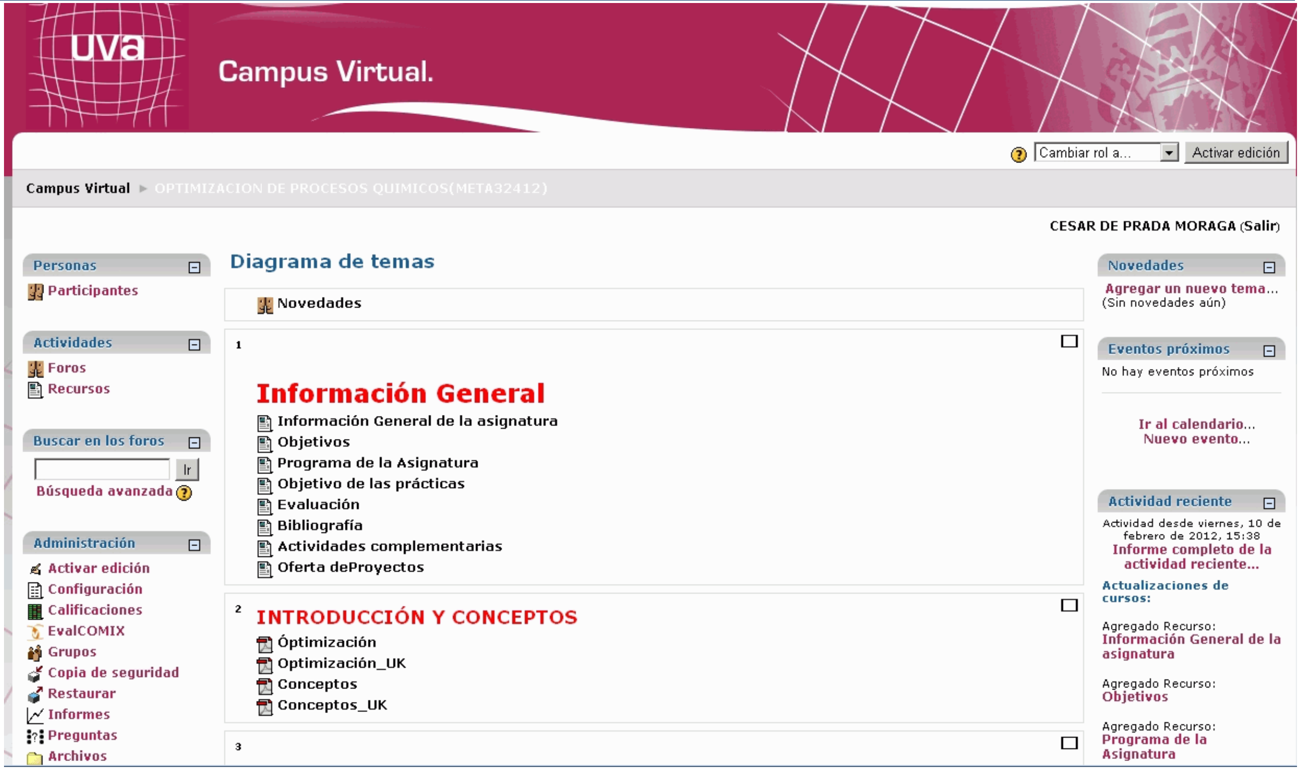
Book


biblioteca de químicas
Nivel 0
Acopio de información
Nivel 1
Rutas químicas
Nivel 2
Estructuras entrada-salida
Nivel 3
Estructura de recirculación
Nivel 4
Sistema de separación
Luis Puigjaner • Pedro Ollero
César de Prada • Laureano Jiménez
Estrategias de modelado, simulación y optimización de procesos químicos
EDITORIAL SINTESIS

http://www.isa.cie.uva.es/~prada/

http://campusvirtual.uva.es

Web + Moodle



Other activities

- Visits:
  - PETRONOR petrol refinery near Bilbao. In cooperation with the ISA student section 8th May 2014 . Refinery operation planning
  - Registration by April the 3rd.
- Conferences:

  Aplicaciones de la Optimización, Prof. Carlos Mendez, INTEC, UNL, Sta. Fe, Argentina
- Research work:
  - A set of topics is offered to those students that wish to develop a research project (1 -15 credits). They cover applications in the petrochemical and sugar industry, LHC accelerator, gas networks, pilot plant development, process design, etc.

Marks / Tutorials

- Exam + reports:
  - Exam (70%):
    - 2 problems (60%)
    - a set of questions (theory + exercises) (40%)
  - Reports: 30% A minimum mark of 4 in the exam is required
  - Exams: 13 June 2014 (9h.) / 30th June 2014 (16h.)
- I shall be available in my room for any question/doubt
  - Dpt. of Systems Engineering and Automatic Control. Ground floor.
  - E-mails:
    - prada@autom.uva.es
    - gloria@autom.uva.es

Dissertation projects

- A set of projects is available for those students wishing to develop his final degree project with the ISA department. They cover applications in the petrochemical and sugar industry, pilot plant development, design, etc.
- Topics in: http://www.isa.cie.uva.es/~prada/
- The doors are open for those students wishing to collaborate in current research projects develop with ISA partners: Repsol-Petronor, CERN, HYCON2, Intergeo Tech., EA, CTA , etc. Topics cover modelling, simulation, advanced control, process optimization, industrial computing, etc.
- Other projects can be developed with pilot plants in the lab.

Complementary courses

They will give you an specialization in the Process Systems Engineering field

- Control por computador
- Informática aplicada a la Ingeniería Química
- Sistemas de supervisión de procesos