Phần 3: Tối ưu hóa

Modeling, simulation and optimization for chemical process

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Bộ môn QT&TB

T. F. Edgar, D. M. Himmelblau. ***Optimization of chemical Processes***. Second edition.

Bùi Minh Trí. ***Tối ưu hóa*** (lý thuyết và bài tập). NXB KHKT, Hà Nội, 2005.

Introduction

- The chemical industry has undergone significant changes during the past 25 years due to the
  - increased cost of energy
  - increasingly stringent environmental regulations
  - global competition in product pricing and quality
  - …
- One of the most important engineering tools for addressing these issues is **optimization**

Decision-making process

Introduction

- As the power of **computers** has increased, the size and complexity of problems that can be solved by **optimization techniques** have correspondingly expanded

- The necessary tools for solving problem
  - We will focus on those **techniques** and discuss **software** that offers the most potential for success and gives reliable results

Outline

- Problem formulation
  - Nature and organization of Optimization problems
  - Developing models for optimization (constraints or process model)
  - Formulation of the objective function
- Optimization theory and methods
  - Optimization of unconstrained functions
  - Linear programming with constraints
  - Nonlinear programming with constraints
  - Multi-objective optimization
- Applications of Optimization

Optimization

- OPTIMIZATION IS THE use of specific methods to determine the most cost-effective and efficient solution to a problem or design for a process
- This technique is one of the major quantitative tools in industrial decision making
- A wide variety of problems in the design, construction, operation, and analysis of chemical plants (as well as many other industrial processes) can be resolved by optimization

Problem formulation

- Formulating the problem is perhaps the most crucial step in optimization (from **verbal statement** of a given application and organizing them into a prescribed **mathematical form**)
  - The objective function (economic criterion)
  - The process model (constraints)
- The objective function represents such factors as profit, cost, energy, and yield in terms of the key variables of the process being analyzed
- The process model and constraints describe the interrelationships of the key variables

Problem formulation

- What optimization is all about
  - Optimization is concerned with selecting the best value by efficient quantitative methods
- Why optimize?
  - Largest production
  - Greatest profit
  - Minimum cost
  - The least energy usage
  - …

Problem formulation

- Examples of applications of optimization
  - Determining the best sites for plant location
  - Routing tankers for the distribution of crude and refined products
  - Sizing and layout of a pipeline
  - Designing equipment and an entire plant
  - Scheduling maintenance and equipment replacement
  - Operating equipment, such as tubular reactors, columns, and absorbers
  - Evaluating plant data to construct a model of a process
  - Minimizing inventory charges
  - Allocating resources or services among several processes
  - Planning and scheduling construction
  - …

Example: See ref.

Problem formulation

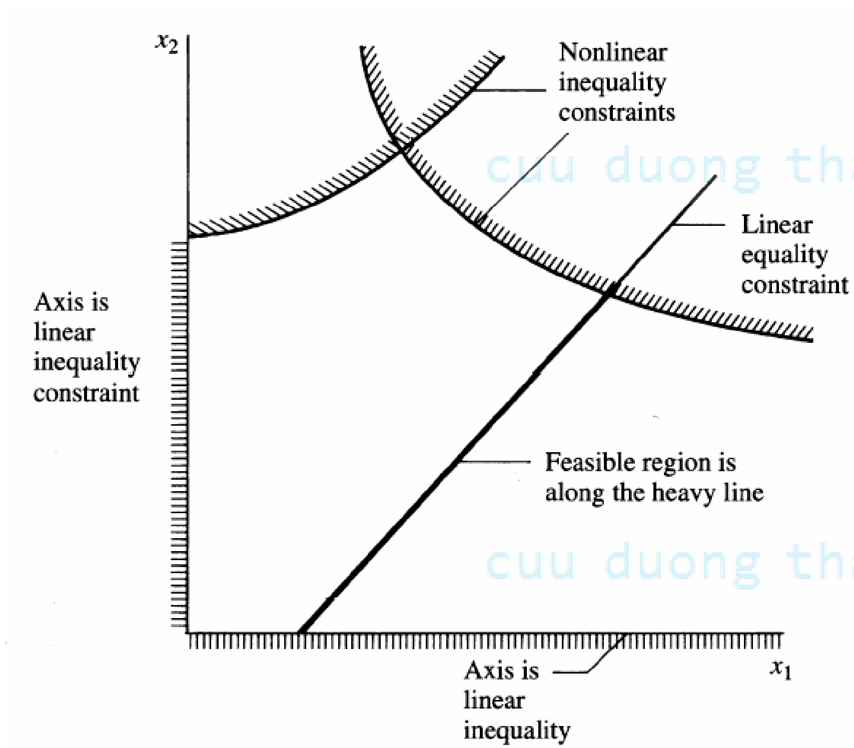
- Main features of optimization problems
  - At least one objective function to be optimized
  - Equality constraints (equations)
  - Inequality constraints (inequalities)

Model of process or equipment

Economic model

Problem formulation

- Main features of optimization problems



Feasible solution/Feasible region

Optimal solution

Degrees of freedom

Underdetermined

Overdetermined

Problem formulation

- An optimization problem:

$$\text{Minimize: } f(x) \text{ objective function}$$

$$\text{Subject to: } h(x) = 0 \text{ equality constraints}$$

$$g(x) \geq 0 \text{ inequality constraints}$$

$$\text{where } \mathbf{x} = (x_1 \cdots x_n) \in X \subset \mathbb{R}^n$$

$$h(x) \text{ is a vector of equations of dim. } m_1$$

$$g(x) \text{ is a vector of equations of dim. } m_2$$

$$D = \left\{ x \in X \middle| h(x) = 0, g(x) \geq 0 \right\}$$

Problem formulation

- Example: optimal scheduling

We want to schedule the production in two plants, *A* and *B*, each of which can manufacture two products: 1 and 2. How should the scheduling take place to maximize profits while meeting the market requirements based on the following data:

t_{A_1} t_{A_2}

Plant	Material processed (lb/day)		Profit ($/lb)	
	1	2	1	2
A	M_{A1}	M_{A2}	S_{A1}	S_{A2}
B	M_{B1}	M_{B2}	S_{B1}	S_{B2}

How many days per year (365 days) should each plant operate processing each kind of material?

t_{B_1} t_{B_2}

Problem formulation

- What is the objective function?

$$f(t) = \quad t_{A_1} M_{A_1} S_{A_1} + t_{A_2} M_{A_2} S_{A_2} \\ + t_{B_1} M_{B_1} S_{B_1} + t_{B_2} M_{B_2} S_{B_2}$$

$$t_{A_1} + t_{A_2} = 365 \qquad t_{Ai} \geq 0$$

$$t_{B_1} + t_{B_2} = 365 \qquad t_{Bi} \geq 0$$

Problem formulation

- Các loại bài toán tối ưu (quy hoạch toán học)
  - Quy hoạch tuyến tính (**QHTT**)

    $$f(x), g(x), h(x)$$ là tuyến tính

    Ví dụ thuộc dạng này có Bài Toán Vận Tải
  - Quy hoạch tham số (**QHTS**) là QHTT mà các hệ số trong

    $$f(x), g(x), h(x)$$ phụ thuộc tham số
  - Quy hoạch động (**QHĐ**):

    - Là quá trình có nhiều giai đoạn nói chung, hay các quá trình phát triển theo thời gian nói riêng

Problem formulation

- Các loại bài toán tối ưu (quy hoạch toán học)
  - Quy hoạch phi tuyến (**QHPT**)

    $f(x)$ hoặc $g(x)$ hoặc $h(x)$ là các hàm phi tuyến

  - Quy hoạch rời rạc (**QHRR**)

    Nếu miền ràng buộc D là tập rời rạc

  - Quy hoạch đa mục tiêu (**QHĐMT**)

    - Nếu trên cùng một miền ràng buộc *D* ta xét nhiều hàm mục tiêu khác nhau

Formulation of the objective function

- Translate a verbal statement or concept of the desired objective into mathematical terms
- Example

Let us return to the chemical plant of Example 2.10 with three products (E, F, G) and three raw materials (A, B, C) in limited supply. Each of the three products is produced in a separate process (1, 2, 3); Figure E3.1 illustrates the process.

Process data

Process 1: $A + B \rightarrow E$

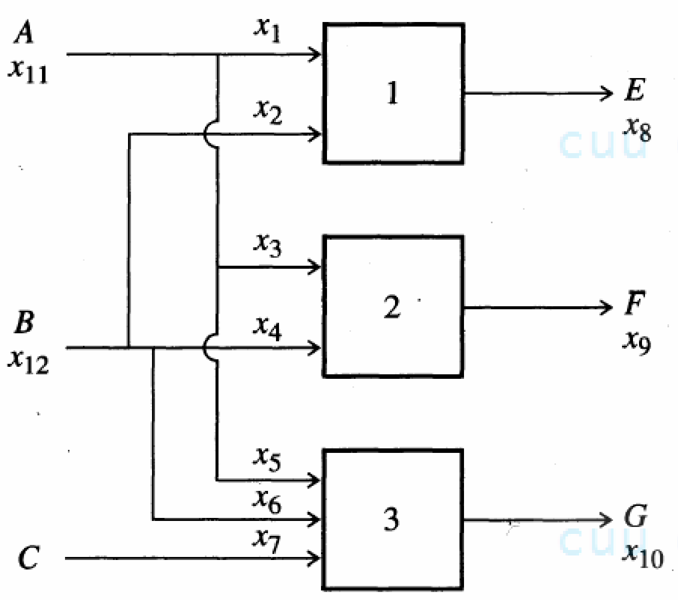
Process 2: $A + B \rightarrow F$

Process 3: $3A + 2B + C \rightarrow G$

Raw material	Maximum available (kg/day)	Cost (¢/kg)
A	40,000	1.5
B	30,000	2.0
C	25,000	2.5

Formulation of the objective function

- Example



Process	Product	Reactant requirements (kg/kg product)	Processing cost (product) (¢/kg)	Selling price (product) (¢/kg)
1	E	$\frac{2}{3}A, \frac{1}{3}B$	1.5	4.0
2	F	$\frac{2}{3}A, \frac{1}{3}B$	0.5	3.3
3	G	$\frac{1}{2}A, \frac{1}{6}B, \frac{1}{3}C$	1.0	3.8
		(mass is conserved)		

Formulate the objective function to maximize the total operating profit per day in the units of \$/day.

Formulation of the objective function

- Example

The notation for the mass flow rates of reactants and products is the same as in Example 2.10.

The income in dollars per day from the plant is found from the selling prices $(0.04E + 0.033F + 0.038G)$. The operating costs in dollars per day include

Raw material costs: $0.015A + 0.02B + 0.025C$

Processing costs: $0.015E + 0.005F + 0.01G$

$$\text{Total costs in dollars per day} = 0.015A + 0.02B + 0.025C + 0.015E + 0.005F + 0.01G$$

The daily profit is found by subtracting daily operating costs from the daily income:

$$\boxed{\begin{aligned} f(\mathbf{x}) &= 0.025E + 0.028F + 0.028G - 0.015A - 0.02B - 0.025C \\ &= 0.025x_8 + 0.028x_9 + 0.028x_{10} - 0.015x_{11} - 0.02x_{12} - 0.025x_7 \end{aligned}}$$

Formulation of the objective function

- Example

Note that the six variables in the objective function are constrained through material balances, namely

$$x_{11} = 0.667x_8 + 0.667x_9 + 0.5x_{10}$$

$$x_{12} = 0.333x_8 + 0.333x_9 + 0.167x_{10}$$

$$x_7 = 0.333x_{10}$$

Also

$$0 \le x_{11} \le 40{,}000$$

$$0 \le x_{12} \le 30{,}000$$

$$0 \le x_7 \le 25{,}000$$

The optimization problem in this example comprises a linear objective function and linear constraints, hence linear programming is the best technique for solving it

Problem formulation

- **The six steps used to solve optimization problems**
  - Make a list of all of the process variables
  - Determine the criterion for optimization, and specify the objective function in terms of the variables defined in step 1 together with coefficients (**Economic model**)
  - Using mathematical expressions, develop a valid process or equipment model (**Process model**) that relates the input-output variables of the process and associated coefficients

Problem formulation

Problem formulation

- **The six steps used to solve optimization problems**
  - If the problem formulation is too large in scope
    - Break it up into manageable parts or
    - Simplify the objective function and model
  - Apply a suitable optimization technique to the mathematical statement of the problem
  - Check the answers, and examine the sensitivity of the result to changes in the coefficients in the problem and the assumptions

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Scope of course