METHODOLOGY AND USE OF MULTIPLE-OBJECTIVE DECISION MAKING IN CHEMICAL ENGINEERING

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Introduction

Increases in the scale and complexity of chemical plants and a reevaluation of their performance criteria have meant that in recent years their operability, reliability, and environmental impacts have become as important as their economic efficiency, and this must obviously be reflected in process design, production planning and control. During the last decade, therefore many methods for studying optimization problems with multiple objectives have been developed to deal with the resulting problems. The aim of this paper is to look at Multiple-Objective Decision Making (MODM) from the point of view of the type of optimization problems which must be solved in the design, control, and production planning of chemical engineering systems. We will survey existing methods, provide an overview of computer codes (especially IIASA software), and discuss applications in this field.

Statement of the Problem

The performance of chemical engineering systems should be evaluated using various criteria which include both economic factors (like profit, capital investment, and operating cost) and non-economic criteria such as environmental quality and safety. In the past, this has meant taking one criterion, usually representing economic efficiency, as a single objective in optimization problems and incorporating the other criteria as inequality constraints indicating permissible levels. Since the chemical industry is characteristically very intensive in its use of energy and feedstocks, economic efficiency is generally pursued through policies involving the minimization of energy consumption , maximization of energy production and and minimization of feedstock consumption.

However, there is an increasing awareness of the importance of non-economic performance criteria. This has meant that systems analysts working in chemical engineering have been faced with multiobjective optimization problems in which two or more non-commensurable and conflicting objectives must be considered simultaneously. In this paper we will study the multiobjective optimization problems arising in process design, control of existing plants, and production planning in the chemical industry.

We assume that these *Multiple-Objective Optimization* (MOO) problems may be defined as follows:

$$\min_{x \in X_0} f(x) \tag{1}$$

where $x = (x_1, x_2, \ldots, x_n)$; $x \in R^n$ is the vector of decision variables. This decision vector generally consists of different combinations of values for structural, equipment size, and control variables. The vector

$$f(x) = (f_1(x), f_2(x), \ldots, f_p(x)) \in R^p$$

represents the objective function and X_0 is the set of feasible decisions satisfying the constraints:

$$X_0 = \left\{ x \in R^n \mid h_1(x) = 0, \ldots, h_k(x) = 0 \, , \, g_{k+1}(x) \leq 0 \, , \, \ldots \, , \, g_m(x) \leq 0 \right\} \qquad (2)$$

The constraining functions $h_i(x) = 0$; $i = 1,2,\ldots,k$ represent the mathematical model of the process being designed, controlled or planned. The second subset of constraining functions $g_i(x) \leq 0$; $i = k+1, k+2, \ldots, m$ expresses the technological and possibly also the environmental limitations on input and output variables and on state and decision variables. Appendix A2 contains a selected bibliography of works dealing with multiple-objective optimization problems of type (1) and some applications in chemical engineering.

Because the objective function $f(x)$ is a vector, the possible values that it can take must be ordered in some way. A decision x^1 is usually considered better than x^2 if:

$$f(x^1) \leq f(x^2) :\Longleftrightarrow \quad f_i(x^1) \leq f_i(x^2) \quad \forall \; i = 1,2,\ldots,p \qquad f(x^1) \, , \, f(x^2) \in R^p$$

and at least one of the inequalities is strict. This is known as ***partial order***.

Using this notion of order we can state the condition that must be met for $f(\hat{x})$ to be a solution of problem (1), (the definition of Pareto-optimality):

$f(\hat{x}) \in R^p$ is Pareto-optimal (a solution of (1)):$\Longleftrightarrow$ $\not\exists$ $f(x) \neq f(\hat{x})$ with $f(x) \leq f(\hat{x})$ and $x \in X_0$

This means that there is no attainable $f(x)$ that scores better than $f(\hat{x})$ in at least one criterion i , $(f_i(x) < f_i(\hat{x}))$ without worsening all other components of $f(\hat{x})$.

The ordering introduced above is special in that it is incomplete, i.e., it is only a partial ordering. This means that problem (1) does not have only one solution, as in classical mathematical optimization; the solution of (1) is a set of an often infinite number of nondominated solutions or efficient points, which are not comparable with each other. At this point it seems natural to limit the analysis of the optimization problem to consideration of the set (or even a subset) of efficient (nonimprovable) decisions [$f(\hat{x})$, $\hat{x} \in X_0$] rather than considering the whole set of feasible decisions [$f(x)$, $x \in X_0$] . This more highly focused analysis then based on information which could not be included in the original formulation of the problem. The identification and evaluation of efficient solutions can be viewed as an indirect improvement of the partial ordering relation and is assumed to lead to a global compromise solution or a new problem formulation.

The order relation can be improved through the use of techniques involving aspiration points (reference points), preferences, trade-offs, or of utility or value theory during the course of the decision-making process; the actual method adopted will depend on the particular circumstances of each situation. This learning process is accompanied by the modification or respecification of one or more objectives, of the mathematical model used and/or of the technological or other constraints. The problem is therefore solved by progressive formulation of the decision maker's (chemical engineer, control engineer, manager) order relation, and the engineer or manager thus becomes an integral part of the interactive decision-making procedure.

Against this background decision making can be seen as a dynamic process [1] : complex, with an intricate network of feedbacks and information flows, occasionally directed into information gathering and filtering activities, fueled by fluctuating uncertainty, fuzziness, and conflict. This process can be divided into *predecision* and *postdecision* stages separated by overlapping regions where *partial* decision making takes place. In the *predecision* stage the objectives, the model and the constraints are formulated using as a basis the desired (but not genarally attainable) alternative which makes the decision process necessary. *Partial* decision making involves the numerical generation of alternatives which are both feasible and efficient , given the desired levels of each objective. Studying the problem in this way results in the displacement of the aspiration levels (reference point) and/or the reformulation and reevaluation of the objectives, model, and constraints. In the *postdecision* situation it is necessary to find information that supports a given *partial* decision as the best compromise among all feasible efficient alternatives. We will examine the second stage in this three-stage model of the decision-making process and present a number of methods for decision analysis and support.

Overview of Methods for Multiple-Objective Decision Making (MODM)

An exhaustive classification of existing MODM methods according to the stage at which preference information is needed and the type of information required is given in [2] and reproduced in Figure 1.

All of these MODM methods are discussed and illustrated using a simple numerical example in [2]. We would argue that branches 3 and 4 are the most important classes of MODM methods because here the process of decision analysis and support involves man/machine interaction.

We will now describe the reference point approach to multiobjective decision making, comparing it with one of the first applications of multiple-objective analysis in chemical engineering [3]. In this paper, problem (1) is solved using the classical approach, i.e., the use of weighting coefficients in Lagrange-type scalarization (method 4.1.1 in Figure 1) . This method is based on the fact that if we choose a vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_p) > 0$ with all components positive, and minimize the following Lagrange-type function:

$$L(\lambda, x) = \sum_{i=1}^{p} \lambda_i f_i(x) = \langle \lambda , f(x) \rangle \tag{3}$$

then every minimal point in X_0 , $\hat{x} = arg \min_{x \in X_0} L(\lambda, x)$ is an efficient solution of

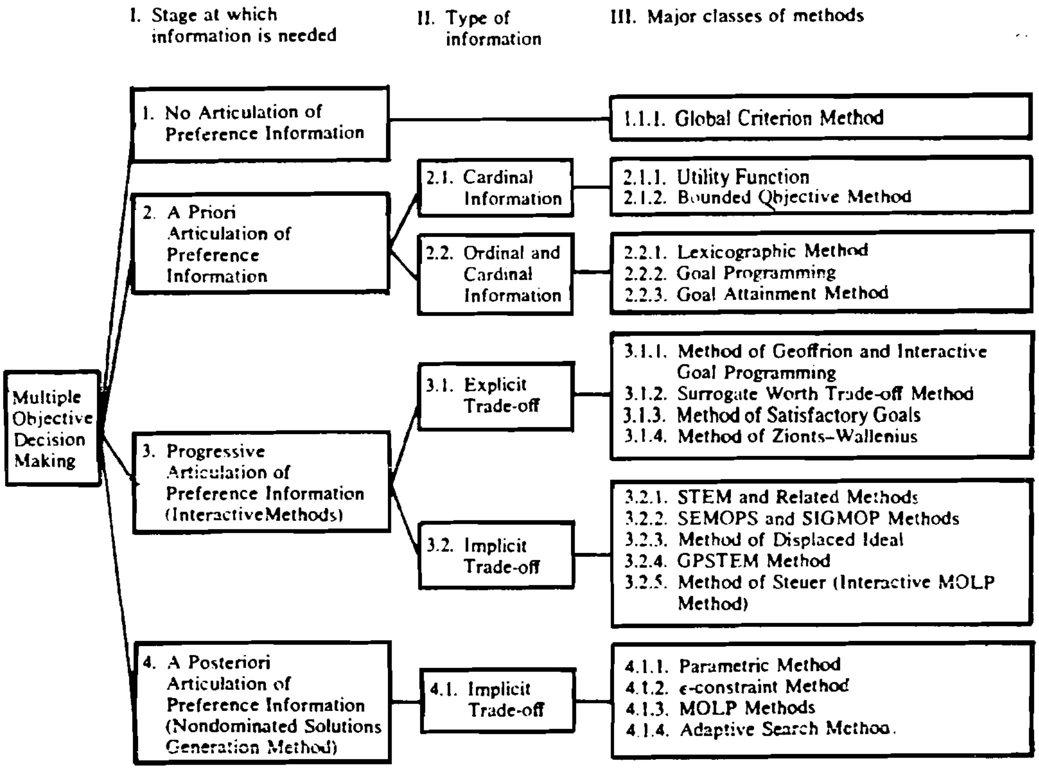


Figure 1 A taxonomy of methods for multi-objective decision making [2].

(1). Unfortunately this is true only if the solution of (1) is identical with its convex hull, and this is the exception rather than the rule in chemical engineering MODM problems. A more practical approach would be to use the reference level method introduced by Wierzbicki [4] , which leads to the following scalarizing function for problem (1):

$$s_1(x,\rho,\bar{f}) = -\,\| f(x) - \bar{f} \|^2 + \rho \| (f(x) - \bar{f})_+ \|^2 \tag{4}$$

where $\bar{f}$ denotes a reference vector of objectives defined by the decision maker, $(f(x) - \bar{f})_+$ denotes the vector with components $\max\{\,0\,,\, f_i(x) - \bar{f}_i(x)\,\}$, i.e., is the positive part of this vector, and ρ is a scalar penalty coefficient. If $\rho > 1$ each minimal point of $s_1(x,\rho,\bar{f})$ is an efficient point regardless of whether $\bar{f}$ is attainable or not. This condition also holds for nonconvex problems. The method involving a displaced ideal (method 3.2.3 in Figure 1) [5] and the goal programming method [6] can be treated as special cases of (4) [7].

The interactive procedure during which reference points $\{\bar{f}^1, \bar{f}^2, \bar{f}^3, \ldots\}$ are formulated by the decision maker and the corresponding efficient points $\{\hat{f}^1, \hat{f}^2, \hat{f}^3, \ldots\}$ are generated by the computer is illustrated in Figure 2.

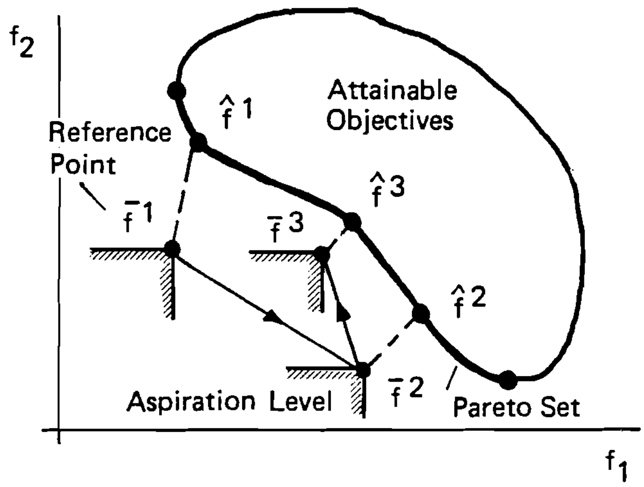


Figure 2 Reference point method : interactive procedure for multiple objective decision making.

The basic idea of the method is quite simple -- it assumes that the decision maker can express his preferences in terms of aspiration levels, i.e., that he can specify the required values of individual objectives. Our experience of actual decision makers has shown that it is easier and more convenient for them to think in these terms than to estimate the trade-off coefficients or utilities required by other methods.

Two situations can occur:

(I) The decision maker overestimates the possibilities -- he sets the reference level too high, so that it cannot be achieved by the system (aspiration level is unattainable).

(II) The decision maker underestimates the possibilities -- he sets the reference level too low, so that the system could do better than required (aspiration level is attainable).

Of course, a third situation can theoretically occur -- the aspiration level is a point in the Pareto set. However, the probability of such a choice is low and we do not consider this case here.

There is an obvious and clear course of action in both situations:

(I) If the aspiration level is not attainable, the computer should report this fact and calculate the nearest point in the Pareto set (see Figure 3(a)).

(II) When the aspiration level is attainable, the computer should find the point in the Pareto set which improves each objective as much as possible and report it to the decision maker (see Figure 3(b)).

The second situation is especially interesting for the decision maker, because the computer is basically saying "you have underestimated the possibilities. aI propose a new solution which not only fulfills your wishes for each objective but also exceeds them."

In either situation, the solution obtained is presented to the decision maker, who must then decide whether to accept it. If he does not, he must decide why this solution cannot be accepted and propose a new aspiration level which reflects his wishes more accuratly. These iterations ("sessions") are continued until the decision maker accepts the solution (usually about 10-20 sessions).

This approach has already been used successfully to solve some of the multiple-objective problems encountered in the design and steady-state control of chemical engineering systems [8, 9] .

It is often necessary to consider the behavior of the system over time when making decisions concerning planning and control in chemical-engineering processes. In this case the goals of the decision maker are also time-dependent and the objective function is therefore a trajectory. One method of solution involves the use of reference trajectories [10]. For example, a national goverment might wish to minimize the use of imported oil and indiginious coal in energy production to save them as feedstocks for the chemical industry, to minimize investment in this industry. This is illustrated in Figure 4, which shows the reference trajectories (goals) for oil and coal supply ($\bar{f}^1$, $\bar{f}^2$) and also the corresponding cost trajectory ($\bar{f}^3$).

By analogy to (4) , the problem may be formulated as follows:

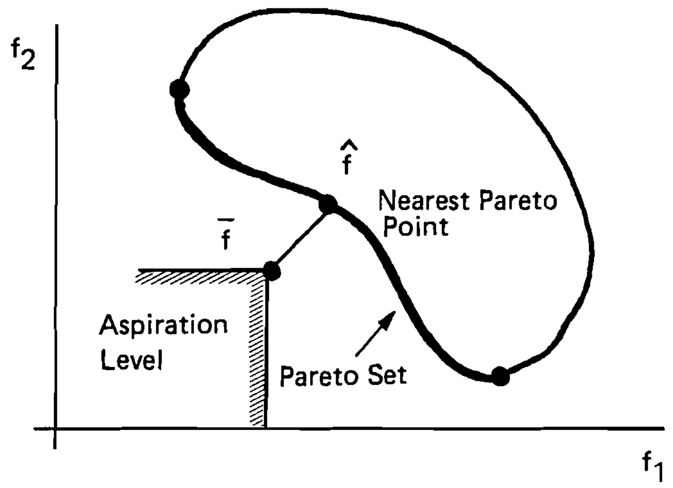
$$s_2(f(t),\bar{f}(t),\rho) = -\int_0^T \left[f(t) - \bar{f}(t) \right]^2 dt + \rho \int_0^T \left[f(t) - \bar{f}(t) \right]^2 dt \qquad (5)$$

where $f(t) = (f^1(t), f^2(t), f^3(t))$ and T is the planning horizon.

Computer Codes

Table 1 (derived from [2]) gives an overview of MODM computer codes. It is virtually impossible to compare and evaluate the codes because of the different approaches taken by the authors, the different assumptions concerning starting information, and the different sizes and kinds of problems considered. We have therefore taken this information directly from [2] and refer the reader to the exhaustive description of 44 MODM computer codes given in [12]. The interactive MODM software developed at IIASA for the linear multiple criteria case is briefly described and illustrated with a hypothetical example in Appendix A1; a list of related IIASA publications is given in Appendix A3.

(a)



(b)

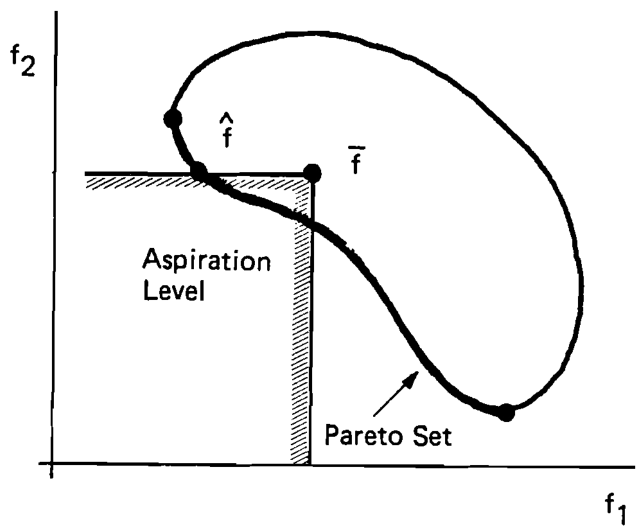


Figure 3 Reference point method : (a) unattainable reference point and (b) attainable reference point.

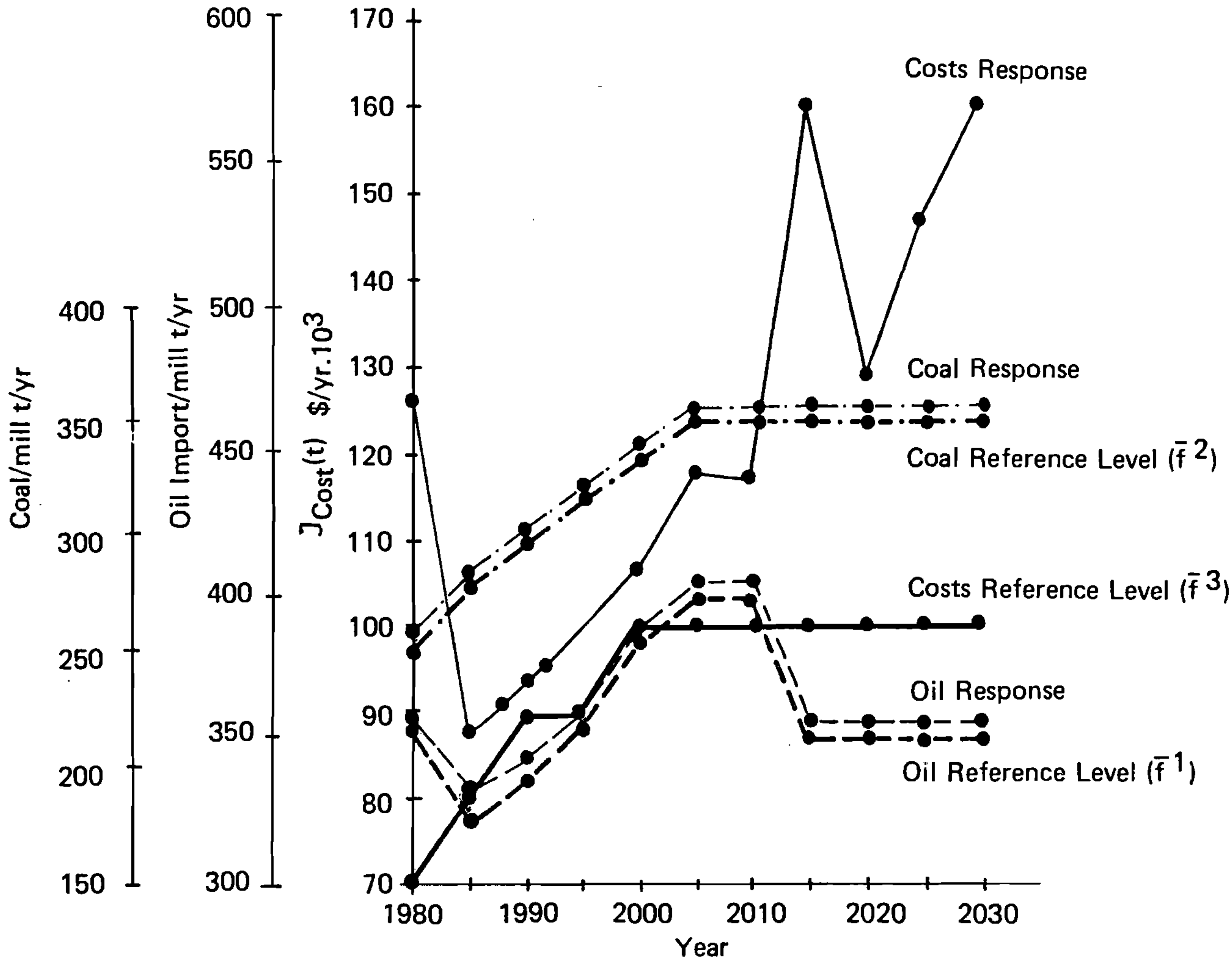


Figure 4 Reference trajectories (objectives) for imported oil supply, indiginous coal supply,and cost [11].

In this section we will first give a general overview of the applications of multiobjective optimization and decision making, and then consider some applications in chemical engineering in more detail.

A large number of publications dealing with multiple-objective decision making are concerned with *water resources management and applications in*

Table 1. Selected list of MODM computer codes [2]

Code number	MODM method	Author(s)	Remarks
1	Linear goal programming	Lee	Not an efficient code for a large scale problem
2	Linear goal programming and linear integer goal programming	Ignizio	Not an efficient code for a large scale problem
3	Linear goal programming	Arthur and Ravindran	
4	Iterative linear goal programming	Dauer and Krueger	Use a basic simplex algorithm code, an efficient code for a large scale problem
5	Nonlinear goal programming	Ignizio	
6	Iterative nonlinear goal programming	Hwang *et al.*	An efficient code for a large scale problem
7	Geoffrion method	Geoffrion *et al.*	An interactive method
8	Zionts–Wallenius method	Wallenius	An interactive method
9	SEMOPS	Monarchi *et al.*	Not for a large scale problem, an interactive method
10	SIGMOP	Monarchi *et al.*	An interactive method
11	Multicriteria simplex	Zeleny	Nondominated solutions generation method for MOLP
12	MOLP (ADBASE)	Steuer	Adjacent basis approach, interval weights
13	MOLP (ADEX)	Steuer	Adjacent efficient extreme point
14	MOLP (ADBASE/FILTER)	Steuer	An extension of code 12
15	MOLP	Iserman	In Algol language

general environmental systems [*13, 14*]. The multiple conflicting objectives in this field are genarally derived from one- dimensional monetary thinking, and thus the goals, besides costs, include aims concerning the quality and quantity of water, the flexibility and socioeconomic impact of the system. Conflicting goals also arise from the need to consider the use of water for various purposes (irrigation, power generation, industrial cooling, recreation, etc.).

Multiple-objective decision making is also important in a number of other fields; these include *planning processes in academic departments*, *econometrics and economic development*, *financial management*, *health-care systems*, *and production and transportation systems*. MODM techniques have been adopted in these araes because of the need for a reasonable compromise between the capital invested and the operating costs [15].

In the field of *System Reliability* the conflicting goals are the maximization of system reliability and the minimization of system cost. In [16] is considered a reliability problem with four objectives (system reliability, cost, weight, and volume); problems of this type often arise in the design of electronic circuits.

Previous applications of multiple-objective decision making in the analysis of engineering systems included the choice of location for an underground power plant and the design of an aircraft lateral control system. In [17] the authors point out that the MOO technique provides the designer with a high level of flexibility in choosing between various design options. This has been demonstrated in the design of lateral control systems for a heavy re-entry vehicle and a fighter aircraft [17].

In the last few years a number of publications have described applications of multiple-objective decision making in chemical engineering (see Appendix A2). One of the first of these was the use of multiple-objective techniques for planning production in a refinery [3]. In this case the MOO problem was basically to maximize total yearly profit while minimizing the sensitivity of the profit to variations in refinery conditions.

We will now illustrate the importance of MODM in chemical engineering by discussing three case studies.

Design using MOO

The problem of the optimal design for a twin-screw extruder (see Figure 5) when more than one objective is specified is discussed in [9] . The components of the objective vector are

- The throughput of thermoplastics ($\max V$)

- The electrical energy demand (min P)
- The quality of the thermoplastics (measured by the attainable deformation ($\max \Gamma$)).

The nonlinear multiple-criteria optimization problem is then solved using the approach presented in eqn(4). An analysis of the efficient points (see Figure 6) provides insight into the extrusion process, and shows that a computer-aided design can increase the quality and quantity of thermoplastics produced while simultaneously reducing the electrical energy required.

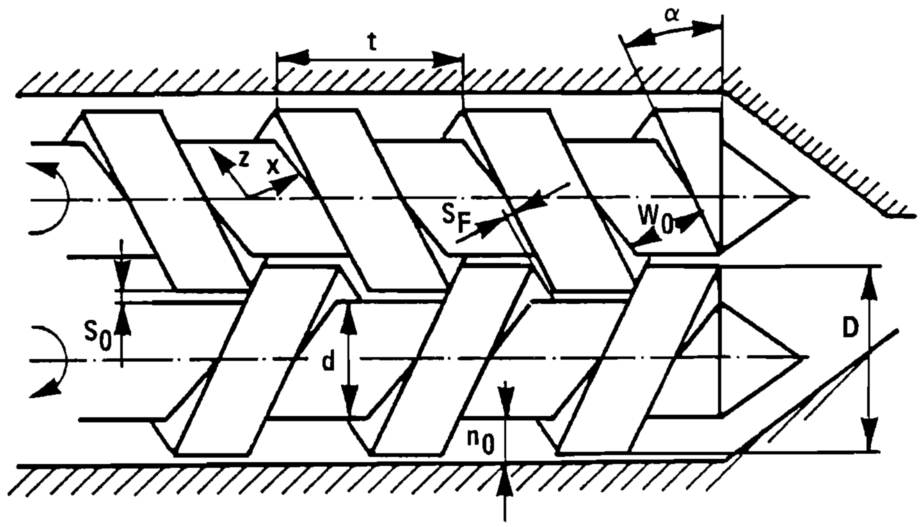


Figure 5 The twin-screw extruder [9].

Control using MOO

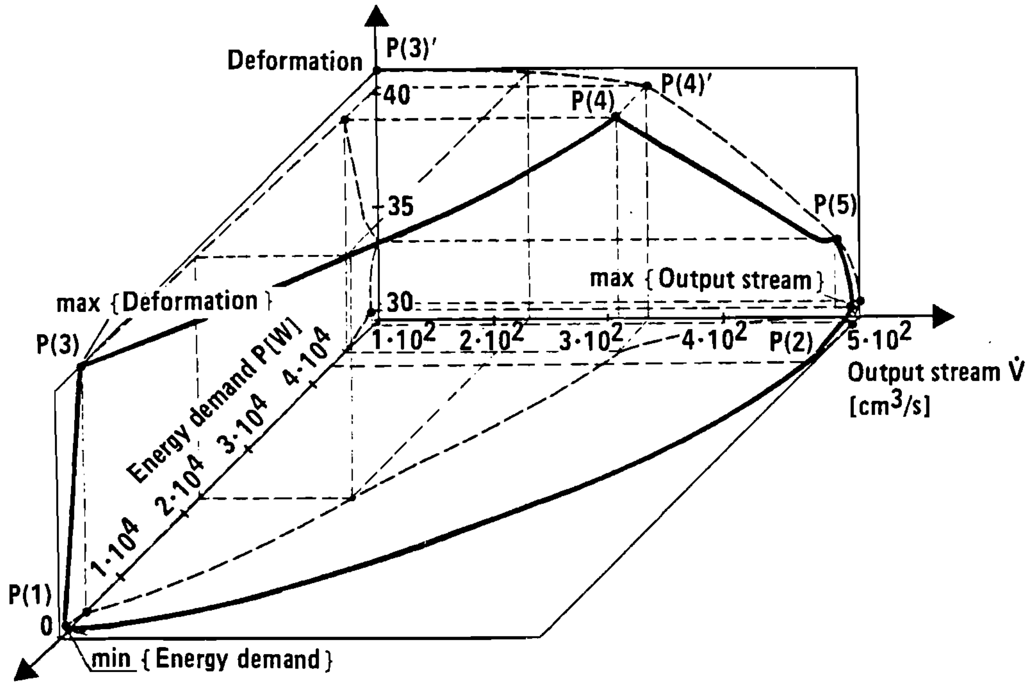


Figure 6 Geometrical interpretation of the problem of extruder design as a multiple objective optimization problem with three objectives [9].

The problem of optimal control in a film-hardening process is treated in [8] as a steady-state MOO problem with two criteria: the amount of the solvent recycled (a measure of the economy of the process) and the quality of the photographic film (see Figure 7). The problem assumes that both the quality of the film and the economy of the process should be maximized. Thus, in Figure 8 the amount of recycling should be maximized and the dimensionless number inversely proportional to the quality should be minimized. The numerical solution of this MOO problem is the curve between points A and B in Figure 8. The other sections, i.e., the curves BC, CD, and DA have been computed only for the sake of completeness. Using the set of efficient points (curve AB), it is now

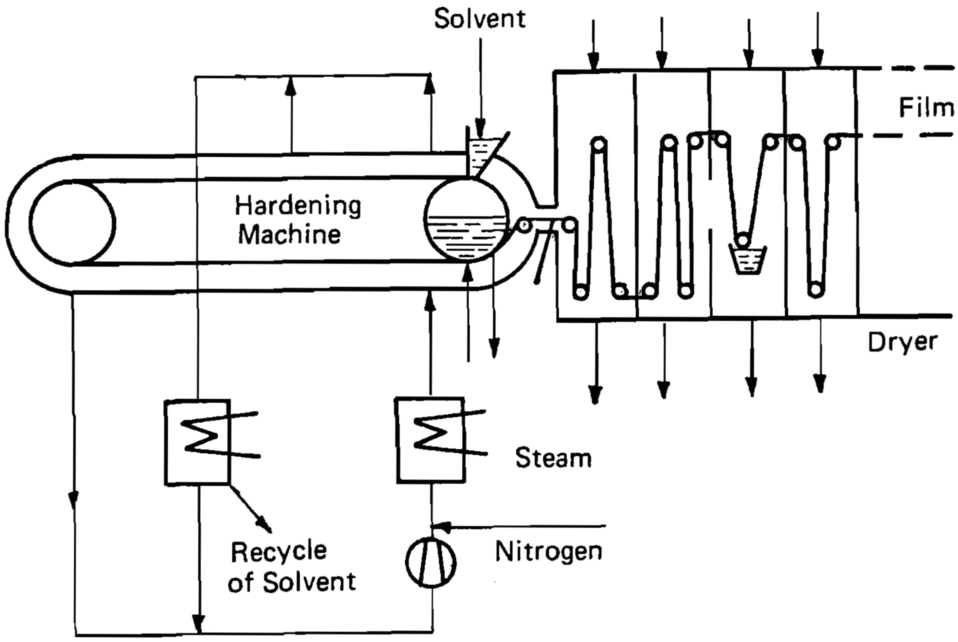


Figure 7 The film-hardening-process [8].

possible to determine the most economic operating conditions for a given film quality.

Planning using MOO

Our MOO planning problem is taken from [18]. The goal is to plan the structure of the chemical industry sector by answering the basic questions dealing with investment policy -- what to produce, what equipment is necessary, whether to build new production units or adapt existing ones, and so on. This is a difficult task because of the complex structure of the chemical industry -- the byproducts of one factory are often used as starting materials in another -- and a sophisticated network-type model has been built to study these relationships.

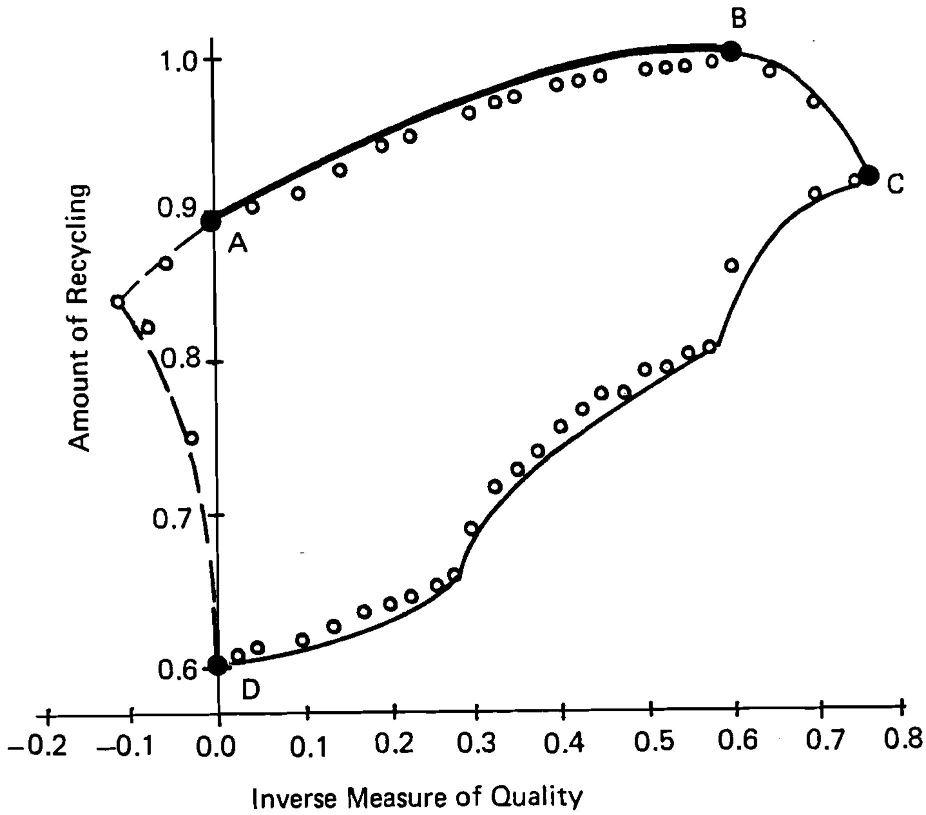


Figure 8 Set of efficient solutions (curve AB) for a model of the film-hardening process[8].

However, the most important factors affecting any decisions are the total cost of production, the energy consumption, and employment. These factors are actually used as performance indexes and the reference point optimization approach seems to be the suitable way of treating such a problem. The other approaches are less convenient; for example, it is difficult or even impossible to determine the scalar performance function using weighting factors. There has been considerable success in solving this type of problem -- selected results are presented in the above mentioned paper.

Conclusion

We have described the use of the reference point optimization method in typical chemical engineering decision problems with multiple objectives that arise in process design, plant control and production planning. We believe that multiobjective decision making methods of this type should be used in conjunction with data-processing tools to provide computer-based decision support systems which could help engineers in exploring and generating various courses of action, structering and modeling different situations, interpreting results, and implementing solutions. Thus the formal optimization procedure should be viewed as only one step toward the solution, as only one stage in the whole creative engineering decision process.

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Appendix A1

Software based on the reference point optimization approach has been developed at IIASA for use in solving linear problems (the development of software for the nonlinear case is underway). This software consists of three basic programs. These are:

(1) The interactive "editor", which is used for manipulating the reference points and the objectives (lpmod).

(2) The preprocessor, which converts the input file (containing the description of the model) from standard MPSX format into its single criterion equivalent (lpmulti).

(3) The postprocessor, which extracts the information from the output file, computes the values of the objectives, and displays the necessary information (lpsol).

The general structure of the system is presented in Figure A1. The fact that the LP problems are pre- and postprocessed means that the system is very flexible and may transferred to different computers without difficulty. The only machine-dependent point is the format of the output file, which is different for different LP packages, but this can be overcome by the simple modification of three FORMAT statements.

All of the programs work in the interactive mode; however, the efficiency of the interaction depends on the size of the LP model. For example, one session with a model of dimension 150 x 100 currently takes 5-10 minutes CPU time on the VAX 11/780 using the MINOS LP system. This makes it possible to solve quite difficult multiple criteria problems using the interactive procedure. More details of the system and the theory underlying the algorithm can be found in the reports listed in Appendix A3.

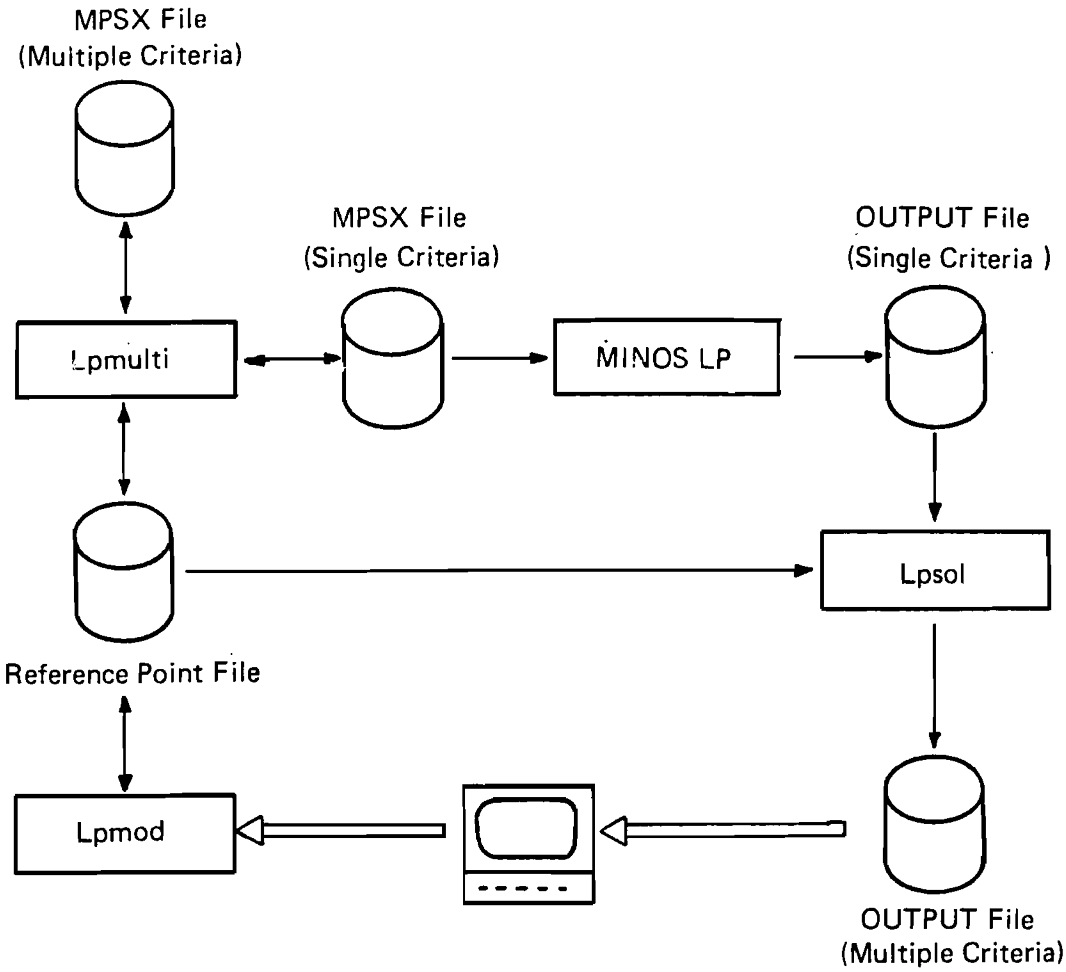

Figure A1. Structure of the reference point optimization system.

We will now demonstrate the use of the system by applying it to a simple linear multiple-criteria optimization problem.

The problem is :

$$\max \left\{ \begin{array}{l} x_1 + 2x_2 - x_3 + 3x_4 + 2x_5 + x_7 = obj1 \\ x_2 + x_3 + 2x_4 + 3x_5 + x_6 = obj2 \\ x_1 + x_3 - x_4 - x_6 - x_7 = obj3 \end{array} \right\}$$

subject to :

$$\begin{array}{l} +x_1 + 2x_2 + x_3 + x_4 + 2x_5 + x_6 + 2x_7 \le 16 \\ -2x_1 - x_2 + x_4 + 2x_5 + x_7 \le 16 \\ -x_1 + x_3 + 2x_5 - 2x_7 \le 16 \\ + x_2 + 2x_3 - x_4 + x_5 - x_6 - x_7 \le 16 \end{array}$$

$$x_i \ge 0, \ i=1,2,\dots,7$$

The results of several interactive sessions are presented below. The first column (obj) gives the names of the components of the vector of objectives, the second (objval) the efficient point, the third (refpt) the corresponding reference point value, the fourth (dif) the difference between the objective value and the reference point component while the fifth gives the dual variable.

The first session gives the so-called neutral solution, in which the reference point is zero.

--obj--	---objval---	---refpt---	----dif----	---dual---
obj1	10.7	0.	10.7	0.500
obj2	10.7	0.	10.7	1.00
obj3	10.7	0.	10.7	1.50

The positive and negative infinite solutions may be obtained by using $+10^5$ or -10^5 as a reference point:

--obj--	---objval---	---refpt---	----dif----	---dual---
obj1	10.7	0.100e+06	-0.100d+06	0.501
obj2	10.7	0.100e+06	-0.100d+06	1.00
obj3	10.7	0.100e+06	-0.100d+06	1.50

--obj--	---objval---	---refpt---	----dif----	---dual---
obj1	48.0	-0.100e+06	0.100d+06	1.000
obj2	32.0	-0.100e+06	0.100d+06	1.000
obj3	-16.0	-0.100e+06	0.100d+06	1.000

Sessions of this type are characteristic of the beginning of the interactive process, when only a little information is available.

The next session assumes a nonzero but "finite" reference point:

--obj--	---objval---	---refpt---	----dif----	---dual---
obj1	37.3	50.0	-12.7	0.
obj2	29.3	60.0	-30.7	2.00
obj3	-10.7	20.0	-30.7	1.00

We may then use information derived from the differences and the dual variables in further analysis:

--obj--	---objval---	---refpt---	----dif----	---dual---
obj1	0.	50.0	-50.0	0.
obj2	8.00	60.0	-52.0	0.
obj3	16.0	70.0	-54.0	3.00

--obj--	---objval---	---refpt---	----dif----	---dual---
obj1	0.	30.0	-30.0	0.
obj2	8.00	40.0	-32.0	0.
obj3	16.0	50.0	-34.0	3.00

Finally a session will produce a "good compromise" solution leading to a "well-balaced" decision (see below).

--obj--	---objval---	---refpt---	----dif----	---dual---
obj1	14.0	50.0	-36.0	0.501
obj2	4.00	40.0	-36.0	1.00
obj3	14.0	50.0	-36.0	1.50

Appendix A2

It is virtually impossible to produce a complete bibliograhpy of works dealing with multiple-objective decision making. Therefore we have attemted to list selected references in three categories. The first group [1-17] contains articles taken from journals and reports, which introduce the methodology and describe some applications in chemical engineering. References [18-20] are bibliographies; one of the most complete bibliographies on MODM (1138 entries) which also contains works in languages other than English (over 100 refernces in Russian)is [18]. The third category [21-28] lists books and monographs. In each group the refernces are ordered by the first author and the date.

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Appendix A3

This appendix contains IIASA publications which are related to multiple-criteria optimization and decision making problems.

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