MULTIPLE-OBJECTIVE DECISION ANALYSIS APPLIED TO CHEMICAL ENGINEERING

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FOREWORD

The Interactive Decision Analysis Project at IIASA is studying both the theoretical basis of interactive decision support systems and their applications in a number of different fields. Such systems are of most use when decisions have to be made against a background of multiple and conflicting objectives, and they are therefore largely based on the theory of multiobjective decision analysis.

This paper looks at the uses of multiobjective decision analysis in the chemical engineering industry. This is a particularly interesting area from the point of view of multiobjective decision making because recent developments have forced chemical plants to give increased weight to noneconomic criteria such as environmental quality and safety at the expense of economic criteria such as profit, capital investment, and operating costs. In addition, it is more necessary than ever for the industry to be able to adapt its production strategy to take into account changes in the economic situation (changing prices, patterns of demand, etc.). The complexity of this system is such that it is now no longer possible to determine the best course of action without some formal analysis.

The techniques of multiobjective decision analysis can usefully be employed to help the plant manager find the best solution to these problems. Specific applications in process design, plant control, and production planning are described. Special emphasis is given to the reference-point approach to multiobjective decision making, and to an interactive software package (DIDASS) based on this approach which has been developed at IIASA.

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Multiple-objective decision analysis applied to chemical engineering

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Zusammenfassung

Die wachsende Komplexität von Anlagen der chemischen Industrie und die Umbewertung von Leistungskriterien für ihren Betrieb zwingen die Ingenieure in der Verfahrenstechnik, mehrere Zielgrößen in ihren Entscheidungen zu berücksichtigen. So gewinnen in den Bereichen des Entwurfs von Anlagen, deren Steuerung und der Produktionsplanung neben ökonomischen Kriterien mehr und mehr Forderungen der Sicherheit und des Umweltschutzes an Bedeutung.
Dieser Beitrag zeigt, wie zur Lösung dieser Probleme Methoden der mehrkriteriellen Optimierung genutzt werden können und gibt einen Überblick zu vorhandener Software auf diesem Gebiet. Im Anschluß daran wird der Nutzen aus der Anwendung der mehrkriteriellen Entscheidungsanalyse am Beispiel eines Extruderentwurfes, der Steuerung einer Anlage zur Herstellung von Filmunterlage und der Planung einer Produktionsstruktur diskutiert.

Multiple-objective decision analysis applied to chemical engineering

Abstract

Chemical engineers are now being faced with new decisions involving multiple (and often conflicting) objectives as a result of increases in the scale and complexity of chemical plants and a re-evaluation of their performance criteria. Reliability and environmental impacts are now considered to be as important as economic efficiency, and this must be taken into account in process design, production planning and control.
This paper describes methods for solving these multiple-objective optimization problems and gives an overview of the existing software. Selected applications of multiple-objective analysis are discussed – these include the design of a twin-screw extruder, the control of a film-hardening process and a production planning problem.

Analyse des décisions à objectifs multiples dans l'industrie chimique

Résumé

A l'heure actuelle, en raison de la complexité croissante des installations et de la réévaluation de leurs critères de rendement, les ingénieurs chimistes ont à prendre de nouvelles décisions impliquant des objectifs multiples (et souvent contradictoires).
Les facteurs de sécurité et les impacts sur la protection de l'environnement sont à présent considérés comme étant tout aussi importants que le rendement économique et doivent être pris en compte dans la conception des installations, dans leur conduite ou dans le planning de production.
L'exposé donne une description des méthodes visant à résoudre les problèmes d'optimisation à objectifs multiples et apporte une vue d'ensemble sur le logiciel existant. Quelques applications d'analyses à objectifs multiples font l'objet d'une discussion. Elles concernent un projet de machine à extruder, le contrôle d'un processus d'alunage de film ou encore des problèmes de planning de production.

1 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; this must obviously be reflected in process design, production planning and control. During the last decade, therefore, many methods have been developed to deal with the multiobjective problems created as a result of this change of priorities. Some of these methods are summarized in several books [1, 2, 3, 4, 5]. In general terms, these methods deal with a situation in which one or more persons must generate and choose between various alternatives that cannot be evaluated on the basis of a scalar performance measure (a "single objective") alone. Instead, the evaluation must involve a number of performance characteristics ("multiple objectives") which are often not commensurable. This kind of multiobjective decision making has been an integral part of human behavior for thousands of years, but the term has recently acquired a new and much more specific meaning with the introduction of mathematical methods into the decision-making area. These methods are generally designed to clarify the decision-making situation and to help in generating useful alternatives; they sometimes involve considerable use of computers and mathematical models. However, it is unrealistic to try to make practical engineering decisions without the involvement and approval of the people concerned in implementing them. Thus, these methods are designed to assist the engineer by illustrating the trade-offs between different conflicting objectives and to help him make a final decision without taking it out of his hands. In this sense we can describe this group of methods as being concernd with multiple-objective decision analysis.

The aim of this paper is to look at multiple-objective decision analysis 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.

2 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 production and minimization of feedstock consumption.

However, there is an increasing awareness of the importance of non-economic performance criteria (like [6]). 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:

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

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:

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

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 $g_i(x) \leqslant 0; i = k+1, k+2, \ldots, m$ expresses the technological and possibly also the environmental limitations on input and output variables and on state and decision variables.

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

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

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 $f(x)$ to be a solution of problem (1), (the definition of Pareto-optimality):

$$\boxed{\begin{array}{c} f(\hat{x}) \in R^p \text{ is Pareto-Optimal (a solution of (1)):} \\ \Longleftrightarrow \nexists \; f(x) \neq f(\hat{x}) \text{ with } f(x) \leqslant f(\hat{x}) \text{ and } x \in X_0 \end{array}}$$

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 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 non-dominated 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 (non-improvable) 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 is 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 utility or value theory or techniques involving aspiration points (reference points), preferences, or trade-offs 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 (preference structure), and the engineer or manager thus becomes an integral part ot the interactive decision-making procedure.

Against this background decision making can be seen as a dynamic process [7]: 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 *post-decision* steps separated by overlapping regions where *partial* decision making takes place. In the *predecision* step the objectives, the model and the constraints are formulated by considering the desired (but not generally attainable) alternative which would be the ideal outcome of the decision process. *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 points) and/or the reformulation and reevaluation of the objective, model, and constraints. In the *post-decision* situation it is necessary to find information that supports a given *partial* decision as the best compromise among all feasible efficient alternatives.

This paper examines the second step in this three-step model of the decision-making process (partial decision making), and presents a number of methods for decision analysis and support.

3 Overview of methods for Multiple-Objective Decision Analysis (MODA)

An exhaustive classification of existing MODA methods according to the stage at which preference information is needed and the type of information required is given in [8] and reproduced in Figure 1.

All of these MODA methods are discussed and illustrated using a simple numerical example in [8]. We would argue that branches 3 and 4 are the most important classes of MODA 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 analysis, comparing it with one of the first applications of multiple-objective analysis in chemical engineering [9]. 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 components positive, and minimize the following Lagrange-type function:

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

then every minimal point in X_0, $\hat{x} = \arg \min\limits_{x \in X_0} L(\lambda, x)$ is an efficient solution of (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 MODA problems. A more practical approach would be to use the reference level method introduced by Wierzbicki [10], which leads to the following scalarizing function for problem (1):

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

where $\bar{f}$ denotes a reference vector of objectives defined by the decision maker, $(f(x) - \bar{f})_{\pm}$ denotes the vector with components $\max \{0, f_i(x) - \bar{f}_i(x)\}$, i. e., 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 non-convex problems. The method involving a displaced ideal (method 3.2.3 in Figure 1) [11] and the goal programming method [12] can be treated as special cases of (4) [13].

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. 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

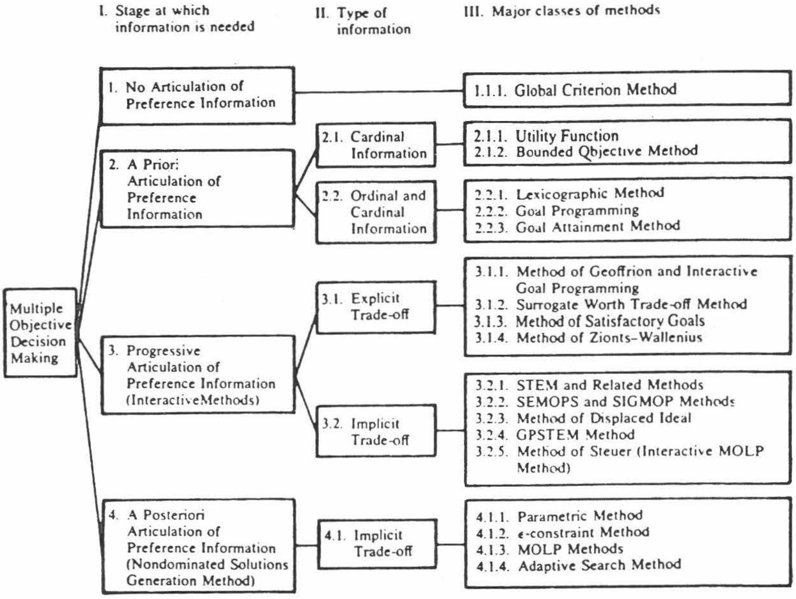

Figure 1: A taxonomy of methods for multi-objective decision analysis [8]

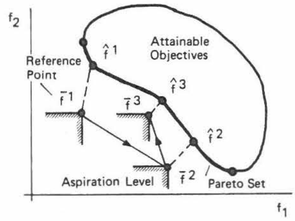

Figure 2: Reference point method; interactive procedure for multiple objective decision analysis

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. I 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 accurately. 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

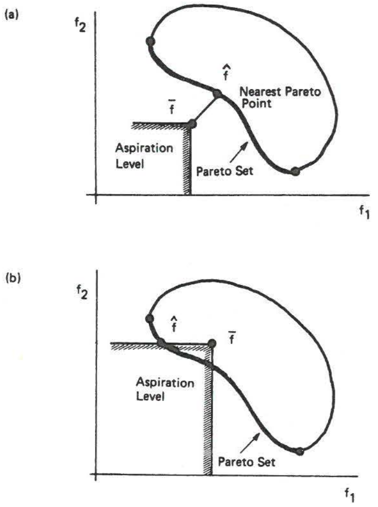

Figure 3: Reference point method: (a) unattainable reference point and (b) attainable reference point

solve some of the multiple-objective problems encountered in the design and steady-state control of chemical engineering systems [14, 15].

It is often necessary to consider the behavior of the system over time when making decisions concerning planning and control in chemical engineering processes.

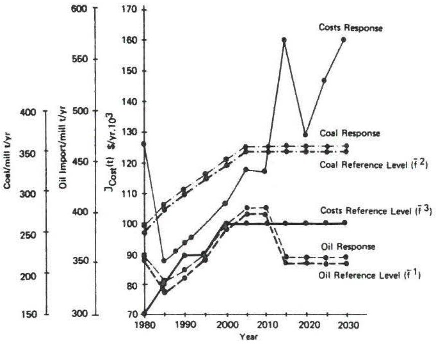

Figure 4: Reference trajectories (objectives) for imported oil supply, indiginous coal supply, and cost [17]

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 [16]. For example, a national goverment might wish to minimize the use of imported oil and indigenous coal in energy production to save them as feedstocks for the chemical industry, thereby minimizing 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 $(\bar{f}^3)$.

Table 1: Selected list of MODA computer codes [8]

Code number	MODA method	Authors	Remarks
1	Linear goal programming	Lee	Not an efficient code for a large scale problem
2	Linear goal programming and linear integer goal pr.	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	Uses 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	Not for a large scale problem, an interactive method
10	SIGMOP	Monarchi	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

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

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

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

4 Computer codes

Table 1 (derived from [8]) gives an overview of MODA 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 [8] and refer the reader to the exhaustive description of 44 MODA computer codes given in [18].

We will concentrate here on the software package DIDASS (Dynamic Interactive Decision Analysis and Support System) developed by the authors at IIASA to deal with linear and nonlinear multiple-objective optimization problems. This software consists of three basic parts. These are:

(1) The interactive "editor", which is used to manipulate the reference points and the objective (Lpmod in Figure 5).

(2) The preprocessor, which converts the multiple-objective problem file into its single criterion equivalent (Lpmulti in Figure 5).

(3) The postprocessor, which extracts the information from the output file, computes the values of the objectives, and displays the necessary information (Lpsol in Figure 5).

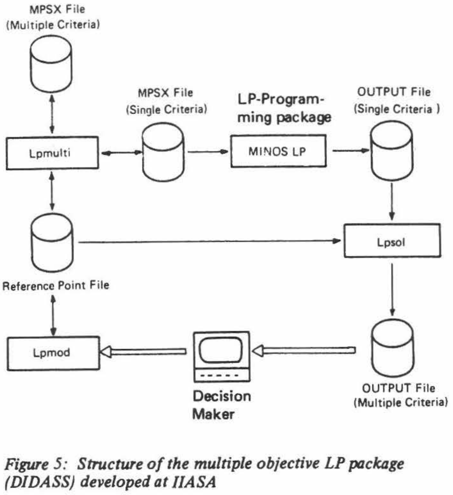

Figure 5: Structure of the multiple objective LP package (DIDASS) developed at IIASA

The general structure of this software package for the linear multiple-objective case is presented in Figure 5. More details of the system and the theory underlying the algorithm can be found in [19].

5 Overview of applications

In this section we give a general overview of the applications of multiobjective optimization and decision analysis in many different fields.

A large number of publications dealing with multiple-objective decision making are concerned with *water resources management and applications in general environmental systems* [20, 21]. The multiple conflicting objectives in this field are generally 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 various possible uses of water (irrigation, power generation, industrial cooling, recreation, etc.).

Multiple-objective decision analysis 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.* MODA techniques have been adopted in these areas because of the need for a reasonable compromise between the capital invested and the operating costs [22].

In the field of *system reliability* the conflicting goals are the maximization of system reliability and the minimization of system cost. In [23] a reliability problem with four objectives (system reliability, cost, weight, and volume) is considered; problem 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 [24] the authors point out that multiple-objective analysis 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 [24].

In the last few years a number of publications have also described applications of multiple-objective decision making in *chemical engineering*. One of the first of these applications was the use of multiple-objective techniques for planning production in a refinery [9]. In this case the problem was basically to maximize total yearly profit while minimizing the sensitivity of the profit to variations in refinery conditions. Another characteristic example of the use of MODA-methods is the multiobjective analysis of the petrochemical industry for a whole nation. In [25] three functions have been considered: the maximization of thermodynamic availability change, the minimization of lost work and and the minimization of the feedstock consumption. The first two objectives aim at structuring the industry for "optimum" energy utulization, while the third aims at the optimum utilization of raw materials. The advantage of the multiobjective analysis in this case is that any combination of mass and energy utilization efficiencies can be selected by the decision maker and the corresponding structure of the petrochemical industry can be found.

6 Selected applications in chemical engineering

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

6.1 Design using multiple-objective analysis

The first example we shall consider is a very general engineering problem: i. e. to design a machine (or a plant) with maximum throughput, minimum energy demand and output of the highest quality. We will demonstrate how to deal with these conflicting objectives by considering how best to design a twin-screw extruder (see Figure 6) for the production of thermoplastics [15].

Extrusion accounts for about 60 % of thermoplastic processing, and about 60 % of extrusion processing relies in twin-screw extruders. Extrusion also requires the expenditure of considerable amounts of energy. Thus, it is both technically interesting and economically profitable to analyse the design and operation of the twin-screw extruder using multiobjective techniques.

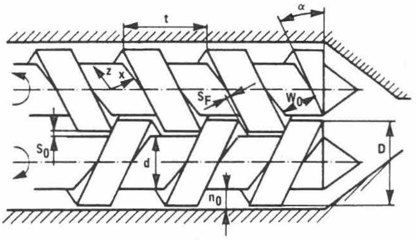

Figure 6: The twin-srew extruder [15]

The conflicting objectives in this problem are

- the throughput of thermoplastics (max $\dot{V}$)
- the electrical energy demand (min P)
- the quality of the thermoplastics (measured by the attainable deformation, max Γ).

The non-linear multiple-criteria optimization problem is then solved using the approach presented in eq. (4). An analysis of the efficient points (see Figure 7) 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.

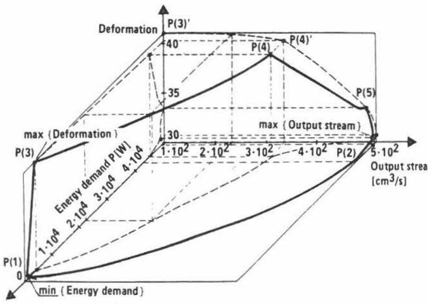

Figure 7: Geometrical interpretation of the problem of extruder design as a multiple objective optimization problem with three objectives [15]

6.2 Control using multiple-objective analysis

The problem of optimal control in a film-hardening process is treated in [14] a steady-state optimization problem with two criteria: the amount of solvent recycled (a monetary measure of the economy of the process) and the quality of the photographic film (see Figure 8). The problem assumes that both the quality of the film and the economy of the process should be maximized. Thus, in Figure 9 the amount of recycling should be maximized and the dimensionless number inversely proportional to the quality should be minimized. The numerical solution of this problem is the curve between points A and B in Figure 9. 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 possible to determine the most economic operating conditions for a given film quality.

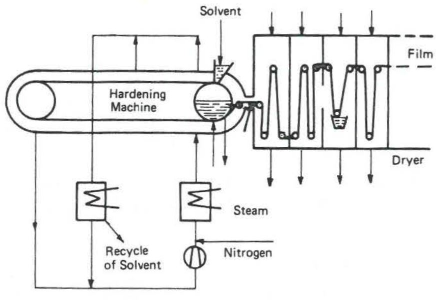

Figure 8: The film-hardening process [14]

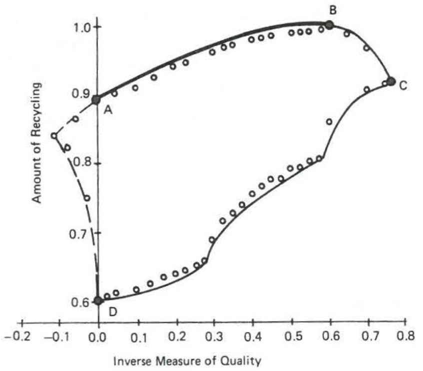

Figure 9: Set of efficient solutions (curve AB) for a model of the film-hardening process [14]

6.3 Planning using multiple-objective analysis

Our multiple-objective planning problem is taken from [26]. 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 structrure of the chemical industry – the by-products of one factory are often used as starting materials in another – and a sophisticated network-type model has been built to study these relationships. However, the most important factors affecting any decissions 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 a 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 also presented in [26].

7 Conclusion

We have described the use of the reference point optimization method in typical chemical engineering decision problems that arise in process design, plant control and production planning. We believe that multiobjective decision analysis of this type should be used in conjunction with data-processing tools to provide computer-based decision support systems for engineers, they could help in exploring and generating various courses of action, structuring 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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