MULTICRITERIA OPTIMIZATION OF CHEMICAL PROCESSES UNDER UNCERTAINTY

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Abstract

In this presentation, we will discuss multicriteria optimization (MCO) under uncertainty. We will consider a number (p) of conflicting criteria which depend on a vector of design variables (e.g. volume of reactor), control variables (e.g. temperature and flowrate) and uncertain parameters (e.g. rate constant and heat transfer coefficient). Our approach exploits the following facts. The design variables are constant at the operation stage, while the control variables can be tuned for satisfaction of process constraints. In addition, the level of accuracy of the uncertain parameters is often different at the design and operation stages. Specifically we will show how to construct a Pareto set (set of inferior points) at the design stage of the chemical process, being mindful that at the subsequent operation stage, there are enough process data for the sufficiently accurate estimation of all of the uncertain parameters. We proceed as follows. We first transform each criterion to a new form, which depends only on the design variables. The formation of new criteria uses a strategy similar to what is generally used for formation of the performance objective function in the two-stage optimization problem. The main difference is that in the internal optimization problem, a convolution of the multiple criteria (discussed earlier) is used instead of the original criteria. The convolution results from using MCO methods. After that the new criteria can be used for construction of a Pareto set. To obtain a point on the Pareto set, we formulate a bi-level optimization problem involving calculation of p multidimensional integrals for each value of the design variable vector. Since the resulting formulation is nondifferentiable and multiextremal, a direct solution is computationally intensive. To avoid this, we transform the bi-level optimization problem to one-level optimization problem, which is then solved using the split and bound method. The latter obtains the global solution if each original criterion satisfies some convexity conditions. At each search point the method requires calculation of only one multidimensional integral. In summary we give a two-stage formulation of the MCO problem under uncertainty and suggest methods for solving the corresponding bi-level optimization problem.

Keywords

Multicriteria optimization, Uncertainty, bi-level optimization.

Introduction

Often the performance of chemical processes cannot be estimated by only one objective function and it is necessary to take into account several conflicting criteria, for example (a) process economics and environmental requirements, and (b) integration of process design and control. Multicriteria optimization (MCO) under uncertainty can be formulated as

$$\begin{aligned} &\min_{d,z}(f_1(d,z,\theta),\ldots,f_p(d,z,\theta)) \\ &g(d,z,\theta)\le 0 \end{aligned} \qquad (1)$$

where d and z are vectors of design and control variables, respectively, θ is a vector of uncertain parameters, $g(x)$ is of dimension m. The main concept in MCO is the *Pareto Set* (PS) (*non-inferior set of points*) (Sophos et al, 1983).

Approach

In the MCO problem under uncertainty, the complexity consists in taking into account the different characteristics of the design and control variables. The main difference between the design and control variables consists in the possibility to change the control variables at the operation stage. To formulate the MCO problem under uncertainty, we will take into account the ability to tune the control variables at the operation stage within the context of extensions of the average criterion (AC) (Sophos et al, 1983) method and the $\varepsilon -$constraint method (Haimes, 1975). In the extended AC method, we employ the following two-level approach. At the first level we transform each criterion $f_i(d,z,\theta)$ to a new criterion, which depends only on design variables. Subsequently, using the AC method, we construct the PS. We formulate the problem as

$$f^*(d,\theta,a) = \min_z f(d,z,\theta,a)$$
$$g(d,z,\theta) \le 0 \quad (2)$$

where

$$f(d,z,\theta,a) = \sum_{k=1}^{p} a_k f_k(d,z,\theta)$$
$$\sum_{k=1}^{p} a_k = 1 \quad a_k \ge 0. \quad (3)$$

Let us construct functions $\bar{f}_i(d,a)$, which employ the optimal solution $z^*(d,\theta,a)$ from (2) as follows

$$\bar{f}_i(d,a) = \int_T f_i(d,z^*(d,\theta,a),\theta)\rho(\theta)d\theta \quad (4)$$
$$(i = 1,...,p)$$

Each new criterion $\bar{f}_i(d,a)$ is a mean value of the original criterion, $f_i(d,z,\theta)$.This mean value is determined at the operation stage such that at each time instant problem (2) is solved as the internal optimization problem. Again we can use the same AC method for the construction of a convolution of the functions $\bar{f}_i(d,a)$. Note that $\bar{f}_i(d,a)$ does not depend on the control variables z, therefore we can directly use the AC method.

$$\min_d \bar{f}(d,a) \quad (5)$$

where

$$\bar{f}(d,a) = \sum_{k=1}^{p} a_k \bar{f}_k(d,a). \quad (6)$$

Solving problem (5) using $\bar{f}_i(d,a)$ for some set of parameters a, we can construct a curve that is an analog of the conventional PS. The decision maker (DM) selects a point$[\bar{d},\bar{a}]$ from the PS. We will refer to this new curve as the DM curve.

Let us analyze the obtained result. For each θ^l the control variables are obtained by solving (2) where $a = \bar{a}$ and $d = \bar{d}$. Thus, the found values of the variables z correspond to one of points on the conventional Pareto set for the functions $f_i(\bar{d},z,\theta^l)$. Solving problem (5) we obtain $\bar{f}_i(\bar{d},\bar{a})$ which correspond to one of the points in the conventional PS for the functions $\bar{f}_i(d,\bar{a})$.

Suppose the decision maker selects the point $(\bar{d},\bar{a})$ from the DM curve as the solution of the MCO problem. This means that if we solve the internal optimization problem (2) at each time instance during the operation stage, the mean of $f_i(\bar{d},z,\theta^l)$ will be equal to $\bar{f}_i(\bar{d},\bar{a})$. It is clear that the solution can be realized, if at each time instant the internal optimization problem (2) will be solved since the same $z^*(d,\theta,\bar{a})$ is used for construction of each $\bar{f}_i(d,a)$. Problem (5) is a bi-level optimization problem since for calculation of $\bar{f}_i(d,a)$ we must use $z^*(d,\theta,a)$, which is the solution of (2). It is known that it is very computationally intensive, requiring the use of global, nondifferentiable optimization methods (Clark and Westerberg, 1983). To make matters worse, during the calculation of the objective function of (6), we must calculate p multidimensional integrals at each value of d.

In connection with this we reduce the problem to a simpler problem as follows. Substitute in $\bar{f}(d,a)$ expressions for $\bar{f}_i(d,a)$ from (4) to obtain

$$\bar{f}(d,a) = \sum_{k=1}^{p} a_k E\{f_k(d,z^*(d,\theta,a),\theta)\}$$
$$= \sum_{k=1}^{p} a_k \int_T f_k(d,z^*(d,\theta,a),\theta)\rho(\theta)d\theta.$$

This is equivalent to

$$\bar{f}(d,a) = \int_T [\sum_{k=1}^{p} a_k f_k(d,z^*(d,\theta,a),\theta)]\rho(\theta)d\theta \quad (7)$$

The term in the square brackets is the optimal value of the objective function of the internal optimization problem (2). Therefore, we can rewrite (7) as

$$\bar{f}(d,a)=\int_T \min_z(\sum_{k=1}^{p} a_k f_k(d,z,\theta)/ \quad g(d,z,\theta)\le 0)\rho(\theta)d\theta$$

Since for a given θ the optimal value at z does not depend on the values of z for other θ, we can rewrite the above as

$$\bar{f}(d,a)=\min_{z(\theta)}\int_T (\sum_{k=1}^{p}\alpha_k f_k(d,z,\theta))\rho(\theta)d\theta$$

$$g(d,z(d,\theta),\theta)\le 0$$

Here $z(\theta)$ is a multivariable function with respect to the uncertain parameters θ. Substitute the expression for $\bar{f}(d,a)$ in problem (5) to obtain

$$\min_{d,z(\theta)}\int_T (\sum_{k=1}^{p}\alpha_k f_k(d,z,\theta))\rho(\theta)d\theta \tag{8}$$

$$g(d,z(\theta),\theta)\le 0 \quad \forall\theta\in T \tag{9}$$

In order to guarantee satisfaction of (9) we must augment (8) with the following constraint

$$\chi_1(d)\le 0 \tag{10}$$

where (Halemane and Grossmann,1983) .

$$\chi_1(d)=\max_{\theta\in T_i}\min_{z\in Z}\max_{j\in J} g_j(d,z,\theta)$$

$$J=(1,...,m).$$

Now consider the $\varepsilon-$constraint method. For simplicity we will look at the case when p=2. In the absence of uncertainty the approach is as follows. The performance criteria are arranged in order of importance, with $f_1(x)$ being the most important. Next the following problem has to be solved

$$f_1^{(1)}=\min_x f_1(x) \qquad g(x)\le 0 \tag{11}$$

Assuming $[x^{(1)}, f_1^{(1)}]$ $(f_1^{(1)}=f_1(x^{(1)})$ is the global solution of the problem; we next solve the following problem

$$f_2^{(2)}=\min_x f_2(x) \tag{12}$$

$$g_j(x)\le 0, \quad j=1,...,m$$

$$f_1(x)\le\varepsilon_1 \tag{13}$$

where $\varepsilon_i>0$ is some parameter satisfying the condition $f_1^{(1)}\le\varepsilon_1$ .Let $[x^{(2)}, f_2^{(2)}]$ be the solution of the problem. We derive an extension of this method to MCO under uncertainty. Here we must formulate two-stage analogs of problems (11), (12).

The analog of problem (11) is the conventional one-criterion optimization problem

$$\bar{f}_1^{(1)}=\min_d E\{f_1^*(d,\theta)\} \qquad \chi_1(d,\theta)\le 0 \tag{14}$$

Here $[z_1^*(d,\theta), f_1^*(d,\theta)]$ is the solution of

$$f_1^*(d,\theta)=\min_z f_1(d,z,\theta)$$

$$g(d,z,\theta)\le 0$$

It is clear that the optimal value of the objective function in (14) can be written as

$$E\{f_1\ (d,z_1^*(d,\theta),\theta)\} \tag{15}$$

Now consider a two-stage analog of (12), for which the internal optimization problem is

$$f_2^*(d,\theta)=\min_z f_2(d,z,\theta) \qquad g(d,z,\theta)\le 0 \tag{16}$$

Let $z_2^*(d,\theta)$ be the solution of (16). To formulate an analog of the constraint (13), we note that $E\{f_1(d,z_2^*(\theta),\theta)\}$ is a mean value of the first criterion when $z(\theta)$ is the control variable vector, obtained by solving problem (16). It is reasonable to require that $E\{f_1(d,z_2^*(\theta),\theta)\}$ would not exceed ε_1 , where ε_1 must satisfy the condition

$$\bar{f}_1^{(1)}\le\varepsilon_1 \tag{17}$$

In other words the following inequality must be met $E\{f_1\ (d,z_2^*(d,\theta),\theta)\}\le\varepsilon_1$ .Finally, the two-stage analog of (12) will be

$$\bar{f}_2=\min_z E\{f_2(d,\theta)\}$$

$$\chi_1(d)\le 0 \tag{18}$$

$$E\{f_1(d,z_2^*(d,\theta),\theta)\}\le\varepsilon_1$$

Substitute into (18) the expressions for mathematical expectation

$$\bar{f}_2=\min_d\int_T \min_z\{f_2(d,z,\theta)/ \quad g(d,z(\theta),\theta)\le 0\}\ \rho(\theta)d\theta$$

$$\bar{\chi}_1(d)\le 0$$

$$\int_T f_2(d,z(\theta),\theta)\rho(\theta)d\theta-\varepsilon_1\le 0. \tag{19}$$

Note that it is very difficult to solve (19) since it requires solving (16) at each point θ. To circumvent this, change the order of operations in the objective function to obtain

$$\bar{\bar{f}}_2 = \min_{d,z(\theta)} \int_T f_2(d,z,\theta)\rho(\theta)d\theta \quad (20)$$

$$g(d,z(\theta),\theta) \le 0), \quad \forall \theta \in T$$

$$\chi_1(d) \le 0$$

$$\int_T f_2(d,z(\theta),\theta)\rho(\theta)d\theta - \varepsilon_1 \le 0 . \quad (21)$$

Problems (19) and (20) are not equivalent since the variables $z(\theta)$ corresponding to different points θ are not independent (they are connected by condition (21)). However, there exists inequality

$$\sum_{i=1}^{n} \min_{x^i}\{f_i(x^i)/g_i(x^i) \le 0, g(x) \le 0\} \le$$

$$\min_x\{\sum_{i=1}^{n} f_i(x^i)/g_i(x^i) \le 0, g(x) \le 0\}$$

where

$x = \{x^i\} \quad (i = 1,...,n)$,

$g(x) = (g_1(x^1,...,x^n),...,g_p(x^1,...,x^n))$ and x^i is a subvector of *x*. then $\bar{f}_2 \le \bar{\bar{f}}_2$. Thus, problem (20) gives an upper bound of the objective function in (18). Later on we will employ (20) in the MCO problem.

Solving problem (20) for different values of ε_1 we will obtain the curve, which can be used by decision maker for selection a final solution of the MCO problem under uncertainty. As indicated earlier, we refer to the curve as a DM curve.

Also, the extension of the average criterion method permits to obtain some points on a PS. However, for obtaining all points of the PS the region restricted by the PS curve must be convex. The ε -constraint method does not have these drawbacks.

The approach can be easily extended for *p*>2. Also the extended AC method and $\varepsilon - \mathrm{constraint}$ method can be used for of constructing a DM curve. Since the latter is constructed point wise, we need to construct q^{p-1} points for representation of the DM curve. Here *q* is the number of discrete points corresponding to each criterion f_i (*i*=1,…,*p*). This means that problem (8), (9), (10) or problem (20) must be solved q^{p-1} times. Therefore for *q*>3 constructing a DM curve can be computationally intensive. To alleviate this problem, one can construct a subset of points on the DM curve. The implication is that when using the AC method, we need coefficients a_i (*i*=1,…,*p*) which give relative importance of the criteria f_i (*i*=1,…,*p*). Solving problem (8),(9),(10) we obtain a point on the DM curve., which is a solution of the MCO problem.

Example

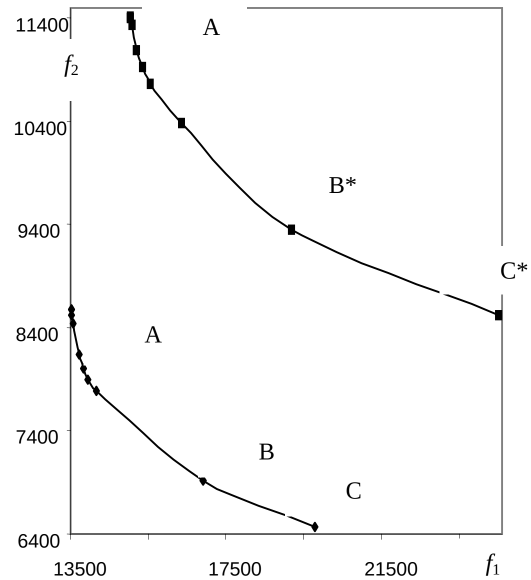

Figure 1 Accounting for Uncertainty - Pareto sets for nominal values of uncertain parameters and DM curve

Consider the MCO problem for a three-stage flowsheet (Ostrovsky et al, 2003). We will suppose that the by-products *C* and *D* are hazardous to the environment. Therefore, it is desirable to decrease the exit flowrate of these products. Thus, here we will have two criteria, which characterize the performance of the chemical process. One criterion (f_1) will represent the economics of the CP. The other criterion (f_2) is flowrate of the undesired by-products. Using the average criterion strategy and $\varepsilon - \mathrm{constraint}$ method, we construct the PS for the case when uncertain parameters take nominal values. In agreement with the theory the points obtained by all methods lie on the curve ABC (Figure 1). For the case when uncertainty is taken into account, we construct the DM curve using the extensions of the AC method and $\varepsilon - \mathrm{constraint}$ method. Both methods gave the same curve $A^*B^*C^*$.

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