Multicriteria Optimization Under Uncertainty – Considering Insufficient Process Data at the Operation Stage
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Multicriteria optimization under uncertainty – considering insufficient process data at the operation stage

I.V. Datskov[a], L.E.K. Achenie[b], G.M. Ostrovsky[c]

[a]*Department of Chemical Engineering, University of Connecticut, Storrs, CT 06269, USA (Current address is: OSISOFT, 777 Davis Street, Suite 250, San Leandro, CA 94577)*
[b]*Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, USA (Author to whom all correspondence should be addressed – achenie@vt.edu)*
[c]*Karpov Institute of Physical Chemistry, Vorontsovo Pole 10, Moscow 103064, Russia*

Abstract

Inherent in chemical process models are parameters that have uncertainty associated with them. In an earlier paper the authors addressed multicriteria optimization in the presence of model and process uncertainty at the design stage. Specifically the authors discussed extensions of the average criterion method, the worst-case strategy and the ε-constraint method under the following conditions: (a) at the design stage the only information available about the uncertain parameters is that they are enclosed in a known uncertainty region *T,* and (b) at the operation stage, process data is rich enough to allow the determination of exact values of all the uncertain parameters. The suggested formulation assumed that at the operation stage, certain process variables (called control variables) could be tuned or manipulated in order to offset the effects of uncertainty. This formulation made the conventional assumption that there was only one type of uncertain parameters. In this follow up paper, the authors consider the more realistic case where the uncertain parameters fall under at least two classes at the operation stage, namely (a) those that can be determined with enough accuracy and (b) those that cannot be determined with such accuracy given the available process data. Three illustrative examples (two benchmark and one direct methanol fuel cell) have been employed.

Keywords: flexibility analysis, uncertain parameter, two-stage optimization, multi-criteria optimization, direct methanol fuel cell

1. Introduction

Often the performance of chemical processes cannot be estimated only by one objective criterion 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. The importance of multiobjective design

has been shown by a small number of researchers (Sophos et al., 1980, Luyben and Floudas, 1994, Palazoglu and Arkun, 1987, Keeney and Raiffa, 1976 and Caballero et al., 1997).

Process simulations are further complicated by the presence of uncertainty in the process models and some process variables. Therefore, we cannot reliably carry out MCO without simultaneously considering process and model uncertainty. Furthermore, under an industrially-relevant scenario we cannot rely on commonly used assumption that any uncertain parameter can be determined accurately enough given the available process data at any time instant during the operation stage. For convenience let us refer to the last assumption as *Assumption 1*.

In the chemical engineering open literature, to our knowledge, the MCO problem under uncertainty has been considered only by Palazoglu and Arkun (1987) and Chakraborty and Linninger (2003). Palazoglu and Arkun considered the MCO problem within the context of the design of robust chemical plant under uncertainty. Here an economic objective function and dynamic operable measure are employed as criteria. The authors formulated the two-stage optimization problem in which as the inner optimization problem they solved a one-criterion optimization problem, using the ε-constraint method. Chakraborty and Linninger (2003) investigated the trade-off between expected cost and flexibility of plant-wide waste management. These investigations were based on *Assumption 1*, meaning that only one type of uncertainty was present; this is very restrictive and often not satisfied in practice.

In an earlier paper by us (Ostrovksy et al., 2006) we employed *Assumption 1*. In this paper we remove this assumption and identify two types of uncertainty at the operation stage. The first type represents the parameters which can be determined accurately enough, meaning that accurate and fast responsive sensors are present. The second type represents the parameters which cannot be determined accurately enough. This is the case when sensors have significant measurement error, delay in response or there are no sensors present to make measurements from which specific parameters can be inferred. In this paper we have to consider mathematical formulations with both types of uncertain parameters simultaneously.

2. Problem Formulation

The MCO problem under parametric uncertainty at the design stage can be formulated as

$$
\begin{aligned}
&\min_{d,z}(f_1(d,z,\theta),...,f_p(d,z,\theta))\\
&g_j(d,z,\theta) \le 0, \quad j=1,...,m
\end{aligned}
\tag{1}
$$

where d is a n_d-vector of design variables, z is a n_z-vector of control variables and θ is a vector of uncertain parameters over the domain T. The minimization is over a set of p (possibly conflicting) performance criteria $f_i(d,z,\theta)$. Constraints $g_j(d,z,\theta)$ in the problem are design specifications. The design variables (associated with the design stage of the chemical process) are fixed during the operation stage. Examples of design variables are reactor volume, heat exchanger area, length and diameter of the flow pipes. The control variables primarily represent tunable parameters that can

be adjusted during the operation of the chemical process; examples are temperatures, flow rates and pressures.

When the set of uncertain parameters is divided into two sets reflecting their level of accuracy at the operation stage (as discussed earlier), the MCO under uncertainty becomes

$$\min_{d,z}(f_1(d,z,\theta^1,\theta^2),...,f_p(d,z,\theta^1,\theta^2))$$
$$g_j(d,z,\theta^1,\theta^2) \leq 0, \quad j=1,...,m$$

(2)

Here θ^1 is a set of vectors of the first type of uncertain parameters over the domain T^1 and θ^2 is a set of vectors of the second type of uncertain parameters over the domain T^2.

When *Assumption 1* holds, the vector of uncertain parameters θ in (1) is considered known at the operation stage and becomes the conventional MCO problem, referred to in this paper as the *nominal MCO problem*. For simplicity we omit θ from the formulation in (1) and introduce the notation $x = (d,z)$. The main concept in the MCO problem is the *Pareto Set* (PS) (*non-inferior set of points*) defined as follows: any point $\bar{x}$ (such that $g(\bar{x}) \leq 0$) belongs to PS if in the small vicinity of $\bar{x}$ we cannot find a point $\bar{\bar{x}}$ (such that $g(\bar{\bar{x}}) \leq 0$) at which there is at least one criterion j such that

$$f_j(\bar{\bar{x}}) < f_j(\bar{x})$$
$$f_i(\bar{\bar{x}}) \leq f_i(\bar{x}) , \ i \neq j$$

This means that at any point in a PS, it is not possible to improve a criterion $f_i(x)$ without making another criterion $f_j(x)$ $(j \neq i)$ worse.

3. Review of Solution Approaches for the Nominal MCO

There are several methods for solving the nominal MCO problem (i.e. absence of parametric uncertainty) and building the PS curve under the following condition: *there is complete information about uncertain parameters at the design stage.* We consider the following methods: the average criterion (AC) (Sophos et al., 1980), the worst case strategy (WCS) (Clark and Westerberg, 1983) and ε-constraint method (Haimes, 1975). All these methods reduce the MCO problem to a one-criterion optimization problem. There are two general approaches for this reduction. In the first approach (employed by AC and WCS) a convolution of the original criteria $f_1(x),...,f_p(x)$ $(i=1,...,p)$ serves as the objective function. In the second approach (employed by the ε-constraint method) one of the original criteria serves as the objective function and the other criteria are used as constraints. A review of these methods can be found in our paper Ostrovksy et al. (2006). For convenience we are including the review below. In order to link the corresponding equations we have used a new designation. Thus Eqn. (a3) is equivalent to Eqn. (3) in the previous paper.

Average Criterion (AC) method

In the AC method each criterion $f_i(x)$ is assigned a weight coefficient a_i, reflecting its importance relative to the other criteria. The resulting problem formulation is given by

$$f^{1*} = \min_x f^1(x,a)$$
$$g(x) \leq 0$$

(a3)

where

$$f^1(x,a) = \sum_{i=1}^{p} a_i f_i(x)$$

$$a_i \geq 0; \ \sum_{i=1}^{p} a_i = 1.$$

(a4)

Here $g(x) = (g_1(x),...,g_m(x))$ is an m-vector of constraints and $a = (a_1,...,a_p)$. A solution $[\bar{x}, \bar{f}_1..., \bar{f}_p]$ of (3) belongs to the PS (Sophos et al., 1980). Changing the values of the weight coefficient a_i and solving problem (3) will generate different points of the PS. Thus a solution $[a^*, x^*]$ of problem (3) generates a point in the PS. This method generates all the points in the PS only if the region bounded by the PS is convex (Sophos et al., 1980).

Worst case strategy

In the worst case strategy (WCS) (Clark and Westerberg, 1983), as in the previous case, each criterion $f_i(z)$ is assigned a weight coefficient a_i, reflecting its importance relative to the other criteria. The key difference here is that the worst weighted criterion is minimized. The resulting problem is given by

$$f^{2*}(a) = \min_x f^2(x,a)$$
$$g_j(x) \leq 0, j = 1,...,m$$

(a5)

where $f^2(x,a) = \max_{j \in J}(a_j f_j(x))$ $J = (1,...,p)$ and $\sum_{j=1}^{p} a_j = 1$, $a_j \geq 0$. One can show that the problem can be reduced to the following problem (Clark and Westerberg, 1983)

$$\min_{x,y} y$$
$$a_i f_i(x) \leq y \quad i = 1,...,p$$
$$g(x) \leq 0.$$

(a6)

It can be shown that the method permits to obtain all the points of the PS. However, for $p > 3$ the method is computationally intensive (the same as for the AC method).

ε-constraint method

First we need to solve the following p problem formulations

$$f_k^{(p)} = \min_x f_k(x)$$
$$g(x) \leq 0 \quad\quad\quad\quad\quad\quad (a7)$$
$$k = 1,...,p$$

Assume $[x^{(k)}, f_k^{(p)}]$ $(f_k^{(p)} = f_k(x^{(k)}))$ is the global solution of the problem. The next step is to form a one-criterion problem, in which one criterion (for example the p-th criterion) is employed as the objective function and the remaining criteria serve as constraints. Note that the criteria are re-ordered such that the p-th criterion is the objective function. Thus

$$\min_x f_p(x)$$
$$g(x) \leq 0$$

(a8)

$$f_i(x) \leq \varepsilon_i, \quad i = 1,...,(p-1)$$ (a9)

where $\varepsilon_i > 0$ are parameters satisfying

$$f_k^{(p)} \leq \varepsilon_k \quad k = 1,...,p-1.$$

Note that ε_i is the allowable deterioration of the optimal value of $f_i(x)$ from the optimal value $f_i^{(p)}$. It can be shown that a solution of the problem belongs to the PS of the set $\{f_1(x),...,f_p(x)\}$. Solving problem (8) for different values of parameters ε_i yields all the points of the PS (Haimes, 1975). For $k=2$ Eqn. (a8) becomes

$$\min_x f_2(x)$$
$$g_j(x) \leq 0, j = 1,...,m \quad\quad\quad (a10)$$

$$f_1(x) \leq \varepsilon_1$$ (a11)

such that ε_1 satisfies $f_1^{(2)} \leq \varepsilon_1$

In this paper we will consider some approaches to address the issues of uncertainty within the MCO framework at the design stage of the CP. We will develop extensions of mathematical formulations for average criterion method, worst-case strategy, ε-constraint method based on *direct approach,* and new extended ε-constraint method while taking into account the presence of both types of uncertainty. It will be shown that the use of the *direct* multicriteria approach results in a conservative design of chemical process under uncertainty. We will show how the new MCO formulations can be reduced to sets of one-criterion problems under uncertainty, which can be solved by TSOP (two-stage optimization problem) algorithm, described in detail in Ostrovsky et al., (2003a). Two cases have been considered. In the first case, we know exact values of the uncertain parameters (at the design stage) that would be employed at the operation stage. This was considered in an earlier paper by us (Ostrovksy et al., 2006).   In the second case we suppose that at the operation stage, there are sufficient process data that can be used to obtain accurate values of the uncertain parameters, which implies that at the design stage the only available information to us is the domain of uncertain parameters.

4. Proposed Solution Approaches for MCO under Uncertainty

We distinguish between two types of variables, namely the design and control variables. The design variables correspond to design stage and can vary only at this stage. While the control variables can be tuned during both stages of CP. This work is focused on the case when at the operation stage we have incomplete information about uncertain parameters. This means that at the operation stage we do not have enough process data for determination of accurate values for all uncertain parameters. In this case we define two groups of uncertain parameters. The first group represents parameters which can be determined exactly at any time instant at the operation stage; at the design stage the only available information about this group is given by the associated domain T^1.   The second group represents uncertain parameters which cannot be determined accurately enough at any time instant at the operation stage. Thus the only information at both stages is given by the associated domain T^2. The presence of the second group of uncertain parameters complicates derivations of MCO under uncertainty. To solve the resulting MCO problem under uncertainty, we will employ extensions of the average criterion (AC) method, the worst-case strategy (WCS) and the ε-constraint method.

We will use the following general approach for the extension of the AC and the WCS methods. First, we will transform each criterion $f_i(d, z, \theta^1, \theta^2)$ to a new criterion $\bar{f}_i(d)$, which depends only on the design variables. With $\bar{f}_i(d)$ $(i = 1, ..., p)$ we will be able to use either the AC method or the WCS method for solving the MCO problem under uncertainty. From now on we will use the phrase "convolution method" to denote the phrase "AC or WCS method".

Consider the following optimization problem

$$\min_{z} \int_{T^2} F(f_1,...,f_p,\alpha)\mu(\theta^2)d\theta^2$$

$$\max_{\theta^2 \in T^2} g_j(d,z,\theta^1,\theta^2) \leq 0 \quad j=1,...,m \tag{3}$$

Here $F(f_1,...,f_p,\alpha)$ is a convolution of p criteria $f_1,...,f_p$, which is constructed using the convolution method and a is a vector of parameters (see (a3) and (a5)). We will suppose that at the operation stage, Eqn. (3) is solved for each θ^1. Let us construct new criteria $\bar{f}_i(d,\alpha)$,

$$\bar{f}_i(d,\alpha) = \int_{T^1} f_i(d,z^*(d,\theta^1,\alpha),\theta^1)\mu(\theta^1)d\theta^1 \tag{4}$$

These criteria employ the optimal solution $z^*(d,\theta^1,a)$ obtained from (3).

The function $\bar{f}_i(d,\alpha)$ is a mean value of the original criterion $f_i(d,z,\theta^1,\theta^2)$ at the operation stage since for each θ^1 Eqn. (3) is solved. Again we can use the same convolution method for solving the MCO problem while employing the functions $\bar{f}_i(d,\alpha)$ (here we will use the same parameters α, used in the construction of the convolution $f(f_1,...,f_p,\alpha)$). Designate the solution as $[d^*,\bar{f}_i^*]$ ($\bar{f}_i^* = \bar{f}_i(d^*,\alpha)$). Using the convolution method with $\bar{f}_i(d,\alpha)$ ($i=1,...,p$) for all values of α, satisfying (4) traces a curve (surface) in the space of the $\bar{f}_i$ ($i=1,...,p$). This curve (termed DM curve) is an analog of the conventional PS in the sense that the decision maker (DM) must make a final decision using the curve. From engineering consideration he must select a point $[\bar{d},\bar{a}]$ from this curve as the solution of the MCO problem.

Let us analyze the results. During the operation stage for each $\theta^{1,l}$, $a=\bar{a}$, and $d=\bar{d}$, the control variables z are obtained from (3) using the convolution method (i.e. we solve a conventional MCO problem). Thus, the resulting value of z corresponds to one of the points on the Pareto set for the functions $f_i(\bar{d},z,\theta^{1,l},\theta^2)$. Now consider the values $\bar{f}_i(\bar{d},\bar{\alpha})$ ($i=1,...,p$). These are obtained by solving (a3) or (a5) where the functions $\bar{f}_i(d,\bar{a})$ are used. Again we obtain a solution, which corresponds to one of the points of the conventional PS for $\bar{f}_i(d,\bar{a})$. Therefore, for each $\bar{f}_i(d,\bar{a})$ we cannot obtain a better MCO solution than $\bar{f}_i(\bar{d},\bar{a})$. It is clear that the solution can be realized, since at each time instance, Eqn. (3) is solved and the resulting $z^*(d,\theta^1,\bar{a})$ is used for construction of all $\bar{f}_i(d,a)$. We will apply this general approach for solving the MCO problem using the convolution method.

If Eqn. (3) is a convex program, then a local optimization algorithm is adequate for obtaining a global solution, otherwise a global optimizer is needed. Global optimization algorithms can be classified as either stochastic or deterministic. For example Luh et al. (2003) considered stochastic methods (specifically the genetic algorithm family of algorithms) in order to converge to globally optimal solutions for

an MCO formulation. Several deterministic global optimizers rely on branch and bound and convex/concave estimators (see for example Ostrovsky et al., 2003b).

4.1. Extended Average Criteria Method

In the extended average criteria (AC) method, we formulate Eqn. (a3) using the weighted sum in Eqn. (a4) (see also Eqn. (a3)) as the objective function, thus

$$f^*(d,\theta^1,\alpha) = \min_z \int_{T^2} f(d,z,\theta^1,\theta^2,\alpha)\mu(\theta^2)d\theta^2$$

$$\max_{\theta^2 \in T^2} g(d,z,\theta^1,\theta^2) \leq 0 \quad j=1,...,m$$

(5)

where

$$f(d,z,\theta^1,\theta^2,\alpha) = \sum_{k=1}^{p} \alpha_k f_k(d,z,\theta^1,\theta^2)$$

$$\sum_{k=1}^{p} \alpha_k = 1 \quad \alpha_k \geq 0$$

(6)

Let $z^*(d,\theta^1,\alpha)$ be the solution to the problem. Then $\bar{f}_i(d,a)$ is given by Eqn. (4). The new criteria $\bar{f}_i(d,a)$ $(i=1,...,p)$ do not depend on the control variables z and uncertain parameters $[\theta^1,\theta^2]$. Now we can directly use the method of minimization of the weighted average criterion

$$\min_d \bar{f}(d,\alpha)$$

(7)

where

$$\bar{f}(d,\alpha) = \sum_{k=1}^{p} \alpha_k \bar{f}_k(d,\alpha)$$

(8)

This is a bi-level optimization problem, since for calculation of $\bar{f}_k(d,\alpha)$ we must use $z^*(d,\theta^1,\alpha)$, which is the solution of Eqn. (5). It has been proven that bi-level optimization problem is multi extremal and nondifferentiable. To make matters worse, during the calculation of the objective function of Eqn. (7), we must recalculate p multidimensional integrals at each value of d. Therefore we need to reduce the Eqn. (7) to a simpler problem. By substituting in Eqn. (8) the expression for $\bar{f}_k(d,a)$ from Eqn. (4) and rearranging, we obtain

$$\bar{f}(d,a) = \int_{T^1} [\sum_{k=1}^{p} \alpha_k f_k(d,z^*(d,\theta^1,a),\theta^1,\theta^2)]\mu(\theta^1)d\theta^1$$

(9)

The term inside the square brackets is the optimal value of the objective function of the internal optimization Eqn. (5), and since for a given θ^1 the optimal value of z does not depend on the values of z for other θ^1, we can rewrite Eqn. (9) as

$$\bar{f}(d,\alpha) = \min_{z(\theta^1)} \int_{T^1} \int_{T^2} (\sum_{k=1}^{p} \alpha_k f_k(d,z,\theta^1,\theta^2)) \mu(\theta^2) \mu(\theta^1) d\theta^1 d\theta^2$$

$$\max_{\theta^2 \in T^2} g_j(d,z,\theta^1,\theta^2) \leq 0 \tag{10}$$

Here $z(\theta^1)$ is a multivariable function with respect to the uncertain parameters θ^1 and $j = 1,...,m$. By substituting the expression for $\bar{f}(d,\alpha)$ from (10) in Eqn. (7) we obtain

$$\min_{d,z(\theta^1)} \int_{T^1} \int_{T^2} \sum_{k=1}^{p} \alpha_k f_k(d,z,\theta^1,\theta^2) \mu(\theta^2) \mu(\theta^1) d\theta^1 d\theta^2 . \tag{11}$$

$$\max_{\theta^2 \in T^2} g_j(d,z(\theta^1),\theta^1,\theta^2) \leq 0, \forall \theta^1 \in T^1 \tag{12}$$

In order to guarantee existence of the solution of the problem we must supplement this problem with the following constraint Ostrovsky et al (2003)

$$\chi_2(d) \equiv \max_{\theta^1 \in T^1} \min_{z} \max_{\theta^2 \in T^2} \max_{j \in J} g_j(d,z,\theta^1,\theta^2) \leq 0 \tag{13}$$

The system of equations in Eqns. (11) and (13) constitute a two-stage optimization problem (TSOP2). Therefore, we can use the split and bound method (SB) described in Ostrovsky et al (2003a) to solve this problem.

Suppose the decision maker selects the point $[\bar{d},\bar{a}]$ from the DM curve. This means that if we solve (5) at each time instance during the operation stage, the mean of $f_i(\bar{d},z,\theta^1,\theta^2)$ will be equal to $\bar{f}_i(\bar{d},\bar{\alpha})$. We note that if we apply the direct approach for formulation of an MCO optimization problem on the basis of the AC method we will obtain TSOP as Eqn. (9). Thus in this case the direct approach gives the same result as the extended AC method approach.

4.2. Extended Worst Case Strategy

In the extended worst case strategy (WCS) method internal optimization Eqn. (3) formulated as follows

$$f^*(d,\theta^1,\alpha) = \min_{z} \int_{T^2} f(d,z,\theta^1,\theta^2,a) \mu(\theta^2) d\theta^2$$

$$\max_{\theta^2 \in T^2} g_j(d,z,\theta) \leq 0 \tag{14}$$

where

$$f(d,z,\theta^1,\theta^2 \alpha) = \max_{k}(\alpha_k f_k(d,z,\theta^1,\theta^2)$$

$$\sum_{k=1}^{p} \alpha_k = 1 \quad \alpha_k \geq 0 \tag{15}$$

Let $z^*(d,\theta^1,a)$ be the solution of the problem. As in the previous case $\bar{f}_i(d,\alpha)$ is represented by Eqn. (4), and the new criteria $\bar{f}_i(d,\alpha)$ $(i=1,...,p)$ do not depend on the control variables z, so we can directly use the method of the worst-case strategy for construction of the Pareto Set. In this case we must solve the problem

$$\bar{f}^*(\alpha) = \min_d \bar{f}(d,\alpha) \tag{16}$$

where

$$\bar{f}(d,\alpha) = \max_k a_k \bar{f}_k(d,\alpha) \tag{17}$$

This is a very computationally intensive bi-level optimization problem, which requires calculation of p multidimensional integrals for calculation of the objective function. Also it is nondifferentiable and multi extremal. We cannot simplify the problem the same way as we did in the case of the average criterion strategy in a previous section. We have to consider a different approach in order to reduce the complexity of this problem. Consider the following problem

$$\bar{\bar{f}}^*(a) = \min_d \bar{\bar{f}}(d,a) \tag{18}$$

where

$$\bar{\bar{f}}(d,\alpha) = \int_{T^1}[\int_{T^2}\max_k \alpha_k f_k(d,z^*(d,\theta^1,\alpha),\theta)\mu(\theta^2)d\theta^2]\mu(\theta^1)d\theta^1 \tag{19}$$

From theory there exists the following known inequality

$$\max_k \sum_i f_k(x,i) \le \sum_i \max_k f_k(x,i) \tag{20}$$

From Eqns. (4) and (17) we have

$$\bar{f}(d,\alpha) = \max_k \alpha_k \int_{T^1}\int_{T^2} f_k(d,z^*(d,\theta^1,\alpha),\theta)\mu(\theta^2)d\theta^2 \mu(\theta^1)d\theta^1 \tag{21}$$

Since an integral can be approximated with Gaussian quadrature, the inequality (20) leads to

$$\bar{f}(d,\alpha) \le \bar{\bar{f}}(d,\alpha), \quad \forall d, \forall \alpha \tag{22}$$

Thus $\bar{\bar{f}}$ is an upper bound of $\bar{f}$ for any design variables d and weight coefficients α. Consequently, $\bar{\bar{f}}^*(\alpha)$ is an upper bound for $\bar{f}^*(\alpha)$. The term in the square brackets in (19) is the optimal value of the objective function of the internal optimization Eqn. (14). Therefore, we can rewrite (19) as

$$\overline{\overline{f}}(d,\alpha) = \int\limits_{T^1}\int\limits_{T^2} \min_{z}[\max_{k} \alpha_k f_k(d,z(\theta^1),\theta^1,\theta^2)/\max_{\theta^2} g(d,z,\theta^1,\theta^2) \le 0]\mu(\theta^1)\mu(\theta^2)d\theta^1 d\theta^2$$

This expression is equivalent to the following expressions

$$\overline{\overline{f}}(d,\alpha) = \min_{z(\theta^1)} \int\limits_{T^1}\int\limits_{T^2} \max_{k} \alpha_k f_k(d,z(\theta^1),\theta^1,\theta^2)\mu(\theta^1)\mu(\theta^2)d\theta^1 d\theta^2$$
$$\max_{\theta^2} g(d,z,\theta^1,\theta^2) \le 0]$$

By substituting this expression for $\overline{\overline{f}}(d,\alpha)$ in problem (18) we obtain

$$\min_{d,z(\theta^1)} \int\limits_{T^1}\int\limits_{T^2} \max_{k} \alpha_k f_k(d,z(\theta^1),\theta^1,\theta^2)\mu(\theta^1)\mu(\theta^2)d\theta^1 d\theta^2$$
$$\max_{\theta^2 \in T^2} g_j(d,z(\theta^1),\theta^1,\theta^2) \le 0, \forall \theta^1 \in T^1 \tag{23}$$

In order to guarantee existence of the solution of the problem we must supplement this problem with the following constraint Ostrovsky et al (2003)

$$\chi_2(d) \equiv \max_{\theta^1 \in T^1} \min_{z} \max_{\theta^2 \in T^2} \max_{j \in J} g_j(d,z,\theta^1,\theta^2) \le 0$$

The obtained problem is similar to that of the two-stage optimization problem. We can use Gaussian quadrature to obtain a discrete form for Eqn. (23) as shown below

$$\min_{d,z^i} \sum_{i \in I_1} w_i \sum_{q \in Q} v_q \max_{k} \alpha_k f_k(d,z^i,\theta^{1,i},\theta^{2,q})$$
$$\max_{\theta^2 \in T^2} g_j(d,z^i,\theta^{1,i},\theta^2) \le 0, \quad i \in I_1, q \in Q, j=1,...,m \tag{24}$$
$$\chi_2(d) \le 0$$

This can be transformed to

$$\min_{d,z^i} \sum_{i \in I_1} w_i \sum_{q \in Q} v_q y^{iq}$$

$$\max_{\theta^2 \in T^2} g_j(d,z^i,\theta^{1,i},\theta^2) \le 0, \quad i \in I_1, \, q \in Q, \, j = 1,...,m \tag{25}$$

$$\alpha_k f_k(d,z^i,\theta^{1,i},\theta^{2,q}) \le y^{iq}, \quad i \in I_1, \, q \in Q, \, k = 1,...,p$$

$$\chi_2(d) \le 0$$

Consider the implications of the results. Suppose the parameter α_k reflects the relative importance of the corresponding criterion, then Eqn. (18) provides an upper bound of the objective function of Eqn. (16). Average values of each criterion will have the form in Eqn. (4) in which $z^*(d,\theta^1,\alpha)$ is the solution of Eqn. (14). It is clear that if we apply the direct approach for formulation of an MCO optimization problem using the WCS method we will obtain the TSOP as Eqn. (18), with $\bar{\bar{f}}(d,\alpha)$ as Eqn. (19). Thus, the direct approach can only give an upper bound of $\bar{f}^2(d,a)$ (also see Eqn. (22)) and, consequently, the use of the direct approach will in general lead to a conservative design.

4.3. Extended ε-Constraint Method

In the extended ε-constraint method we must formulate two-stage analogs of Eqns. (a7) and (a8). The analog of Eqn. (a7) is the conventional one-criterion optimization problem

$$f_k^{(p)} = \min_d E\{f_k^*(d,\theta^1)\}$$

$$\chi_2(d) \le 0$$

$$\tag{26}$$

where $f_k^*(d,\theta^1)$ is obtained by solving the problem

$$f_k^*(d,\theta^1) = \min_z \int_{T^2} f_k(d,z,\theta^1,\theta^2)\mu(\theta^2)d\theta^2$$

$$\max_{\theta^2 \in T^2} g(d,z,\theta^1,\theta^2) \le 0 \tag{27}$$

Let $z_k^*(d,\theta^1)$ be the solution of the above problem. Then

$$f_k^*(d,\theta^1) = E_{\theta^2}\{f_k(d,z_k^*(d,\theta^1),\theta^1,\theta^2)\}$$

Let $d^{(k)}$ be the solution of Eqn. (26). Subsequently the optimal value of the objective function in Eqn. (26) can be written as $E_\theta\{f_k(d^{(k)},z_k^*(d^{(k)},\theta^1),\theta^1,\theta^2)\}$. First

consider the case when $p=2$. Next we formulate a two-stage analog of Eqn. (a10). The internal optimization problem has the following form

$$f_2^*(d,\theta^1) = \min_z \int_{T^2} f_2(d,z,\theta^1,\theta^2)\mu(\theta^2)d\theta^2$$

$$\max_{\theta^2 \in T^2} g(d,z,\theta^1,\theta^2) \le 0$$

(28)

Let $z_2^*(d,\theta^1)$ be the solution. Next, we formulate an analog of the constraint in Eqn. (a11). Note that

$$\bar{f}_1 = E\{f_1(d,z_2^*(d,\theta^1),\theta^1,\theta^2)\}$$

(29)

is the mean value of the first criterion when $z_2^*(d,\theta^1)$ is obtained by solving Eqn. (28). From here it is naturally required that the value in Eqn. (29) would not exceed ε_1; in other words the following inequality must be met

$$E\{f_1 (d,z_2^*(d,\theta^1),\theta^1,\theta^2)\} \le \varepsilon_1$$

Finally, the two-stage analog of Eqn. (a10) is

$$f_2 = \min_d \int_{T^1} f_2^*(d,\theta^1)\mu(\theta^1)d\theta^1$$

(31)

Such that

$$\chi_2(d) \le 0$$
$$E\{f_1(d,z_2^*(d,\theta^1),\theta^1,\theta^2)\} - \varepsilon_1 \le 0$$

Substitute in Eqn. (30) the expressions for mathematical expectations

$$f_2^{(2)} = \min_d \int_{T^1} f_2^*(d,\theta^1)\mu(\theta^1)d\theta^1$$

$$\chi_2(d) \le 0$$

(31)

$$E\{f_1(d,z_2^*(\theta^1),\theta^1,\theta^2)\} - \varepsilon_1 \le 0$$

Since $f_2^*(d,\theta)$ is the solution of Eqn. (28), Eqn. (31) can be rewritten as

$$f_2 = \min_d \int_{T^1} \min_z (\int_{T^2} f_2(d,z,\theta^1,\theta^2)\mu(\theta^2)d\theta^2 / \max_{\theta^2} g(d,z(\theta^1),\theta^1,\theta^2) \le 0)\mu(\theta^1)d\theta^1$$

$$\chi_2(d) \le 0$$

$$\int_{T^1}\int_{T^2} f_1(d,z_2(d,\theta^1),\theta^1,\theta^2)\mu(\theta^2)\mu(\theta^1)d\theta^2 d\theta^1 - \varepsilon_1 \le 0$$

$$(32)$$

It is very difficult to solve Eqn. (32) since it requires solving Eqn. (28) at each point θ^1. To alleviate this, let us change the order of execution of the integration and minimization operations in the objective function to obtain

$$\overline{f}_2 = \min_{d,z(\theta^1)} \int_{T^1}\int_{T^2} f_2(d,z,\theta^1,\theta^2)\mu(\theta^2)\mu(\theta^1)d\theta^2 d\theta^1 \tag{33}$$

$$\max_{\theta^2 \in T^2} g(d,z(\theta^1),\theta^1,\theta^2) \le 0), \quad \forall \theta^1 \in T^1 \tag{34}$$

$$\chi_2(d) \le 0 \tag{35}$$

$$\int_{T^1}\int_{T^2} f_1(d,z_2(d,\theta^1),\theta^1,\theta^2)\mu(\theta^2)\mu(\theta^1)d\theta^2 d\theta^1 - \varepsilon_1 \le 0 \tag{36}$$

Eqns. (32) and (33) are not equivalent since the variables $z(\theta^1)$ corresponding to different points θ^1 are not independent (they are connected by Eqn. (36)). Let us employ the relation

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

where $x = \{x^i\}\ i = 1,...,n\}$ and x^i is a subvector of x, then we can write

$$f_2 \le \overline{f}_2$$

Thus Eqn. (33) gives an upper bound of the objective function of Eqn. (30). Later when we refer to the extended ε - constraint method, Eqn. (33) is implied.

Designate as $\overline{\varepsilon}_1$ the minimal possible value ε_1 under which Eqn. (30) has the solution. This means that ε_1 must satisfy the following condition

$$\varepsilon_1 \ge \overline{\varepsilon}_1. \tag{37}$$

It is clear that $\overline{\varepsilon}_1$ can be determined from

$$\overline{\varepsilon}_1 = \min_{d,\varepsilon_1} \varepsilon_1$$

$$\chi_2(d) \le 0 \tag{38}$$

$$E\{f_1(d,z_2^*(d,\theta^1),\theta^1,\theta^2)\} - \varepsilon_1 \le 0$$

This is a bi-level programming problem, which requires methods of nondifferentiable, global optimization. However, there is a simpler way to calculate a lower estimate of $\overline{\varepsilon}_1$. Indeed, since $f_1^{(1)}$ is the solution of Eqn. (26) for $k=1$, then the following inequality holds

$$f_1^{(1)} = E\{f_1(d,z_1^*(d,\theta^1),\theta^1,\theta^2)\} \le E\{f_1(d,z_2^*(d,\theta^1),\theta^1,\theta^2)\}.$$

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Therefore $f_1^{(1)}$ is a lower bound of $\bar{\varepsilon}_1$, thus

$$f_1^{(1)} \le \bar{\varepsilon}_1.$$

Using Gauss quadrature we obtain a discrete variant of Eqn. (33) as

$$\min_{d,z^i} \sum_{i \in I_1} w_i \sum_{q \in Q} v_q f_2(d, z^i, \theta^{1,i}, \theta^{2,q})$$

$$\max_{\theta^2 \in T^2} g_j(d, z^i, \theta^{1,i}, \theta^2) \le 0$$

$$\chi_2(d) \le 0 \quad i \in I_1 \quad q \in Q \quad j = 1, \ldots, m \tag{39}$$

$$\sum_{i \in I_1} w_i \sum_{q \in Q} v_q f_1(d, z^i, \theta^{1,i}, \theta^{2,q}) - \varepsilon_1 \le 0$$

where $\theta^{1,i}, \theta^{2,q}$ and w_i, $(i \in I_1)$, v_q, $(q \in Q)$ are approximation points and weight coefficients, respectively. Solving Eqn. (33) for different values of ε_1 one can construct the DM curve for $p=2$.

Similarly we can formulate two-stage analog of Eqn. (8) for $p=3$. First we need to solve Eqn. (26) for $k=1,2$. After that we must solve the problem

$$\min_d E\{f_3^*(d, \theta^1)\}$$

$$\chi_2(d) \le 0$$

$$E\{f_1(d, z_3^*(d, \theta^1), \theta^1, \theta^2)\} \le \varepsilon_1$$

$$E\{f_2(d, z_3^*(d, \theta^1), \theta^1, \theta^2)\} \le \varepsilon_2 \tag{40}$$

where $[z_3^*(d, \theta^1), f_3^*(d, \theta^1)]$ is the solution of the internal optimization problem

$$f_3^*(d, \theta^1) = \min_z \int_{T^2} f_3(d, z, \theta^1, \theta^2) \mu(\theta^2) d\theta^2$$

$$\max_{\theta^2 \in T^2} g(d, z, \theta^1, \theta^2) \le 0 \tag{41}$$

Again, we have to replace this problem with the corresponding upper bound on the objective function.

At the operation stage, consider the implementation of the optimal operating conditions determined from Eqn. (33) (for $p=2$). Let the decision maker select from the DM curve a point with $\varepsilon_1 = \varepsilon_1^*$ and $d=d^*$. It is seen from Eqn. (33) that at operation stage for each θ^1 the variables $z(\theta^1)$ must be determined by solving the problem

$$\min_{z(\theta^1)} \int_{T^1} \int_{T^2} f_2(d^*, z, \theta^1, \theta^2) \mu(\theta^2) \mu(\theta^1) d\theta^2 d\theta^1$$

$$\max_{\theta^2 \in T^2} g(d^*, z(\theta^1), \theta^1, \theta^2) \le 0), \qquad \forall \theta^1 \in T^1 \tag{42}$$

$$\int_{T^1} \int_{T^2} f_1(d, z(d, \theta^1), \theta^1, \theta^2) \mu(\theta^2) \mu(\theta^1) d\theta^2 d\theta^1 - \varepsilon_1^* \le 0$$

Let us compare the direct ε-constraint method and the extended ε-constraint method for $p=2$. Using the direct approach we must formulate the internal optimization problem as one criterion optimization problem using ε-constraint method. It is reasonable to use one of the criteria (for example, $f_2(d, z, \theta^1, \theta^2)$) as the objective function and use the other criterion within a constraint, namely $f_1(d, z, \theta^1, \theta^2) - \varepsilon_1 \le 0$. In this case the internal optimization problem is given by

$$\bar{f}_2^*(d, \theta^1) = \min_z \int_{T^2} f_2(d, z, \theta^1, \theta^2)$$

$$\max_{\theta^2 \in T^2} g_j(d, z, \theta^1, \theta^2) \le 0, \qquad j = 1, ..., m \tag{43}$$

$$g_{m+1}(d, z, \theta^1, \theta^2) \le 0$$

where $g_{m+1} = f_1(d, z, \theta^1, \theta^2) - \varepsilon_1$. In this case the TSOP is given by

$$\bar{\bar{f}}_2 = E\{f_2^*(d, \theta^1)\} \tag{44}$$

$$\bar{\chi}_2(d) \le 0$$

Note that

$$\bar{\chi}_2(d) = \max_{\theta^1 \in T^1} \min_{z \in Z} \max_{\theta^2 \in T^2} \max_{j \in \bar{J}} g_j(d, z, \theta^1, \theta^2), \quad \bar{J} = \{1, ..., (m+1)\}.$$

Designate as $\bar{\bar{\varepsilon}}_1$ the smallest value of ε_1 for which (44) has a solution. This means that

$$\varepsilon_1 \ge \bar{\bar{\varepsilon}}_1. \tag{45}$$

It is easy to see that (44) has a solution if the following inequality holds

$$\min_d \bar{\chi}_2(d, \varepsilon_1) \le 0.$$

Thus $\bar{\bar{\varepsilon}}_1$ can be found by solving the problem

$$\bar{\bar{\varepsilon}}_1 = \min_{\varepsilon_1} \varepsilon_1 \tag{46}$$

$$\min_d \bar{\chi}_2(d, \varepsilon_1) \le 0$$

Using a theorem from (Ostrovsky et al, 1997) we can reduce the problem to

$$\bar{\bar{\varepsilon}}_1 = \min_{d, \varepsilon_1} \varepsilon_1 \tag{47}$$

$$\bar{\chi}_2(d, \varepsilon_1) \le 0$$

Now we will show that for ε_1 satisfying (37) and (45), the following inequality holds

$$\bar{f}_2 \le \bar{\bar{f}}_2. \tag{48}$$

Using the same strategy which we used for reducing Eqn. (5) to (11), Eqn. (44) becomes

$$\bar{\bar{f}}_2 = \min_{d, z(\theta^1)} \int_{T^1} \int_{T^2} f_2(d, z(\theta^1), \theta^1, \theta^2) \mu(\theta^2) \mu(\theta^1) d\theta^2 d\theta^1 \tag{49}$$

$$\max_{\theta^2 \in T^2} g(d, z(\theta^1), \theta^1, \theta^2) \le 0 \quad \forall \theta^1 \in T^1$$

$$f_1(d, z(\theta^1), \theta^1, \theta^2) \le \varepsilon_1, \quad \forall \theta^1 \in T^1, \forall \theta^2 \in T^2 \tag{50}$$

$$\bar{\chi}_2(d) \le 0 \tag{51}$$

We note that Eqns. (33) and (49) have identical objective functions and constraints. It is easy to show that

$$\chi_2(d) \le \bar{\chi}_2(d) \tag{52}$$

Now compare the constraints from Eqns. (36) and (50). In order to do that, let us take $[d, z(\theta^1)]$ such that (50) holds. Then we have

$$\int_{T^1} \int_{T^2} f_1(d, z(\theta^1), \theta^1, \theta^2) \mu(\theta^2) \mu(\theta^1) d\theta^2 d\theta^1 \le \varepsilon_1 \int_{T^1} \int_{T^2} \mu(\theta^2) \mu(\theta^1) d\theta^2 d\theta^1 \le \varepsilon_1.$$

Thus, if the inequality in Eqn. (50) is met then the inequality in Eqn. (36) is met as well. The reverse is not true, however. To see this, suppose that the mathematical expectation $E\{z\}$ of a random variable z is less than a given value a; however it does not follow that all values of the random value z will be less than a. It follows from here that Eqn. (50) is more stringent than Eqn. (36). From this consideration and Eqn. (52) it follows that the feasible region in Eqn. (49) contains the one in Eqn (33). Therefore, Eqn. (48) holds. Thus, the direct ε-constraint method obtains a more conservative design in comparison with the extended ε-constraint method.

5. Comparison of the Methods

The extension of the average criterion method permits to obtain some points on a DM curve by solving the system (10). However, for obtaining all points of the PS, convexity of the region bounded by a PS is required. The extension of the worst-case strategy requires solving a very computationally intensive problem. To avoid this we calculate $\bar{\bar{f}}^*(a)$ by solving Eqn. (18) which gives only an upper bound of $\bar{f}^*(a)$ (see (16)). The extended ε-constraint method does not have the drawbacks of the first two methods.

6. Computational Experiments

6.1. Example 1: Three-stage flowsheet

Consider the MCO problem for a three-stage flow sheet (Ostrovsky et al, 2003a) (Fig. 1).

Each stage has one CSTR of volume V^i and heat exchanger with heat exchange area A_i. In each CSTR, the reaction is assumed to be first order of the type

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$
$$B \xrightarrow{k_3} D$$
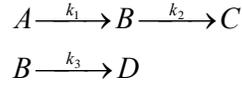
The reaction step $B \to D$ is endothermic and the steps $A \to B$ and $B \to C$ are exothermic. The process models and associated data are given in (Ostrovsky et al, 2003a). The cold stream for each heat exchanger is cold water at a temperature of T_{w1}. There are six design variables $[V_i, A_i](i = 1, 2, 3)$, six control variables $[T_i^1, T_{w2}^i](i = 1, 2, 3)$ and nine uncertain parameters $\theta = [T_0^1, T_{w1} \, F_0, k_1, k_2, k_3, U^1, U^2, U^3]$, where $[V_i, A_i]$ are the volume and heat exchange area of the i-th rector and heat exchanger, $[T_i^1, T_{w2}^i]$ are temperatures inside of the reactor and cold water at outlet of heat exchanger, respectively, $[F_0, T_0^1]$ are the flowrate and temperature of the inlet stream for the first reactor, $[k_1, k_2, k_3]$ are rate constants, and $[U^1, U^2, U^3]$ are heat transfer coefficients. The uncertainty region is given by

$$T(\gamma) = [\theta_i^N (1 - \gamma \, \delta \, \theta_i) \le \theta_i \le \theta_i^N (1 + \gamma \, \delta\theta_i)]$$

where θ_i^N is the nominal value of the i-th uncertain parameter, and $\delta\theta_i$ is a corresponding deviation fraction. Temperatures T_0^1 and T_{w1} deviate by $+\!/\!\_0.03$ each. The deviation for the remaining uncertain parameters is $+\!/\!\_0.1$. Suppose the concentration of B is required to be at least 18.4 kmol/mg, then

$$C_B \ge 18.4 \tag{53}$$

Other constraints are

$$
\begin{aligned}
&-T_2 + 311 \le 0 \\
&-T_{w2}^i + T_{w1} \le 0 && i = 1, 2, 3 \\
&301 \le T_{w2}^i \le 355 && i = 1, 2, 3 \\
&-(T_2^i - T_{w1}) + 11.1 \le 0 && i = 1, 2, 3 \\
&T_2^i - T_1^i \le 0 && i = 1, 2, 3 \\
&311 \le T_1^i \le 389 && i = 1, 2, 3
\end{aligned}
\tag{54}
$$

We assume that we need to minimize capital and operating costs such that all constraints in (53) and (54) are met. Suppose that side products C and D are hazardous to the environment. Therefore, it is desirable to decrease the outlet flowrate of these products. Thus, here we have to construct two conflicting criteria, which characterize performance of the chemical process. One criterion (f_1) will represent the cost of the chemical process and the other will represent the combined flowrate of hazardous side products. The cost function (f_1) is combined from cost of the equipment and process operating cost. It is represented by the following

$$f_1 = 700.0\sum_{i=1}^{3} V_i^{0.7} + 174.7\sum_{i}^{3} A_i^{0.6} + 1.76\sum_{1}^{3} W_i + 7.056\sum_{i=1}^{3} F_l^i \;,\; \$/yr. \tag{55}$$

Second criterion is represented by combined molar flowrate of side products C and D on the exit from third stage of the flowsheet. It is given as

$$f_2 = 24.0F(c_C^3 + c_D^3) \tag{56}$$

In this example we considered three levels of uncertainty. The first level is a nominal optimization when we do not have any uncertainty present in the system. The second level is a two-stage optimization in case of *complete information* about uncertain parameters (TSOP1). Two-stage optimization in case of *incomplete information* (TSOP2) represents the third level of uncertainty. One stage optimization (OSOP) is not considered since it does not have a solution for the given variations in uncertain parameters. We defined two groups of uncertain parameters as $\theta^1 = \{T_0, T_{W1}\}$ and $\theta^2 = \{F_0, k_i, U_i, i = 1,...,3\}$. For TSOP2 we selected 5 approximated points for first group of uncertain parameters: $\theta^{1,1} = \{N, N\}$, $\theta^{1,2} = \{U, U\}$, $\theta^{1,3} = \{L, L\}$, $\theta^{1,4} = \{L, U\}$, $\theta^{1,5} = \{U, L\}$ and one for the second group: $\theta^{2,1} = \{N, N, N, N, N, N, N\}$. Here, N is a nominal value; L and U are lower and upper bounds of corresponding parameter, respectively. Thus, in the full space of parameters θ in order to solve TSOP1 we used five approximation points $(\theta^{1,i}, \theta^{2,1})$ $(i = 1,...,5)$, which are the result of combining approximation points of the first and second types. The following weights were used in objective function for TSOP2: for the first group $w = [0.6, 0.1, 0.1, 0.1, 0.1]$, for the second group $v = [1.0]$.

Using the average criterion strategy, the worst-case strategy and the ε-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 same curve (i.e. curve 1 in Fig. 2). For the second case when we have complete information about uncertain parameters, we construct the DM curve using the extensions of the AC method and the extended ε-constraint method. For the WCS method we construct only the curve obtained by solving the upper bound problem. In order to solve this case we simplified the formulations in Eqns. (11), (23) and (33) by assuming that only θ^1 uncertain parameters were present in the system.

The results are given by profile number 2 in Fig.2. All methods gave the same profile. The third case, which represents incomplete information about uncertain parameters, is given by profile number 3. Again results obtained by different methods fell on the same curve. In agreement with theory, profile number 3 shows worse behavior than profile number 2. Even though the difference between profiles 2 and 3 is not as significant as between 1 and 2, nevertheless for a fixed set of weight coefficients the design obtained under the assumption that we have complete information about uncertain parameters (curve 2) is infeasible under the new supposition that for some uncertain parameters we have incomplete information (curve 3).

6.2. Example 2

Consider the reactor –separator system (Fig. 3) that consists of a continuous stirred tank reactor (1) and separator (2) (Grossmann and Sargent, 1978).

In the reactor a Denbigh type reaction takes place with first order irreversible kinetics.

$$A \xrightarrow{k_B} B \xrightarrow{k_R} R$$
$$A \xrightarrow{k_X} X$$
$$B \xrightarrow{k_Y} Y$$
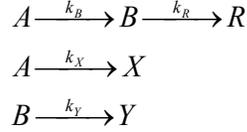
The fresh feed consists of pure A with molar concentration C_{A0} and flowrate F_{A0}. The reactor effluent (which consists of five components A, B, R, X, and Y) has a total flowrate of F. It is assumed that the separator achieves a perfect split with R as the top product. At the bottom, a fraction α of components A and B and a fraction β of components X and Y are recycled to the reactor, where it is mixed with fresh feed.

The steady state process model is as follows

$$F_{A0} - x_A F(1-\alpha) - V(k_B + k_X)c_{A0}x_A = 0$$

$$-Fx_B(1-\alpha) + Vc_{A0}[k_B x_A - (k_R + k_Y)x_B] = 0$$

$$-Fx_X(1-\beta) + Vc_{A0}k_X x_A = 0$$

$$-Fx_Y(1-\beta) + Vc_{A0}k_Y x_B = 0 \qquad (57)$$

$$-Fx_R + Vc_{A0}k_R x_B = 0$$

$$x_A + x_B + x_R + x_X + x_Y - 1 = 0$$

We will assume that reactor is operated isothermally. We select the volume $V\ [m^3]$ of the reactor as the design variable; for control variables we can pick α and β. The uncertain parameters are inlet molar flow rate of component A and rate constant coefficients $\theta = [F_{A0}, k_B, k_R, k_X, k_Y]$. The chemical reaction rate constants have dimensions of $[h^{-1}]$. For fixed F_R, we require the flowrate of R to satisfy the constraints

$$F_R - Fx_R \le 0.$$

In addition, there are the following constraints on the design, control and state variables

$$12 \le V \le 16$$
$$0 \le \alpha \le 1 \quad 0 \le \beta \le 1$$
$$0 \le x_i \le 1 \quad i = \{A, B, R, X, Y\}$$
$$10 \le F \le 1000.$$

Other data for the process are

$$k_B = 0.4h^{-1} \quad k_R = 0.1h^{-1} \quad k_X = 0.02h^{-1} \quad k_Y = 0.01h^{-1}$$
$$F_{A0} = 100\,mole/h \quad c_{A0} = 100\,mole/m^3 \quad F_R = 70\,mole/h.$$

Suppose that products X and Y are hazardous to the environment, and therefore undesirable. In order to design "cheap" chemical process and at the same

reduce molar flowrate of undesired products in outlet stream from separator, we have to construct two conflicting criteria. The first criterion (f_1) will characterize the costs of reactor and separation system, while the second criterion (f_2) will characterize the molar flowrate of products X and Y in outlet stream; these two criteria are given by

$$
\begin{aligned}
f_1 &= c_1 V + c_2 (\alpha F(x_A + x_B) + \beta F(x_X + x_Y)) \quad [=] \$ \\
f_2 &= 10.0(1-\beta)F(x_X + x_Y) \quad [=] \, mole/h
\end{aligned}
\tag{58}
$$

In this example we solved the MCO as (a) nominal optimization, (b) TSOP1 and (c) TSOP2. Note, that TSOP1 is a special case of TSOP2 when there are no uncertain parameters of the second type present. In TSOP1 we assumed that the inlet reactant molar flow rate F_{A0} and the reaction rate constants could be determined accurately using the available process data; therefore $\theta^1 = \{F_{A0}, k_B, k_R, k_X, k_Y\}$ and $\theta^2 = \varnothing$. In TSOP2 we assumed that the reaction rate constants could not be determined using the available process data; therefore $\theta^1 = \{F_{A0}\}$ and $\theta^2 = \{k_B, k_R, k_X, k_Y\}$. As nominal values for uncertain parameters we chose $\theta^N = [F_{A0}, k_B, k_R, k_X, k_Y]^N = [100.0; 0.4; 0.1; 0.02; 0.01]$ and the maximum deviation (as a percentage) from nominal values is $\delta\theta = [5.0; 15.0; 15.0; 15.0; 15.0]$. In TSOP2 we selected three approximated points for θ^1 as $\{\theta^{1,1}, \theta^{1,2}, \theta^{1,3}\} = \{[N], [U], [L]\}$. We also selected three sets of approximation points for θ^2 as $\theta^{2,1} = [N, N, N, N]$, $\theta^{2,2} = [L, L, U, U]$ and $\theta^{2,3} = [U, U, L, L]$. Here, N is a nominal value, while L and U are lower and upper bounds. We employed the same approximation points for TSOP1; therefore there were nine approximation points $(\theta^{1i}, \theta^{2j})$, $(i = 1,...,3; j = 1,...,3)$, as a result of combining approximation points of θ^1 and θ^2. For TSOP1 the weights were calculated as $s_k = w_i v_j$, where for each w_i there were three v_j. The following weights were used in the objective function for TSOP2: for θ^1, $w = \left[\dfrac{2}{3}, \dfrac{1}{6}, 1.6\right]$ while for θ^2, $v = \left[\dfrac{2}{3}, \dfrac{1}{6}, \dfrac{1}{6}\right]$. For TSOP1 the weights for approximation points were $s = \left[\dfrac{4}{9}, \dfrac{1}{9}, \dfrac{1}{9}, \dfrac{1}{9}, \dfrac{1}{36}, \dfrac{1}{36}, \dfrac{1}{9}, \dfrac{1}{36}, \dfrac{1}{36}\right]$.

Using the three strategies, namely the average criterion strategy (AC), the worst-case strategy (WCS) and the ε-constraint method, we constructed the PS for the nominal optimization case. All three methods gave the same results (curve 1 in Fig.4). For TSOP1 we constructed the DM curve using extensions of the AC method and the ε-constraint method. Both methods gave the same results (curve 2 in Fig. 4). For the WCS method we constructed curve 3 (in Fig. 4). For TSOP2 both AC and the ε-constraint methods gave the same results (curve 4 in Fig. 4), while the WCS resulted in curve 5 (in Fig. 4) which as expected is an upper bound on all the curves. It is interesting to note that with decreasing f_2, curves 2 and 3 tend to merge with curve 1 (nominal MCO), while curves 4 and 5 move away from curve 1.

6.3. Example 3

In this case study we will illustrate the effect of uncertainty on multicriteria optimization of the Direct Methanol Fuel Cell (DMFC) (Fig. 5). The DMFC is a power-generation system, which offers a new and promising environmentally friendly source of energy. It has several advantages over other types of fuel cells, such as high efficiency, very low emissions, a potentially renewable fuel source and fast refueling. The DMFC uses methanol in the form of liquid or vapor, to generate electrical energy. The main disadvantage is the voltage drop associated with crossover of methanol through the membrane. The direct methanol fuel cell model is from Scott et al. (1997) and is summarized in the appendix of our paper Ostrovksy et al. (2006). In this case study we will concentrate only on the catalyst and membrane layers in order to analyze the effect of methanol crossover on the DMFC performance. An analysis based on the DMFC can easily be adapted to apply to other fuel cell systems.

As design variables we chose the anode thickness $l_{anode}[cm]$, the cathode thickness $l_{cathode}[cm]$ (in the catalyst layers) and the membrane thickness $t_m[cm]$. For control variables we select the anode methanol pressure $P_{anode}[atm]$, the cathode oxygen (air) pressure $P_{cathode}[atm]$, and overall current density $I[A \cdot cm^{-3}]$. As uncertain parameters we select $\theta = [T, \Delta l_{anode}, \Delta l_{cathode}, \Delta t_m, \chi, D_{m,MeOH}, \lambda_{MeOH}, C_{0,MeOJH}]$. The uncertainty region is given by

$$T(\gamma) = [\theta_i^N(1 - \delta\theta_i/100) \leq \theta_i \leq \theta_i^N(1 + \delta\theta_i/100)]$$

where θ_i^N is the nominal value of the ith uncertain parameter, and $\delta\theta_i$ is a corresponding deviation fraction. The vector of nominal values is given as $\theta^N = [353, 0, 0, 0, 3 \times 10^6, 4.9 \times 10^{-6}, 2.48 \times 10^{-2}, 1.0 \times 10^{-3}]$. The deviations for the uncertain parameters are set equal to $\delta\theta_1 = 5\%$, $\delta\theta_i = 20\%$ $(i = 2,3)$, $\delta\theta_4 = 10\%$, $\delta\theta_i = 20\%$ $(i = 5,...,8)$.

In the DMFC the most important problem is to decrease the cell voltage drop associated with crossover of methanol through the membrane. A proposed solution is to increase the pressure of oxygen (air) on the cathode side. Thus, in the first study case we constructed two conflicting criteria, which characterize the performance of the DMFC. One criterion ($f_1[V]$) represents the crossover overpotential and the other ($f_2[V]$) represents the cost of pressurizing; we employed a correlation similar to one in Douglas (1988).

$$f_1 = \eta_{crossover}$$
$$f_2 = \left(\frac{P_{cathode}}{P_{ref}}\right)^{0.29} - 1 \tag{59}$$

Another important problem is to design a cost efficient fuel cell with minimal loss of power. For the second case one criterion is chosen to be the combined cost of the membrane and the catalyst ($f_1[\$/cm^2]$). The second criterion is ($f_2[Watts]$), which is the power of a single fuel cell. Specifically

$$f_1 = 42 \cdot 10^{-2} \rho_{Pt} l_{anode} + 28.9 \cdot 10^{-2} \rho_{Pt+Ru} l_{cathode} + 7.7 \cdot 10^{-3} e^{32.7 t_m} + 0.38$$
$$f_2 = I \cdot V_{cell}$$

(60)

The process constraints are

$$V_{cell} \geq 0.5$$
$$\upsilon_{water} \leq \upsilon_0$$

(61)

Since, the rate of water being produced is directly proportional to the overall current density we can implement this constraint through simple bounds on the overall current density (see Eqn. (61)).

As in previous examples we solved the MCO as (a) nominal optimization, (b) TSOP1 and (c) TSOP2. For TSOP2 We defined two groups of uncertain parameters $\theta^1 = \{T, \Delta l_{anode}, \Delta l_{cathode}, \Delta t_m\}$ and $\theta^2 = \{\chi, D_{m,MeOH}, \lambda_{MeOH}, C_{0,MeOJH}\}$; in addition we selected 2 approximation points for θ^1, thus $\theta^{1,1} = \{N, N, N, N\}$, $\theta^{1,2} = \{L, L, U, L\}$. We also selected 4 approximation points for θ^2 as $\theta^{2,1} = \{N, N, N, N\}, \theta^{2,2} = \{U, N, U, N\}$, $\theta^{2,3} = \{N, U, N, U\}$ and $\theta^{2,4} = \{U, U, U, U\}$. Since the same approximated points were used for TSOP1, we used a total of 8 approximation points $(\theta^{1,i}, \theta^{2,j})$ $(i = 1, 2; j = 1, ..., 4)$, resulting from combining approximation points of the first and second types. The following weights were used in the objective function for TSOP2: for the first group $w = [0.6, 0.4]$, for the second group $v = [0.4, 0.2, 0.2, 0.2]$. For TSOP1 the weights were $s = [0.24, 0.12, 0.12, 0.12, 016, 0.08, 0.08, 0.08]$.

For both cases we used the AC and ε-constraint methods to obtain the Pareto curves (1). The DM curves 2 and 3 were obtained by using the extended AC and extended ε-constraint method for MCO under uncertainty. Both methods gave identical results. The graphs are given in Fig. 6 and Fig. 7. In both figures the x-axis corresponds to f_1 and its mathematical expectation and the y-axis corresponds to f_2 and its mathematical expectation.

In the first case (Fig. 6) the results were as expected; with an increase in the cost of pressurizing (f_2), the performance (curve 1) of the DMFC drops as a result of increasing crossover overpotential (f_1). Note that for TSOP1 (only one type of parametric uncertainty), a significant increase in crossover overpotential occurred, resulting in poor DMFC performance (curve 2). In TSOP2 (two types of parametric uncertainty), no significant differences were detected (curve 3), except that the feasibility region is reduced significantly. This leads to conservative design, since the design and control variables are very close to their bounds.

In case 2 (Fig. 7) the results were also as expected; an increase in the catalyst and membrane layer thicknesses leads to an increase in the overall performance of the fuel cell (curve 1). An increase in the anode thickness l_{anode} (Eqn. 73) results in an increase in the overpotential associated with the anode; at the same time it provides a lower methanol concentration on the boundary of the anode catalyst layer leading to a

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decrease in the crossover overpotential $\eta_{crossover}$ (Eqns. 79 and 80). The later has a dominating effect on the anode thickness. The membrane thickness t_m also plays a dual role in this model. An increase in t_m leads to an increase in the ohmic overpotential η_{ohmic} (Eqn.71) while resulting in a decrease in the crossover overpotential $\eta_{crossover}$ (Eqns. 79 and 80). The latter has a greater effect on the fuel cell performance. In TSOP1 (curve 2), we have similar results as in the nominal case. The performance of the fuel cell dropped by 50 [mWatts], which is very significant to fuel cell design. In TSOP2 the performance of the fuel cell dropped by 80 [mWatts], which is almost twice as large as the TSOP1 results. As result, multicriteria optimization of DMFC model showed the significant effect of uncertainty based on the drop in fuel cell performance when there are two types of uncertainty in the system.

Table 1. Direct Methanol Fuel Cell model constants			
Constant	**value**	**Constant**	**value**
E^0_{cell}	1.214 V	F	96,488 $C \cdot equiv^{-1}$
$dE/dT, gas$	$1.043 \cdot 10^{-3}$ $V \cdot K^{-1}$	$n\,(anode)$	6
ΔN	0.5	$n\,(cathode)$	4
σ^{ref}_m	0.073 $S \cdot cm^{-1}$	R	8.314 $J \cdot mol \cdot K^{-1}$
$(\gamma \dot{i}_0)^{ref}_{anode}$	6.25 $A \cdot cm^{-3}$	ε	0.3
E_{anode}	0.265 V	$(\gamma \dot{i}_0)^{ref}_{cathode}$	7.14 $A \cdot cm^{-3}$
D^{ref}_{anode}	$2.8 \cdot 10^{-5}$ $cm^2 \sec^{-1}$	$E_{cathode}$	0.355 V
$C_{0,MeOH}$	$1.0 \cdot 10^{-3}$ $mol \cdot cm^{-3}$	$D^{ref}_{cathode}$	$2.8 \cdot 10^{-5}$ $cm^2 \sec^{-1}$
$\upsilon_{m,anode}$	0.17	$\upsilon_{m,cathode}$	0.05
λ_{MeOH}	$2.48 \cdot 10^{-2}\ {}^{MeOH}/_{H^+}, mol \cdot equiv^{-1}$	χ	$3.0 \cdot 10^6$ $[V \cdot cm^2 \sec \cdot mol^{-1}]$

7. Conclusion

We developed extensions of the average criterion method (AC), the worst case strategy (WCS) and the ε-constraint method for solving the multicriteria optimization problem under uncertainty for a chemical process when there are two distinct types of uncertainty present. Specifically we have considered the more realistic case where the uncertain parameters fall under at least two classes at the operation stage, namely (a) those that can be determined with enough accuracy and (b) those that cannot be determined with such accuracy given the available process data.

In all three approaches we exploit the degrees of freedom afforded by the presence of the control variables at the operation stage. It is shown that the extended

methods have significant advantages over the direct approach for the multicriteria optimization problem (MCO). Through three illustrative examples (two benchmark and one direct methanol fuel cell) we have seen the implications of being able to distinguish among the types of uncertain parameters.

8. Acknowledgements

9. Notation

a_i	Scalar constant
a , a^*	Vector constant
d	Vector of design variables (with dimension n_d)
$f_i(*)$, $f^i(*)$	Performance criterion
$\overline{f}^2(*)$, $\overline{f}_i(*)$, $\overline{\overline{f}}^2(*)$	Performance criterion
f^{i*} , $f_k^{(p)}$, $\overline{f}^{2*}(*)$, $\overline{\overline{f}}^{2*}(*)$	Optimal value of performance criterion
$g_j(*)$	Scalar constraint
$g(*)$	Vector constraint
$E\{*\}$	Expected value
J , $\overline{J}$	Index set
w_i	Weight (scalar)
x , $\overline{x}$, $\overline{\overline{x}}$, x^* , $x^{(k)}$	A point
z	Vector of control variables (with dimension n_z)
$z^*(*)$	Optimal vector of control variables (with dimension n_z)
z^i	$z(\theta^i)$

Greek

ε_i , $\overline{\overline{\varepsilon}}_i$, α_k , β , γ	Scalar constant
θ	Vector of uncertain parameters over the domain T
θ^l	A given value of θ
θ_i^N	Nominal value of θ
$\delta\theta_i$	Deviation fraction
$\rho(*)$	Probability density function
$\chi_1(*)$, $\overline{\chi}_1(*)$	Feasibility function

Example Problems

A_i	Heat exchanger area
c_i	Concentration or cost
F_i, F	Flow rate
I	Overall current density
k_i	Rate constant
l_{anode}	Anode thicknesses
$l_{cathode,}$	Cathode thickness
P_{anode}, $P_{cathode}$	Pressure of methanol at anode or cathode
P_{ref}	Reference pressure
t_m	Membrane thickness
T_{w1}	Cold water temperature
T_i^1	Temperature
U^i	Heat transfer coefficient
V_i, V	Volume
V_{cell}	Cell voltage
x_i	Mole fraction (used in examples)

References

Clark, P.A., A.W. Westerberg. Optimization for design problems having more than one objective. *Comput. Chem. Eng.*, 7: 259, 1983.

Chakraborty, A., A.A. Linninger. Plant-wide waste management. 2. Decision making under uncertainty. *Ind. Eng. Chem. Res.*, 42: 357, 2003.

Caballero, R., F. Ruiz, R.E. Steuer. Advances in multiple objective and goal programming. *Berlin: Springer-Verlag*, 1997.

Douglas, J. Conceptual Design of Chemical Processes. *McGraw-Hill*, 1988

Haimes, Y., W.A. Hall, N.J. Friedman. Multi-objective optimization in water resource systems: the surrogate worth trade-off method. *Amsterdam: Elsevier*, 1975.

Keeney, R.L., H. Raiffa. Decisions with Multiple Objectives. *New York: John Wiley*, 1976.

Luh, G.C., C.H. Chueh, W. W. Liu. MOIA: Multi-Objective Immune Algorithm, *Eng. Opt.,* 35(2):143–164, 2003.

Luyben, M.L., C.A Floudas. Analysing the interaction of design and control-1., a multiobjective framework and application to binary distillation synthesis. *Comp. Chem. Eng.* 18: 933, 1994.

Ostrovsky, G., Achenie, L. E. K., Datskov, I. and Volin, Y., "An Approach to Multicriteria Optimization under Uncertainty," (accepted by Chemical Engineering Science, 2006).

Ostrovsky, G.M., I.V. Datskov, L.E.K. Achenie, Yu.M. Volin. Process uncertainty: the case of insufficient process data at the operation stage. *AIChE Journal*, 49: 1216-1240, 2003a.

Ostrovsky, G.M., Achenie, L. E. K., and Sinha, M. "A Reduced Dimension Branch-and-Bound Algorithm for Molecular Design," *Comp. Chem. Eng*, **27**(4), 551-567, 2003b.

Ostrovsky, G.M., Yu.M. Volin, M.M. Senyavin. An approach to solving a two-stage optimization problem under Uncertainty, *Comp. Chem. Eng*, 21: 311, 1997.

Palazoglu, A., Y. Arkun. Design of chemical plants with multiregime capabilities and robust dynamic operability characteristics. *Comp. Chem. Eng*, 11: 205, 1987.

Scott, K., W. Taama, J. Cruickshank. Performance and modeling of a direct methanol solid polymer electrolyte fuel cell. *Journal of Power Sources*, 65: 159-171, 1997.

Sophos, A., F. Rodstein, C. Stephanopoulos. Multi-objective analysis in modeling the petrochemical Industry. *Chem. Eng. Sci.*, 35: 2415, 1980.
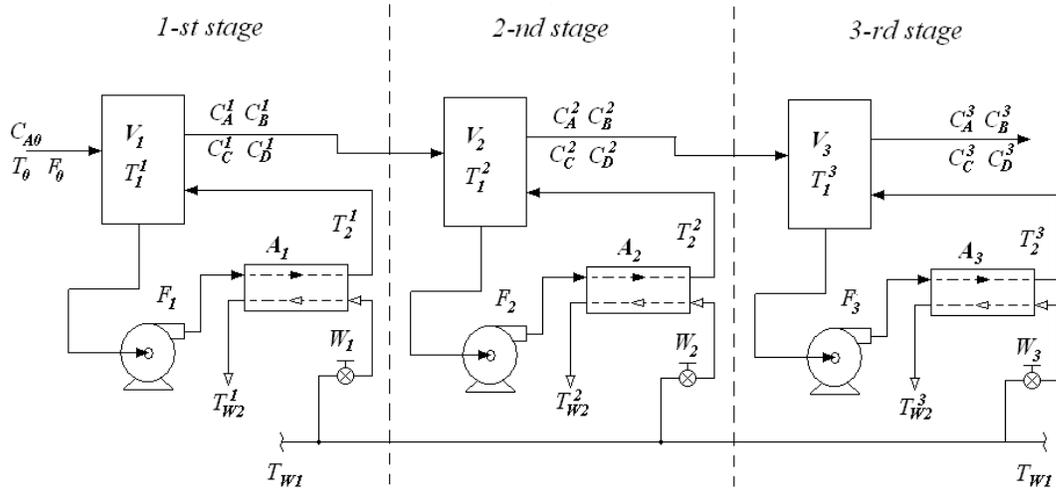
Figure 1: Three-stage flowsheet
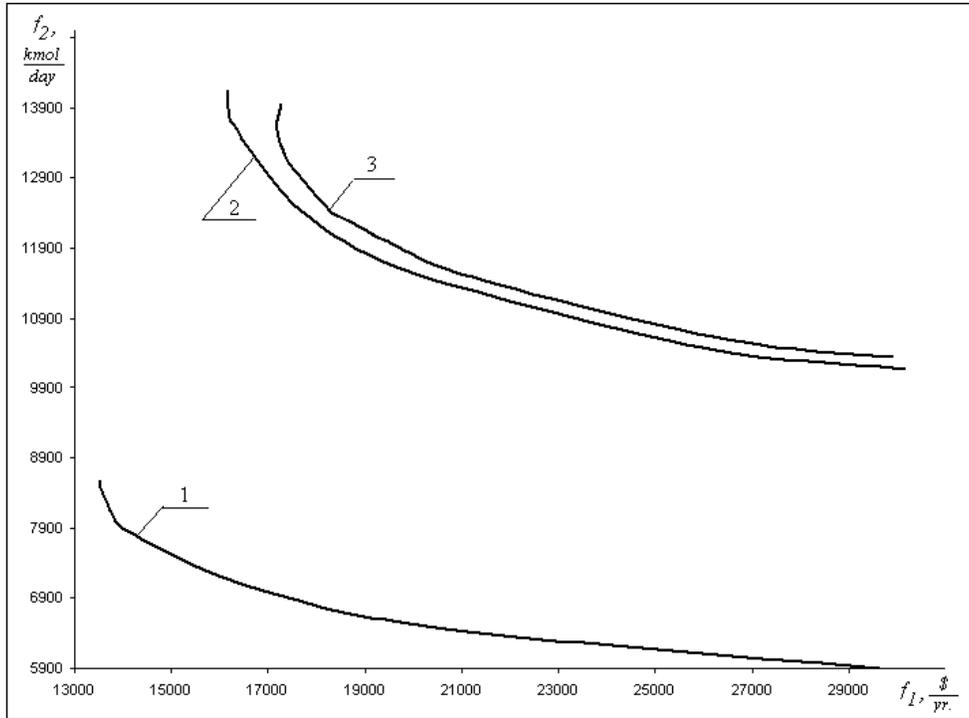
Figure 2: Results for Example 1

Nominal case (all 3 methods) = curve # 1, TSOP 1 (all 3 methods) = curve # 2, TSOP 2 (all 3 methods) = curve # 3
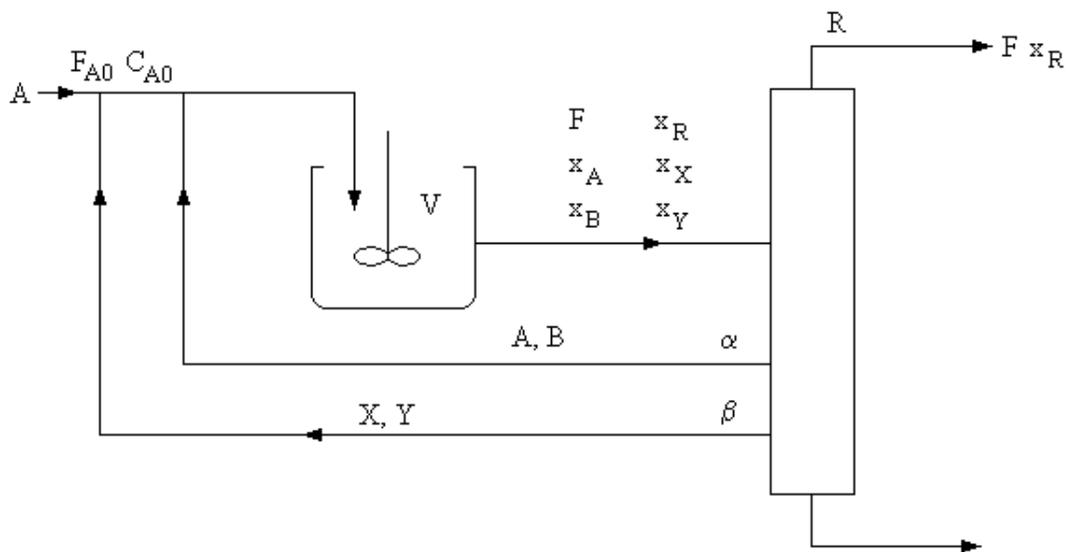
Figure 3: Reactor-separator system
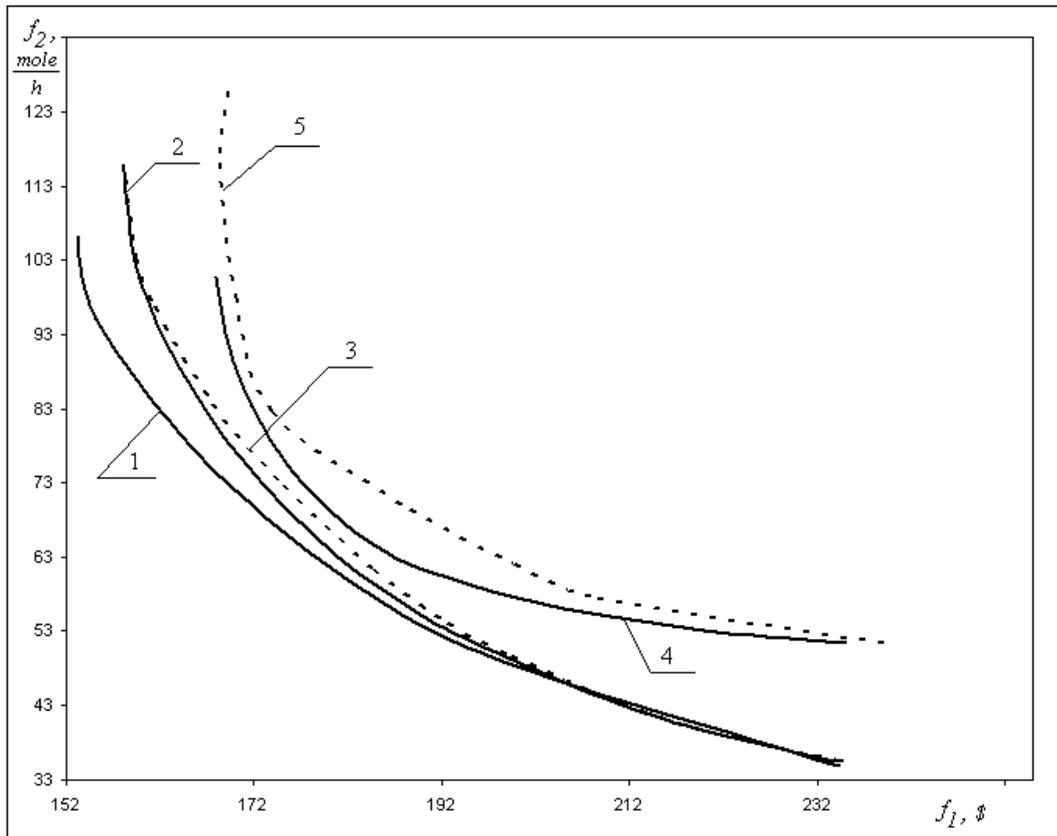
Figure 4: Results for Example 2

Nominal case (all 3 methods) = curve # 1, TSOP1 (AC & ε-constraint methods) = curve # 2, TSOP1 (WCS method) = curve # 3, TSOP2 (AC & ε-constraint methods) = curve # 4, TSOP2 (WCS method) = curve # 5
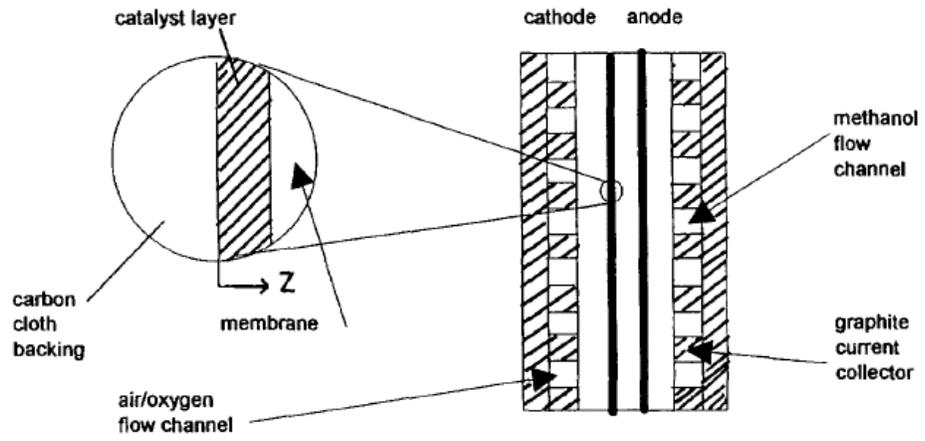
Figure 5: Direct Methanol Fuel Cell (DMFC)
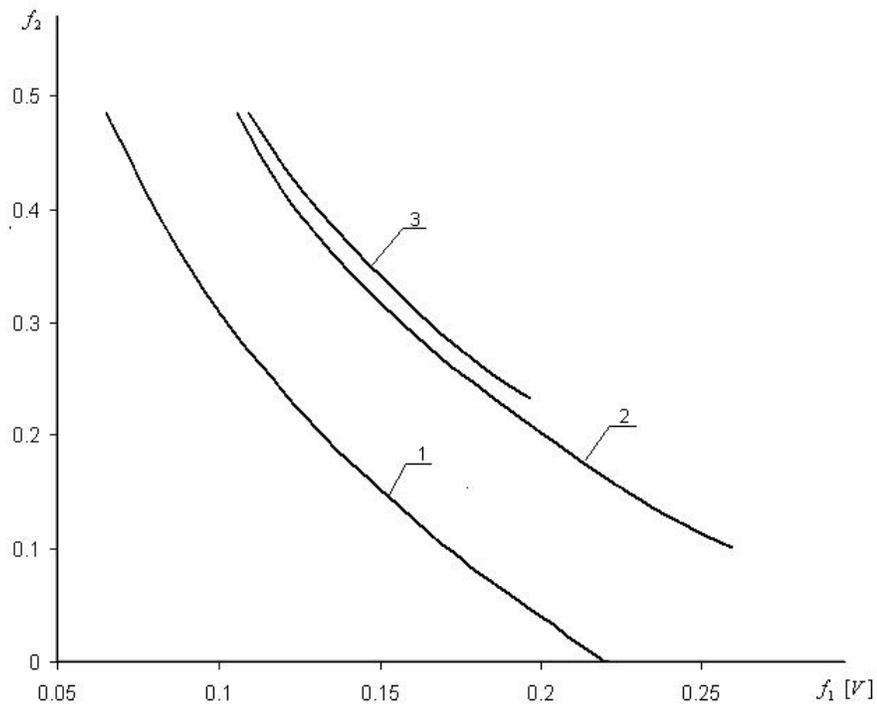
Figure 6: Pareto curve and DM curves for Example 3-Case 1.

WCS was not done. Nominal case (both methods) = curve # 1, TSOP 1 (both methods) = curve # 2, TSOP 2 (both methods) = curve # 3
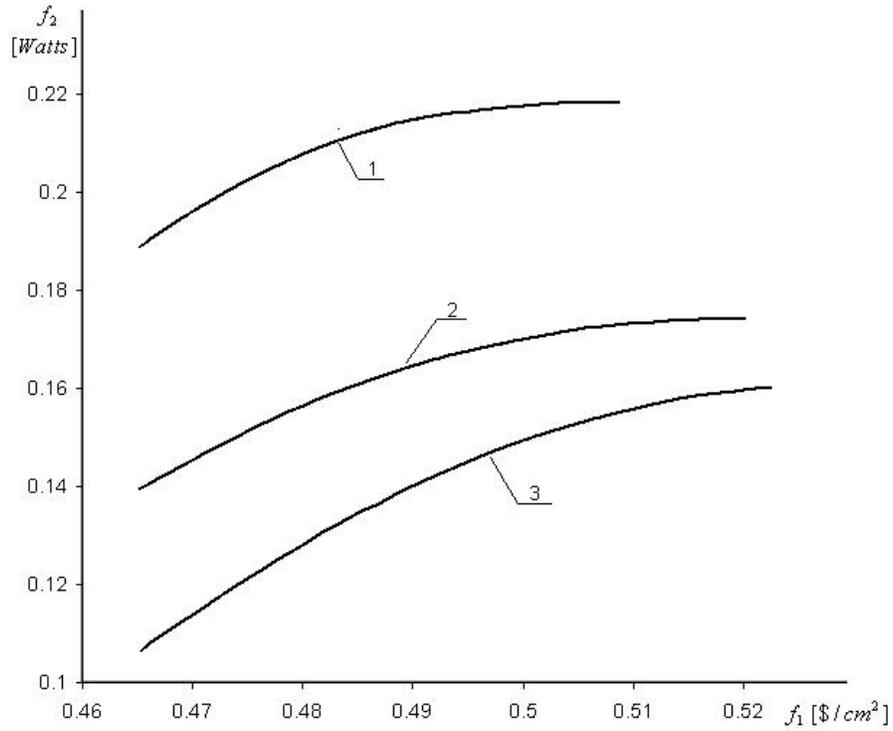
Figure 7: Pareto curve and DM curves for Example 3-Case 2.

WCS was not done. In the MCO $(-f_2)$ instead of (f_2) was employed. Nominal case (both methods) = curve # 1, TSOP 1 (both methods) = curve # 2, TSOP 2 (both methods) = curve # 3