Process Uncertainty: Case of Insufficient Process Data at the Operation Stage

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Flexibility analysis is of prime importance in chemical process systems, since it permits the creation of chemical processes, which can satisfy all design specifications in spite of changes in internal and external factors during the operation stage. The modern foundations of flexibility analysis were developed in the 1980s by Grossman and coworkers. They formulated solution approaches for the main problems of flexibility analysis (feasibility test), flexibility index, and the two-stage optimization problem. All the formulations are based on the supposition that during the operation stage there are enough experimental data to accurately determine uncertain parameter values, but in practice, these assumptions are not likely to be met. This article discusses extensions of the feasibility test and the two-stage optimization problem (TSOP), which take into account the possibility of accurately estimating some of the uncertain parameters while estimating with less accuracy the remaining uncertain parameters. To solve the TSOP, the split and bound approach was developed based on a partitioning of the uncertainty region and estimation of bounds on the performance objective function. Three computational experiments show the importance of taking into account the possibility (or lack thereof) of obtaining values of greater accuracy for uncertain parameters at the operation stage.

Introduction

Design specifications usually have to be met during the design and synthesis of chemical processes (CP). However, the satisfaction of such design specifications is complicated by the presence of uncertainty in the process model parameters. The issue then is how could one guarantee satisfaction of all design specifications at the operation stage? Flexibility analysis addresses this problem. The first articles in flexibility analysis appeared in the 1970s (Takamatsu et al., 1973; Grossmann and Sargent, 1978; Johns et al., 1978). However, foundations of the modern theory of flexibility analysis were laid in the 1980s (Halemane and Grossmann, 1983; Swaney and Grossmann; 1985; Grossmann and Floudas, 1987). Formulations of the feasibility test and the flexibility index (all subproblems of flexibility analysis), and the two-step optimization problem were given in these articles. In addition, some solution approaches were suggested.

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The feasibility test (Halemane and Grossmann, 1983) is defined as

$$\chi_1(d) \le 0 \tag{1}$$

such that the feasibility function $\chi_1(d)$ is given by

$$\chi_1(d) = \max_{\theta \in T} \min_{z \in Z} \max_{j \in J} g_j(d, z, \theta) \qquad J = (1, \ldots, m). \tag{2}$$

Here d is a vector of design variables, z is a vector of control variables, and T is the region for the uncertain parameters such that

$$T = \{\theta : \theta^L \le \theta \le \theta^U\}. \tag{3}$$

The reduced process constraints

$$g_j(d, z, t) \le 0, \qquad j = 1, \ldots, m \tag{4}$$

are obtained from the original mathematical models

$$h(d, x, z, \theta) = 0 \tag{5}$$

$$\bar{g}(d, x, z, \theta) \leq 0, \tag{6}$$

where x is a vector of state variables, z is a vector of control variables, and θ is a vector of uncertain variables. Equation 5 describes the state of the CP (i.e., material and energy balances), while the inequalities in Eq. 6 are design specifications. Here, dim $h =$ dim x and x can be obtained from Eq. 5, either analytically or numerically using fixed values of the variables d, z, θ. Thus

$$x = x(d, z, \theta), \tag{7}$$

leading to the reduced process constraints

$$g(d, z, \theta) \equiv \bar{g}[d, x(d, z, \theta), z, \theta]. \tag{8}$$

The feasibility test (Eq. 1) is a necessary and sufficient condition for flexibility of the CP if and only if the global solution of problem (Eq. 2) is obtained. Floudas et al. (2001) suggest an approach for obtaining the global solution of the problem.

With the preceding definitions, the two-stage optimization problem (designated here as TSOP1) is given as (Halemane and Grossmann, 1983)

$$f_1 = \min_{d \in D} E_T\{f^*(d,\theta)\} = \min_{d \in D} \int_T f^*(d, \theta)\mu(\theta)\, d\theta,$$

$$\chi_1(d) \leq 0, \tag{9}$$

where $E_T\{\ldots\}$ is the mathematical expectation over the region T, $\mu(\theta)$ is the probability density function, and $f^*(d, \theta)$ is obtained from

$$f^*(d,\theta) = \min_{z \in Z} f(d, z, \theta)$$

$$g_j(d, z, \theta) \leq 0, \qquad j = 1, \ldots, m. \tag{10}$$

Solving the preceding problem permits determination of optimal values of design margins guaranteeing satisfaction of all design specifications during the operation stage. The discrete variant of the problem is obtained by discretizing (Halemane and Grossmann, 1983) as follows

$$f_1 = \min_{z^i,\, d \in D} \sum_{i \in I_1} w_i f(d, z^i, \theta^i) \tag{11}$$

$$g_j(d, z^i, \theta^i) \leq 0, \qquad i \in I_1$$

$$\chi_1(d) \leq 0, \tag{12}$$

where w_i is a weight coefficient, θ^i is an approximation point, z^i is a vector of control variables associated with the point θ^i, and I_i is a set of indices associated with the approximation points. The discrete variant can be used even in the case when probability distribution functions are unknown. In this case, the approximation points, θ^i, and weight coefficient, w_i, are given from engineering considerations.

Note that

$$\chi_1(d) = \max_{\theta \in T} \psi^{(1)}(d,\theta), \tag{13}$$

where

$$\psi^{(1)}(d,\theta) = \min_{z} \max_{j \in J} g_j(d, z, \theta). \tag{14}$$

The following methods for solving the main problems of flexibility analysis have been developed.

(1) The feasibility test and flexibility index (evaluation): Methods for these can broadly be classified under (a) explicit and implicit enumeration methods (Halemane and Grossmann, 1985; Swaney and Grossmann, 1985), and (b) active constraints set (ACS) methods (Grossmann and Floudas, 1987).

(2) TSOP1 evaluation: Methods for TSOP1 are (a) those based on the outer approximation algorithm (Reemtsen and Gorner, 1998) using an explicit enumeration method (Halemane and Grossmann, 1983) for evaluating the feasibility function, and (b) the solution of the retrofit design problem using the active constraints set method (Pistikopoulos and Grossmann, 1989).

A number of flexibility analysis methods (Pistikopoulos and Ierapetritiou, 1995; Ostrovsky et al., 1994, 1997; Paules and Floudas, 1992; Bernardo et al., 1999; Raspanti, 2000; Straub and Grossman, 1995; Ahmad et al., 2000; Biegler et al., 1997; were since developed. These approaches took into account uncertainty at the design stage, but not at the operation stage, since they used the implicit assumption that at the operation stage, uncertain parameter values could be determined exactly.

There is a principal difference between the design and control variables; specifically, while the design variables are constant (i.e., fixed) during the operation stage, the control variables can be tuned in order to satisfy process constraints and to improve the performance of the CP. This property of the control variables is used in the formulation of TSOP1.

In fact, according to Eq. 9 we must solve Eq. 10 for each value of the uncertain parameters. Thus, in order to realize the optimal solution of TSOP1, we must optimize the CP at each time point (to solve Eq. 10) using process models with uncertain parameter values corresponding to the state of the CP. Consequently, at each time point we must have accurate values of the uncertain parameters. This is possible only if there is enough process data for precise determination of all uncertain parameter values. This condition is very restrictive and it is often not satisfied in practice (Walsh and Perkins, 1996). Often it is difficult or impossible to have on-line measurements of some of the input process variables and parameters (e.g., concentrations, rate constants, and heat-transfer coefficients) (Bahri et al., 1996). Compounding this problem is the possibility that some of the sensors are not accurate enough.

To address these problems, we need to identify the following three groups of uncertain parameters. The first group of uncertain parameters $\theta^1 \in T^1$ contains parameters whose values can be determined to within any desired accuracy at the operation stage. This means that the appropriate sensors are available to sufficiently determine accurate values of all the uncertain parameters (by direct measurement or by solving parameter estimation problems). The second group $\theta^2 \in T^2$ cannot be made any more precise (due to the lack of appropriate sensors) during the operation stage. The parameters $\theta^3 \in T^3$ of the third group can be made more precise at the operation stage; however, the precision is not sufficient. In this case, we need to take into account sensor measurement errors.

Motivating Example

Suppose we must design a CP that consists of a CSTR and an external countercurrent heat exchanger (Figure 2). The reaction is assumed to be first-order exothermal of the type $A \rightarrow B \rightarrow C$, with B as product. The flow rate through the heat exchanger loop is adjusted to maintain the reactor temperature below some $T_{1\max}$. The flow sheet was considered in Halemane and Grossmann (1983) for the first-order reaction $A \rightarrow B$. The process model of the reactor (material and energy balance) is

$$\begin{aligned} \rho c_p F_0(T_0 - T) + k_1 \exp(-E_A/RT) C_A(-\Delta H_1) V \\ + k_2 \exp(-E_B/RT) C_B(-\Delta H_2) V - Q_{HE} = 0 \\ F(C_{A0} - C_A) - k_1 \exp(-E_A/RT) C_A V = 0 \\ F(C_{B0} - C_B) + k_1 \exp(-E_A/RT) C_A V \\ - k_2 \exp(-E_B/RT) C_B V = 0, \quad (15) \end{aligned}$$

while for the heat exchanger (heat balance and design equations) the process model is

$$\begin{aligned} Q_{HE} = F_1 C_p (T_1 - T_2) = C_{pw}(T_{w2} - T_{w1}) W, \\ Q_{HE} = AU \frac{(T_1 - T_{w2}) - (T_2 - T_{w1})}{\ln\{(T_1 - T_{w2})/(T_2 - T_{w1})\}}. \quad (16) \end{aligned}$$

Here F_0, T_0, C_{A0}, and C_{B0} are the feed flow rate, temperature of the feed, and the concentration of the reactant in the feed, respectively; V, T_1, C_A, and C_B are the reactor volume, the reactor temperature, and the concentrations of the reactants A and B in the product, respectively; E_A and E_B are activity energies; ΔH_1 and ΔH_2 are the heats of reaction; F_1 is the flow rate of the recycle; T_2 is the recycle temperature; C_p and C_{pw} are the heat capacities of the recycle mixture and the cooling water, respectively; T_{w1}, T_{w2}, and W are the inlet and outlet temperatures and the flow rate of the cooling water, respectively; A is the heat-transfer area of the heat exchanger; and U is the overall heat-transfer coefficient.

We select two design variables, V and A, two control variables (T_1 and T_{w2}), and six uncertain parameters $\theta = (F_0, T_0, T_{w1}, k_1, k_2, U)$. In this problem, there are the following constraints

$0.9 \le \text{conv}$	reactor conversion
$311 \le T_1 \le 389$	reactor temperature
$301 \le T_{w2} \le 355$	heat exchanger
$-T_2 + 311 \le 0$	heat exchanger
$-(T_2 - T_{w1}) + 11.1 \le 0$	minimum temperature approach
$T_2 - T_1 \le 0$	thermodynamic constraint for heat exchanger
$-T_{w2} + T_{w1} \le 0$	thermodynamic constraint for heat exchanger (17)

where $\text{conv} = (A_0 - A_1)/A_0$. We will suppose that the performance objective function $f = f(V, A, T_1\ T_{w2})$ takes into account all capital and operating costs.

Many parameters in the process model have experimentally determined values and are only accurate to some degree. The errors in these parameters can be traced to sources

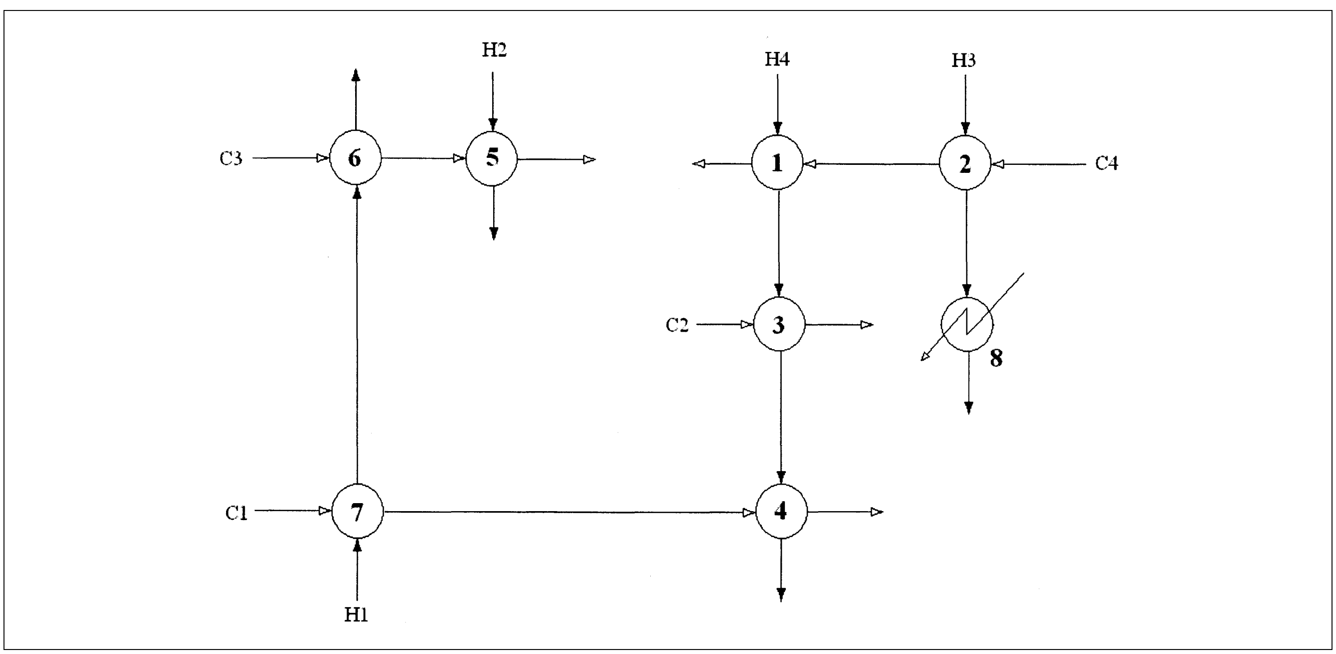

Figure 1. Heat-exchanger network.

such as model structure, parameter estimation, or inherent changes in the process over time. Therefore, the parameters are uncertain at the design stage. We consider the uncertain parameters (F_0, T_0, T_{w1}, k_1, k_2, U). In order to obtain an optimal design, the conventional approach is to solve Eq. 10 with nominal values of all the uncertain parameters. This results in "optimal" values of the design variables V and A, which are then used to size the reactor and heat exchanger. However, during the operation stage, the values of the inlet flow F_0, its temperature T_0, and the temperature of the cooling water T_{w1} can change. In addition, the actual values of the rate constant and heat-transfer coefficient can differ from the nominal values. Consequently, we cannot ensure that all the constraints in Eq. 17 will be met. For example, a violation of the reactor temperature constraints can lead to an unsafe operation of the CP.

Therefore, it is very important to find an optimal design d^*, which guarantees satisfaction of all the process constraints for all probable values of the uncertain parameters (that is, from a given uncertainty region). In theory, such a solution is afforded by solving TSOP1. However, TSOP1 assumes that at each time point accurate values of all the uncertain parameters are known. Very often, this assumption is not valid. We are not aware of sensors that do on-line measurement of rate constants and heat-transfer coefficients. Even if such sensors are on the market, they are not available on most process systems. Therefore, during the operation stage it is safe to assume that one cannot make the parameters k_1, k_2, and U any more accurate than they already are. In addition, if some sensors for measurement of flow rates and temperatures are absent, one cannot obtain accurate values of some of the parameters F_0,T_0,T_{w1} at the operation stage. Therefore, only some of the uncertain parameters can be corrected. In summary, the optimal design d^* found by solving TSOP1 cannot guarantee flexibility of the chemical process.

For obtaining a flexible chemical process, we can solve a one-step optimization problem (OSOP) (Bahri et al., 1996). The formulation of the OSOP supposes that none of the uncertain parameter can be corrected during the operation stage. This means that tuning using control variables is impossible. Of course, the use of the OSOP for the case when we can correct only some of the uncertain parameters permits determination of a feasible design, but it will be more conservative since the OSOP does not take into account the possibility of tuning using the control variables. Therefore, there is a need to formulate the two-stage optimization problem for the case when at the operation stage one can only correct some of the uncertain parameters.

New Feasibility Test and TSOP Formulation

We first consider the feasibility test and two-step optimization problem when there are only two groups of uncertain parameters and θ^1 and θ^2 [such that $\theta=(\theta^1, \theta^2)$] in the process models; denote this problem as TSOP2. In what follows, we will discuss the development of TSOP2.

For simplicity, we will assume that the parameters in the two groups are independent. Therefore, the joint probability density function is $\mu(\theta)=\mu_1(\theta^1)\mu_2(\theta^2)$. The new feasibility test and the optimization problem under uncertainty will be based on the following supposition. At each time instant during the operation stage, one carries out CP optimization using process models in which at least one uncertain parameter is made more precise using available process information. We refer to the CP optimization problem at the current time instant as an internal optimization problem.

The new feasibility test must guarantee the satisfaction of all process constraints for all values of uncertain parameters. Let us consider some time instant during the operation stage. According to our supposition, the accurate values of the components of θ^1 can be determined at this time instant, while the values of the components of θ^2 cannot be determined. Subsequently the feasibility condition for fixed θ^1 takes the form

$$\exists z \forall \theta^2 \in T^2 \forall j \in J\left[g_j(d, z, \theta) \leq 0\right]. \tag{18}$$

It is clear that a CP will be flexible if the condition is met for all possible values of θ^1. Consequently, the following condition must be met

$$\forall \theta^1 \in T^1 \exists z \forall \theta^2 \in T^2 \forall j \in J\left[g_j(d, z, \theta) \leq 0\right]. \tag{19}$$

Using Eqs. A1 and A2, one can transform the logical relation to the following analytical relation

$$\chi_2(d) \leq 0, \tag{20}$$

where

$$\chi_2(d) \equiv \max_{\theta^1 \in T^1} \min_{z} \max_{\theta^2 \in T^2} \max_{j \in J} g_j(d, z, \theta^1, \theta^2). \tag{21}$$

Introduce the feasibility function $\chi_2^i(d)$ on T_i^1 (a subregion of T^1) as

$$\chi_2^i(d) \equiv \max_{\theta^1 \in T_i^1} \min_{z} \max_{\theta^2 \in T^2} \max_{j \in J} g_j(d, z, \theta^1, \theta^2). \tag{22}$$

This is the *feasibility test* for the case of *incomplete* information about uncertain parameters at the operation stage. Using (A4) one can show that the following inequality holds

$$\chi_2(d) \geq \chi_1(d). \tag{23}$$

In addition, the less information about uncertain parameters at the operation stage, the harder the requirements on the design variables.

Now let us consider a new formulation of the TSOP. First, we will formulate the internal optimization problem. Recall that for some fixed time instant the value of θ^1 is known, while θ^2 is not. Therefore, for fixed z and θ^1 the following logical condition must be met

$$\theta^2 \in T^2 \forall j \in J\left[g_j(d, z, \theta) \leq 0\right]. \tag{24}$$

The equivalent analytical condition is

$$\max_{\theta^2 \in T^2} g_j(d, z, \theta^1, \theta^2) \leq 0, \qquad j=1, \ldots, m. \tag{25}$$

A suitable objective function is the mathematical expectation of $f(d,z,\theta)$ with respect to θ^2. Subsequently, the internal optimization problem will have the form

$$f_2^*(d,\theta^1) = \min_z E_{\theta^2}\{f(d, z, \theta^1, \theta^2)$$

$$\max_{\theta^2 \in T^2} g_j(d, z, \theta^1, \theta^2) \le 0, \qquad (j=1, \ldots, m). \quad (26)$$

The condition in Eq. 20 guarantees the existence of a solution to the problem for all values of $\theta^1 \in T^1$. The mathematical expectation of $f_2^*(d, \theta^1)$ characterizes the future performance of the CP. Therefore, it is suitable as the performance objective function for the two-step optimization problem. Since Eq. 20 guarantees the existence of a solution for Eq. 26 for all $\theta^1 \in T^1$, the feasibility test (Eq. 20) must be included as a constraint in the two-step optimization problem under uncertainty. Therefore, the TSOP (designated here as TSOP2) is given by

$$f_2 = \min_d E_{\theta^1}\{f^*(d,\theta^1)\} \quad (27)$$

$$\chi_2(d) \le 0. \quad (28)$$

We rewrite Eq. 27 using the expressions for mathematical expectation as

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

$$\chi_2(d) \le 0. \quad (29)$$

Note that the optimal value of z (the control variable) in Eq. 26 for a fixed value of the parameter θ^1 does not depend on the optimal values of the control variable corresponding to other values of the parameter. Therefore, we can change the order of operations in the integration and minimization in Eq. 29. Then Eq. 27 takes the form

$$f_2 = \min_{d, z(\theta^1)} \int_{T^1}\int_{T^2} f\left[d, z(\theta^1), \theta^1, \theta^2\right] \mu(\theta^1)\mu(\theta^2)\, d\theta^1\, d\theta^2$$

$$\max_{\theta^2 \in T^2} g_j\left(d, z(\theta^1), \theta^1, \theta^2\right) \le 0 \qquad j=1, \ldots, m$$

$$\chi_2(d) \le 0. \quad (30)$$

Since the search variable z in Eq. 30 depends on θ^1, z is a multivariate function $z(\theta^1)$.

Using Gaussian quadrature (Carnahan, 1969), the discrete variant of the optimization problem (designated here as TSOP2) is given as

$$f_2 = \min_{d,z^1} \sum_{i \in I_1} w_i \sum_{j \in Q_1} \nu_j f(d, z^i, \theta^{1i}, \theta^{2j}) \quad (31)$$

$$\max_{\theta^2 \in T^2} g_j(d, z^i, \theta^{1i}, \theta^2) \le 0, \qquad j=1, \ldots, m \qquad i \in I_1 \quad (32)$$

$$\chi_2(d) \le 0, \quad (33)$$

where w_i and ν_j are weight coefficients, satisfying the conditions

$$\sum_{i \in I_1} w_i = 1, \qquad \sum_{j \in Q_1} \nu_j = 1. \quad (34)$$

If the probability density function is not known, the weight coefficients and the sets of approximation points $S_1 = \{\theta^{1i}: i \in I_1\}$ and $S_2 = \{\theta^{2j}: j \in Q_1\}$ need to be specified *a priori*.

Let us compare TSOP1 and TSOP2. If we employ the same approximation points in the discrete variants of the problems, then the same expressions for the objective functions will be obtained. The following inequality holds

$$\max_{\theta^2 \in T^2} g_j(d, z^i, \theta^{1i}, \theta^2) \ge g_j(d, z^i, \theta^{1i}, \theta^2) \forall \theta^2 \in T^2.$$

Therefore, from this inequality and Eq. 23 the feasible region of TSOP2 is smaller. Thus, $f_2 \ge f_1$. In addition, the less the information about uncertain parameters at the operation stage, the more conservative the CP design.

Now consider the case when all three groups of uncertain parameters are present (that is, θ^3 is also present). We will show that this case can be reduced to the previous case. Indeed, let $\theta^{3,1}$ be the value of θ^3 determined at the operation stage. Then the exact value of θ^3 can be represented as

$$\theta^3 = \theta^{3,1} + \theta^{3,2},$$

where $\theta^{3,2}$ is measurement error. The latter can take any value from the region T^{3*}, determined by the accuracy of the sensors. Thus, at the operation stage, we can determine values of $\theta^{3,1}$, while $\theta^{3,2}$ can take any values in T^{3*}. Consequently, $\theta^{3,1}$ and $\theta^{3,2}$ can be considered as parameters of the first and second groups, respectively; the problem with three groups of uncertain parameters is reduced to one with only the first two groups of uncertain parameters, in which the first group contains the parameters θ^1 and $\theta^{3,1}$, and the second group contains the parameters θ^2 and $\theta^{3,2}$. The uncertainty region is determined by

$$\theta^1 \in T^1, \qquad \theta^{3,1} \in T^3, \qquad \theta^2 \in T^2, \qquad \theta^{3,2} \in T^{3*}, \qquad \theta^{3,1} + \theta^{3,2} \in T^3.$$

Split-and-bound method for solving TSOP2

The split-and-bound (SB) method for solving TSOP2 uses a two-level iterative procedure, which is based on a partition of the uncertainty region, T^1, into subregions, $T_i^{1,(k)}$; thus, $T^1 = T_1^{1,(k)} \cup T_2^{1,(k)} \cup \cdots T_{N_k}^{1,(k)}$, where k is an index of iteration. Thus, some collection T^k of N_k subregions $T_i^{1,(k)}$ corresponds to each iteration of the method. The lower level is used for estimating upper and lower bounds of the optimal value, f_2, of the objective function corresponding to the given collection, T^k. The upper level serves to partition (at each iteration) some subregions from T^k using information obtained from the lower level. The procedure stops when the difference between upper and lower bounds is less than a given tolerance ϵ.

In Appendices C and D, we discuss how to calculate upper and lower bounds. Properties 2 and 3 of the upper-bound problem (Appendix D) form the basis of the SB method. At the kth iteration, suppose we have a collection T^k of subregions. Then according to the Property 2, splitting some subregions of T^k improves the upper bound corresponding to T^k. In addition, according to Property 3, in the limit as the sizes of all subregions tend to zero, the solution of the upper-bound problem tends to the solution of TSOP2. The rationale for the name split and bound is as follows: at each iteration it is necessary to split some subregions and estimate the upper bound for a new collection of subregions. In addition to the upper- and lower-bound algorithms, we need a *partitioning* strategy, the choice of which strongly affects the computational complexity of TSOP2. We showed previously that a partition of T^1 improves the upper bound $f_2^{U,(k)}$ (see Eq. D7). The question is how must we partition T? A direct way is to partition all the subregions such that each of them is small enough. In this case, we obtain a solution according to Property 3 of the upper-bound problem (see Eq. D8). This strategy for solving the TSOP2 is not efficient, since we will have to solve optimization problems of very large dimensionality. We consider here a more efficient way of partitioning that uses the following heuristic at the kth iteration: only those $T_l^{(k)}$ $(l=1,\ldots,N_k)$ are partitioned for which the constraints (Eqs. D2) in the upper bound problem (Eqs. D1) are active. Justification of the partitioning strategy is discussed in Appendix E.

Define $L^{(k)}$ as the set of subregions $T_i^{(k)}$ such that

$$L^{(k)} = \{T_i^{(k)}: r(T_i^{(k)}) > \delta\} \tag{35}$$

for small δ, where $r(T_i^{(k)})$ is a measure of the size of $T_i^{(k)}$ .We propose the following algorithm for solving TSOP2.

Algorithm 1

Step 1. Set $k=1$. Choose an initial partition of T^1 into subregions $T_i^{(1)}$, $(i=1, \ldots, N^{(1)})$, and fix the set of approximation points, initial values $d^{(0)}$, $z^{i,(0)}$, $z^{l,(0)}$ $(l=1, \ldots, N^{(1)})$ and δ.

Step 2. Calculate an upper bound by solving (Eq. D1) using Algorithm D1 from Appendix D. Let $d^{(k)}$, $z^{i,(k)}(i \in I_1)$, $z^{l,(k)}(l=1, \ldots, N^{(k)})$ be the solution of the problem.

Step 3. Determine the set $Q^{(k)}$ of indices of subregions with active constraints in Eqs. D2

$$\chi_2^{U,i}(d^{(k)}) = 0, \qquad i \in Q^{(k)}. \tag{36}$$

Step 4. If $Q^{(k)}$ is empty, STOP (solution of TSOP2 (Eq. C1) is found).

Step 5. Calculate a lower bound by solving Eq. C11, using $S_2^{(k)} = S_{A.P}^{(k)}$ (from Step 9 of Algorithm D1).

Step 6. *If*

$$f_2^{U,(k)} - f_2^{L,(k)} \le \epsilon, \tag{37}$$

for a small enough ϵ, then STOP (the solution of TSOP2 is found).

Step 7. If

$$r(T_i^{(k)}) \le \delta, \qquad i=1, \ldots, N_k \tag{38}$$

go to Step 9.

Step 8. Set $R^{(k)} = L^{(k)} \cap Q^{(k)}$. Replace each $T_i^{(k)} \in R^{(k)}$ by its partition $T_{i_1}^{(k+1)}$ and $T_{i_2}^{(k+1)}$ (that is, $T_i^{(k)} = T_{i_1}^{(k+1)} U T_{i_2}^{(k+1)}$). With these replacements $T^{(k)}$ now becomes $T^{(k+1)}$. The strategy for partitioning each T_l^1 into two subregions $T_{l_1}^1$ and $T_{l_2}^2$ is through the addition of the constraints $\theta_s \le a_s$ and $\theta_s \ge a_s$, respectively. Here θ_s is the sth component of θ. Thus $T_{l_1} = \{\theta : \theta \in T_l;\ \ \theta_s \le a_s\}$ and $T_{l_2} = \{\theta : \theta \in T_l\}$, where a_s is chosen as $a_s = 0.5(\bar{\theta}_s + \bar{\bar{\theta}}_s)$. Each θ_i will take a turn at being the branching variable. Go to Step 10.

Step 9. Set $\delta = \delta/2$ and go to Step 7.

Step 10. Set $k = k+1$ and go to Step 2.

The proof for the stopping criterion in Step 4 is similar to the proof for that in TSOP1 (see Ostrovsky et al., 1997). It is clear that any solution found in Algorithm 1 is also a solution to TSOP2 since, according to (Eq. C7) the difference between upper and lower bounds at termination of Algorithm 1 is less than the tolerance ϵ. In addition, in Appendix F we show that Algorithm 1 converges. This statement is correct in a local sense, that is, the SB method will obtain at least a local minimum of TSOP2. To obtain the global minimum, the following conditions are sufficient (see Ostrovsky et al., 2002):

(1) Each $g_j(d, z, \theta)$ is quasi concave in θ.

(2) Each $g_j(d, z, \theta)$ is quasi convex in d and z.

(3) The function $f(d, z, \theta)$ is convex.

Obviously, it is difficult to verify the convexity conditions in practice. Therefore, one can use one of the following approaches. The first is a modification of the SB method in order to guarantee flexibility of the CP in a global sense. This is similar to the modification for TSOP1 developed in Ostrovsky et al. (2002). The second approach is as follows. Suppose we obtain a design d^* by solving TSOP2. We can verify the flexibility of the CP by computing $\chi_2(d^*)$ using a global optimization method (see, for example, Floudas et al., 2001). If d* is infeasible, then the worst point θ^* must be added to the set of critical points.

Let us compare the SB method and the outer approximation (OA) algorithm (Reemtsen and Gorner, 1998), which is one of the main methods for solving TSOP1 (see Halemane and Grossmann, 1983). The OA algorithm can be extended for solving TSOP2. Indeed, since $\chi_2(d)$ is given by Eq. B1, the TSOP2 has the structure, which permits application of the OA algorithm. At each iteration of the algorithm, we will have to calculate the feasibility function $\chi_2(d)$. Calculation of $\chi_2(d)$ can be reduced to the maximization of $\psi^{(2)}(d)$. Halemane and Grossmann (1983) showed that $\psi^{(1)}(d)$ (see Eq. 12) is nondifferentiable and multiextremal. It is clear that $\psi^{(2)}$ is nondifferentiable and multiextremal as well. This means that the use of a computationally intensive nondifferentiable, global optimization method may be needed. In contrast, the SB method solves relatively simple upper- and lower-bound problems. We note, however, that if the number, T_l^1, of subregions is large, the dimension of the upper- and lower-bound problems can become very large. This can cause problems for standard NLP software. However, since Eqs. C11 and D3 have special sparse structures, one can exploit this knowledge in a special-purpose NLP software.

Computational Experiments

We considered three examples. The uncertainty region in all three cases is given as

$$T(\gamma) = \{\theta_i : \theta_i^N(1-\gamma\delta\theta_i) \le \theta_i \le \theta_i^N(1+\gamma\delta\theta_i)\}, \tag{39}$$

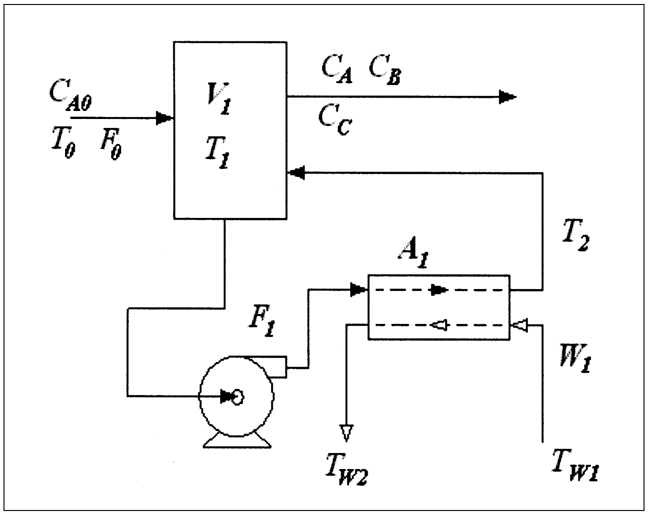

Figure 2. CSTR and external heat exchanger.

where θ_i^N is a nominal value of parameter θ_i, $\delta\theta_i$ is the maximal deviation from the nominal values, and γ is a scalar coefficient. For solving all NLP problems in Algorithms 1 and D1 we employed FSQP (Craig, 1997). All the examples were solved on a 2-GHz Pentium 4 PC.

Example 1: heat-exchanger network

Here we consider the heat-exchanger network (HEN) (Figure 1) consisting of seven heat exchangers, one cooler, four hot streams ($H_i, i=1, \ldots, 4$), and four cold streams (C_i, $i=1, \ldots, 4$). Here design variables are heat-exchanger areas A_i; control variable F_w is a cooler cold-water flow rate. The cost function f (\$/yr) is

$$f = 145.6 \sum_{i=1}^{8} A_i^{0.6} + 1530 F_w. \tag{40}$$

Specific data for the HEN are in Table 1. Uncertain parameters are heat-transfer coefficients, U_i; input temperatures, T_{Hi}^{in} ($i=1, \ldots, 4$) and T_{Cj}^{in} ($j=1, \ldots, 4$) of the hot and cold streams, respectively. Let $T^{\text{in}} = (T_{Hi}^{\text{in}}, T_{Cj}^{\text{in}}, i,j=1, \ldots, 4)$. For design specifications, bounds on the outlet temperatures of the hot (T_{Hi}^{out}) and cold streams (T_{Cj}^{out}) are enforced as

$$T_{Hi}^{\text{out}} - \overline{T}_{Hi}^{\text{out}} \le 0, \qquad i=1, \ldots, 4 \tag{41}$$

$$-T_{Cj}^{\text{out}} + \overline{T}_{Cj}^{\text{out}} \le 0, \qquad j=1, \ldots, 4, \tag{42}$$

Table 1. Specific Data for Example 1

Heat capacity of water C_{PW}	4.19 kJ/kg·K
Max. water output temp. T_W	355.37 K
Cooling water temp. T_W	310.93 K
Min. allowable approach ΔT:	
Heat exchanger: ΔT_{He}	11.1 K
Water cooler: ΔT_C	11.1 K
Overall heat transfer coeff.:	
Heat exchanger: U_{He}	0.203 kcal/m^2·s K
Water cooler: U_C	0.203 kcal/m^2·s K

Table 2. Stream Information for Example 1

Stream	FCp [=] kcal/(s K)	Input Temp. [=] K	$\overline{T}_{Cj}^{\text{out}}$[=] K	$\overline{T}_{Hi}^{\text{out}}$[=] K
C_1	1.818	333	433	—
C_2	1.454	389	495	—
C_3	2.016	311	494	—
C_4	3.312	366	478	—
H_1	2.106	433	—	366
H_2	2.52	522	—	411
H_3	3.528	500	—	339
H_4	3.006	544	—	422

where $\overline{T}_{Hi}^{\text{out}}$ and $\overline{T}_{Cj}^{\text{out}}$ are given in Table 2. In addition, bounds on the temperature approach driving forces are enforced. Thus

$$T_H^{\text{in},(k)} - T_C^{\text{out},(k)} \ge \delta, \qquad k=1, \ldots, 8, \tag{43}$$

where $T_H^{\text{in},(k)}$, $T_C^{\text{out},(k)}$ are inlet and outlet temperatures of the hot and cold streams for the kth heat exchanger; and δ is the minimum approach temperature difference. The maximum water output temperature does not exceed 82.2 K. Here we suppose that $\gamma=1$. The design problem then consists of selecting the optimal heat-exchanger areas, A_i, so that for heat-transfer coefficients within $\pm 20\%$ of the nominal values, and inlet stream temperatures within $\pm 5\%$ of the nominal values, all the design specifications are satisfied by a suitable choice of the cooling-water flow rate. The process model of a heat exchanger is given in Eq. 16, which can be transformed as

$$T_H^{\text{out}} = T_H^{\text{in}} - \gamma\left(T_C^{\text{out}} - T_C^{\text{in}}\right),$$

$$T_C^{\text{out}} = \frac{T_H^{\text{in}}(\exp\alpha - 1) + T_C^{\text{in}}(\gamma - 1)\exp\alpha}{\gamma\exp\alpha - 1},$$

where $\alpha = AU(\gamma-1)/F_C c_{pC}$, $\gamma = F_C c_{pC}/F_H c_{pH}$, c_{pH}, and c_{pC} are heat capacities of hot and cold streams, respectively. The process model permits calculation of the outlet temperatures of the streams if we know the inlet temperatures. It should be noted that one cannot obtain explicit expressions for the reduced constraints $g_j(d,z,\theta)$ in Eq. 3. However, for given values of T_{Hi}^{in}, T_{Cj}^{in} (i, $j=1, \ldots, 4$), F_i, A_i, U_i ($i=1, \ldots, 8$), and F_w, the heat-exchanger network can be simulated to yield the temperatures T_{Hi}^{out}, T_{Cj}^{out} (i, $j=1, \ldots, 4$). All the constraints (Eqs. 41–43) depend indirectly on A_i, U_i ($i=1, \ldots, 8$) F_w, and $T_{Hi}^{\text{in}} T_{Cj}^{\text{in}}$ (i, $j=1, \ldots, 4$), and they can be represented in the form

$$g_j\left(A_i, F_w, U_i, T_{Hi}^{\text{in}}, T_{Cj}^{\text{in}}\right) \le 0, \qquad j=1, \ldots, 16, \tag{44}$$

where constraints with indices $i=1, \ldots, 4$ correspond to Eq. 41, constraints with indices $i=5, \ldots, 8$ correspond to Eq. 42, and constraints with indices $i=9, \ldots, 16$ correspond to Eq. 43.

We consider three cases. In the first case, we suppose that at the operation stage we can determine exact values of all the uncertain parameters. We need to solve TSOP1 in order to obtain the optimal HEN design. In the second case, we suppose that during the operation stage we cannot determine any of the uncertain parameters any more precisely. In this case, we need to solve the one-step optimization problem (OSOP) (Bahri et al., 1996). In the third case, we assume that during the operation stage (a) we can find the exact values for the inlet temperatures of the streams, and (b) we cannot determine the heat-transfer coefficients any more precisely. Thus $\theta^1 = T^{\text{in}} = (T_{Hi}^{\text{in}}, T_{Cj}^{\text{in}}, i, j = 1, \ldots, 4)$ and $\theta^2 = \{U_i, i = 1, \ldots, 8\}$. The uncertainty regions T^1 and T^2 for the vectors θ^1 and θ^2 are of the form $T^1 = \{T_j^{\text{in}} : 0.95T_j^{\text{in},N} \le T_j^{\text{in}} \le 1.05T_j^{\text{in},N}\}$ and $T^2 = \{U_i : 0.8U_i^N \le U_i \le 1.2U_i^N\}$, where $T_j^{\text{in},N}$ and U_i^N are the nominal values of input temperatures and heat-transfer coefficients, respectively.

Here we need to solve TSOP2 in order to obtain an optimal HEN design. We employ three approximation points $\theta^{1,1} = N,N,N,N$; $\theta^{1,2} = L,L,L,L$; $\theta^{1,3} = U,U,U,U$ for the vector θ^1, where N, U, and L denote nominal value, upper, and lower bounds, respectively. The following weight coefficients were used for the first group, $w_1 = 0.8$; $w_2 = w_3 = 0.1$. Now the objective function (Eq. 31) does not depend directly on the uncertain parameters. Therefore, using Eq. 34, the objective function in TSOP2 can be represented as

$$145.6 \sum_{i=1}^{8} A_i^{0.6} + 1530 \sum_{i=1}^{3} w_i F_w^i,$$

where F_w^i is the cold-water flow rate, corresponding to the ith approximation point. In this case, TSOP2 becomes

$$\min_{A_i, F_w^i, F_w^l} \left(145.6 \sum_{i=1}^{8} A_i^{0.6} + 1530 \sum_{i=1}^{3} w_i F_w^i \right),$$

$$\max_{U \in T^2} g_j\big(A_i, F_w^i, T^{in,i}, U\big) \le 0, \qquad j = 1, \ldots, 16; \qquad i = 1,2,3$$

$$\max_{T^{in} \in T^1} \min_{F_w} \max_{U \in T^2} \max_{j \in J} g_j\big(A_i, F_w, T^{\text{in}}, U\big) \le 0. \tag{45}$$

Consider realization of the SB method (Algorithm 1) in the preceding case. At each iteration of the algorithm, calculation of the lower and upper bounds are the main operations. It is necessary to solve Eqs. D3 and C11. Consider in detail Algorithm D1 intended for solving Eq. D3. Suppose the uncertainty region T^1 is partitioned into N_k subregions T_l^1 ($l = 1, \ldots, N_k$), then the upper-bound problem (Eq. D3) becomes

$$\min_{A_w^i, F_w^l, F_w^l} \left(145.6 \sum_{i=1}^{8} A_i^{0.6} + 1530 \sum_{i=1}^{3} w_i F_w^i \right) \tag{46}$$

$$\max_{U \in T^2} g_j\big(A_i, F_w^i, T^{\text{in},i}, U\big) \le 0, \qquad j = 1, \ldots, 16; \qquad i = 1,2,3 \tag{47}$$

$$\max_{T^{in} \in T_l^1, U \in T^2} g_j\big(A_i, F_w^i, T^{\text{in},i}, U\big) \le 0, \qquad l = 1, \ldots, N_k; \qquad j = 1, \ldots, 16. \tag{48}$$

In Eq. 46 there are $3n_z + N_k n_z + n_d$ search variables z^i ($i = 1, 2, 3$), $z^l(l = 1, \ldots, N_k)$ and d where n_z and n_d are the dimensions of z and d, respectively. Algorithm A1 for solving the upper-bound problem (Eq. 46) is

Step 1. Initialize the search variables and the sets S_2^i and S_2^l (critical points for Eqs. 47 and 48).

Step 2. Solve Eq. D9 given explicitly as

$$\min_{A_i, F_w^i, F_w^l} \left(145.6 \sum_{i=1}^{8} A_i^{0.6} + 1530 \sum_{i=1}^{3} w_i F_w^i \right) \tag{49}$$

$$g_j\big(A_i, F_w^i, T^{in,i}, U^{i,q}\big) \le 0; \qquad i = 1,2,3; \qquad U^{i,q} \in S_2^i; \qquad j = 1, \ldots, 16 \tag{50}$$

$$g_j\big(A_i, F_w^l, T^{in,l,s}, U^{l,s}\big) \le 0; \qquad j = 1, \ldots, 16; \qquad \big(T^{in,l,s}, U^{l,s}\big) \in S_2^l, \qquad l = 1, \ldots, N_k. \tag{51}$$

Remember that in order to calculate the lefthand side of Eqs. 50 and 51 we must carry out calculations of HEN for the given values of A_i, F_w^i, T^{in}, and U^q.

Step 3. For each $T^{\text{in},i}$, solve Eq. D12, which in this case takes the form

$$\max_{U \in T^2} g_j\big(\overline{A_i}, \bar{F}_w^l, T^{\text{in},i}, U\big), \tag{52}$$

such that $[\overline{A_i}, \bar{F}_w^i]$ is the solution of Eq. 49. This is optimization of HEN where the objective function is $g_j(\overline{A_i}, \bar{F}_w^l, T^{\text{in},i}, U)$. Note that Eq. 52 is solved $3 \times 16 = 48$ times.

Step 4. For each subregion $T_l^1 (l = 1, \ldots, N_k)$, solve

$$\max_{T^{\text{in}} \in T_l^1, U \in T^2} g_j\big(A_i, F_w^l, T^{\text{in}}, U\big). \tag{53}$$

This requires solving Eq. 51 $16N_k$ times. If the condition in Step 5 is not met, then in Steps 6 and 7 new critical points are added to the sets S_2^i and S_2^l. In Step 9 the set of active points of Eq. 46 is formed. The latter serves as the set $S_2^{(k)}$ in the lower-bound problem.

The lower-bound problem (see Appendix C) is

$$\min_{A_i, F_w^i, F_w^r} \left(145.6 \sum_{i=1}^{3} A_i^{0.6} + 1530 \sum_{i=1}^{3} F_w^i \right)$$

$$\max_{U \in T^2} g_j\big(A_i, F_w^i, T^{\text{in},i}, U\big) \le 0, \qquad j = 1, \ldots, 16; \qquad i = 1,2,3$$

$$\max_{U \in T^2} g_j\big(A_i, F_w^r, T^{\text{in},r}, U\big) \le 0, \qquad j = 1, \ldots, 16; \qquad i = 1,2,3; \qquad T^{\text{in},r} \in S_2^{(k)}. \tag{54}$$

The algorithm for solving the lower bound problem is similar to that of the upper bound problem as discussed earlier. The lower- and upper-bound problems are used in the SB algorithm (Algorithm 1) as follows:

Step 1. Give an initial partition of the uncertainty region T^l, and initialize the search variables A_i, F_w^i, and F_w^l.

Step 2. Solve Eq. 46.

Step 3. Determine the set of active constraints in Eq. 46.

Step 4. If the set is empty, then STOP with the solution.

Step 5. Calculate a lower bound by solving Eq. 54.

Step 6. If |upper bound − lower bound| is less than a given tolerance ϵ, then STOP with the solution.

Table 3. Results for Nominal Optimization, TSOP1, and TSOP2 for Example 1

		F	A_1(m^2)	A_2(m^2)	A_3(m^2)	A_4(m^2)	A_5(m^2)	A_6(m^2)	A_7(m^2)	A_c(m^2)
1	Nominal	43,124.13	$1e-3$	81.3	11.5	25.9	37.8	8.71	2.74	29
2	TSOP1	56,619.94	8.2	91.1	34.3	53.7	96.7	11.4	5.26	30.2
3	Design margins,%		—	11.95	197.53	107.47	155.93	31.06	92.06	4.17
4	TSOP2	59,335.09	8.63	103	34	53.8	96.9	11.4	5.26	34
5	Design margins,%		—	27.19	194.64	107.93	156.37	31.13	91.84	17.22
6	OSOP	61,216.76	8.48	99	34.1	53.8	96.8	11.4	5.26	34.9
7	Design margins, %		—	21.721	195.65	107.77	156.21	31.11	91.92	20.47

Step 7. If the size of each subregion is less than a given tolerance δ, go to Step 9.

Step 8. Consider subregions with size greater than δ. Partition these subregions if they have active constraints.

Step 9. Decrease δ and go to Step 2.

In Table 3, we give optimal values of the objective functions and the heat-transfer areas obtained by solving the nominal optimization problem, TSOP1, TSOP2, and OSOP. We also give the optimal values of design margins ΔA_i calculated through $\Delta d_i\% = 100(d_i^{\text{TSOP}} - d_i^{\text{nom}})/d_i^{\text{nom}}$. Here d_i^{TSOP} and d_i^{nom} are the values of the ith design variable obtained by solving TSOP and the nominal optimization problem, respectively.

Let us discuss the results in Table 3. From TSOP1, it is seen that the presence of uncertainty (in the heat-transfer coefficients and the stream inlet temperatures) leads to the need to provide significant design margins (see row 3) in order to guarantee flexibility of the HEN. This requires a significant increase (31%) in the HEN cost from \$43,124/yr up to \$56,629/yr. The inability to correct the heat-transfer coefficients during the operation stage leads to an increase in the heat-exchanger areas of the second heat exchanger and the cooler (see rows 3 and 5). This increases (by 4%) the cost of the network from \$56,619/yr to \$59,335/yr.

Next, let us consider the implications of using the optimal HEN design variables d^{TSOP1} (from TSOP1) in the case when the heat-transfer coefficients cannot be corrected at the operation stage. We first evaluate the modified feasibility function $\chi_2(d)$ to obtain $\chi_2(d^{\text{TSOP1}}) = 7.09$. Since $\chi_2(d^{\text{TSOP1}})$ is greater than zero, the design d^{TSOP1} will be infeasible. This means that if d^{TSOP1} is employed in the design of the HEN, then the latter will not be flexible. On the other hand, if d^{OSOP} (from the one-step optimization problem) is employed, then a flexible HEN will result. However, in this case a more conservative design will result. Actually, the cost of the HEN for $d = d^{\text{OSOP}}$ is equal to \$61,216/yr, which represents a 5% increase over that obtained from TSOP2.

Table 4. Specific Data for Example 2

ρC_p	167.4 kJ/(m$^3\cdot$K)	k_1	314.0 L/h
C_{PW}	4.19 kJ/(kg$\cdot$K)	k_2	40.0 L/h
F_0	45.36 m^3/h	U_1	1635.0 kJ/ (m$^2\cdot$h$\cdot$K)
C_{A0}	32.04 kmol/m^3	ΔH_1	-725.97 kJ/kg$\cdot$mol
C_{b0}	0.0 kmol/m^3	ΔH_2	-2176.03 kJ/kg$\cdot$mol
E_A/R	560.0 K	T_0	333.0 K
E_B/R	500.0 K	T_{w1}	300.0 K

Example 2: continuous stirred-tank reactor and external heat exchanger

The process (Figure 2) is described as the motivating example. Process models of the reactor and heat exchanger are given by Eqs. 15 and 16, while the constraints are given by Eq. 17. Here there are two design variables, V and A, two control variables T_1, T_{w2}, and six uncertain parameters $\theta = (F_0, T_0, T_{w1}, k_1, k_2, U)$. Specific data for the example are in Table 4. The cost of the separation is given by 12.5 $(e^{0.3C_c} - 1)$ (Fogler, 1999). The performance objective is the maximization of income f (\$/yr) as follows

$$f = 100F_0C_B - \big[345.6V^{0.7} + 436.8A^{0.6} + 0.88W + 3.528F_1 + 12.5(e^{0.3C_c} - 1)\big].$$

Nominal values of uncertain parameters are $\theta^N = [45.36, 333, 300, 314, 40, 1{,}635]$ and $\delta\theta_i = [0.08, 0.1, 0.1, 0.1, 0.1, 0.1]$.

We consider two cases. In the first case, we suppose that all uncertain parameters can be determined with enough precision at the operation stage. In the second case, we suppose that there is no sensor for measurement of the input flow rate, F_0. In addition, we noted already that k_1, k_2, and U cannot be measured at the operation stage. In this case, for optimal design we must solve TSOP2 for which $\theta^1 = [T_0, T_{w1}]$ and $\theta^2 = [k_1, k_2, F_0, U]$. We used four approximation points for the vector θ^1: $\theta^{1,1} = N, N$; $\theta^{1,2} = L,L$; $\theta^{1,3} = U,U$; $\theta^{1,4} = L,U$. For each approximation in θ^1, we employed five approximation points for θ^2 ($\theta^{2,1} = N,N,N,N$; $\theta^{2,2} = L, U, U, L$; $\theta^{2,3} = L, L, L, L$; $\theta^{2,4} = U, L, L, U$; $\theta^{2,5} = U, U, U, U$). Thus in the space of parameters θ we employ 20 approximation points. The following weight coefficients were used: first group $w_1 = 0.7$; $w_2 = w_3 = w_4 = 0.1$; second group $\nu_1 = 0.6$; $\upsilon_2 = \upsilon_3 = \upsilon_4 = \upsilon_5 = 0.1$.

In Table 5, we give the results for the nominal optimization, TSOP1 and TSOP2. According to TSOP1, we must use the following design margins to obtain a flexible CP. $\Delta V = 25.71\%$, $\Delta A = 17.61\%$. On the other hand, TSOP2 suggests the following design margins: $\Delta V = 30.69\%$, $\Delta A = 31.79\%$.

Table 5. Results for nominal optimization, TSOP1 and TSOP2 for Example 2

	F (\$/yr)	V (m^3)	A (m^2)	ΔV (%)	ΔA (%)
Nominal	40,231.12	5.485	32.421		
TSOP1	29,065.01	6.895	38.132	25.71	17.61
TSOP2	27,808.68	7.169	42.727	30.69	31.79

Table 6. Results for Nominal Optimization, TSOP1 and TSOP2 for Example 2a

γ	TSOP Version	f [=] \$/yr	V [=] m^3	A [=] m^2	ΔV (%)	ΔA (%)	CPU [=] s
Nominal (i.e. $\gamma = 0$)		9769.25	5.42	7.20			0.005
1.00	TSOP1	10547.54	6.63	8.25	22.22	14.66	0.52
	TSOP2	10554.80	6.63	8.42	22.22	17.02	0.14
1.25	TSOP1	10815.43	6.97	8.72	28.57	21.14	1.56
	TSOP2	10855.25	6.97	9.09	28.57	26.28	0.49
1.50	TSOP1	11127.69	7.33	9.13	35.29	26.89	5.3
	TSOP2	11230.99	7.39	9.74	36.23	35.24	1.67
1.75	TSOP1	11522.28	7.83	9.81	44.40	36.25	14.61
	TSOP2	11670.52	7.91	10.74	45.93	49.23	3.96

Similar to Example 1 we investigated the feasibility of design d_i^{TSOP1} for the case when the parameters k_1, k_2 F_0, and U cannot be corrected at the operation stage. We obtain $\chi_2(d^{\text{TSOP1}}) = 0.0017 > 0$, that is, the value of the feasibility function is a small positive number. Consequently, the design d_i^{TSOP1} is infeasible. It is interesting to note that the OSOP in this case does not have a solution, since the feasibility region of the OSOP is empty.

Next, we consider Example 2 for a reaction of the type $A \rightarrow B$; refer to this case as Example 2a. Here the design, control variables, and the uncertain parameters are the same, except for k_2. Specific data for the example are in Table 4. We consider two cases. In the first case, we suppose that all uncertain parameters can be determined with enough precision at the operation stage. In the second case, we suppose that there is no process data (at the operation stage) to determine with enough precision k_1, k_2, and U. For optimal design, we need to consider TSOP2. Here θ^1 consists of T_0, T_{w1}, F_0, and θ^2 consists of k_1 and U. We used four approximation points for the vector θ^1 : ($\theta^{1,1} = N,N,N$; $\theta^{1,2} = L, L, L$; $\theta^{1,3} = U, U, U$; $\theta^{1,4} = U, U, L$); and for each approximation point of θ^1, we used five approximation points for θ^2: ($\theta^{2,1} = N, N$; $\theta^{2,2} = L, U$; $\theta^{2,3} = L, L$; $\theta^{2,4} = U, L$; $\theta^{2,5} = U, U$). In Table 6, we give the results for the nominal optimization, TSOP1 and TSOP2, for different sizes of the uncertainty region. Note that Halemane and Grossmann (1983) considered the case $\gamma = 1$ (CPU time of 162 s on a DEC-20). We obtained the same results with a CPU time of 0.5 s on a 2-GHz Pentium 4 PC. Note that it is difficult to compare the CPU for different computers that are separated by several years.

Example 3: three-stage flow sheet

Consider the reactor/heat-exchanger network in Figure 3. Each stage has one CSTR of volume V_i and a heat exchanger with heat-exchange area A_i. In each CSTR the reaction is

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$
$$B \xrightarrow{k_3} D.$$

Here $B \rightarrow D$ is endothermic, while $A \rightarrow B$ and $B \rightarrow C$ are exothermic. Moreover, each reaction step is first order. The process models of the reactor and heat exchanger are given as follows.

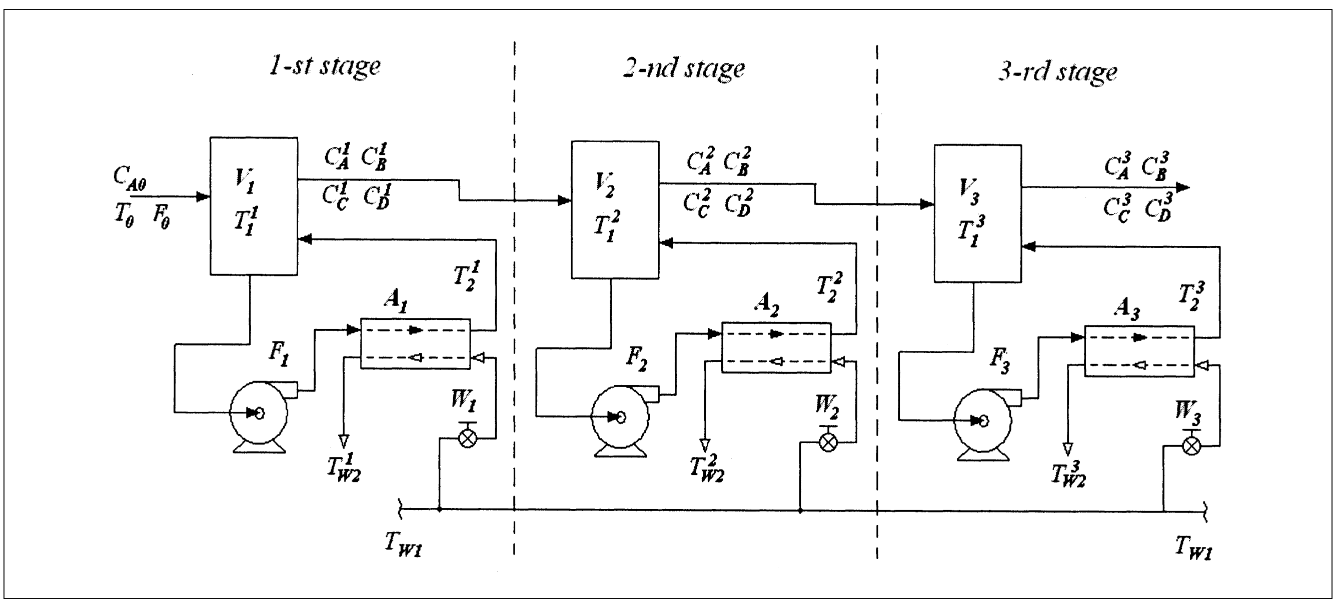

Figure 3. Three-stage flow sheet.

Table 7. Specific Data for Example 3

$\rho_p C_p$	100.0 kJ/(m^3 K)	k_1	98.0 L/h
C_{PW}	4.19 kJ/(kg K)	k_2	25.0 L/h
F_0	90.0 m^3/h	k_3	110.0 L/h
C_{A0}	32.0 kmol/m^3	ΔH_1	−725.0 kJ/kmol
E_A/R	500.0 K	ΔH_2	−781.25 kJ/kmol
E_B^1/R	1200.0 K	ΔH_3	625.0 kJ/kmol
E_B^2/R	1300.0 K	T_0	350.0 K
$U_1 = U_2 = U_3$	1400.0 kJ/ (m^2 h K)	T_{w1}	300.0 K

CSTR. For the ith stage

$$\rho c_p F_0 (T_0^i - T_1^i) + k_1 \exp(-E_A/RT^i) C_A(-\Delta H_1) V_i + k_2 \exp(-E_B/RT) C_B(-\Delta H_2) V_i - Q_{HE}^i = 0$$

$$F(C_{A0}^i - C_A^i) - k_1 \exp(-E_A/RT^i) C_A^i V^i = 0$$

$$F(C_{B0}^i - C_{B_i}^i) + k_1 \exp(-E_A/RT^i) C_A^i V^i - k_2 \exp(-E_B^1/RT) C_B V - k_3 \exp(E_B^1/RT^i) = 0$$

$$F(C_{D0}^i - C_D^i) + k_3 \exp(E_B^2/RT^i) C_B V = 0. \quad (55)$$

The design equation for the heat exchanger is given by (Eq. 16). Neighboring stages are connected by $T_0 = T_0^1$; $C_{j0} = C_{j0}^1$; $C_j^i = C_{j0}^{i+1}$; T_0^{i+1} T_i^1: $j = A, B, C, D$; $i = 1, 2$ such that $C_{B0} = C_{C0} = C_{D0} = 0$. The cooling-water temperature in each heat exchanger is T_{w1}. We employ the same notation as in Example 2. 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 $\theta = (T_0^1, T_{w1}\ F_0, k_1, k_2, k_3, U^1, U^2, U^3)$. Specific data for this example are given in Table 7. Deviations are equal to $\delta\theta_i = [0.03;0.03;0.1;0.1;0.1;0.1;0.1;0.1;0.1]$. The production of B should be at least 18.4 kmol/mg. Thus

$$C_B \geq 18.4. \quad (56)$$

In addition, all the constraints in Eq. 17 (excluding $0.9 \leq$ conv) are also enforced here. Thus

$$-T_2^i + 311 \leq 0 \qquad T_{w2}^i - T_{w1} \leq 0 \qquad 301 \leq T_{w2}^i \leq 355 \qquad i = 1,2,3$$

$$-(T_2^i - T_{w1}) + 11.1 \leq 0 \qquad T_2^i - T_1^i \leq 0 \qquad 311 \leq T_1^i \leq 389. \quad (57)$$

In this study, minimization of cost is required such that all constraints in Eqs. 56 and 57 are met. The capital costs include cost of reactors and heat exchangers, while operating costs include the cost of cold water, recycles, and separation of byproducts C and D after the third stage. As in Example 2, the separation of the byproducts is very difficult. The cost of separation is given by 2.5 ($e^{0.3C_C} - 1$) (Fogler, 1999). The performance objective is finally given by

$$f = 700(V_1^{0.7} + V_2^{0.7} + V_3^{0.7}) + 174.72(A_1^{0.6} + A_2^{0.6} - A_3^{0.6}) \\ 1.76(W_1 + W_2 + W_3) + 7.056(F_1 + F_2 + F_3) \\ + 100(e^{0.5(Cc3 + Cd3)} - 1).$$

We solved TSOP1 and TSOP2. In the latter, $\theta^1 = (T_0, T_{w1})$ and $\theta^2 = (F_0, k_i, U_i, i = 1,2,3)$. For TSOP2 we used five approximation points $[\theta^{1,1}, \theta^{1,2}, \theta^{1,3}, \theta^{1,4}, \theta^{1,5}] = [NN, UU, LL, LU, UL]$. Moreover, for each approximation point of θ^1 we used one approximation point: $\theta^{2.1} = [N, N, N, N, N, N]$. The following weight coefficients were used for the first group $w_1 = 0.6$, $w_2 = w_3 = w_4 = w_5 = 0.1$.

The results are given in Table 8. If during the operation stage, values of all uncertain parameters can be determined accurately enough, then from TSOP1 we need to use the design margins given in row 3 of Table 7 in order to guarantee flexibility of the flow sheet. If during the operation stage the uncertain parameters from θ^2 cannot be corrected, then it is necessary to use design margins from row 5. It is clear that design margins must be increased for V_1, A_1, and A_2. On the other hand, the design margins for V_3 and A_2 must be decreased. Here the total costs increase from \$16,351 to \$16,670 (a 2% increase).

As before, we investigated the feasibility of the design d_i^{TSOP1} for the case when k_1, k_2, k_3, U_1, U_2, U_3 cannot be corrected at the operation stage. For this case, the feasibility function $\chi_2(d^{TSOP1})$ is 0.008, indicating d_i^{TSOP1} is not feasible (since it is positive). It is interesting to note that the corresponding OSOP does not have a solution, since the feasible region is empty.

Discussion of the SB Method

The efficiency of the SB methods was explored using several examples. The number of iterations for the upper-bound problem was usually 2 or 3. The number of iterations (equal to the number of partitions) in the SB method usually ranged from 10 to 15. The following were encountered:

(1) In some cases when using the SB method for solving examples 2 and 3, the search point strayed into the infeasible region (specifically, the constraint $T_2 - T_1 \leq 0$ was violated), after which it remained in the infeasible region and we ob-

Table 8. Results for Nominal Optimization, TSOP1 and TSOP2 for Example 3

		F[=] \$/yr	V_1[=] m^3	V_2[=] m^3	V_3 [=]m^3	A_1 [=] m^2	A_2 [=] m^2	A_3 [=] m^2
1	Nominal	14146.86	1.605	1.687	1.611	7.168	10.596	5.966
2	TSOP1	16351.34	1.923	2.034	2.141	9.367	11.01	6.172
3	Design margins, %		19.81	20.57	32.9	30.68	3.91	3.45
4	TSOP2	16670.5	2.183	2.134	1.938	11.5	11.5	3.473
5	Design margins, %		36.01	26.5	20.3	60.44	8.53	−41.79

tained incorrect results. The behavior is apparently associated with the code FSQP that we used. This is because when we replaced FSQP with Knitro (Waltz and Nocedal, 2002), the problem disappeared.

(2) When the uncertainty region is expanded, the complexity of solving TSOP2 is increased, since the dimensions of Eqs. C11 and D3 become rather large. Apparently, such behavior is explained by the fact that for some critical size of the uncertainty region the TSOP2 does not have a solution (the process is not flexible). In order to solve successfully TSOP of large dimension it is necessary to take into account the structure of TSOP2.

Conclusions

So far, in the open literature, two extreme approaches, namely, two-step optimization problem (TSOP) and one-step optimization problem (OSOP), have been developed for solving the optimization problem under uncertainty. At the operation stage, in TSOP, one assumes that there is enough process data for determining accurate values of the uncertain parameters. This permits tuning the control variables in order to optimize the chemical process (CP) for each measured value of the uncertain parameters. On the other hand, in OSOP, one assumes that accurate values of uncertain parameters cannot be determined during the operation stage. In this case, we cannot tune the control variables during the operation stage. It is reasonable to expect that available process data at the operation stage can permit us to determine with enough accuracy only a subset of the uncertain parameters. If this is the case, then the TSOP cannot guarantee flexibility of the CP, since the optimal regime found by solving the problem cannot be realized. On the other hand, OSOP results in designs that are more conservative, since the control variables cannot be tuned at the operation stage. In connection with this, we developed extensions of the feasibility test and TSOP, which take into account the possibility (a) to determine with enough precision some of the uncertain parameters, and (b) to improve the remaining uncertain parameters, although the required precision cannot be attained.

We developed the split-and-bound method for solving the extended TSOP. Computational experiments show that if it is not possible to correct some of the uncertain parameters during the operation stage, then it is necessary to increase the design margins (with a concurrent increase in costs) beyond what would be done by solving the conventional TSOP.

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Literature Cited

Ahmad, S., N. V. Sahinidis, and E. N. Pistikopoulos, "An Improved Algorithm for Optimization Under Uncertainty," *Comput. Chem. Eng.*, **23**, 1589 (2000).

Bahri P. A., J. A. Bandony, and J. A. Romagnoli, "Effect of Disturbances in Optimizing Control: Steady-State Open-Loop Back Off Problem," *AIChE J.*, **42**, 983 (1996).

Bernardo, F. P., E. N. Pistikopoulos, and P. M. Saraiva, "Integration and Computational Issues in Stochastic Design and Planning Optimization Problems," *Ind. Eng. Chem. Res.*, **38**, 3056 (1999).

Biegler, L. T., I. E. Grossmann, and A. W. Westerberg, *Systematic Methods of Chemical Process Design*, Prentice Hall, Upper Saddle River, NJ (1997).

Carnahan, B., H. A. Luther, and J. O. Wilkes, *Applied Numerical Methods*, Wiley, New York (1969).

Craig, L., J. L. Zhou, and A. L. Tits, *User's Guide for CFSQP Version 2.5*, Institute for Systems Research, University of Maryland, College Park (1997).

Floudas, C. A., Z. H. Gumu, and M. R. Ierapetritou, "Global Optimization in Design Under Uncertainty: Feasibility Test and Feasibility Index Problems," *Ind. Eng. Chem*, **40**, 4267 (2001).

Fogler, H. S., *Elements of Chemical Reaction Engineering*, Prentice Hall, Upper Saddle River, NJ (1999).

Grossmann, I. E., and R. W. H. Sargent, "Optimum Design of Chemical Plants with Uncertain Parameters," *AIChE J.*, **24**, 1021, (1978).

Grossmann, I. E., and C. A. Floudas, "Active Constraints Strategy for Flexibility Analysis in Chemical Processes," *Comput. Chem. Eng.*, **11**, 675 (1987).

Halemane, K. P., and I. E. Grossmann, "Optimal Process Design Under Uncertainty," *AIChE J.*, **29**, 425 (1983).

Johns, W. R., G. Marketos, and D. W. T. Rippin, "The Optimal Design of Chemical Plants to Meet Time-Varying Demands in the Presence of Technical and Commercial Uncertainty," *Trans. Inst. Chem. Eng.*, **56**, 249 (1978).

McKinsey, J. C. C., *Introduction to the Theory of Games*, McGraw-Hill, New York (1952).

Ostrovsky, G. M., Y. M. Volin, E. I. Barit, and M. M. Senyavin, "Flexibility Analysis and Optimization of Chemical Plants," *Comput. Chem. Eng.*, **18**, 755 (1994).

Ostrovsky, G. M., Y. M. Volin, and M. M. Senyavin "An Approach to Solving a Two-Stage Optimization Problem Under Uncertainty," *Comput. Chem. Eng.*, **21**, 311 (1997).

Ostrovsky, G. M., L. E. K. Achenie, A. M. Karalapakkam, and Y. M. Volin, "Flexibility Analysis of Chemical Processes: Selected Global Optimization Subproblems, *Optim. Eng.*, **3**, 31 (2002).

Paules, G. E., and C. A. Floudas, "Stochastic Programming in Process Synthesis: A Two-Stage Model with MINLP Recourse for Multiperiod Heat-Integrated Distillation Sequences," *Comput. Chem. Eng.*, **16**, 189 (1992).

Pistikopoulos, E. N., and I. E. Grossmann, "Optimal Retrofit Design for Improving Process Flexibility in Nonlinear Systems—1. Fixed Degree of Flexibility," *Comput. Chem. Eng.*, **12**, 1003 (1989).

Pistikopoulos, E. N., and M. G. Ierapetritou, "Novel Approach for Optimal Process Design under Uncertainty," *Comp. Chem. Eng.*, **19**, 1089 (1995).

Raspanti, C. G., J. A. Bandoni, and L. T. Biegler, "New Strategies for Flexibility Analysis and Design Under Uncertainty," *Comput. Chem. Eng.*, **24**, 2193 (2000).

Reemtsen, R., and S. Gorner, "Numerical Methods for Semi-Infinite Programming: A Survey," *Semi-infinitive Programming*, R. Reemtsen and J.-J. Ruckman, eds., Kluwer, Norwell, MA, p. 195 (1998).

Straub, D. A., and I. E. Grossmann, "Design Optimization of Stochastic Flexibility," *Comput. Chem. Eng.*, **17**, 339 (1993).

Takamatsu, T. Y., I. Hashimoto, and S. Shioya, "On Design Margin for Process Systems with Parameters Uncertainty," *J. Chem. Eng. Jpn.*, **6**, 453 (1973).

Walsh, S., and J. Perkins, "Operability and Control in Process Synthesis and Design," *Process Synthesis*, J. L. Anderson, ed., Academic Press, New York, p. 301 (1996).

Waltz, R. A., and J. Nocedal, *Knitro 2.0 User's Guide*, Northwestern Univ., Evanston, IL (2002).

Appendix A: Auxiliary Relations

We need the following equivalence relations and inequalities

$$\max_{x \in X} \varphi(x) \leq 0 \Leftrightarrow \varphi(x) \leq 0, \qquad \forall x \in X \qquad \text{(A1)}$$

$$\exists x \qquad f(x) \leq 0 \Leftrightarrow \min_{x} f(x) \leq 0 \qquad \text{(A2)}$$

$$\max_x \max_y f(x, y) = \max_y \max_x f(x, y) \tag{A3}$$

$$\min_x \max_y f(x, y) \geq \max_y \min_x f(x, y), \tag{A4}$$

where x is a vector of continuous or discrete variables. The relations in Eqs. A1, A2, and A3 are obvious, while Eq. A4 is proved in McKinsey (1952).

Theorem A.1. Consider the problem

$$f = \min_{x \in X} f(x)$$

$$\min_{y \in Y} \varphi_i(x, y) \leq 0, \qquad i = 1, \ldots, m. \tag{A5}$$

Here there are n_x search variables ($n_x = \dim\ x$). Consider the auxiliary problem

$$\bar{f} = \min_{x, y^i} f(x)$$

$$\varphi_i(x, y^i) \leq 0, \qquad i = 1, \ldots, m, \tag{A6}$$

where y^i, $(i = 1, \ldots, m)$ are vectors of new search variables. Thus in Eq. A6 there are $n_x + mn_y$ variables. It is shown in Ostrovsky et al. (1997) that if x^*, y^{i*} is the solution of Eq. A6, then x^* is the solution of Eq. A5.

Theorem A.2. Let x^* be the solution of

$$\min_x f(x) \tag{A7}$$

$$\varphi_i(x) \leq 0 \qquad i \in I. \tag{A8}$$

Let the constraints in Eq. A8 with indices $i \in I_A$ be active at x^*, that is,

$$\varphi_i(x^*) = 0 \qquad i \in I_A \qquad \varphi_i(x^*) < 0 \qquad i \in I/I_A. \tag{A9}$$

Then x^* is a local minimum of

$$\min_x f(x) \tag{A10}$$

$$\varphi_i(x) = 0 \qquad i \in I_A.$$

Indeed, since x^* is the solution of Eq. A7 in which conditions in Eq. A9 hold, there exists a vicinity C of x^* in which

$$f(x^*) \leq f(x) \qquad x \in C \tag{A11}$$

$$\varphi_i(x) = 0, \qquad i \in I_A, \qquad \varphi_i(x^*) < 0 \qquad i \in I/I_A.$$

However, Eq. A11 is the condition for x^* to be a local minimum of Eq. A10. Now consider the proof of the inverse statement. Let x^* be the solution of Eq. A10 and consider the set of functions $\varphi_i(x)$, $i \in \bar{I}$, that satisfy

$$\varphi_i(x^*) < 0 \qquad i \in \bar{I} \tag{A12}$$

Then x^* is a local minimum of Eq. A7 such that $I = I_A \cup \bar{I}$. We prove this statement as follows. Since x^* is also a local minimum of Eq. A10, there is a vicinity $\overline{C}$ of x^* such that

$$f(x^*) \leq f(x) \qquad x \in \overline{C} \tag{A13}$$

$$\varphi_i(x^*) = 0 \qquad i \in I_A. \tag{A14}$$

However, at x^* the condition in Eq. A12 is met. Note that Eqs. A12 and A14 coincide with Eq. A8, with $I = I_A \cup \bar{I}$. However, Eqs. A13 and A8 indicate that x^* is a local minimum of Eq. A7.

Theorem A.3. Let x^* be the solution of

$$f^* = \min_x f(x) \tag{A15}$$

$$\varphi_i(x) \leq 0 \qquad i = 1, \ldots, k, \ldots, m. \tag{A16}$$

We will suppose that Eq. A15 has a unique global minimum. Consider a problem in which the kth constraint is deleted from the constraints in Eq. A16:

$$f^{k*} = \min f(x) \tag{A17}$$

$$\varphi_i(x) \leq 0 \qquad i = 1, \ldots, k-1, k+1, \ldots, m. \tag{A18}$$

Let x^* be the unique global minimum of the problem. Since the feasible region of Eq. A17 encloses that of Eq. A15, $f^{k*} \leq f^*$ holds.

Suppose that the global minimum of Eq. A15 does not coincide with the global minimum of Eq. A17 $x^* \neq x^{k*}$. Then on

$$D_k = \{x : \varphi_i(x) \leq 0 \qquad i = 1, \ldots, k-1, \qquad k+1, \ldots, m\},$$

where x^* does not coincide with the global minimum of Eq. A17. Therefore, at the global minimum of Eq. A.17 the objective function value must be less than at x^*. Consequently, the strong inequality $f^{k*} < f^*$ holds. Since the equality $x^* = x^{k*}$ is rare, the deletion of some constraints improves the optimal objective function value in general.

Appendix B: Upper Bound of the Feasibility Function and Its Properties

The feasibility function can be represented as

$$\chi_2(d) = \max_{\theta^1 \in T^1} \psi^{(2)}(d, \theta^1), \tag{B1}$$

where

$$\psi^{(2)}(d, \theta^1) = \min_z \max_{\theta^2 \in T^2} \max_{j \in J} g_j(d, z, \theta^1, \theta^2).$$

Introduce auxiliary functions $\chi_2^U(d)$ and $\chi_2^{U,i}(d)$ for the region T^1 and the subregion T_i^1, respectively,

$$\chi_2^U \text{-} \min_z \max_{\theta^1 \in T^1} \max_{\theta^2 \in T^2} \max_{j \in J} g_j(d, z, \theta) \tag{B2}$$

$$\chi_2^{U,i} = \min_z \max_{\theta^1 \in T_i^1} \max_{\theta^2 \in T^2} \max_{j \in J} g_j(d, z, \theta). \tag{B3}$$

These are obtained by changing the order of the first two operations in Eqs. B2 and B3. Consider some properties of χ_2^U and $\chi_2^{U,i}$ as follows:

Property 1. The function $\chi_2^U(d)$ is the upper bound of $\chi_2(d)$ on T^1, thus

$$\chi_2^U(d) \geq \chi_2(d). \quad \text{(B4)}$$

This is easily proved using Eqs. A4 in 21. From Eq. B1 we have

$$\chi_2^U(d) \geq \psi^{(2)}(d, \theta^1) \qquad \forall \theta^1 \in T^1. \quad \text{(B5)}$$

Similarly, for $\chi_2^{U,i}$ we have

$$\chi_2^{U,i}(d) \geq \psi^{(2)}(d, \theta^1) \qquad \forall \theta^1 \in T_i^1. \quad \text{(B6)}$$

Property 2. There is the following relation

$$\chi_2^{U,i}(d) \leq \chi_2^{U,j}(d) \qquad \text{if} \qquad T_i^1 \in T_j^1. \quad \text{(B7)}$$

The relation follows directly from $\chi_2^{U,i}(d)$ (see Eq. B3).

Property 3. The following holds

$$\chi_2^U(d) = \min_z \max_{j \in J} \max_{\theta \in T} g_j(d, z, \theta). \quad \text{(B8)}$$

Indeed, it is clear that the following equality holds:

$$\max_{\theta^1 \in T_1} \max_{\theta^2 \in T_2} \max_{j \in J} g_j(d, z, \theta) = \max_{\theta \in T} \max_{j \in J} g_j(d, z, \theta).$$

Using the preceding equality and Eq. A3, we can obtain Eq. B8 from Eq. B2. It should be noted that the upper bound $\chi_1^U(d)$ of the feasibility function $\chi_1(d)$, introduced in (Ostrovsky et al., 1994), is equal to the righthand side of Eq. B8 as well. Therefore, we have $\chi_1^U(d) = \chi_2^U(d)$. Due to this fact, calculation of the feasibility function in this case is similar to that in the case when there is complete information about uncertain parameters at the operation stage.

Property 4. Let T^1 be partitioned into N_k subregions $T_i^{1,k}$ such that

$$T^1 = T_1^{1,(k)} \cup T_2^{1,(k)} \cup \cdots T_{N_k}^{1,(k)}, \quad \text{(B9)}$$

where k is an iteration index to be discussed later. Then

$$\max_i \chi_2^{U,i} \geq \chi_2. \quad \text{(B10)}$$

This follows from the fact that for all T_i^1, Eq. B6 holds.

Property 5. The following holds

$$\lim_{r(T_1^i) \to 0} \chi_2^{U,i} = \min_z \max_{j \in J} \max_{\theta^2 \in T^2} g_j(d, z, \theta^{1,i}, \theta^2) = \psi^{(2)}(d, \theta^{1,i}), \quad \text{(B11)}$$

where $\theta^{1,i}$ is a point to which T_i^1 tends. The property follows directly from the form of $\chi_2^{U,i}$ (see Eq. 22). From here for a small enough T_i^1 we have

$$\chi_2^{U,i} \cong \min_z \max_{j \in J} \max_{\theta^2 \in T^2} g_j(d, z, \theta^{1,i}, \theta^2) \qquad \text{if} \qquad r(T_i^1) \leq \epsilon, \quad \text{(B12)}$$

where $r(T_i^1)$ characterizes the size of T_i^1, and ϵ is a small positive number.

Appendix C: Lower-Bound Estimate

Using the expression for $\chi_2(d)$ from Eq. B1, we can rewrite TSOP2 (Eq. 31) as

$$f_2 = \min_{d, z^i} \sum_{i \in I_1} w_i \sum_{j \in Q_1} \nu_j f(d, z^i, \theta^{1i}, \theta^{2j}) \quad \text{(C1)}$$

$$\max_{\theta^2 \in T_2} g_j(d, z^i, \theta^{1i}, \theta^2) \leq 0, \qquad j = 1, \ldots, m \quad \text{(C2)}$$

$$\max_{\theta^1 \in T^1} \psi^{(2)}(d, \theta^1) \leq 0. \quad \text{(C3)}$$

Transforming the constraint in Eq. C3 according to Eq. A1, we can reduce Eq. C1 to

$$f_2 = \min_{d, z^i} \sum_{l \in I_2} w_i \sum_{l \in I_2} \nu_i f(d, z^i, \theta^{1i}, \theta^{2l}) \quad \text{(C4)}$$

$$\max_{\theta^2 \in T^2} g_j(d, z^i, \theta^{1i}, \theta^2) \leq 0 \qquad j = 1, \ldots, m; \qquad i \in I_1 \quad \text{(C5)}$$

$$\psi^{(2)}(d, \theta^{1,p}) \leq 0 \qquad \forall \theta^{1,p} \in T^1. \quad \text{(C6)}$$

Let d^*, z^{i*} be the solution. We need additional definitions. The approximation point $\theta^{1,i}$ will be called active if at least one constraint in Eq. C5 corresponding to the point is active. By this definition, $\theta^{1,i}$ is active if: $\exists j \max_{\theta^2 \in T^2} g_j(d^*, z^{i*}, \theta^{1i}, \theta^2) = 0$. We will call the point $\theta^{1,p}$ from Eq. C6 active if the corresponding inequality in Eq. C6 is active. Thus for the active point $\theta^{1,p}$, we have $\psi^{(2)}(d^*, \theta^{1,p}) = 0$.

Now we introduce for TSOP2 the concept of an active points set $S_{A.P}$

$$S_{A.P} = S_{A.P}^{(1)} \cup S_{A.P}^{(2)}. \quad \text{(C7)}$$

Here $S_{A.P}^{(1)}$ contains all the active approximation points and $S_{A.P}^{(2)}$ contains all the active points $\theta^{1,p}$ from Eq. C6. Thus

$$S_{A.P}^{(1)} = \left\{ \theta^{1,i} : \exists j, \max_{\theta^2 \in T^2} g_j(d^*, z^{i*}, \theta^{1,i}, \theta^2) = 0, i \in I_1 \right\},$$

$$S_{A.P}^{(2)} = \left\{ \theta^{1,p} : \psi^{(2)}(d^*, \theta^{1,p}) = 0 \right\}.$$

Introduce the set $S_2^{(k)} = \{\theta^{1,r}: r \in I_2^{(k)}\}$ at the kth iteration of the SB method and the set $I_2^{(k)}$ of indices of the points belonging to $S_2^{(k)}$. We refer to these points as *critical points*.

Introduce the following problem.

$$f_2^{L,(k)} = \min_{d,z^i} \sum_{i \in I_1} w_i \sum_{r \in Q_2} \nu_i f(d, z^i, \theta^{l1,i}, \theta^{1,r}) \quad \text{(C8)}$$

$$\max_{\theta^2 \in T^2} g_j(d, z, \theta^{1,i}, \theta^2) \le 0 \qquad j = 1, \ldots, m; \qquad i \in I_1 \quad \text{(C9)}$$

$$\psi^{(2)}(d, \theta^{1,l}) \le 0 \qquad \forall \theta^{1,l} \in S_2^{(k)}. \quad \text{(C10)}$$

Taking into account the form of $\psi^{(2)}$ (d,θ^1) (see Eq. B1) and using Theorem A1 and relation Eq. A3, we can transform the problem in Eq. C8 to the form

$$f_2^{L,(k)} = \min_{d,z^i,\, z^r} \sum_{i \in I_1} w_i \sum_{r \in Q_1} \nu_l f(d, z^{1,i}, \theta^{1,i}, \theta^{2r}) \quad \text{(C11)}$$

$$\max_{\theta^2 \in T_2} g_j(d, z^{1,i}, \theta^{1i}, \theta^2) \le 0 \qquad j = i, \ldots, m, \qquad i \in I_1 \quad \text{(C12)}$$

$$\max_{\theta^2 \in T^2} g_j(d, z^{1,r}, \theta^{1,r}, \theta^2) \le 0, \qquad \theta^{1,r} \in S_2^{(k)} \qquad j = 1, \ldots, m.$$

A rule of the selection of critical points for the problem is considered in Appendix D. Consider properties of lower-bound problem and TSOP2.

Property 1. The value $f_2^{L,(k)}$ is a lower bound on the optimal value f_2 of the objective function in TSOP2. Since $S_2^{(k)} \in T^1$, the feasible region of Eq. C8 will be enclosed in the feasible region of Eq. C4. Therefore,

$$f_2^{L,(k)} \le f_2. \quad \text{(C13)}$$

That is, $f_2^{L,(k)}$ is a lower bound for TSOP2.

Property 2. Let the set $S_2^{(p+1)}$ be obtained from $S_2^{(p)}$ by the addition of at least one point. Then

$$f_2^{L,(p+1)} \ge f_2^{L,(p)} \qquad \text{if} \qquad S_2^{(p)} \subset S_2^{(p+1)}. \quad \text{(C14)}$$

In fact, since $S_2^{(p)} \subset S_2^{(p+1)}$, then the feasible region of Eq. C11 for $k = p+1$ will be less than the feasible region of the problem for $k = p$. Thus Eq. C14 holds. Therefore, adding points to the set of critical points improves the lower bound.

Property 3. If $S_2^{(k)}$ covers T densely enough, then the lower bound $f_2^{L,(k)}$ is close to the solution of TSOP2 (the solution of (A34)). In fact, if $S_2^{(k)}$ covers T^1 densely enough then there exists the condition $\forall \theta^1 \in \mathrm{T}^1 \exists \theta^{1,i}$ such that $|\theta^1 - \theta^{1,i}| \le \epsilon$, where ϵ is small. It is clear that in this case the solution of Eq. C1 will be close to that of Eq. C11.

Property 4. The solution d^*, z^{i*} of TSOP2 (see Eq. C4) is the solution of

$$f_2 = \min_{d \in D . z^i} \sum_{i \in I_1} w_i \sum_{r \in Q_1} \nu_i f(d, z^i, \theta^{l,i}, \theta^{2,r}) \quad \text{(C15)}$$

$$\max_{\theta^2 \in T^2} g_j(d, z, \theta^{1,i}, \theta^2) = 0 \qquad \theta^{1,i} \in S_{A.P}^{(1)}$$

$$\psi^{(2)}(d, \theta^{1,p}) = 0 \qquad \theta^{1,p} \in S_{A.P}^{(2)}.$$

The property follows from Theorem A2.

Appendix D: Upper-Bound Problem and Its Properties

Let the region T^1 be partitioned into N_k subregions $T_i^{l,(k)}$ (see Eq. B9) at the kth iteration of iterative procedure of the SB method. Designate as T^k the collection of the subregions $T_i^{1,(k)}$ $(i = 1, \ldots, N_k)$. Introduce the problem

$$f_2^{U,(k)} = \min_{d,z^i} \sum_{i \in I_1} w_i \sum_{r \in Q_1} \nu_i f(d, z^i, \theta^{1i}, \theta^{2r}) \quad \text{(D1)}$$

$$\max_{\theta^2 \in T^2} g_j(d, z^i, \theta^{1i}, \theta^2) \le 0, \qquad j = 1, K, m, \qquad i \in I_1$$

$$\chi_2^{U,1}(d) \le 0, \ldots, \chi_2^{U,N_k}(d) \le 0, \quad \text{(D2)}$$

where $\chi_2^{U,i}(d)$ is determined by Eq. B3. Using $\chi_2^{U,i}(d)$, Theorem A1, Eq. A1, and Eq. A3, we can transform Eq. D1 through Eq. D2 as

$$f_2^{U,(k)} = \min_{d,z^i,\, z^l} \sum_{i \in I_1} w_i \sum_{r \in Q_1} \nu_i f(d, z^i, \theta^{1i}, \theta^{2r}) \quad \text{(D3)}$$

$$\max_{\theta^2 \in T^2} g_j(d, z^i, \theta^{1i}, \theta^2) \le 0, \qquad j = 1, K, m, \qquad i \in I_1$$

$$\max_{\substack{\theta^1 \in T_l^1 \\ \theta^2 \in T^2}} g_j(d, z^l, \theta^1, \theta^2) \le 0, \qquad l = 1, K, N_k, \qquad j = 1, \ldots, m. \quad \text{(D4)}$$

Let $d^{(k)}$, $z^{i,(k)}$, $z^{l,(k)}$ be the solution of the problem. Similar to what we did for TSOP2, the active approximation point $\theta^{1,i}$ at the kth iteration is such that

$$\exists j \max_{t^2 \in T^2} g_j(d^{(k)}, z^{i,(k)}, \theta^{1i}, \theta^2) = 0.$$

Let $\theta^{1,p}$, $\theta_j^{2,p}$ be the solution of

$$\max_{\theta^1 \in T_p^1, \theta^2 \in T^2} g_j(d^{(k)}, z^{p,(k)}, \theta^1, \theta^2).$$

Also, as in TSOP2, the points $\theta_j^{1,p}$, $\theta_j^{2,p}$ are active at the kth iteration if

$$g_j\left(d^{(k)}, z^{p,(k)}, \theta_j^{1,p}, \theta_j^{2,p}\right) = 0.$$

Similar to the active points set $S_{A.P}$ of the TSOP2 we introduce an active points set $S_{A.P}^{(k)}$ at the kth iteration

$$S_{A.P}^{(k)} = S_{A.P}^{(k)1} \cup S_{A.P}^{(k)2}, \quad \text{(D5)}$$

where

$$S_{A.P}^{(k),1} = \left\{\theta^{1,i} : \exists j \in J \max_{\theta^2 \in T^2} g_j(d^{(k)}, z^{i,(k)}, \theta^{1,i}, \theta^2) = 0\right\}$$

$$S_{A.P}^{(k),2} = \left\{\theta^{1,p} : g_j\left(d^{(k)}, z^{p,(k)}, \theta_j^{1,p}, \theta_j^{2,p}\right) = 0\right\}.$$

Let $T_l = \{\theta^1, \theta^2 : \theta^1 \in T_l^1;\ \theta^2 \in T^2\}$. Introduce a critical point set S_2^l for each T_l:

$$S_2^l = \left\{\theta^{1,l,s}, \theta^{2,l,s} : (\theta^{1,l,s}, \theta^{2,l,s}) \in T_l,\ s \in I_2^l\right\},$$

where I_2^l is a set of indices of critical points in T_l, and the critical point set S_2^l corresponds to each point $\theta^{1,i}$, $S_2^i = \{\theta^{2,i,q}: q \in I_1^i\}$.

Consider some properties of the problem.

Property 1. The value $f_2^{U,(k)}$ is an upper bound on the optimal value of the objective function f_2 in TSOP2. Since Eq. B10 is met, the feasible region of Eq. D1 is less than that of TSOP2 (see Eq. 31). Consequently

$$f_2^{U,(k)} \geq f_2. \tag{D6}$$

Property 2. If the collection $T^{(p+1)}$ is obtained from $T^{(p)}$ by partitioning some subregions from $T^{(p)}$ (that is, $\forall T_i^{(p+1)}$ $\exists T_j^{(p)}$, such that $T_i^{(p+1)} \subset T_j^{(p)}$, then

$$f_2^{U,(p+1)} \leq f_2^{U,(p)}. \tag{D7}$$

From (Eq. B7), it follows that the feasible region of Eq. D1 for $k = p$ is contained in the feasible region for $k = p + 1$, therefore Eq. D7 is valid. Thus, partitioning of the collection $T^{1,(k)}$ improves the upper bound of TSOP2.

Property 3. The following holds

$$\lim_{\forall r(T_i^{1,(k)}) \to 0} f_2^{U,(k)} = f_2. \tag{D8}$$

From Eq. B11, Eq. D1 is reduced to Eq. C4 when $r(T_i^1) \to 0$, $(i = 1, \ldots, N_k)$. Therefore, if T^1 is partitioned into small enough subregions $T_i^{1,(k)}$, then the solution of Eq. D1 is close enough to that of TSOP2 (see Eq. 31).

Property 4. If the sizes of all the subregions $T_i^{1,(k)}$ strive to zero, then the set $S_{A.P}^{(k)}$ of active points strives to the set $S_{A.P}$ of active points of TSOP2.

According to *Property 3* of the upper-bound problem, if the size of each $T_i^{1,(k)}$ tends to zero, then Eq. D1 becomes TSOP2 (Eq. 31). Therefore, the set $S_{A.P}^{(k)}$ of active points of the collection T^k tends to set $S_{A.P}$ of active points of TSOP2. Now we consider a method for solving the semi-infinite programming problem, Eq. D2. To solve the latter, we will use the outer approximation algorithm (Reemtsen and Gorner, 1998). We propose the following upper-bound algorithm.

Algorithm D1

Step 1. Set $p = 1$. Give initial values of the variables d, z^i, z^l; give the set S_1 and initial sets

$$S_2^i, (i \in I_1) \qquad \text{and} \qquad S_2^l \qquad (l = 1, \ldots, N_k)$$

Step 2. Solve the problem

$$\min_{d,z^i,z^l} \sum_{i \in I_2} w_i \sum_{r \in Q_1} \nu_r f(d,z^i,\theta^{1,i},\theta^{2,r}) \tag{D9}$$

$$g_j(d, z^i, \theta^{1,i}, \theta^{2,i,q}) \leq 0 \qquad i \in I_1, \qquad \theta^{2,i,q} \in S_2^i, \qquad j = 1,K, m \tag{D10}$$

$$g_j(d, z^l, \theta^{1,l,s}, \theta^{2,l,s}) \leq 0, \qquad j = 1,K, m \qquad (\theta^{1,l,s}, \theta^{2,l,s}) \in S_2^l, \qquad l \in 1,K, N_k. \tag{D11}$$

Let the solution of the above system be $\bar{z}^i, \bar{z}^l$, $\bar{d}$.

Step 3. For each point, $\theta^{1,i}$ solve

$$\max_{\theta^2 \in T_2} g_j(\bar{d}, \bar{z}^{1,i}, \theta^{1,i}, \theta^2). \tag{D12}$$

Step 4. For each subregion $T_l (l = 1, \ldots, N_k)$ solve

$$\max_{\substack{\theta^1 \in T_l^1, \\ \theta^2 \in T^2}} g_j(\bar{d}, \bar{z}^l, \theta^1, \theta^2). \tag{D13}$$

Designate as $\bar{\theta}^{2,i,j}$ the solution of Eq. D12 and $\bar{\theta}^{l,j} = (\bar{\theta}^{1,l,j}, \bar{\theta}^{2,l,j})$ the solution of Eq. D13.

Step 5. Check the conditions

$$g_j(\bar{d}, \bar{z}^{1,i}, \theta^{1,i}, \bar{\theta}^{2,i,j}) \leq \epsilon, \qquad j = 1,K, \qquad m,i \in I_1 \tag{D14}$$

$$g_j(\bar{d}, \bar{z}^l, \bar{\theta}^{l,j,}) \leq \epsilon, \qquad j = 1,K,m, \qquad 1 = 1, K, N_k. \tag{D15}$$

If Eqs. D14 and D15 are met (that is, the solution has been found), go to Step 9.

Step 6. Construct the sets R^l and R^i:

$$R^l = \left\{\theta^{l,j} : g_j(\bar{d}, \bar{z}^l, \bar{\theta}^{1,l,s}, \bar{\theta}^{2,l,s}) \geq \epsilon\right\}$$

$$R^i = \left\{\bar{\theta}^{2,i,j} : g_j(\bar{d}, \bar{z}^i \theta^{1,i}, \bar{\theta}^{2,i,j}) \geq \epsilon\right\},$$

where R^l and R^i contain all the points in which Eqs. D14 and D15 are violated.

Step 7. Create the new sets of critical points:

$$S_2^l = \{S_2^l \cup R^l\}, \qquad S_2^i = \{S_2^i \cup R^i\}.$$

Step 8. Set $p = p + 1$ and go to Step 2.

Step 9. Construct the set $S_{A.P}^{(k)}$ and stop.

Let us now consider a rule of selection of critical points for lower-bound estimation. We showed that: (a) the set $S_{A.P}^{(k)}$ of active points at the kth iteration tends to the set of active points $S_{A.P}$ of TSOP2 if the size of each subregion tends to zero (*Property 4* of the upper-bound problem), and (b) only the set $S_{A.P}$ of active points determines the solution of TSOP2 (*Property 4*, Appendix C) (see Eq. C15). Therefore, since the proposed algorithm is based on a partition of T_1, it is reasonable to select $S_{A.P}^{(k)}$ as the set of critical points for the lower-bound estimation in Eq. C8.

Appendix E

Here we give justification for using the suggested partitioning strategy. A partition of an active constraint deletes the constraint from the set of constraints corresponding to the k-iteration. However, we showed (see Theorem A3) that (with the exception of unusual cases) deletion of the active constraint improves the optimal value of the objective function. On the other hand, partitioning of $T_i^{(k)}$ corresponding to inactive constraints in Eq. D2 certainly does not improve the upper bound $f_2^{U,(k)}$.

To prove the previous statement, suppose for a set $T^{(k)}$ of subregions $T_i^{(k)}$ we obtain the solution $[d^{(k)}, z^{i,(k)}, f_2^{U,(k)}]$ to Eq. D1. For illustration, suppose also that only one of the constraints in Eq. D2 corresponding to the lth subregion is inactive, which means that for the solution $d^{(k)}$, the following condition holds:

$$\chi_2^{U,1}(d^{(k)}) = 0, \ldots, f_2^{U,l-1}(d^{(k)}) = 0, \chi_2^{U,l}(d^{(k)}) < 0, \chi_2^{U,1+1}(d^{(k)}) = 0, \ldots, \chi_2^{U,N_k}(d^{(k)}) = 0.$$

It follows from Theorem A2 that $[d^{(k)}, z^{i,(k)}]$ is the solution of Eq. D1 for which the constraints in Eq. D2 are replaced by the constraints $\chi_2^{U,1}(d) = 0, \ldots, \chi_2^{U,l-1}(d) = 0, \chi_2^{U,1+1}(d) = 0, \ldots, \chi_2^{U,N_k}(d) = 0$. Now, suppose we partition the lth subregion into two subregions p and q. At the $k+1$-st iteration, we must solve Eq. D1, in which the constraints in Eq. D2 take the form

$$\chi_2^{U,1}(d) \le 0, \ldots, \chi_2^{U,l-1}(d) \le 0, \chi_2^{U,p}(d) \le 0, \chi_2^{U,q}(d) \le 0, \chi_2^{U,1+1}(d) \le 0, \ldots, \chi_2^{U,N_k}(d) \le 0.$$

Since $T_p \subset T_l$ and $T_q \subset T_l$, then

$$\chi_2^{U,l}(d) \ge \chi_2^{U,p}(d) \chi_2^{U,1}(d) \ge \chi_2^{U,q}(d).$$

Consequently, the constraints corresponding to the pth and qth subregions will be inactive again. Therefore, it is clear that $[d^{(k)}, z^{i,(k)}]$ will also be a solution to this new problem, and we obtain $f_2^{U,(k+1)} = f_2^{U,(k)}$. Thus partitioning the subregions having inactive constraints has no effect.

Appendix F: Convergence of the SB Method

Now we will show that Algorithm 2 always converges. Since the algorithm partitions only subregions with indices in $Q^{(k)}$, then for sufficiently small ϵ (see Eq. 37) the values of $r(T_i)(i \in Q^{(k)})$ will be sufficiently small. Let k^* be the index of the last iteration in Algorithm 2 and d^*, z^{i*}, z^{l*} be the values of the variables d, z^i, z^l at the last iteration. Also, let Q_ϵ^* be a limit set for $Q^{(k)}$. Since $Q^{(k)}$ is a set of indices of active constraints in Eq. D1, $[d^*, z^{i*}]$ is the solution of the problem (Theorem A2)

$$f_2^{U,(k)} = \min_{d \in D, z} \sum_{i \in I_1} w_i \sum_{j \in I_i} \nu_i f(d, z^i, \theta^{1i}, \theta^{1r})$$

$$\max_{\theta^2 \in T^2} g_j(d, z^i, \theta^{1i}, \theta^{2r}) \le 0 \qquad i \in I_1, \qquad j = 1, \ldots, m \tag{F1}$$

$$\chi_2^{U,i}(d) = 0, \forall i \in Q^{(k)}.$$

Here

$$\chi_2^{U,i}(d^*) < 0, \qquad \forall i \notin Q^{(k)}. \tag{F2}$$

From here $f_2^{U,(k^*)}$ from Eq. D1 is the solution of Eq. F2 for $k = k^*$ and $Q^{(k)} = Q^*$. Earlier we showed that when the size of all subregions is small enough, then the solution of upper-bound problem Eq. D1 is close to the solution of TSOP2. However, Algorithm 1 partitions only those subregions that have at least one active constraint in Eq. D2. Nevertheless, Algorithm 1 will always converge to the solution of TSOP2. To prove this, note that Algorithm 1 partitions all active subregions whenever Eq. 37 is violated. Subsequently from Algorithm 1 for some $k = k^*$ either Eq. 37 is met, or in Eq. D1 each $T_i^{(k)}$ $(i \in Q^*)$ is small enough. If Eq. 37 is met, then our claim is correct. Consider the last scenario. For a small enough $T_i^{(k)}$ Eq. B12 holds. Substituting the expressions of $\chi_2^{U,i}(d)$ from Eq. B12 into Eq. F1 we obtain

$$f_2^{U,(k)} = \min_{d \in D, z} \sum_{i \in I_1} w_i \sum_{j \in I_i} \nu_i f(d, z^i, \theta^{1i}, \theta^{1r})$$

$$\max_{\theta^2 \in T^2} g(d, z^i, \theta^{1i}, \theta^2) \le 0, \qquad i \in I_1, \qquad j = 1, \ldots, m \tag{F3}$$

$$\psi^{(2)}(d, \theta^{1,s}) = 0 \qquad \forall s \in Q^{(k)}.$$

It follows from Eq. B6 that if $\chi_2^{U,i}(d^*) < 0$, then $\psi^{(2)}(d, \theta^{1,j}) < 0$ for $\forall \theta^{1,j} \in T_i^1$. Consequently, it follows from Eq. F2: $\psi^{(2)}(d, \theta^{1j}) < 0$, $\theta^{1,j} \notin T_i^1$, $i \in Q_\epsilon^*$. Thus, according to Theorem A2, $[d^*, z^{i*}]$ is the solution of

$$f_2^{U,(k)} = \min_{d \in D, z} \sum_{i \in I_1} w_i \sum_{r \in I_i} \nu_i f(d, z^i, \theta^{1i}, \theta^{2r})$$

$$\max_{\theta \in T^2} g(d, z^i, \theta^1, \theta^2) \le 0 \qquad i \in I_1$$

$$\psi^{(2)}(d, \theta^i) = 0 \qquad \forall i \in Q_\epsilon^*$$

$$\psi^{(2)}(d, \theta^j) < 0 \qquad \forall \theta^j \notin T_i^1, \qquad i \in Q_\epsilon^*.$$

However, the problem coincides with TSOP2 in the form Eq. C4. Consequently, d^*, z^{i*} is the solution of TSOP2.

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