Optimization Problem with Normally Distributed Uncertain Parameters

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The issue of chemical process optimization when at the operation stage the design specification should be met with some probability and the control variables can be changed has been considered. A common approach for solving the broad class of optimization problems with normally distributed uncertain parameters were developed. This class includes the one-stage and two-stage optimization problems with chance constraints. This approach is based on approximate transformation of chance constraints into deterministic ones. © 2013 American Institute of Chemical Engineers *AIChE J*, 59: 2471–2484, 2013

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Introduction

We will consider the problem of chemical process (CP) optimal design for the case when inexact mathematical models are used. The inexactness of mathematical models arises because of the original uncertainty of chemical, physical, and economic data which are used during the CP design. The optimization problem of a CP design in the case of the use of an exact mathematical model can be expressed as

$$\min_{d,z} f(d,z,\theta) \tag{1}$$
$$g_j(d,z,\theta) \le 0 \quad j=1,\ldots,m$$

where $f(d,z,\theta)$ is the goal function, d is an n_d-vector of design variables, z is an n_z-vector of control variables, and θ is a p-vector of parameters. We suppose that the functions $f(d,z,\theta)$, $g_j(d,z,\theta)$, $j=1,\ldots,m$ are continuously differentiable and the uncertain parameters θ_i are random variables having the multivariate normal distribution $N_p(E[\theta],\Lambda)$ with the probability density function "probability density function"

$$\rho(\theta) = \frac{1}{(2\pi)^{n_\theta/2}(\det\Lambda)^{1/2}} \exp\left\{-\frac{1}{2}(\theta-\mu)^T\Lambda^{-1}(\theta-\mu)\right\} \tag{2}$$

where μ is the vector of the mean values of the parameters $\theta_i(\mu_i = E[\theta_i])$ and Λ is the covariance matrix: $\Lambda = (\lambda_{ij})$, where $\lambda_{ij} = \rho_{ij}\sigma_i\sigma_j$, $(\sigma_i)^2$ is the variance of the parameter θ_i, ρ_{ij} is the correlation coefficient of the parameters θ_i and θ_j, $\rho_{ij}=1$, if $i=j$. In the case of independent uncertain parameters θ_i, the probability density function of the j-th uncertain parameter has the following form

$$\rho_j(\theta_j) = \frac{1}{\sigma_j\sqrt{2\pi}}\exp\left[-\frac{(\theta_j-\mu_j)^2}{2\sigma_j^2}\right] \tag{3}$$

The problem of the optimal design of a CP under uncertainty can be formulated as follows: it is necessary to create an optimal CP that would guarantee the satisfaction (exact or with some probability) of all design specifications in the case when inexact mathematical models are used and internal and external factors change during the CP operation stage. Usually, the following two formulations of this problem are used

1. The *formulation of the two-stage optimization problem* (TSOP) takes into account possibility of the control variables change at the operation stage.[1] Here, we suppose that at each time instant during the operation stage (a) values of all or some of the uncertain parameters can be either measured or calculated using the experimental data (thus at each time instant the process model is corrected) and (b) during the operation stage, the control variables are adjusted depending on a CP state. This formulation can be used if it is possible to accurately estimate all or some of the uncertain parameters at the operation stage of CP.

2. The *formulation of the one-stage optimization problem* (OSOP) supposes that the control variables are constant at the operation stage. Since the formulation of TSOP has more freedom degrees, a CP design obtained by solving the TSOP is, generally speaking, "better" in comparison with a design obtained by solving the OSOP.

The formulation of the optimization problem under uncertainty depends on the type of constraints. The constraints can be "hard" or "soft".[2] Hard constraints must never be violated during the operation stage. Conversely, if occasional violations are allowed then the constraints are said to be soft.

We consider methods of solving the one-stage optimization problems with chance constraint (OSOPCC) and two-

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stage optimization problems with chance constraint (TSOPCC). Methods of solving the two-stage optimization problem with hard constraints (TSOPHC) and the OSOP with soft constraints (with chance constraints) were developed significantly. Methods of solving TSOPHC have been developed in Refs. 3–7. Methods of solving the OSOPs for CP with chance constraints have been developed in Refs. 8 and 9.

The main issue in solving optimization problems under uncertainty is the computation of multiple integrals for calculation of the expected value of the objective function and probabilities of constraints satisfaction. The known methods of nonlinear programming (e.g., sequential quadratic programming (SQP)) (see, e.g., Ref. 10) require calculation of the multiple integrals at each iteration. This operation is very intensive computationally even when the dimensionality of the uncertain parameters vector θ is low. Three approaches are used to overcome this difficulty. The first way is the improvement of the Gauss quadrature.[11] Acevedo and Pistikopoulos[12] suggested three alternative integration schemes. For normally distributed uncertain variables, Bernardo et al.[13] obtained a special quadrature formula that significantly decreases the number of required evaluation points (knot points) for the multidimensional integrals. One must note that the articles,[14,15] where methods of the approximate evaluation of multidimensional integral are considered. The second way is based on one of the sampling techniques (Monte–Carlo, Latin Hypercube, or Hammersley Sequence Sampling).[8,16] The third approach is the transformation of chance constraints into deterministic ones. It is clear that this transformation allows us to avoid calculation of multiple integrals First of all, one must note that linear chance constraints can be transformed into deterministic ones.[17] Maranas[18] used the transformation of chance constraints into deterministic constraints for the case when the constraints are nonlinear with respect to search variables and linear with respect to uncertain parameters. Wendt et al.[19] have developed a method of solving the steady-state OSOPCC based on the use of the monotone relationship between constrained output and one of input uncertain parameters. Later on, the group of Wozny[20] applied this strategy to solve the problems of optimal design, nonlinear dynamic systems, optimal production planning, and optimal control of chemical processes under uncertainty. However, their approach still requires the calculation of multiple integrals at each iteration. Ostrovsky et al.[21,22] have developed a series of approaches to solving optimization problems with chance constraints based on the transformation of chance constraints into deterministic ones.

Significantly less attention has been given to formulation and solution of the TSOP for chemical processes with soft constraints. Wellons and Rekleitis[2] consider the approach based on the penalty method. Here, difficulties arise with the assignment of a penalty coefficient. In the articles,[13,23,24] the TSOP with soft constraints is formulated by relaxing the soft constraints and penalizing the objective function (using Taguchi loss function). Here also one can encounter difficulties when assigning the penalty coefficient. Bernardo and Saraiva[25] consider the TSOP with the following soft constraint: the expected value of the variance of a variable y characterizing the process quality must be less than or equal to some given value. Ostrovsky et al.[22] formulated the TSOPCC.

On the basis of the approaches developed in Refs. 21 and 22, we will develop here a common approach for solving a broad class of optimization problems of chemical processes with normally distributed uncertain parameters. This class includes the OSOPCC and TSOPCC in the cases of independent and dependent, normally distributed uncertain parameters.

Formulation of TSOPCC

The TSOPCC has the following form[22]

$$f^1 = \min_{d,z(\theta)} E[f(d, z(\theta), \theta)] \tag{4}$$

$$\Pr\{g_j(d, z(\theta), \theta) \le 0\} \ge \alpha_j \quad j = 1, \ldots, m \tag{5}$$

where

$$0 \le \alpha_j < 1, \quad j = 1, \ldots, m \tag{6}$$

It is seen that in this case the search variables $z(\theta)$ are multivariable functions. Here $\Pr\{g_j(d, z(\theta), \theta) \le 0\}$ is the probability of satisfaction of the constraint $g_j(d, z(\theta), \theta) \le 0$, that is, it is the probability measure of the region $\Omega_j = \{\theta : g_j(d, z, \theta) \le 0\}$

$$\Pr\{g_j(d, z, \theta) \le 0\} = \int_{\Omega_j} \rho(\theta) d\theta \tag{7}$$

$E[f(d, z(\theta), \theta)]$ is the expected value of a goal function $f(d, z(\theta), \theta)$

$$E[f(d, z, \theta)] = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} f(d, z, \theta) \rho(\theta) d\theta \tag{8}$$

To avoid integrating over regions with infinite limits we introduce the concept of an *uncertainty region* T_θ. The region T_θ is an uncertainty region if its probability measure is close to 1

$$\Pr[\theta \in T_\theta] \ge \bar{\alpha} \tag{9}$$

where $\bar{\alpha}$ is close to 1. Thus, the uncertainty region is the region a point θ hits with a large probability. We will use $\bar{\alpha} = 0.999$. This means that all values of the vector θ are found in the region T_θ with probability 0.999. We will use the following approximate expression for the expected value $E\{f(d, z(\theta), \theta)\}$

$$E_\theta[f(d, z(\theta), \theta)] = \int_{T_\theta} f(d, z(\theta), \theta) \rho(\theta) d\theta \tag{10}$$

Thus, we will consider problem (4) in which the expected value $E[f(d, z(\theta), \theta)]$ is replaced by its approximation $E_\theta[f(d, z(\theta), \theta)]$

$$\bar{f} = \min_{d,z(\theta)} E_\theta[f(d, z(\theta), \theta)] \tag{11}$$

$$\Pr\{g_j(d, z(\theta), \theta) \le 0\} \ge \alpha_j \quad j = 1, \ldots, m \tag{12}$$

where

$$0 \le \alpha_j < 1, \quad j = 1, \ldots, m \tag{13}$$

Suppose we solved problem (11) and obtained the optimal value $\bar{f}$. This means that the optimal value of the objective function of problem (4) will be equal to $\bar{f}$ with probability 0.999.

If $z(\theta)$ does not depend on θ, that is, $z(\theta) = z = \text{const}$ $\forall \theta \in T_\theta$, then TSOPCC (11) is transformed into the one-stage optimization problem with chance constraints (OSOPCC)

$$f^* = \min_{d,z} E_\theta[f(d,z,\theta)] \tag{14}$$

$$\Pr\{g_j(d,z,\theta) \le 0\} \ge \alpha_j \quad j = 1,\ldots,m,$$

where the variables z do not depend on θ.

We noted already that the main issue in solving optimization problems under uncertainty is the computation of multiple integrals for calculation of the expected value of the objective function and probabilities of constraints satisfaction. In connection with this, we have transformed problem (11) into the following form[22]

$$\bar{f} = \min_{d,z(\theta),T_{\alpha_j}} E_\theta[f(d,z(\theta),\theta)] \tag{15}$$

$$\max_{\theta \in T_{\alpha_j}} g_j(d,z(\theta),\theta) \le 0 \quad j = 1,\ldots,m \tag{16}$$

$$\Pr\{\theta \in T_{\alpha_j}\} \ge \alpha_j \quad j = 1,\ldots,m \tag{17}$$

Thus, in this problem, we look for the optimal values of the variables $d, z(\theta)$ and the optimal regions T_{α_j}, $(j = 1,\ldots,m)$. In other words, we look for the optimal form and location of the regions T_{α_j}. For the sake of simplicity of description, we will call both $d, z(\theta)$ and T_{α_j} as search variables and any set of values of the search variables as a point. Designate the solution of problem (15) as $d^*, z^*(\theta)$, $T^*_{\alpha_j}$, $j = 1,\ldots,m$. Thus, we have reduced an optimization problem with chance constraints (11) to an optimization problem (15) with deterministic (16) and chance constraints (17).

General Description of an Approximate Method of Solving the Optimization Problem with Chance Constraints

These are the main difficulties of solving problem (15):

1. As it is very difficult to look for the optimal forms and locations of the regions T_{α_j}, we will restrict the class of possible forms of the regions T_{α_j}. The form of the regions T_{α_j} will be selected in such a way that we can simply transform chance constraint (17) into deterministic ones.

2. We have noted already that the calculation of the expected value of the goal function (calculation of a multiple integral) is very intensive computationally.

3. Search variables are present in the form of multivariate functions, therefore problem (15) is the infinite programming problem. So long as there exist efficient methods of solving optimization problems with finite number of search variables, it is desirable to reduce problem (15) to an optimization problem with finite number of search variables.

We will develop an iteration method which will be based on a partition of the uncertainty region T_θ into subregions. Let at the k-iteration the region T_θ be partitioned into a set $R^{(k)}$ of subregions (multidimensional rectangles) $R_l^{(k)}$

$$R_l^{(k)} = \{\theta_i : \theta_{i,l}^{(k)L} \le \theta_i \le \theta_{i,l}^{(k),U}, l = 1,\ldots,N_k\} \tag{18}$$

where N_k is the number of the regions $R_l^{(k)}$ at the k-th iteration and l is the index of a subregion in the set $R^{(k)}$. Let $(R_l^{(k)})$ designate the set of interior points of the region $R_l^{(k)}$. We will construct the regions $R_l^{(k)}$ in the such a way that the following conditions will be met

$$R_1^{(k)} \cup \ldots \cup R_{N_k}^{(k)} = T \tag{19}$$

$$(R_l^{(k)}) \cap (R_q^{(k)}) = \varnothing, \quad \forall l,q\ 1 \le l \le N_k, \quad 1 \le q \le N_k \tag{20}$$

At each iteration of this procedure, we will use the following approximations:

1. Approximation of the region T_{α_j}

2. Approximation of multivariate functions. We will approximate multivariate functions with the help of functions of finite number of variables.

3. Approximate representation of the expected value of the goal function $f(d, z(\theta), \theta)$.

At the k-th iteration, we will designate approximations of the region T_{α_j}, multivariate functions $z(\theta)$ and expected value of the function $f(d, z(\theta), \theta)$ as $\tilde{T}_{\alpha_j}$, $\tilde{z}(\theta)$ and $E_{\text{ap}}^{(k)}[f(d, \tilde{z}(\theta), \theta)]$, respectively. Thus, at the k-th iteration, we will solve the following problem

$$f^{(k)} = \min_{d,\tilde{z}(\theta),\tilde{T}_{\alpha_j}} E_{\text{ap}}^{(k)}[f(d,\tilde{z}(\theta),\theta)] \tag{21}$$

$$\max_{\theta \in \tilde{T}_{\alpha_j}} g_j(d,\tilde{z}(\theta),\theta) \le 0 \quad j = 1,\ldots,m \tag{22}$$

$$\Pr\{\theta \in \tilde{T}_{\alpha_j}\} \ge \alpha_j \quad j = 1,\ldots,m. \tag{23}$$

Consider the following problem which differs from problem (21) only by the objective function

$$\tilde{f} = \min_{d,\tilde{z}(\theta),\tilde{T}_{\alpha_j}} E_\theta[f(d,\tilde{z}(\theta),\theta)] \tag{24}$$

$$\max_{\theta \in \tilde{T}_{\alpha_j}} g_j(d,\tilde{z}(\theta),\theta) \le 0 \quad j = 1,\ldots,m \tag{25}$$

$$\Pr\{\theta \in \tilde{T}_{\alpha_j}\} \ge \alpha_j \quad j = 1,\ldots,m \tag{26}$$

It is clear that problem (24) is obtained from problem (15) by substitution of $z(\theta)$, T_{α_j} with their approximations $\tilde{z}(\theta)$, $\tilde{T}_{\alpha_j}$. Designate the solution of problem (24) as $\tilde{d}^*, \tilde{z}^*(\theta)$, $\tilde{T}^*_{\alpha_j}$, $j = 1,\ldots,m$. Compare problems (15) and (24). Let S be the feasibility region of problem (15), that is, the set of points where constraints (16), (17) are met. Since the point $d^*, z^*(\theta)$, $T^*_{\alpha_j}$, $j = 1,\ldots,m$ is the minimum of problem (15) then the following inequality holds

$$\bar{f} \le E_\theta[f(d,z(\theta),\theta)] \text{ if } (d,z(\theta),T_{\alpha_j}) \in S) \tag{27}$$

Since the point $d^*, \tilde{z}^*(\theta)$, $\tilde{T}^*_{\alpha_j}$, $j = 1,\ldots,m$ is the solution of problem (24), constraints (25), (26) are met. However, constraints (25), (26) coincide with constraints (16), (17). This means that the point $\tilde{d}^*, \tilde{z}^*(\theta)$, $\tilde{T}^*_{\alpha_j}$, $j = 1,\ldots,m$ belongs to the set S. Consequently, using (27), we obtain

$$\bar{f} \le E_\theta[f(\tilde{d}^*,\tilde{z}^*(\theta),\theta)] = \tilde{f}$$

Thus, the solution of problem (24) gives an upper bound of the solution of problem (15)

$$\bar{f} \le \tilde{f} \tag{28}$$

At each iteration, all the approximations $\tilde{d}, \tilde{z}(\theta)$, $\tilde{T}_{\alpha_j}$, $j = 1,\ldots,m$, will be made more exact with the help of a partition procedure. Consider ways of construction of these approximations.

Approximation of the region T_{α_j}

We will construct the region $\tilde{T}_{\alpha_j}$ in the following form

$$\tilde{T}_{\alpha_j} = T_{\alpha_j,1} \cup T_{\alpha_j,2} \cup \ldots \cup T_{\alpha_j,N_k} \tag{29}$$

where $T_{\alpha_j,l}$ is the l-th subregion of the region $\tilde{T}_{\alpha_j}$, and N_k is the number of the subregions $T_{\alpha_j,l}$ at the k-th iteration. Note that the number of the regions $T_{\alpha_j,l}$ is equal to the number of

the regions $R_l^{(k)}$. We will construct the regions $T_{\alpha_j,l}$ in such a way that the following conditions are met

$$(T_{\alpha_j,s}) \cap (T_{\alpha_j,t}) = \varnothing, \quad \forall s,t = 1,\ldots,N_k \tag{30}$$

To guarantee the satisfaction of conditions (30), we require each region $T_{\alpha_j,l}$ to belong to only one region $R_l^{(k)}$. Thus, we require the satisfaction of the following conditions

$$T_{\alpha_j,l} \in R_l^{(k)}, \quad l = 1,\ldots,N_k \quad j = 1,\ldots,m. \tag{31}$$

It is clear that the greater N_k is the more adjusted parameters (search variables) correspond to the region $\tilde{T}_{\alpha_j}$. Therefore, the greater N_k is, the better the optimal region $T^*_{\alpha_j}$ is approximated by $\tilde{T}_{\alpha_j}$. Since the regions $T_{\alpha_j,l}$, $(l = 1,\ldots,N_k)$ do not have common parts (see Eq. 30), the following equality holds

$$\Pr\{\theta \in \tilde{T}_{\alpha_j}\} = \Pr\{\theta \in T_{\alpha_j,1}\} + \Pr\{\theta \in T_{\alpha_j,2}\} + \ldots + \Pr\{\theta \in T_{\alpha_j,N_k}\} \tag{32}$$

Since equality (29) holds, the following evident equality holds

$$\max_{\theta \in \tilde{T}_{\alpha_j}} g_j(d, z(\theta), \theta) = \max_l \max_{\theta \in T_{\alpha_j,l}} g_j(d, z(\theta), \theta) \tag{33}$$

Consequently, inequality (22) can be rewritten in the following form

$$\max_l \max_{\theta \in T_{\alpha_j,l}} g_j(d, z(\theta), \theta) \le 0, \quad j = 1,\ldots,m, \tag{34}$$

Using Statement A1 (Appendix), we can transform inequalities (34) into the following form

$$\max_{\theta \in T_{\alpha_j,l}} g_j(d, z(\theta), \theta) \le 0, \quad j = 1,\ldots,m,\ l = 1,\ldots,N_k \tag{35}$$

Approximation of multivariate functions

We will look for an approximate solution of problem (15) supposing that the control variables $z(\theta)$ are piece-wise constant functions $\tilde{z}(\theta)$ of the following form

$$\tilde{z}(\theta) = z_l \quad \text{if } \theta \in R_l^{(k)},\ l = 1,\ldots,N_k \tag{36}$$

where z_l is the vector of the control variables. Now searching for the optimal functions $z(\theta)$ is reduced to searching for the optimal values of the components z_{il}, $i = 1,\ldots,n_z$ of the vectors $\tilde{z}(\theta)$. If at each iteration $N_k = 1$, $k = 1,\ldots,r,\ldots$ then the method of solving the TSOPCC is transformed into the method of solving OSOPCC (14).

Approximation of the expected value of the objective function

When we solve problem (15) we have to calculate a multiple integral in order to find the expected value of the function $\tilde{f}(d, \tilde{z}(\theta), \theta)$. Calculating this integral exactly at each iteration leads to significant computational expenditures. Therefore we suggest an approach when at each iteration an approximation of this integral is improved. Let at the k-th iteration, the region T_θ be partitioned into N_k subregions (multidimensional rectangles) $R_r^{(k)}, r = 1,\ldots,N_k$ (see (19)). For the approximate calculation of the expected value of the function $f(d, \tilde{z}(\theta), \theta)$, we will use the piecewise linear approximation $\tilde{f}(d, \tilde{z}(\theta), \theta)$ of the function $f(d, \tilde{z}(\theta), \theta)$ of the following form

$$\tilde{f}(d, \tilde{z}(\theta), \theta) = \tilde{f}(d, z_r, \theta, \theta_r) \quad \text{if } \theta \in R_r^{(k)}\ r = 1,\ldots,N_k$$

where

$$\tilde{f}(d, z_r, \theta, \theta_r) = f(d, z_r, \theta_r) + \sum_{i=1}^{p} \frac{\partial f(d, z_r, \theta_r)}{\partial \theta_i} (\theta_i - \theta_{\text{ir}}) \tag{37}$$

the point θ_r is a linearization point in the subregion $R_r^{(k)}$, θ_{ir} is the i-th component of the vector θ_r. The right-hand side of formula (37) is the linear part of the Taylor's expansion of the function $f(d, z_r, \theta)$ at the point θ_r. Introduce the following designation

$$E_\theta[\tilde{f}(d, z_r, \theta, \theta^r); R_r^{(k)}] = \int_{R_r^{(k)}} \tilde{f}(d, z_r, \theta, \theta_r)\rho(\theta)d\theta$$

We showed (Ostrovsky et al.[22]) that the value $E[\tilde{f}(d, z_r, \theta); T_r^{(k)}]$ has the following form

$$E_\theta[\tilde{f}(d, z_r, \theta, \theta_r); R_r^{(k)}] = a_r f(d, z_r, \theta_r) + \sum_{i=1}^{p} \frac{\partial f(d, z_r, \theta_r)}{\partial \theta_i} (E_\theta[\theta_i; R_r^{(k)}] - a_r \theta_{\text{ir}}) \tag{38}$$

where

$$a_r = \int_{R_r^{(k)}} \rho(\theta)d\theta \quad E_\theta[\theta_i; R_r^{(k)}] = \int_{R_r^{(k)}} \theta_i \rho(\theta)d\theta \tag{39}$$

If we use the point $E_\theta[\theta_i; T]$ as a linearization point, then we have

$$E_\theta[\tilde{f}(d, z_r, \theta, \theta_r); R_r^{(k)}] = a_r f(d, z_r, \theta_r) + (1 - a_r) \sum_{i=1}^{p} \frac{\partial f(d, z_r, \theta_r)}{\partial \theta_i} E_\theta[\theta_i; R_r^{(k)}] \tag{40}$$

Since all the subregions $R_r^{(k)}$ do not have common points (see (20)), then the integral of the function $f(d, \tilde{z}(\theta), \theta)\ \rho(\theta)$ over the region T_θ is equal to the sum of the integrals of the function $f(d, z^r, \theta)\ \rho(\theta)$ over the regions $R_r^{(k)}$

$$\int_{T_\theta} f(d, \tilde{z}(\theta), \theta)\rho(\theta)d\theta = \sum_{r=1}^{N_k} \int_{R_r^{(k)}} f(d, z_r, \theta)\rho(\theta)d\theta \tag{41}$$

Introduce the following designation

$$E_\theta[f(d, z_r, \theta); R_r^{(k)}] = \int_{R_r^{(k)}} f(d, z_r, \theta)\rho(\theta)d\theta$$

Then Eq. 41 can be rewritten in the following form

$$E_\theta[f(d, \tilde{z}(\theta), \theta); T_\theta] = \sum_{r=1}^{N_k} E_\theta[f(d, z_r, \theta); R_r^{(k)}] \tag{42}$$

The value $E_\theta[\tilde{f}(d, z_r, \theta, \theta_r; R_r^{(k)}]$ is an approximation of the value $E_\theta[f(d, z_r, \theta); R_r^{(k)}]$.

Therefore, since equality (42) holds, the sum of the values $E_\theta[\tilde{f}(d, z_r, \theta, \theta_r); R_r^{(k)}]$ is an approximation of the value $E_\theta[f(d, \tilde{z}(\theta), \theta); T_\theta]$. Thus, the approximation $E_{\text{ap}}^{(k)}[f(d, \tilde{z}(\theta), \theta)]$ of the expected value of the function $f(d, \tilde{z}(\theta), \theta)$ has the following form

$$E_{\text{ap}}^{(k)}[f(d, \tilde{z}(\theta), \theta)] = \sum_{r=1}^{N_k} E_\theta[\tilde{f}(d, z_r, \theta, \theta_r); R_r^{(k)}] \tag{43}$$

Substituting $z(\theta)$ with $\tilde{z}(\theta)$ from (36), and using conditions (31), (35) we can transform problem (21) into the following form

$$f^{(k)} = \min_{d,z_l,T_{\alpha_j,l}} E_{\text{ap}}^{(k)}[f(d,\tilde{z}(\theta),\theta);T_\theta] \tag{44}$$

$$\max_{\theta\in T_{\alpha_j,l}} g_j(d,z_l,\theta) \le 0, \quad j=1,\ldots,m, \;\; l=1,\ldots,N_k$$

$$\sum_{l=1}^{N_k} \Pr\{\theta \in T_{\alpha_j,l}\} \ge \alpha_j, \quad j=1,\ldots,m, \tag{45}$$

$$T_{\alpha_j,l} \in R_l^{(k)}, \quad l=1,\ldots,N_k, \;\; j=1,\ldots,m \tag{46}$$

where $E_{\text{ap}}^{(k)}[f(d,\tilde{z}(\theta),\theta);T_\theta]$ is given by (43). Let $d^{(k)}, \tilde{z}(k)(\theta), T_{\alpha_j}^{(k)}, j=1,\ldots,m, f^{(k)}$ be the solution of problem (44), $f^{(k)} = E_{\text{ap}}^{(k)}[f(d^{(k)},\tilde{z}^{(k)}(\theta),\theta);T_\theta]$. This problem will be solved at the k-th iteration. Compare the solution of this problem with the solution of original problem (15). Substituting $z(\theta)$ with $\tilde{z}(\theta)$ from (36) and using conditions (31), (35) we can transform problem (24) into the following form

$$\tilde{f}^{(k)} = \min_{d,z_l,T_{\alpha_j,l}} E_\theta[f(d,\tilde{z}(\theta),\theta);T] \tag{47}$$

$$\max_{\theta\in T_{\alpha_j,l}} g_j(d,z_l,\theta) \le 0, \quad j=1,\ldots,m, \;\; l=1,\ldots,N_k$$

$$\sum_{l=1}^{N_k} \Pr\{\theta \in T_{\alpha_j,l}\} \ge \alpha_j, \;\; j=1,\ldots,m \tag{48}$$

$$T_{\alpha_j,l} \in R_l^{(k)}, \quad l=1,\ldots,N_k \quad j=1,\ldots,m.$$

Let $\tilde{d}^*, \tilde{z}^*(\theta), \tilde{T}_{\alpha_j}^*, j=1,\ldots,m, \tilde{f}^{(k)}$ be the solution of problem (47), $\tilde{f}^{(k)} = E_\theta[f(\tilde{d}^*,\tilde{z}^*(\theta),\theta);T]$.

Since problems (44) and (47) are obtained from problems (15) and (24) with the help of identical transformations (36) and (31), (35) we obtain using inequality (28)

$$\bar{f} \le \tilde{f}^{(k)} = E_\theta[f(\tilde{d}^*,\tilde{z}^*(\theta),\theta);T] \tag{49}$$

We will show that the solution of problem (44) produces an upper bound of the solution of problem (15) if the function $f(d,z,\theta)$ is concave with respect to variables θ_i. For the sake of simplicity, we prove this statement only for the first iteration and $N_1 = 1$. For concave functions, the following inequality holds[26]

$$f(d,z_1,\theta) \le f(d,z_1,\theta_1) + \sum_{i=1}^{p} \frac{\partial f(d,z_1,\theta_1)}{\partial\theta_i}(\theta_i - \theta_{i1}) \quad \forall\theta\in T$$

Hence, we have

$$E_\theta[f(d,z_1,\theta);T_\theta] \le a_1 f(d,z_1,\theta_1) + (1-a_1)\sum_{i=1}^{p} \frac{\partial f(d,z_1,\theta_1)}{\partial\theta_i} E_\theta[\theta_i;T_\theta] \tag{50}$$

Since $k=1$, $N_1=1$, we have $\tilde{z}(\theta)=z_1$. Using equality (43), we obtain

$$E[f(d,\tilde{z}(\theta),\theta);T_\theta] \le E_\theta[f(d,\tilde{z}(\theta),\theta_1) + (1-a_1)\sum_{i=1}^{p} \frac{\partial f(d,\tilde{z}(\theta),\theta_1)}{\partial\theta_i} E_\theta[\theta_i;T_\theta] = E_{\text{ap}}^{(1)}[f(d,\tilde{z}(\theta),T]$$

This inequality holds for any $d,\tilde{z}(\theta)$. Hence, the following inequality also holds $E[f(\tilde{d}^*,\tilde{z}^*(\theta),\theta);T] \le E_{\text{ap}}^{(1)}[f(d^{(k)}, \tilde{z}^{(k)}(\theta),\theta);T]$. From this inequality, we obtain

$$\bar{f} \le E[f(\tilde{d}^*,\tilde{z}^*(\theta),\theta);T] \le E_{\text{ap}}^{(1)}[f(d^{(k)},\tilde{z}^{(k)}(\theta),\theta);T] = f^{(k)}$$

Thus, the solution of problem (44) produces an upper bound of the solution of problem (15) if the function $f(d,z,\theta)$ is concave with respect to variables θ.

Approximate Method of Solving the TSOPCC; Case of Independent Uncertain Parameters

We suppose that the uncertain parameters θ_i are mutually independent, random variables having the normal distribution. In this case[27]

$$\rho(\theta) = \rho(\theta_1)\rho(\theta_2)\ldots\rho(\theta_p) \tag{51}$$

where the function $\rho_i(\theta_i)$ is the probability density function of the random parameter θ_i. We will use the following form of the uncertainty region T_θ: $T_\theta = \{\theta_i : \theta_i^L \le \theta_i \le \theta_i^U, i=1,\ldots,p\}$. The values $\theta_i^L, \theta_i^U, i=1,\ldots,p$ have the following form $\theta_i^L = E[\theta_i] - k_i\sigma_i$, $\theta_i^U = E[\theta_i] + k_i\sigma_i$, where $E[\theta_i]$ and $(\sigma_i)^2$ are the expected value and variance of the random parameter θ_i, respectively, k_i, is a coefficient. It is clear that the region T_θ is a multidimensional rectangle. If the values k_i, $i=1,\ldots,p$ are large enough, then the probability measure of the region T_θ is close to 1. Let us consider the aforementioned approximations in details.

Approximation of the region T_{α_j}

We will suppose that the regions $T_{\alpha_j,l}$ have the form of multidimensional rectangle

$$T_{\alpha_j,l} = \{\theta_i : \theta_{ijl}^L \le \theta_i \le \theta_{ijl}^U, i=1,\ldots,p\} \;\; j=1,\ldots,m \tag{52}$$

As we will see later such form of the regions $T_{\alpha_j,l}$ allows simple transformation of chance constraints (48) into deterministic ones. In this case the form and location of the region $T_{\alpha_j}^l$ are specified by the variables $\theta_{ijl}^L, \theta_{ijl}^U$, $i=1,\ldots,p$. Therefore, the search for the optimal forms and locations of the regions T_{α_j}, $j=1,\ldots,m$ is reduced to the search for the optimal values of the upper and lower bounds $\theta_{ijl}^L, \theta_{ijl}^U$ of sides of the multidimensional rectangles $T_{\alpha_j,l}$. It is easy to see that conditions (46) are equivalent to the following conditions

$$\theta_{il}^{(k)L} \le \theta_{ijl}^L, \; \theta_{ijl}^U, \le \theta_{il}^{(k)U}, \quad i=1,\ldots,p, \; l=1,\ldots,N_k, \; j=1,\ldots,m \tag{53}$$

Let us transform chance constraints (45) into deterministic ones. Since all the parameters θ_i have the normal distribution, the probability measure of the interval $[\theta_{ijl}^L \le \theta_i \le \theta_{ijl}^U]$ is equal to

$$I_{ijl} = \int_{\theta_{ijl}^L}^{\theta_{ijl}^U} \rho(\theta_i)d\theta_i \tag{54}$$

Let us make the following variable change in integral (54)

$$\vartheta_i = (\theta_i - E[\theta_i])(\sigma_i)^{-1} \tag{55}$$

Using (3) and making simple transformations we obtain

$$I_{ijl} = \int_{\vartheta_{ijl}^L}^{\vartheta_{ijl}^U} \rho(\vartheta_i)d\vartheta_i$$

where

$$\vartheta_{ijl}^L = (\theta_{ijl}^L - E[\theta_i])(\sigma_i)^{-1}, \quad \vartheta_{ijl}^U = (\theta_{ijl}^U - E[\theta_i])(\sigma_i)^{-1} \tag{56}$$

$$\rho(\vartheta_i) = (2\pi)^{-0.5}\exp\left[-0.5\vartheta_i^2\right]$$

Using expression for a definite integral

$$\Phi(\bar{\vartheta}) = \int_{-\infty}^{\bar{\vartheta}} \rho(\vartheta) d\vartheta$$

we obtain finally

$$I_{ijl} = \Phi(\vartheta_{ijl}^U) - \Phi(\vartheta_{ijl}^L). \tag{57}$$

The function $\Phi(\bar{\vartheta})$ is the standard normal distribution function. There is the table of values of the function $\Phi(\bar{\vartheta})$.[26] Therefore the use of the formulae (57) permits to avoid numerical integration for calculation of I_{ijl}. Since all the parameters θ_i are independent, the probability measure of the rectangle $T_{\alpha_j,l}$ is equal to the product of the probability measures of the intervals $[\theta_{ijl}^L \le \theta_i \le \theta_{ijl}^U]$, $i = 1, \ldots, p$

$$\Pr\{\theta \in T_{\alpha_j,l}^l\} = \prod_{i=1}^{p} [\Phi(\vartheta_{ijl}^U) - \Phi((\vartheta_{ijl}^L)] \tag{58}$$

Substituting the expressions for $\Pr\{\theta \in T_{\alpha_j,l}\}$ from (58) into (48), we obtain

$$\Pr\{\theta \in \tilde{T}_{\alpha_j}^{(k)}\} = \sum_{l=1}^{N_k} \prod_{i=1}^{p} [\Phi(\vartheta_{ijl}^U) - \Phi(\vartheta_{ijl}^L)] \tag{59}$$

Approximation of the expected value of the objective function

For the calculation of the expected value of the objective function we will use expression (43). To calculate the values a_r and $E[\theta_i; T_r^{(k)}]$ in expression (38) we must calculate $2N_k$ multivariate integrals (39). One can significantly simplify the calculation of these values. Indeed, it is clear that a_r is the probability measure of the region $T_r^{(k)}$

$$a_r = \Pr[\theta \in T_r^{(k)}] \tag{60}$$

Taking into account the independence of the uncertain parameters θ_i, $i = 1, \ldots, p$ and using formulae (58), we obtain

$$a_r = [\Phi(\vartheta_{1jr}^U) - \Phi(\vartheta_{1jr}^L)][\Phi(\vartheta_{2jr}^U) - \Phi(\vartheta_{2jr}^L)] \ldots [\Phi(\vartheta_{pjr}^U) - \Phi(\vartheta_{pjr}^L)]$$

Transform the expression $E[\theta_i; T_r^{(k)}]$ (see (39)). Substitute in (39) the expression for $\rho(\theta)$ from (51)

$$E[\theta_i; T_r^{(k)}] = \int_{\theta_{1r}^L}^{\theta_{1r}^U} \int_{\theta_{2r}^L}^{\theta_{2r}^U} \ldots \int_{\theta_{pr}^L}^{\theta_{pr}^U} \theta_i \rho(\theta_1)\rho(\theta_2)\ldots$$
$$\rho(\theta_i)\ldots\rho(\theta_i) d\theta_1 d\theta_2 \ldots d\theta_p = I_{1r}\ldots I_{ir}\ldots I_{pr}$$

where

$$I_{1r} = \int_{\theta_{1r}^L}^{\theta_{1r}^U} \rho(\theta_1) d\theta_1, I_{2r} = \int_{\theta_{2r}^L}^{\theta_{2r}^U} \rho(\theta_2) d\theta_2, \ldots I_{ir}$$
$$= \int_{\theta_{ir}^L}^{\theta_{ir}^U} \theta_i \rho(\theta_i) d\theta_i, \ldots, I_{pr} = \int_{\theta_{pr}^L}^{\theta_{pr}^U} \rho(\theta_p) d\theta_p.$$

Above we have obtained the expression for integral $I_{sr}, (s \ne i)$ (see (57)). Using these expressions we can obtain the following expression for $E[\theta_i; T_r^{(k)}]$.

$$E[\theta_i; T_r^{(k)}] = I_{r,(1,i-1)} \left(\int_{\theta_{ir}^L}^{\theta_{ir}^U} \theta_i \rho(\theta_i) d\theta_i \right) I_{r,(i+1,p)}$$

where

$$I_{r,(1,i-1)} = [\Phi(\vartheta_{1r}^U) - \Phi(\vartheta_{1r}^L)] \ldots [\Phi(\vartheta_{i-1,r}^U) - \Phi(\vartheta_{i-1,r}^L)]$$
$$I_{r,(1,i+1)} = [\Phi(\vartheta_{i+1,r}^U) - \Phi(\vartheta_{i+1,r}^L)] \ldots [\Phi(\vartheta_{pr}^U) - \Phi(\vartheta_{pr}^L)]$$

For the calculation of N_k values $E[\theta_i; T_r^{(k)}]$, we must calculate the following N_k univariate integrals

$$\int_{\theta_{ir}^L}^{\theta_{ir}^U} \theta_i \rho(\theta_i) d\theta_i \tag{61}$$

It is clear that calculating univariate integral (61) is significantly simpler than calculating multivariate integral (see (39)). Moreover, one can avoid the calculation of univariate integrals if the following function is tabulated beforehand

$$G(\bar{\vartheta}) = \int_{-\infty}^{\bar{\vartheta}} \vartheta \rho(\vartheta) d\vartheta$$

where ϑ is a random variable having standard normal distribution. Indeed, by making variable change (55) one can express a value of integral (61) with help of the function $G(\bar{\vartheta})$.

Let us replace in problem (44) $\Pr\{\theta \in \tilde{T}_{\alpha_j}^{(k)}\}$ by its expression from (59) and conditions (46) by conditions (53). Then problem (44) takes the following form

$$f^{(k)} = \min_{d, z_l, \theta_{ijl}^L, \theta_{ijl}^U} E_{\text{ap}}^{(k)}[f(d, \tilde{z}(\theta), \theta); T_\theta] \tag{62}$$

$$\max_{\theta \in T_{\alpha_j,l}} g_j(d, z_l, \theta) \le 0, \quad j = 1, \ldots, m,\ l = 1, \ldots, N_k,\ j = 1, \ldots, m$$

$$\sum_{l=1}^{N_k} \prod_{i=1}^{p} [\Phi(\vartheta_{ijl}^U) - \Phi(\vartheta_{ijl}^L)]\} \ge \alpha_j, \quad j = 1, \ldots, m, \tag{63}$$
$$\theta_{il}^{(k)L} \le \theta_{ilj}^L, \quad i = 1, \ldots, p,\ l = 1, \ldots, N_k,\ j = 1, \ldots, m$$
$$\theta_{ilj}^U \le \theta_{il}^{(k)U}, \quad i = 1, \ldots, p,\ l = 1, \ldots, N_k,\ j = 1, \ldots, m$$

where $E_{\text{ap}}^{(k)}[f(d, z^{(k)}(\theta), \theta); T]$ is given by (43), $\vartheta_{ijl}^L = (\theta_{ilj}^L - E[\theta_i])(\sigma_i)^{-1}$, $\vartheta_{ijl}^U = (\theta_{ilj}^U - E[\theta_i])(\sigma_i)^{-1}$. In this problem, the values $\theta_{il}^{(k)L}$, $\theta_{il}^{(k)U}$ are constant at the k-th iteration. Note that the system of inequalities (63) consists of N_k groups and the l-th group corresponds to the l-th subregion $R_l^{(k)}$. Each of these N_k groups consists of m inequalities. Problem (62) is a semi-infinite programming problem. To solve it we can use the outer approximations method.[28] It is easy to see that $2p$ search variables $\theta_{ijl}^U, \theta_{ijl}^L$, $i = 1, \ldots, p$ correspond to one subregion $T_{\alpha_j,l}$ for fixed j and l. Consequently, problem (62) has $n_d + n_z N_k + 2\text{p}N_k$ search variables: d, z, $\theta_{ijl}^U, \theta_{ijl}^L$. n_d is a dimensionality of the vector d, n_z is a dimensionality of the vector z. Thus, a number of search variables increases proportionally to a number of subregions $R_l^{(k)}$. The dimensionality of

problem (62) can become very large if n_z, p, N_k are large. For example, for a comparatively small problem with $n_d = 5$, $n_z = 5$, $p = 10$ and N_k subregions ($N_k = 8$) the number of search variables will be equal to 205. The use of usual algorithms of nonlinear programming methods can require significant computational time, therefore it is necessary to develop additional means of decreasing it. There are three ways to decrease significantly computational time of solving problem (62):

1. Problem (62) has a sparse structure. Indeed, constraints (63) for fixed $l = \bar{l}$ depend explicitly only on the variables $d, z_{\bar{l}}$, $\theta^U_{ij\bar{l}}, \theta^L_{ij\bar{l}}$ and do not depend on the variables z_l, $\theta^U_{ijl}, \theta^L_{ijl}$, $(l \neq \bar{l})$. Therefore, the use of sparse nonlinear optimization algorithms[29,30] that take into account the sparse structure of an optimization problem can significantly decrease computational time.

2. The outer approximations algorithm requires repeated solutions of nonlinear programming problems. We use the sequential quadratic programming for solving these problems. However, these algorithms require significant computational time for calculation (by differences) of gradients of the objective function and the left-hand sides of constraints. The use of the "conjugate process" method to calculate the gradients can significantly decrease computational time.[31]

3. The use of a family of orthogonal functions for approximation of the expected value of the objective function can decrease a number of subregions $R^{(k)}_l$

Designate initial and optimal values (the solution of problem (62)) of the search variables and the objective function at the k-th iteration as $(d^{(k)})^0, (z^{l,(k)})^0$, $(\theta_i^{(k),L,j,l})^0$, $l = 1, \ldots, N_k$, $f^{(k)0} = E^{(k)}_{ap}[f((d^{(k)})^0, (\tilde{z}^{(k)}(\theta))^0, \theta)]$ and $d^{(k)}$, $z^{(k)}_l$, $\theta^{(k)L}_{ijl}$, $\theta^{(k)U}_{ijl}$, $l = 1, \ldots, N_k$, $f^{(k)} = E^{(k)}_{ap}[f((d^{(k)})^*, (\tilde{z}^{(k)}(\theta))^*, \theta)]$, respectively. Similarly, designate initial and optimal forms of the regions $T_{\alpha_j,l}$, $j = 1, \ldots, m$ as $(T^{(k)}_{\alpha_j,l})^0$, and $T^{(k)}_{\alpha_j,l}$, respectively.

In the case of solving an OSOPCC control variables do not depend on θ and we have $z_l = z$ $l = 1, \ldots, N_k$. In this case, problem (62) has the following form

$$f^{(k)} = \min_{d,z,\theta^L_{ijl},\theta^U_{ijl}} E^{(k)}_{ap}[f(d,z,\theta);T]$$

$$\max_{\theta \in T_{\alpha_j,l}} g_j(d,z,\theta) \leq 0, \quad j = 1, \ldots, m, \quad l = 1, \ldots, N_k$$

$$\sum_{l=1}^{N_k} \prod_{i=1}^{p} [\Phi(\vartheta^U_{ijl}) - \Phi(\vartheta^L_{ijl})]\} \geq \alpha_j, \quad j = 1, \ldots, m$$

$$\theta^{(k)L}_{il} \leq \theta^L_{ilj}, \quad i = 1, \ldots, p, \ l = 1, \ldots, N_k, j = 1, \ldots, m$$

$$\theta^U_{ilj} \leq \theta^{(k)U}_{il}, \quad i = 1, \ldots, p, \ l = 1, \ldots, N_k, j = 1, \ldots, m$$

Partition of the Subregions $R^{(k)}_q$

The iteration procedure is based on a partition of the uncertainty region. The aim of the partition is an improvement of the approximation of the regions T_{α_j}, multivariate functions $z(\theta)$, and the expected value of a goal function $f(d, z(\theta), \theta)$. Consider at first a technique of partition of the regions $R^{(k)}_l$. Suppose the region $R^{(k)}_{l_k}$ should be partitioned. This region is partitioned into two regions $R^{(k+1)}_{p_k}$ and $R^{(k+1)}_{q_k}$ $(R_{l_k} = R^{(k+1)}_{p_k} \cup R^{(k+1)}_{q_k})$ as follows

$$R^{(k+1)}_{p_k} = \{\theta : \theta \in R^{(k)}_{l_k}, \theta_s \leq c^{(k)}_{\mathrm{sp}_k}\}, R^{(k+1)}_{q_k} = \{\theta : \theta \in R^{(k)}_{l_k}, \theta_s \geq c^{(k)}_{\mathrm{sp}_k}\} \quad (64)$$

Here, θ_s and $c^{(k)}_{\mathrm{sl}}$ are referred to as a *splitting variable* and a *splitting point*. Thus, we partition the region $R^{(k)}_{l_k}$ with the help of a hyperplane $\theta_s = c^{(k)}_{\mathrm{sp}_k}$. At the following iterations the value $c^{(k)}_{\mathrm{sp}_k}$ does not change. Thus, to execute a partition we should select a subregion which must be partitioned, a splitting variable and a splitting point. We will select these values to improve the solution obtained at the k-th iteration. For the sake of simplicity we will suppose that at each iteration only one subregion $R^{(k)}_l$ will be partitioned. Suppose we solved problem (62) at the k-th iteration. Designate the solution of problem (62) as $d^{(k)}$, $\tilde{z}^{(k)}$, $\theta^{(k)}_{ijl}$, $\theta^{(k)}_{ijl}$, $j = 1, \ldots, m$. We will call the p-th constraint (63) in the region $R^{(k)}_q$ active if the following equality holds

$$\max_{\theta \in T^{(k)}_{\alpha pq}} g_j(d^{(k)}, \tilde{z}^{(k)}, \theta) = 0$$

Later on we will call the subregion $T^{(k)}_{\alpha_j l}$ *active* if a group of constraints (63) corresponding to this region contains the active constraints and the region $R^{(k)}_l$ *active* if it contains at least one active subregion $T^{(k)}_{\alpha_j l}$. Consider a heuristic rule of selection of a subregion which must be partitioned. In Statement A2, we show that removal of active constraints generally speaking improves the obtained optimal solution. Therefore, we will partition one of the subregions $R^{(k)}_l$ with at least one corresponding active subregion $T^{(k)}_{\alpha_j l}$. In addition, we should partition the subregion $R^{(k)}_l$ in such a way that at least one active subregion $T^{(k)}_{\alpha_j s}$ (belonging to $R^{(k)}_l$) is partitioned. It is clear that if we partition an active subregion $T^{(k)}_{\alpha_j l}$ (belonging to $R^{(k)}_l$) we remove all constraints which are active at the k-th iteration and correspond to the subregion $T^{(k)}_{\alpha_j s}$. Suppose $S^{(k)}$ is a set of active subregions $R^{(k)}_l$ at the k-th iteration. To select a region from the set $S^{(k)}$ for partition we can use the following heuristic rule. We will partition the subregion where the *approximation quality* of the function $f(d,z,\theta)$ by the function $\tilde{f}(d,z,\theta,\theta_q)$ (see (37)) will be the worst. The approximation quality will be defined by the value μ_q

$$\mu_q = \max_{\theta \in R^{(k)}_q} (f(d^{(k)}, z_q, \theta) - \tilde{f}(d^{(k)}, z_q, \theta, \theta_q))^2 \quad (65)$$

Thus, the region $R^{(k)}_s$ is selected for partition if:

1. It contains at least one active subregion $T^{(k)}_{\alpha_j l}$.
2. *Approximation quality* of the function $f(d, z_s, \theta)$ by the function $\widehat{f}\ (d, z_s, \theta, \theta_s)$ is the worst, that is, $\mu_s \geq \mu_l, \forall R^{(k)}_l \in S^{(k)}$ (see (65)).

Consider now the rule of selection of the splitting variable. We will use the following rule: each component of the vector θ will be used in turn as a splitting variable.

The splitting point will be selected as follows. Suppose we have to partition the subregion $R^{(k)}_s$. We have already noted that removal of active constraints, generally speaking, improves the obtained optimal solution Therefore, one must select such value $c^{(k)}_{rs}$ as the splitting point that hyperplane $\theta_r = c^{(k)}_{rs}$ partitions the largest number of the active regions $T^{(k)}_{\alpha_j l}$ belonging to the region $R^{(k)}_l$.

Consider the relationship between the search variables at the k-th and $(k+1)$-th iterations. We will use the following rule: the values of the search variables obtained at the k-th iteration will be initial values of this variables at the $(k+1)$-th iteration. Thus, we have

$$(d^{(k+1)})^0 = d^{(k)} \quad (66)$$

Designate the set of the regions $T^{(k)}_{\alpha_j l}$ that are partitioned at the k-th iteration as $\mathrm{T}^{(k)}$ and the set of the regions $T^{(k)}_{\alpha_j l}$ that are not

partitioned at the k-th iteration as $\bar{\mathrm{T}}^{(k)}$. If a region $T_{\alpha_j l}^{(k)}$ belongs to the set $\bar{\mathrm{T}}^{(k)}$, then the initial form $(T_{\alpha_j l}^{(k+1)})^0$ of the region $T_{\alpha_j l}$ at the iteration $(k+1)$ will be the same as $T_{\alpha_j l}^{(k)}$ and the values of the search variables $z_l^{(k)}$ obtained at the k-th iteration will be initial values of these variables at the $(k+1)$-th iteration

$$(z_l^{(k+1)})^0 = z_l^{(k)}, \quad T_{\alpha_j l}^{(k)} \in \bar{\mathrm{T}}^{(k)} \tag{67}$$

$$(T_{\alpha_j l}^{(k+1)})^0 = T_{\alpha_j l}^{(k)}, \quad T_{\alpha_j l}^{(k)} \in \bar{\mathrm{T}}^{(k)} \tag{68}$$

Suppose the region $T_{\alpha_j l}^{(k)}$ belongs to the set $\mathrm{T}^{(k)}$. In this case the region $T_{\alpha_j l}^{(k)}$ is partitioned into two subregions: $T_{\alpha_j p_k}^{(k+1)}$ and $T_{\alpha_j q_k}^{(k+1)}$. The initial values of these variables $z_{p_k}^{(k+1)}$, $z_{q_k}^{(k+1)}$ at the $(k+1)$-th iteration will be equal to $z_{l_k}^{(k)}$

$$(z_{p_k}^{(k+1)})^0 = (z_{q_k}^{(k+1)})^0 = z_{l_k}^{(k)} \quad \forall T_{\alpha_j l}^{(k)} \in \mathrm{T}^{(k)} \tag{69}$$

The initial forms $(T_{\alpha_j p_k}^{(k+1)})^0$ and $(T_{\alpha_j q_k}^{(k+1)})^0$ of the regions $T_{\alpha_j p_k}$ and $T_{\alpha_j q_k}$ at the $(k+1)$-th iteration are linked with the region $T_{\alpha_j l}^{(k)}$ by the following relation

$$T_{\alpha_j l}^{(k)} = (T_{\alpha_j p_k}^{(k+1)})^0 \cup (T_{\alpha_j q_k}^{(k+1)})^0 \quad \forall T_{\alpha_j l}^{(k)} \in \mathrm{T}^{(k)} \tag{70}$$

Using this relation and the equation of a straight line $\theta_r = c_{rl}^{(k)}$ it is easy to obtain the equations relating the initial values of the variables θ_{ijl}^L, θ_{ijl}^U at the $(k+1)$-th iteration and the optimal values of these variables at the k-th iteration. Below we will consider an example of this operation.

Let us illustrate this consideration with the help of Figure 1. Suppose that the number of constraints that are inequalities is equal to 2. Here, the region $A_1A_2A_3A_4$ is the uncertainty region. Suppose at the first iteration we partitioned the uncertainty region into two subregions $R_1^{(2)}$ (the region A_1A_2BC) and $R_2^{(2)}$ (the region CBA_3A_4) with the help of a straight line $\theta_1 = c_1^{(1),1}$. The regions $A_5A_6A_7A_8$ and $A_9A_{10}A_{11}A_{12}$ are the optimal regions $T_{\alpha_1}^{(1),1}$ and $T_{\alpha_2}^{(1),2}$ that correspond to the region $R_2^{(2)}$. Suppose that at the second iteration we partition the subregion $R_2^{(2)}$ and the variable θ_2 is the splitting variable. Let us consider three cases

1. Both regions $T_{\alpha_1 1}^{(1)}$ and $T_{\alpha_2 2}^{(1)}$ are active
2. The region $T_{\alpha_1 1}^{(1)}$ is active and the region $T_{\alpha_2 2}^{(1)}$ is not active
3. The region $T_{\alpha_2 2}^{(1)}$ is active and the region $T_{\alpha_1 1}^{(1)}$ is not active

In the first case, it is reasonable to select any point in the interval DE as a splitting point $c_{2,2}^{(2)}$ since in this case the straight line $\theta_2 = c_{2,2}^{(2)}$ partitions both regions $T_{\alpha_1 1}^{(1)}$ and $T_{\alpha_2 2}^{(1)}$. Suppose that the straight line FG (the designation of interval in Figure 1) corresponds to the straight line $\theta_2 = c_{2,2}^{(2)}$, this straight line partitions the region $R_2^{(2)}$ into two subregions $R_1^{(3)}$ (the region FBA_3G) and $R_2^{(3)}$ (the region CFGA_4). Besides, the straight line FG partitions the regions $T_{\alpha_1 1}^{(1)}$ and $T_{\alpha_2 2}^{(1)}$ into two subregions each: HA_6A_7J, A_5HJA_8 and L$A_{10}A_{11}M$, A_9LMA_{12}, respectively. When solving problem (63) at the third iteration, the subregions HA_6A_7J and L$A_{10}A_{11}M$ belong to the $R_1^{(3)}$ (the region FBA_3G) and subregions A_5HJA_8 and A_9LMA_{12} belong to the $R_2^{(3)}$ (the region CFGA_4). The subregions HA_6A_7J and L$A_{10}A_{11}M$ will be used as initial forms of the regions $T_{\alpha_1 1}^{(3)}$, $T_{\alpha_2 1}^{(3)}$, respectively, the subregions A_5HJA_8 and A_9LMA_{12} will be used as initial forms of the regions $T_{\alpha_1 2}^{(3)}$, $T_{\alpha_2 2}^{(3)}$, respectively. At the third iteration, the approximation $\tilde{T}_{\alpha_1}^{(3)}$ of the region $T_{\alpha_1}^*$ has the following form

$$\tilde{T}_{\alpha_1}^{(3)} = T_{\alpha_1 1}^{(3)} \cup T_{\alpha_1 2}^{(3)}$$

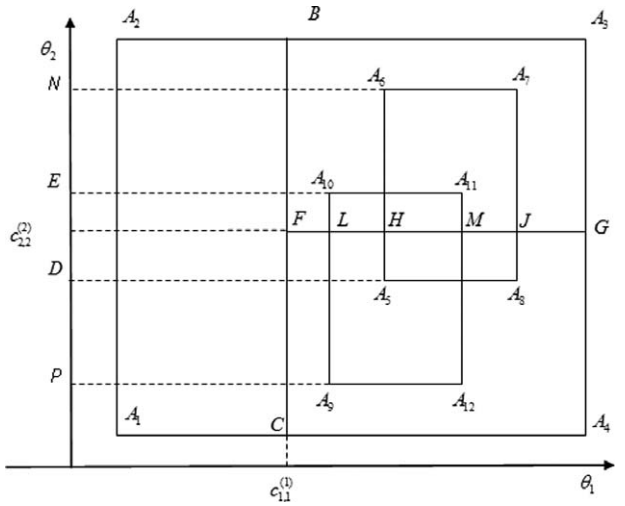

Figure 1. Illustration of the rule of selection of a splitting point.

and the approximation $\tilde{T}_{\alpha_2}^{(3)}$ of the region $T_{\alpha_2}^*$ has the following form

$$\tilde{T}_{\alpha_2}^{(3)} = T_{\alpha_2 1}^{(3)} \cup T_{\alpha_2 2}^{(3)}$$

In the second case, it is reasonable to partition only the region $T_{\alpha_1 1}^{(1)}$ and not to partition the region $T_{\alpha_2 2}^{(1)}$. In this case, one must select any point in the interval EN as the splitting point $c_{2,2}^{(2)}$ since in this case the straight line $\theta_2 = c_{2,2}^{(2)}$ partitions only region $T_{\alpha_1 1}^{(1)}$ and does not partition the region $T_{\alpha_2}^{2*}$. In the third case, one must select any point in the interval DP as the splitting point $c_{2,2}^{(2)}$ since in this case the straight line $\theta_2 = c_{2,2}^{(2)}$ partitions only region $T_{\alpha_2 2}^{(1)}$ and does not partition the region $T_{\alpha_1 1}^{(1)}$. We will call this approach an iteration procedure with *the fixed partition structure*.

Variable partition structure

The iteration procedure with *the fixed partition structure* has the following drawback: we select the splitting variables and splitting points arbitrarily and the values $c_{\mathrm{rl}}^{(k)}$ selected at the k-th iteration are constant at all following iterations. It is not very good since the selection of the values $c_{rl}^{(k)}$ can strongly impact the velocity of convergence of the iteration procedure. To overcome this drawback, we will include the values $c_{rl}^{(k)}$ in the set of the search variables. In this case, the values $\theta_{il}^{(k)L}$, $\theta_{il}^{(k)U}$ are added to the search variables. In addition, as before, we will use each component of the vector θ in turn as a splitting variable. Besides, we should add to problem (62) equations characterizing the connection of the variables $c_{rl}^{(k)}$ with the variables $\theta_{il}^{(k)L}, \theta_{il}^{(k)U}$.

Let us illustrate this consideration with the example of a CP with two uncertain parameters (Figure 2). Here the region ABCD is an uncertainty region. Let $R_1^{(1)}$ coincide with the region ABCD. Suppose at the first iteration the parameter θ_1 is a splitting variable and $c_{1,1}^{(1)}$ is a splitting point. Thus, at the second iteration we will have two regions—$R_1^{(2)}$ (ABEF) and $R_2^{(2)}$ (EFCD). Suppose at the second iteration we have to partition the region $R_1^{(2)}$ using θ_2 as a spitting variable and $c_{2,2}^{(2)}$ as a splitting point. Thus, at the third iteration we will have three regions—$R_1^{(3)}$ (AGHF), $R_2^{(3)}$ (GBEH) and $R_3^{(3)}$ (FECD). These regions have the following forms

$$R_1^{(3)} = \{\theta : \theta_{1,1}^{(3)L} \le \theta_1 \le \theta_{1,1}^{(3)U}, \theta_{2,1}^{(3)L} \le \theta_2 \le \theta_{2,1}^{(3)U}\} \tag{71}$$

$$R_2^{(3)} = \{\theta : \theta_{1,2}^{(3)L} \le \theta_1 \le \theta_{1,2}^{(3)U}; \theta_{2,2}^{(3)L} \le \theta_2 \le \theta_{2,2}^{(3)U}\} \tag{72}$$

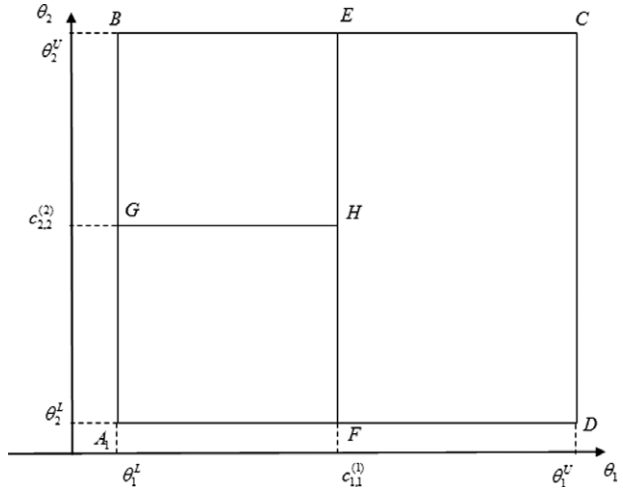

Figure 2. Illustration of the case when elements of the matrix *C* are search variables.

$$R_3^{(3)} = \{\theta : \theta_{1,3}^{(3)L} \le \theta_1 \le \theta_{1,3}^{(3)U}; \theta_{2,3}^{(3)L} \le \theta_2 \le \theta_{2,3}^{(3)U}\},\ i = 1, \ldots, p \tag{73}$$

where

$$\theta_{1,1}^{(3)L} = \theta_1^L; \theta_{1,1}^{(3)U} = \mathrm{c}_{1,1}^{(1)}; \theta_{2,1}^{(3)\mathrm{L}} = \theta_2^{\mathrm{L}}; \theta_{2,1}^{(3)\mathrm{U}} = c_{2,2}^{(2)}$$
$$\theta_{1,2}^{(3)L} = \theta_1^L; \theta_{1,2}^{(3)U} = \mathrm{c}_{1,1}^{(1)}; \theta_{2,2}^{(3)\mathrm{L}} = c_{2,2}^{(2)}; \theta_{2,2}^{(3)U} = \theta_2^U$$
$$\theta_{1,3}^{(3)L} = c_{1,1}^{(1)}; \theta_{1,3}^{(3)U} = \theta_1^{\mathrm{U}}; \theta_{2,1}^{(3)\mathrm{L}} = \theta_2^{\mathrm{L}}; \theta_{2,1}^{(3)\mathrm{U}} = \theta_2^{\mathrm{U}}$$

Then the following equalities hold

$$\theta_{1,1}^{(3)U} = \theta_{1,2}^{(3)U} = \theta_{1,3}^{(3)\mathrm{L}} = \mathrm{c}_{1,1}^{(1)} \tag{74}$$

$$\theta_{2,1}^{(3)U} = \theta_{2,2}^{(3)L} = c_{2,2}^{(2)} \tag{75}$$

Since here the parameters $\mathrm{c}_{1,1}^{(1)}$, $c_{2,2}^{(2)}$ are the new search variables, the parameters $\theta_{1,1}^{(3)U}\theta_{1,2}^{(3)U}$, $\theta_{1,3}^{(3)L}$, $\theta_{2,1}^{(3)U}$, $\theta_{2,2}^{(3)L}$ become new search variables. Similarly, in the general case at the k-th iteration some values $\theta_{il}^{(k)L}, \theta_{il}^{(k)U}, i = 1, \ldots, p$ become search variables. Thus, problem (63) will have the following form

$$f^{(k)} = \min_{d, z_l, \theta_{ijl}^L, \theta_{ijl}^U, c_i^{(k)}} E_{ap}^{(k)}[f(d, \tilde{z}(\theta), \theta); T] \tag{76}$$

$$\max_{\theta \in T_{z_jl}} g_j(d, z_l, \theta) \le 0, \quad j = 1, \ldots, m,\ l = 1, \ldots, N_k$$
$$\sum_{l=1}^{N_k} \prod_{i=1}^{p} [\Phi(\vartheta_{ijl}^U) - \Phi(\vartheta_{ijl}^L)]\} \ge \alpha_j, \quad j = 1, \ldots, m$$
$$\theta_{il}^{(k)L} \le \theta_{ijl}^L, \quad i = 1, \ldots, p, l = 1, \ldots, N_k, j = 1, \ldots, m$$
$$\theta_{ijl}^U \le \theta_{il}^{(k)U}, \quad i = 1, \ldots, p, l = 1, \ldots, N_k, j = 1, \ldots, m,\ i = 1, \ldots, p$$
$$\theta_{il}^{(k)U} \le \theta_i^U, \quad \theta_i^L \le \theta_{il}^{(k)L},\ i = 1, \ldots, p$$

$$\mathrm{c}_{i_r l}^{(r)} = \theta_{i_r l}^{(k)L}, \quad l \in S_r^{(k)L},\ r = 1, \ldots, k-1 \tag{77}$$

$$\mathrm{c}_{i_r l}^{(r)} = \theta_{i_r l}^{(k)U}, \quad l \in S_r^{(k),U},\ r = 1, \ldots, k-1 \tag{78}$$

$$\theta_i^L \le \mathrm{c}_{i_r l}^{(r)} \le \theta_i^U, \quad i = 1, \ldots, p$$

where $S_r^{(k)L}$ is a set of indexes of lower bounds $\theta_{i_r l}^{(k)L}$ that became variables since the values $\mathrm{c}_{il}^{(k)}$ became search variables, $S_r^{(k),U}$ is a set of indexes of upper bounds $\theta_{i_r l}^{(k)U}$ that became variables when the values $\mathrm{c}_{il}^{(k)}$ became search variables, equalities (77), (78) represent the relationship of the variables $\mathrm{c}_{il}^{(k)}$ with the corresponding upper and lower bounds of the regions $R_l^{(k)}$. For the example considered above, they have form (74), (75).

Now let us compare these approaches. Suppose we use the approach with the fixed partition structure. Then at the first iteration we can use either θ_1 or θ_2 as the splitting variable. Suppose at the first iteration θ_1 is the splitting variable and $c_{1,1}^{(1)}$ is the splitting point; then at the second iteration the set $R^{(2)}$ will consist of the following subregions $R_1^{(2)} = \{\theta : \theta_1^L \le \theta_1 \le c_{1,1}^{(1)}, \theta_2^L \le \theta_2 \le \theta_2^U\}$ and $R_2^{(2)} = \{\theta : c_{1,1}^{(1)} \le \theta_1 \le \theta_1^U, \theta_2^L \le \theta_2 \le \theta_2^U\}$. Now let θ_2 be the splitting variable and $c_{2,1}^{(1)}$ be the splitting point at the first iteration; then at the second iteration the region $R^{(2)}$ will consist of the subregions $R_1^{(2)} = \{\theta : \theta_1^L \le \theta_1 \le \theta_1^U, \theta_2^L \le \theta_2 \le c_{2,1}^{(1)}\}$ and $R_2^{(2)} = \{\theta : \theta_1^L \le \theta_1 \le \theta_1^U, c_{2,1}^{(1)} \le \theta_2 \le \theta_2^U\}$. It is clear that we do not know beforehand which variable should be selected as a splitting variable, since we do not know which one will make the iteration procedure converge faster.

Let us now use the approach with a variable partition structure. At the third iteration the set $R^{(3)}$ will consist of three subregions $R_1^{(3)}$ (AGHF), $R_2^{(3)}$ (GBEH) and $R_3^{(3)}$ (FECD) (see Figure 2).

$$R_1^{(3)} = \{\theta : \theta_1^L \le \theta_1 \le c_{1,1}^{(1)}, \theta_2^L \le \theta_2 \le c_{2,2}^{(2)}\},$$
$$R_2^{(3)} = \{\theta : \theta_1^L \le \theta_1 \le c_{1,1}^{(1)}; c_{2,2}^{(2)} \le \theta_2 \le \theta_2^U\}$$

Since the parameters $\mathrm{c}_{1,1}^{(1)}$, $\mathrm{c}_{2,2}^{(2)}$ are the search variables they can assume at the third iteration any values belonging to the following intervals $[\theta_1^L; \theta_1^U]$, $[\theta_2^L; \theta_2^U]$, respectively. If the variable $\mathrm{c}_1^{(1),1}$ assumes the value θ_1^U then the subregion $R_3^{(3)}$ is empty and the subregions $R_1^{(3)}$, $R_2^{(3)}$ coincide with the subregions obtained at the second iteration of the approach with the fixed partition structure when using variable θ_2 as the splitting variable at the first iteration. If the variable $\mathrm{c}_{2,2}^{(2)}$ assumes the value θ_2^U then the subregion $R_2^{(3)}$ is empty and the subregions $R_1^{(3)}$, $R_3^{(3)}$ coincide with the subregions obtained at the second iteration of the approach with the fixed partition structure when using the variable θ_1 as the splitting variable at the first iteration. Similarly, one can show that it is possible to obtain all the sets $R^{(3)}$ (obtained at the third iteration of the first method) from the set $R^{(4)}$ by changing the splitting variables. Thus, the second approach permits to diminish to a certain degree the arbitrariness in

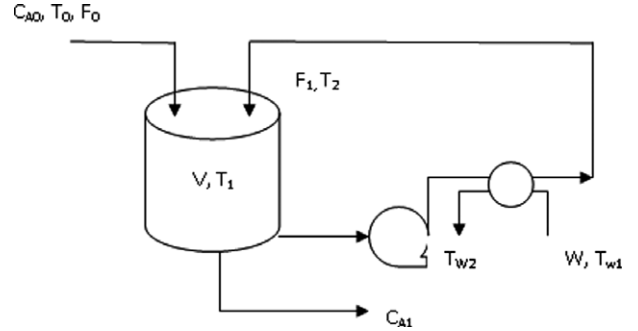

Figure 3. Flowsheet of a chemical process with reactor and heat exchanger.

the selection of splitting variables and splitting points. In other words the approach with the variable partition structure determines the optimal partition structure at each iteration.

Stop criterion

The iteration procedure stops at the k-th iteration if the following two conditions are met

$$\max_k \mu_k \le \varepsilon_1$$
$$|f^{(k)} - f^{(k-1)}| \le \varepsilon_2$$

where $\varepsilon_1, \varepsilon_2$ are small enough. The first criterion guarantees a given accuracy of the approximation of the function $f(d,z,\theta)$ by the piecewise linear approximation $\tilde{f}(d,z,\theta)$ (37).

Illustrative example

Consider the following problem

$$\min_{d\ge 0, z} (d + 0.5 z\theta^2) \tag{79}$$
$$-d - z - \theta + 2 \le 0 \tag{80}$$
$$-3 \le z \le 1$$

d, z, and θ are scalars. Let the parameter θ have the normal distribution and $E[\theta] = 2$, $\sigma = 0.303$. We will suppose that constraint (80) is a soft constraint. The uncertainty region has the following form: $T_\theta = \{\theta : 1 \le \theta \le 3\}$. In this case, the probability measure of the region T_θ is equal to 0.999. Let the probability of satisfaction of constraint (80) be equal to 0.7. We consider the form of problem (62) for the first two iterations of solving TSOP (15) for this example. The TSOP has the following form

$$\min_{d\ge 0, z(\theta)} E[d + 0.5 z(\theta)\theta^2]$$
$$\Pr\{-d - z(\theta) - \theta + 2 \le 0\} \ge 0.7$$
$$-3 \le z \le 1$$

Consider the form of problem (62) at the first iteration. Let $N_1 = 1$, then $R_1^{(1)} = T$ and $z(\theta) = z_1 (1 \le \theta \le 3)$ (see (36)). The region $T_{\alpha_1 1}$ approximating the region T_{α_1} will have the form $T_{\alpha_1 1} = \{\theta : \theta_{1,1}^L \le \theta \le \theta_{1,1}^U\}$. Take the middle point of the intervals $T_1^{(1)}$ as the linearization point $(\theta_1 = 2)$. Then $E_\theta[\tilde{f}(d, z_1, \theta, \theta_1); R_1^{(1)}] = d + 2z_1$. Performing the optimization operation of the left-hand sides of the constraints of problem (62) we obtain in this case

$$f^{(1)} = \min_{d\ge 0, z_1, \theta_{1,1}^L, \theta_{1,1}^U} d + 2z_1$$
$$-d - z_1 - \theta_{1,1}^L + 2 \le 0$$
$$-3 \le z_1 \le 1$$
$$[\Phi((\theta_{1,1}^U - 2)3) - \Phi((\theta_{1,1}^L - 2)3)] \ge 0.7$$
$$1 \le \theta_{1,1}^L, \theta_{1,1}^U \le 3$$

The solution of problem (81) has the following form $f^{(1)} = -2.866$, $z = -3$, $d = 3.134$, $\theta_{1,1}^L = 1.86$ $\theta_{1,1}^U = 3.0$. Consider the second iteration. We partition the interval [1; 3] into two intervals $R_1^{(2)} = \{\theta : \theta_1^{(2)L} \le \theta \le \theta_1^{(2)U}\}$ $R_2^{(2)} = \{\theta : \theta_2^{(2)L} \le \theta \le \theta^{\,2(2)U}\}$ where $\theta_1^{(2)L} = 1$, $\theta_1^{(2)U} = 2$ $\theta_2^{(2)L} = 2$, $\theta_2^{(2)U} = 3$. In this case

$$\tilde{z}^{(2)}(\theta) = \begin{cases} z_1 & \text{if } \theta \in R_1^{(2)} \\ z_2; & \text{if } \theta \in R_2^{(2)} \end{cases}$$

Take the middle points of the intervals $R_1^{(2)}, R_2^{(2)}$ as the linearization points $(\theta_1^{(2)} = 1.5, \theta_2^{(2)} = 2.5)$. In this case, $a_1 = a_2 = 0.5$, $E_\theta[\theta; R_1^{(2)}] = 0.75$, $E_\theta[\theta; R_2^{(2)}] = 1.25$

$$E_\theta[\tilde{f}(d, z_1, \theta, \theta_1); R_1^{(2)}] = 0.5(d + 1.125 z_1),$$
$$E_\theta[\tilde{f}(d, z_2, \theta, \theta_2); R_2^{(2)}] = 0.5(d + 3.125 z_2)$$

At the second iteration, problem (62) has the following form

$$f^{(2)} = \min_{d\ge 0, z_1, z_2, \theta_{1l}^L, \theta_{1l}^U} [0.5(d + 1.125 z_1) + 0.5(d + 3.125 z_2)]\ l = 1; 2$$
$$-d - z_l - \theta_{1,l}^L + 2 \le 0 \quad l = 1; 2$$
$$-3 \le z_1 \le 1, \quad -3 \le z_2 \le 1$$
$$[\Phi((\theta_{1,1}^U - 1.5)3) - \Phi((\theta_{1,1}^L - 1.5)3)]$$
$$+ [\Phi((\theta_{1,2}^U - 2.5)3) - \Phi((\theta_{1,2}^L - 2.5)3)] \ge 0.7,$$
$$1 \le \theta_{1,1}^L, \theta_{1,1}^U \le 2 \quad 2 \le \theta_{1,2}^L, \theta_{1,2}^U \le 3$$

The solution of this problem has the following form: $f^{(2)} = -3.339, z = -3, d = 2.94$

Method of Solving TSOPHC; Case of Independent Uncertain Parameters

Generally speaking, the optimal region $T_{\alpha_j}^*$ is not a multidimensional rectangle. However, the optimal region $T_{\alpha_j}^*$ will be a multidimensional rectangle for values α_j close to 1. Let us solve the following problem

$$\bar{f} = \min_{d, z(\theta), T_{\alpha_j}} E_\theta[f(d, z(\theta), \theta)] \tag{81}$$
$$\max_{\theta \in T_\theta} g_j(d, z(\theta), \theta) \le 0 \quad j = 1, \ldots, m \tag{82}$$

where T_θ satisfies the condition (9) and $\bar{\alpha}$ is close to 1. Problem (81) is obtained from problem (15) by the removal of inequalities (17) and the use of the region T_θ as $T_{\alpha_j}\, j = 1, \ldots, m$. Suppose the solution of problem (81) is $d^*, z^*(\theta)$. Then $d^*, z^*(\theta)$, $T_{\alpha_j}^* = T_\theta$, $(j = 1, \ldots, m)$ is the solution of problem (15) for $\alpha_j = \bar{\alpha}$, $j = 1, \ldots, m$. Indeed, let us add inequalities (9) to problem (81).

$$\bar{f} = \min_{d, z(\theta), T_{\alpha_j}} E_\theta[f(d, z(\theta), \theta)] \tag{83}$$
$$\max_{\theta \in T_\theta} g_j(d, z(\theta), \theta) \le 0 \quad j = 1, \ldots, m$$
$$\Pr\{\theta \in T_\theta\} \ge \bar{\alpha} \tag{84}$$

It is clear that the solution of problem (83) coincides with the solution of problem (81) since inequality (84) is always met. Problem (83) is the same as problem (15), given $T_{\alpha_j}^* = T_\theta$, $\alpha_j = \bar{\alpha}\ j = 1, \ldots, m$. Hence $d^*, z^*(\theta)$, $T_{\alpha_j}^* = T_\theta$, $j = 1, \ldots, m$ is the solution of problem (15) for $T_{\alpha_j}^* = T_\theta$, $\alpha_j = \bar{\alpha}\ j = 1, \ldots, m$. T_θ is a multidimensional rectangle, therefore, for $\alpha_j = \bar{\alpha}$ the regions $T_{\alpha_j}^*$ are multidimensional rectangles.

Transform inequalities (82) using Statement A1

$$g_j(d, z, \theta) \le 0 \quad \forall \theta \in T_\theta\ j = 1, \ldots, m$$

This means that the constraints $g_j(d, z, \theta) \le 0\ j = 1, \ldots, m$ must hold at all the points of the uncertainty region T_θ. Thus, if we take $\bar{\alpha}$ close enough to 1 and solve problem

(81), we will obtain the solution which guarantees the satisfaction of the constraints $g_j(d,z,\theta) \le 0 \;\; j=1,\ldots,m$ with probability close enough to 1. Thus, for solving TSOP with hard constraints we can solve problem (15) for $T^*_{\alpha_j} = T_\theta$, $\alpha_j = \bar{\alpha}$, $j=1,\ldots,m$. At the k-th iteration, we will solve problem (62). In addition, since we know the optimal forms of the regions $T^*_{\alpha_j}$, we must exclude the variables $\theta^L_{ijl}, \theta^U_{ijl}$, $i=1,\ldots,p$, $j=1,\ldots,m$, $l=1,\ldots,N_k$ from search variables. Therefore, in this case problem (62) takes the following form

$$f^{(k)} = \min_{d,z_l} E^{(k)}_{ap}[f(d,\tilde{z}(\theta),\theta);T]$$
$$\max_{\theta \in T_\theta} g_j(d,z_l,\theta) \le 0,$$
$$j=1,\ldots,m,\; l=1,\ldots,N_k$$

Approximate Method of Solving TSOP with Chance Constraints; Case of Dependent Uncertain Parameters

We consider a method of solving problem (4) in the case when uncertain parameters θ_i are random, dependent parameters having multivariate normal distribution (2). We develop the method which is based on a reduction of a problem with dependent, normally distributed, random parameters into a problem with independent random parameters having normal distribution. Suppose we have p random parameters $\theta_i, i=1,\ldots,p$ having multivariate normal distribution (2). It is known that the dependent random parameters $\theta_i, i=1,\ldots,p$ can be represented in the following form[26]

$$\theta_i = a_i + c_{i1}\eta_1 + c_{i2}\eta_2 + \ldots + c_{ip}\eta_p, \quad i=1,\ldots,p \tag{85}$$

where $a_i = E[\theta_i]$, random parameters η_i are independent and have standard normal distribution $N_1(0,1)$. The matrix $C=(c_{ij})$ satisfies the condition

$$CC^T = \Lambda \tag{86}$$

where the matrix Λ is a covariance matrix (see (2)). It is clear that in the case of independent uncertain parameters the matrix Λ is diagonal. Rewrite equality (84) in the following matrix form

$$\theta = a + C\eta \tag{87}$$

where $a=(a_1,\ldots,a_p)^T$, $\eta=(\eta_1,\ldots,\eta_p)^T$. We can consider matrix equality (86) as a system of p^2 nonlinear equations with p^2 unknown elements c_{ij} of the matrix C. However, a number of independent equations is equal to $0.5\,p^2$ since the matrices Λ and CC^T are symmetric. Thus, generally speaking, an infinite number of matrices C satisfies condition (86). Suppose we found a matrix C that satisfies condition (86). We can make the change of variables θ in problem (1) using equations (87)

$$\min_{d,z} F(d,z,\eta) \tag{88}$$
$$G_j(d,z,\eta) \le 0 \quad j=1,\ldots,m,$$

where $F(d,z,\eta,C) \equiv f(d,z,a+C\eta)$, $G_j(d,z,\eta,C) \equiv g_j(d,z,a+C\eta)$ $j=1,\ldots,m$. The TSOPCC for problem (88) for fixed values c_{ij} is of the form

$$F^* = \min_{d,z(\eta)} E_\eta[F(d,z(\eta),\eta,C)] \tag{89}$$
$$\Pr\{G_j(d,z(\eta),\eta,C) \le 0\} \ge \alpha_j \quad j=1,\ldots,m,$$

However, the obtained value F^* depends on the selected values c_{ij}. In order to obtain the optimal value F^*, we should include the values c_{ij} in the set of search variables and use matrix equality (86) as a constraint. Thus, we should solve the following problem

$$F^* = \min_{d,z(\eta),c_{ij}} E_\eta[F(d,z(\eta),\eta,C)] \tag{90}$$
$$\Pr\{G_j(d,z(\eta),\eta,C) \le 0\} \ge \alpha_j \quad j=1,\ldots,m,$$
$$CC^T = \Lambda$$

Formulation (90) includes a broad class of optimization problems of chemical processes with normally distributed uncertain parameters. Indeed, if the matrix Λ is diagonal, then problem (90) is an optimization problem with chance constraints and independent uncertain parameters (OSOP if $z(\eta) = \text{const}, \forall \eta \in T_\eta$ and TSOP if $z(\eta)$ is multivariate function). If the matrix Λ is not diagonal then problem (90) is an optimization problem with chance constraints and dependent uncertain parameters. Since in problem (90) the random parameters η_i are independent with the normal distribution $N_1(0;1)$ we can use the iteration procedure developed in General description of an approximate method of solving the optimization problem with chance constraints section, Approximate method of solving the TSOP with chance constraints; case of independent uncertain parameters section, and Partition of the Subregions $R^{(k)}_q$ section to solve this problem. If $\alpha_j = 1, j=1,\ldots,m$, then problem (90) is an optimization problem with hard constraints. Therefore using developed approach for solving problem (90) for $\alpha_j = 1, j=1,\ldots,m$, we can solve OSOPHC and TSOPHC.

Computational Experiment

Example 1. *For illustration let us consider the production of species B from A as $A \rightarrow B$ in a continuous stirred tank reactor in the flowsheet in Figure 3.*[3] *We solved the optimal design problem for this CP. The performance equations of this system are as follows. The material and energy balance equations for the reactor are*

$$F_0(C_{A0}-C_{A1})/C_{A0} = Vk_0\exp(-E/RT_1)C_{A1}$$
$$(-H)F_0(C_{A0}-C_{A1})/C_{A0} = F_0C_p(T_1-T_0)+Q_{HE}.$$

For the heat exchanger the energy balances are

$$Q_{HE} = F_1C_p(T_1-T_2) = C_{pw}(T_{w2}-T_{w1})W,$$
$$Q_{HE} = AU(0.5((T_1-T_{w2})+(T_2-T_{w1}))) \tag{92}$$

where F_0, T_0, and C_{A0} are the feed flow rate (kmol h^{-1}), the temperature of the feed (°K) and the concentration of the reactant in the feed (kmol h^{-1}), respectively; V, T_1, and C_{A1} are the values of the reactor volume (m^3), the reaction temperature (K) and the concentration of reactant A in the product (kmol m^{-3}); k_0 is the rate constant, E is the activation energy; H is the heat of reaction (kJ $kmol^{-1}$); Q_{HE} is the value of heat transfer (heat exchange), F_1 is the flow rate of the recycle (kmol h^{-1}); T_2 is the recycle temperature; C_p and C_{pw} (kJ $kmol^{-1)}$ are the heat capacity of the recycle mixture and the cooling water, respectively; T_{w1}, T_{w2}, and W are the inlet, outlet temperatures and the flow rate (kmol h^{-1}) of the cooling water, respectively; A is the heat transfer area of the heat exchanger (m^2); and U is the overall heat transfer coefficient (kJ m^{-2} h^{-1} K^{-1}).

In this problem, V and A are the design variables, and T_1 ($311 \le T_1 \le 389$) and T_{w2} ($301 \le T_{w2} \le 355$) are the

Table 1. Results of Solving Nominal Optimization Problem, OSOPCC, and TSOPCC (Independent Parameters)

		OSOPCC				TSOPCC			
γ	α_j	f	V	A	CPU-time (s)	f	V	A	CPU-time (s)
0		9003	5.42	5.21	0.1				
1.0	0.5	9878	5.63	7.37	2	9852	557	735	5.5
1.0	0.75	9957	5.79	7.41	2	9937	5.73	7.39	6
1.0	1	10,405	6.7	7.84	6	10,380	6.69	7.82	6
1.25	0.5	9886	5.66	7.35	2	9781	5.30	7.21	5
1.25	0.75	10,096	5.87	7.75	2	9956	5.70	7.40	6
1.25	1	18,475	20.25	22.17	6	10,636	8.25	7.34	6.0
1.5	0.5	9941	5.7	7.54	3	9786	5.78	8.40	7
1.5	0.75	10,190	5.95	7.98	4	10,010	5.80	8.50	8.5
1.5	1.0	–	–	–	–	10,500	6.1	8.65	9.0
2.5	0.5	–	–	–	–	11,025	7.42	8.78	10
2.5	0.75	–	–	–	–	10,040	5.71	8.34	10
2.5	1.0	–	–	–	–	11,350	8.42	9.5	12

control variables. The state variables are C_{A1}, T_2, F_1, W, and the vector θ of uncertain parameters has the following form $\theta = (F_0 T_0, T_{w1}, k_0, U)$. We suppose that during the operation stage there is enough experimental data that allows us either to measure or to calculate the values of all the uncertain parameters.

We solved two variants of this problem. In the first case the uncertain parameters θ_i are independent, random parameters, having the normal distribution $N_1(E[\theta_i], \sigma_i)$, where $E[\theta_i] = \theta_i^N$, θ_i^N is the nominal value of the uncertain parameter θ_i. The vector θ^N of the nominal values is of the form $\theta^N = (45.36; 333; 300; 9.8; 1635)$. The values σ_i are determined from the condition $3.3\sigma_i = \gamma\Delta\theta_i$, where $\Delta\theta_i$ is the i-th component of the vector $\Delta\theta = (0.1; 0.02; 0.03; 0.1; 0.1)^3$ and γ is a coefficient. The uncertainty region is $T_\theta = \{\theta_i : \theta_i^N - \gamma\Delta\theta_i \le \theta_i \le \theta_i^N + \gamma\Delta\theta_i, i = 1, \ldots, p\}$ and $\gamma\Delta\theta_i$ is the maximal deviation of the parameter θ_i from the nominal value. With the help of the parameter γ we can change the region T_θ. We chose σ_i so that the probability measure of the interval T_θ is equal to 0.999. In the second case the uncertain parameters θ_i are random dependent parameters θ_i having the normal distribution $N_p(E[\theta], \Lambda)$. The values of the standard deviations σ_i were the same as in the case of the independent parameters and the correlation coefficients have the following forms

$$\rho_{12} = 0.7; \rho_{13} = 0.5; \rho_{14} = 0.5; \rho_{15} = 0.1; \rho_{23} = 0.7; \rho_{24} = 0.5; \rho_{25} = 0.3$$
$$\rho_{23} = 0.7; \rho_{24} = 0.5; \rho_{25} = 0.3; \rho_{34} = 0.7; \rho_{35} = 0.5; \rho_{45} = 0.5$$

The objective function is $f = 691.2V^{0.7} + 873.6A^{0.6} + 1.76W + 7.056F_1$. Design specifications are given by the following constraints

$$0.9 - (c_{A0} - c_{A1})/c_{A0} \le 0 \quad 311 - T_2 \le 0 \quad T_2 - 389 \le 0 \quad T_{w1} - T_2 + 11.1 \le 0 \tag{93}$$

$$T_{w2} - T_1 + 11.1 \le 0, \quad T_{w2} - 355 \le 0 \quad 301 - T_{w2} \le 0 \quad T_2 - T_1 \le 0 \tag{94}$$

$$311 - T_1 \le 0 \quad T_1 - 389 \le 0, \quad 301 - T_{w2} \le 0, \quad T_{w2} - 355 \le 0 \tag{95}$$

By using the state equations (91), (92) we can analytically eliminate the state variables $[C_{A1}, T_2, F, W]$ and obtain problem (1).

We solved three problems. In the first problem the uncertain parameters were equal to their nominal values θ^N (their expected values). This is the nominal optimization problem. It has form (1) in which $\theta = \theta^N$. The second problem is the one-stage optimization problem with chance constraints (OSOPCC). It has form (64). The third problem is the TSOPCC (62).

In Tables 1 and 2, we give the results of solving the nominal optimization problem, the OSOPCC and the TSOPCC for the cases of independent and dependent uncertain parameters, respectively. It is clear that the line $\gamma = 0$ corresponds to the nominal optimization problem.

A dash in the Table 1 means that the OSOPHC and OSOPCC for relevant α and γ do not have a solution. This means that if all the control variables are constant at the operation stage then in case $\alpha_j = 1$ we cannot guarantee the satisfaction of all the constraints for all values of the uncertain parameters and in case $\alpha_j < 1$ we cannot guarantee the satisfaction of all the constraints with a given probability. Table 1 shows that if $\gamma = 1.0$ and $\alpha_j = 0.5, 0.75, 1.0$ the two-stage optimization strategy improves (in comparison with the OSOP) the optimal value of the objective function insignificantly (approximately by 0.2%); if $\gamma = 1.25; 1.5$ and $\alpha_j = 0.5, 0.75$, the two-stage optimization strategy improves the optimal value of the objective function approximately by 1% -2%; if $\gamma = 1.25$ and $\alpha_j = 1$, the optimal value (10636) of the objective function of the TSOPCC is significantly less than the optimal value (18475) of the objective function of the OSOPCC; if $\gamma = 1.5; 2.5$ and $\alpha_j = 1$, only the two-stage

Table 2. Results of Solving Nominal Optimization Problem, OSOPCC, and TSOPCC (Dependent Parameters)

		OSOPCC				TSOPCC			
γ	α_j	f	V	A	CPU-time (s)	f	V	A	CPU-time (s)
0		9003	5.42	5.21	0.1	9003	5.42	5.21	0.1
1.0	0.5	10,111	5.7	7.51	2	9985	5.64	7.45	5
1.0	0.75	10,040	5.76	7.61	2	10,009	5.78	7.49	5
1.5	0.5	10,380	5.78	8.40	3	10,130	5.98	8.69	8.5
1.5	0.75	10,450	5.80	8.50	3	10,265	6.04	8.82	9

optimization strategy guarantees satisfaction of all the constraints for all values of the uncertain parameters and if $\gamma = 2.5$ and $\alpha_j = 0.5$ the one-stage optimization strategy cannot guarantee satisfaction of the chance constraints. Table 2 shows that the optimal value of the goal function obtained by solving the TSOPCC is less than the optimal value of the goal function obtained by the OSOPCC approximately by 1–2%.

Compare the developed approach with the straightforward way of solving problem (11) when using some method of nonlinear programming (e.g., SQP). Suppose we use the straightforward way of solving problem (11). In this case, it is necessary to calculate at each iteration the values of the objective function, the left-hand sides of constraints of problem (11) and the gradients of these functions. Let us estimate the total CPU-time required for solving problem (11). Using the Monte–Carlo method from the software package "Mathematica" we computed 12 multiple integrals used to determine the values of objective function and the left-hand sides of constraints of problem (11) for $z(\theta) = z^*(\theta)$ where $z^*(\theta)$ is the solution of problem (11) for $\gamma = 1.0$ and $\alpha_j = 0.5$. The total CPU-time (Pentium 4) required for the computation of these multiple integrals is approximately 40 minutes. Therefore, taking into account the necessity of calculating gradients of the objective function and the left-hand sides of constraints of problem (11) at each iteration solving problem (11) can require several hours of computational time. At the same time, the total CPU-time required to solve problem (11) (for $\gamma = 1.0$, $\alpha_j = 0.5$) with help of our approach is equal to 5-10 sec. Thus, developed approach permits to reduce the computational time significantly. The value of the objective function obtained by solving problem (11) by developed method is equal to 9878. At the same time, the value of the expected value $E[f(d, z, \theta)]$ obtained by numerical integration by the Monte–Carlo method is to 9852. Thus, the piece-wise linear approximation of the objective function gives good enough accuracy.

Conclusion

We have developed a common approach for solving a broad class of optimization problems with normally distributed uncertain parameters. This class includes the OSOPCC and TSOPCC. Besides, we showed that this approach can be used for solving the OSOPHC and TSOPHC. This approach is based on four following operations:

1. Transformation of a set of dependent, normally distributed uncertain parameters θ into a set of independent, normally distributed uncertain parameters η.

2. Approximate transformation of chance constraints into deterministic ones.

3. Approximate calculation of the objective function of the two-stage (one-stage) optimization problem with the help of piece-wise linear approximation of a goal function.

4. Approximate representation of control variables $z(\theta)$ as piece-wise constant functions.

The use of these approximations permits us to avoid computationally intensive calculation of multiple integrals to determine the expected value of the objective function and probabilities of constraints satisfaction. On the basis of these approximations we have developed the iteration procedure of solving the aforementioned class of optimization problems. This iteration method is based on the partition of the uncertainty region into subregions in order to improve the accuracy of the used approximations.

Notation

d is an n_d = vector of design variables,
z is an n_z = vector of control variables,
$d^{(k)}, z^{(k)}$ = optimal values of the design and control variables vectors obtained at the k-th iteration (the solution of problem (64)), respectively
θ = p-vector of the uncertain parameters
T_θ = uncertainty region
$E[f(d, z(\theta), \theta)]$ = the expected value of the function $f(d, z(\theta), \theta)$
T_{α_j} = region where the probability of satisfaction of the constraint $g_j(d, z(\theta), \theta) \le 0$ is equal to α_j, $(\Pr\{\theta \in T_{\alpha_j}\} \ge \alpha_j)$
$R_l^{(k)}$ = the l- subregion (multidimensional rectangle) of the region T
N_k = number of regions $R_l^{(k)}$ at the k-th iteration
$R^{(k)}$ = set of subregions $R_l^{(k)}$
$\theta_{il}^{(k)L}$ = lower bound of change of the variable θ_i in the region $R_l^{(k)}$ at the k-iteration
$\theta_{il}^{(k)U}$ = upper bound of change of the variable θ_i in the region $R_l^{(k)}$ at the k-iteration
$\tilde{T}_{\alpha_j}$ = approximation of the region T_{α_j}
$\tilde{z}(\theta)$ = approximation of the multivariate functions $z(\theta)$
$E_{ap}^{(k)}[f(d, \tilde{z}(\theta), \theta)]$ = approximation of the expected value of the function $f(d, z(\theta), \theta)$ at the k-iteration
$T_{\alpha_j l}$ = the l-th subregion of the region $\tilde{T}_{\alpha_j}$
z^l = the l-th component of the vector $\tilde{z}(\theta)$
$\tilde{f}(d, \tilde{z}(\theta), \theta)$ = piecewise linear approximation of the function $f(d, \tilde{z}(\theta), \theta)$
θ_r = linearization point at the subregion$R_r^{(k)}$
$\tilde{f}(d, z_r, \theta, \theta_r)$ = linear part of the Taylor's expansion of the function $f(d, z^r, \theta)$ at the point θ^r
θ_{ijl}^L = lower bound of an interval of a change of the variable θ_i in the multidimensional rectangle $T_{\alpha_j l}$
θ_{ijl}^U = upper bound of an interval of a change of the variable θ_i in the rectangle $T_{\alpha_j l}$
$c_{\mathrm{sl}}^{(k)}$ = splitting point
μ_q = approximation quality of the region $R_q^{(k)}$
$Q_l^{(k)}$ = set of active regions $T_{\alpha_j}^s$ belonging to the region $R_l^{(k)}$
$\mathrm{T}^{(k)}$ = set of regions $T_{\alpha_j}^{(k),l}$, which are partitioned at the k-th iteration
$\bar{\mathrm{T}}^{(k)}$ = set of regions $T_{\alpha_j}^{l,(k)}$, which are not partitioned at the k-th iteration.

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Appendix

Statement A1: There is equivalence between the following two inequalities

$$\max_{x\in X} \phi(x) \le 0 \tag{A1}$$

$$\phi(x) \le 0,\ \forall x \in X \tag{A2}$$

Here x is a vector of continuous or discrete variables. This statement reflects the following evident fact: if the maximum of a function $f(x)$ on feasible region X is less than zero then $f(x)$ is less than zero everywhere on X; the reverse is true as well, thus Statement A1 holds.

Statement A2: Consider the following problem

$$\begin{aligned} f^* &= \min_x f(x) \\ \varphi_i(x) &\le 0 \quad i = 1, \ldots, k, \ldots m \end{aligned} \tag{A3}$$

and problem, in which the k-th constraint is removed

$$\begin{aligned} f^{k*} &= \min_x f(x) \\ \varphi_i(x) &\le 0 \quad i = 1, \ldots, (k-1), (k+1), \ldots m. \end{aligned} \tag{A4}$$

Let $[x^*, f^*]$, $[x^{k*}, f^{k*}]$ be isolated local solutions of problems (A.3),(A.4), respectively.

The following inequality holds

$$f^{k*} \le f^* \tag{A5}$$

If the k-th constraint is not active for the optimal solution of problem (A.3) ($\varphi_k(x^*) < 0$), then inequality (A5) is transformed into equality

$$f^{k*} = f^* \quad \varphi_k(x^*) < 0 \tag{A6}$$

Indeed, in this case the feasible region $D = \{\varphi_i(x) \le 0, i = 1, \ldots, k, \ldots m\}$ of problem A.3 is a part of the feasible region $D^k = \{\varphi_i(x) \le 0, i = 1, \ldots, k-1, k+1, \ldots m\}$ of problem A4

$$D \subseteq D^k \tag{A7}$$

Consequently, inequality (A.5) holds. Let us prove (A.6). Since x^* is the solution of (A.3), there is a small enough vicinity C of the point x^*

$$C = \{x : \varphi_i(x) \le 0,\ \varphi_k(x) < 0\ i = 1, \ldots, k-1, k+1, \ldots, m\}$$

where

$$f(x^*) \le f(x)\ \forall x \in C \tag{A8}$$

It follows from (A8) that there exists the following small enough vicinity C_k of the point x^*

$$C_k = \{x : \varphi_i(x) \le 0, i = 1, \ldots, k-1, k+1, \ldots, m\},$$

where the following condition holds: $f(x^*) \le f(x) \forall x \in C_k$. It is clear that this condition is the condition that the point x^* is the minimum of problem (A4). Consequently, the minimum of problem (A4) coincides with the minimum of problem (A3) and relation (A6) holds.

Consider the case when the k-th constraint is active at the optimal solution of problem (A3) ($\varphi_k(x^*) = 0$). In this case the feasible region $D = \{\varphi_i(x) \le 0, i = 1, \ldots, k, \ldots m\}$ of problem (A3) is a part of the feasible region $D^k = \{\varphi_i(x) \le 0, i = 1, \ldots, k-1, k+1, \ldots m\}$ of problem (A4) (see (A7)). Therefore, in this case we are more likely to find a solution of problem (A4) that is strictly better than the solution of problem (A3) that is, the following inequality will be held $f^{k*} < f^*$.

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