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An Approach to solve the power and resource-intensive process design problem in a one-stage optimization problem form

T.V. Lapteva[1,2], A.S. Silvestrova[1], N.N. Ziatdinov[1]

1 Kazan National Research Technological University, Russia, Kazan, K.Marx str., 68
2 Kazan State Power Engineering University, Russia, Kazan, Krasnoselskaya Str., 51

tanlapteva@yandex.ru

Abstract: Approach to the solution of a problem of optimal power and resource-intensive process design under uncertainty is proposed. The problem has a form of one-stage optimization problem with separate chance constraints. The approach based on the problem's functions approximations and approximations of the regions of the constraints satisfaction. This allows us to avoid calculation of multiple integrals. Thus we reduce the problem of stochastic nonlinear programming to the sequence of the usual problem of nonlinear programming.

Intrduction

Generally, power and resource-intensive processes are designed with the use of uncertain source data and inaccurate mathematical models. The inexactness of mathematical models arises because of the original uncertainty of chemical, physical, and economic data which are used during a process design. Therefore, it is important to design a process that guarantees the satisfaction of all design specifications either exactly or with some probability. This paper considers the issue of power and resource-intensive process optimization when at the operation stage the design specifications should be met with some probability and the control variables can be changed.

The optimization problem of a optimal process design in the case of the using an exact mathematical model and uncertain source data can be expressed as follows

$$\min_{d,z\in H} f(d,z,\theta)$$

$$g_j(d,z,\theta)\le 0,\ j=1,...,m,\ \forall\theta\in T,$$

where d – n_d-vector of design variables, z – n_z of control variables, and θ – n_θ-vector of uncertain parameters, $\theta\in T$, the region $T=\{\theta_i:\theta_i^L\le\theta_i\le\theta_i^U, i=1,...,n_\theta\}$ characterizes the changing of the operating conditions of the designed process (DP) for the operation period, $f(d,z,\theta)$ – the function of evaluation of the operational efficiency of the designed process at a time that appropriate to the operating conditions of the designed process, specified values of uncertain parameters θ. We cannot solve this problem due to an exact values of uncertain parameters θ.

The problem of the optimal design of a process under uncertainty can be formulated as follows: it is necessary to create an optimal process that would guarantee the satisfaction (exact or with some

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probability) of all design specifications in the case when inexact mathematical models are used and internal and external factors change during the process operation stage. Usually, the following two formulations of this problem are used:

– the formulation of the two-stage optimization problem (TSOP) takes into account possibility of the control variables change at the operation stage. 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 process 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 process.

– the formulation of the one-stage optimization problem (OSOP) supposes that the control variables are constant at the operation stage.

The formulation of the optimization problem under uncertainty depends on the type of constraints. The constraints can be "hard" or "soft". 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)

1. General formulations

Let write OSOPCC with the expected value of the function $f(d,z,\theta)$ criterion during the process operation stage in the form [2]

$$\min_{d,z\in H} E_\theta[f(d,z,\theta)], \tag{1}$$

$$\Pr\{g_j(d,z,\theta)\le 0\}\ge \alpha_j,\ \ j=1,...,m, \tag{2}$$

where $\Pr\{g_j(d,z,\theta)\le 0\} = \int\limits_{\Omega_j} \rho(\theta)d\theta \ge \alpha_j$, $0\le\alpha_j\le 1$, $\Omega_j=\{\theta: g_j(d,z,\theta)\le 0,\ \theta\in T\}$,

$E_\theta[f(d,z,\theta)] = \int\limits_T f(d,z,\theta)\rho(\theta)d\theta$, $\rho(\theta)$ – is the probability density function.

The solution of problem (1)-(2) requires multidimensional integration to calculate the values of constraints (2) and the criterion in (1) at each iteration of the procedure for solving problem (1)-(2). It is computationally time-consuming operation even in the case of a small number of uncertain parameters. Currently, there are proposed a number of approaches for the economic calculation of multidimensional integrals that can be grouped into three groups:

1. Approaches based on the development of Gauss quadratures. Unfortunately, these approaches require extremely large computations with increasing dimension of the integration region.

2. A group of approaches developing ideas for methods of statistical testing. The most advanced approach in this group is currently the method of approximation of the sample-average approximation (SAA) [3]. However, these methods in turn use random variables, and such solution can lead to chance constraints violation.

3. Methods for the transformation chance constraints to deterministic form, which allows to exclude the multidimensional integration procedure. Among the methods of this group, methods for transformation linear constraints are known [4], approaches based on certain properties of constraint functions [5]. There are methods that use known inequalities in the transformation of constraints. However, such methods either impose certain requirements to the form of constraint functions, or still require multidimensional integration.

An overview of the approaches to the solution of the OSOPCC is given in [6].

2. Proposed approach basics

In [2, 7] we proposed an approach to the solution of OSOPCC (1)-(2) for independent indefinite parameters, based on our proposed method of reducing chance constraints to a deterministic form that does not depend on the form of the constraint functions and does not require multidimensional integration. However, the proposed approach required an analytic transformation of the functions of chance constraints, which is not always possible and convenient. In this paper we consider the development of the approach proposed in [2, 7], which allows to avoid preliminary analytical transformations.

2.1. Expected value quantity approximation

To reduce the computations for multidimensional integration for getting the value of the criterion for the problem (1)-(2), in [2] we used at the k -th iteration of the solving procedure the approximation of the value $E_\theta[f(d,z,\theta)]$ by a function $E_{ap}^{(k)}[f(d,z,\theta)]$, relying on the expansion of the function $f(d,z,\theta)$

$$E_{ap}^{(k)}[f(d,z,\theta)] = \sum_{q=1}^{Q^{(k)}}\left(a_q f(d,z,\theta^q) + \sum_{i=1}^{n_\theta} \frac{\partial f(d,\bar{z}^q,\theta^q)}{\partial\theta_i}(E[\theta_i;T_q^{(k)}] - a_q\theta_i^q)\right),$$

$$a_q = \prod_{i=1}^{n_\theta}[\Phi(\tilde{\theta}_i^{(k)U,q}) - \Phi(\tilde{\theta}_i^{(k)L,q})],\ E[\theta_i;T_q^{(k)}] = A_q^{(k)}\cdot I_i^{(k),q}\cdot B_q^{(k)},$$

$$A_q^{(k)} = \prod_{r=1}^{i-1}[\Phi(\tilde{\theta}_r^{(k)U,q}) - \Phi(\tilde{\theta}_r^{(k)L,q})],\ B_q^{(k)} = \prod_{r=i+1}^{n_\theta}[\Phi(\tilde{\theta}_r^{(k)U,q}) - \Phi(\tilde{\theta}_r^{(k)L,q})],$$

$$I_{iq} = \int_{\theta_i^{(k)L,q}}^{\theta_i^{(k)U,q}} \theta_i\rho(\theta)d\theta,\ \tilde{\theta}_i^{(k)L,q} = \frac{\theta_i^{(k)L,q} - E[\theta_i]}{\sigma_i},\ \tilde{\theta}_i^{(k)U,q} = \frac{\theta_i^{(k)U,q} - E[\theta_i]}{\sigma_i},$$

$$T = T_1^{(k)} \bigcup T_1^{(k)} \bigcup \ldots \bigcup T_{Q^{(k)}}^{(k)},\ T_q^{(k)} = \{\theta : \theta_i^{(k)L,q} \le \theta_i \le \theta_i^{(k)U,q}, i=1,\ldots,n_\theta\},\ q=1,\ldots,Q^{(k)},\ i=1,\ldots,n_\theta.$$

The proposed approximation does not require the calculation of multidimensional integrals. To calculate it, one-dimensional integrals values are required. However, the values of these quantities can be obtained before the optimization procedure because the integration elements are independent of the search variables of the problem.

2.2. Approximation of the chance constraints satisfaction region

In [7] we proposed a method for reducing the chance constraints (2) to a deterministic form by approximation the T_{α_j} regions of satisfaction of constraints $g_j(d,z,\theta) \le 0$ by multidimensional rectangles R_{α_j}. For this, the hypersurfaces of the boundaries of the regions T_{α_j} obtained by the expression $\theta_{n_\theta} = \varphi_j(d,z,\theta_1,\ldots,\theta_{n_\theta-1})$ from the equations $g_j(d,z,\theta_1,\ldots,\theta_{n_\theta}) = 0$ were approximated by hyperplanes $\bar{\varphi}_j(d,z,\bar{\theta}_1,\ldots,\bar{\theta}_{n_\theta-1})$, $\bar{\theta}_i = 0.5\cdot(\theta_i^U - \theta_i^L)$, $i=1,\ldots,n_\theta-1$,. As a result, we get the formulation of the problem of evaluation the criterion of the OSOPCC (1)-(2) in form (see [7])

$$\min_{d,z\in H} E_{ap}^{(k)}[f(d,z,\theta)] \tag{3}$$

$$\sum_{l=1}^{N_j^{(k)}}\left(\prod_{i=1}^{n_\theta-1}[\Phi(\tilde{\theta}_r^{(k)U,j,l}) - \Phi(\tilde{\theta}_r^{(k)L,j,l})]\cdot I_{n_\theta,j,l}\right) \ge \alpha_j,\ j=1,\ldots,m, \tag{4}$$

where $\tilde{\theta}_i^{L,j,l} = (\theta_i^{L,j,l} - E[\theta_i])/\sigma_i$, $\tilde{\theta}_i^{U,j,l} = (\theta_i^{U,j,l} - E[\theta_i])/\sigma_i$, $E[\theta_i]$, $(\sigma_i)^2$ – the expected value and dispersion of parameter θ_i, $I_{n_\theta,j,l} = \int_{S_{n_\theta,j,l}} \rho(\theta_{n_\theta})d\theta_{n_\theta}$, $\theta_i^{(k)L,j,l}, \theta_i^{(k)U,j,l}$ – boundaries of $R_{j,l}$ regions, $l=1,\ldots,N_j^{(k)}$, obtained by partitioning the regions R_{α_j} to improve the approximation of the functions $g_j(d,z,\theta_1,\ldots,\theta_{n_\theta})$, $i=1,\ldots,n_\theta$, $j=1,\ldots,m$. In (4) $S_{n_\theta,j,l} = [\theta_{n_\theta}^{(k),L,j,l}; \varphi_j(d,z,\bar{\theta}_1^{j,l},\ldots,\bar{\theta}_{n_\theta-1}^{j,l})]$, $\bar{\theta}_i^{j,l} = 0.5(\theta_i^{(k)L,j,l} + \theta_i^{(k)U,j,l})$, $i=1,\ldots,n_\theta-1$. The calculation of one-dimensional integrals $I_{n_\theta,j,l}$ is conducted according to the expressions:

$$I_{n_\theta,j,l}^{(k)} = \begin{cases} \Phi((\overline{\varphi}_{j,l}^{(k)} - E[\theta_{n_\theta}])/\sigma_{n_\theta}) - \Phi(\widetilde{\theta}_{n_\theta}^{(k)L,j,l}), & \text{if } \partial g_j(d,z,\theta)/\partial\theta_{n_\theta} \geq 0, \\ \Phi(\widetilde{\theta}_{n_\theta}^{(k)U,j,l}) - \Phi((\overline{\varphi}_{j,l}^{(k)} - E[\theta_{n_\theta}])/\sigma_{n_\theta}), & \text{if } \partial g_j(d,z,\theta)/\partial\theta_{n_\theta} \leq 0, \end{cases} \tag{5}$$

где $\overline{\varphi}_{j,l}^{(k)} = \varphi_{j,l}(d,z,\overline{\theta}_1^{j,l},\overline{\theta}_2^{j,l},...,\overline{\theta}_{n_\theta-1}^{j,l})$ вычисляется в подобласти $R_{j,l}$, $l=1,...,N_j^{(k)}$.

However, to calculate the values $\overline{\varphi}_{j,l}^{(k)}$, we need to express them from the equations $g_j(d,z,\overline{\theta}_1^{j,l},...,\overline{\theta}_{n_\theta-1}^{j,l},\overline{\varphi}_{j,l}) = 0$ in the subregion $R_{j,l}$, that is not always possible. Therefore, we will receive values $\overline{\varphi}_{j,l}^{(k)}$ during the execution of the optimization procedure. Let introduce the equations into the number of constraints of problem (3)-(4), add variables to the list of search variables of the problem $\overline{\varphi}_{j,l}^{(k)}$ and obtain a new form of problem (3)-(4)

$$f^{(k)} = \min_{d,z\in H,\overline{\varphi}_{j,l}} E_{ap}[f(d,z,\theta)], \tag{6}$$

$$g_j(d,z,\overline{\theta}_1^{j,l},...,\overline{\theta}_{n_\theta-1}^{j,l},\overline{\varphi}_{j,l}) = 0,\ j=1,...,m,\ l=1,...,N_j^{(k)}, \tag{7}$$

$$\sum_{l=1}^{N_j^{(k)}} \left(\prod_{i=1}^{n_\theta-1} [\Phi(\widetilde{\theta}_r^{(k)U,j,l}) - \Phi(\widetilde{\theta}_r^{(k)L,j,l})] \cdot I_{n_\theta,j,l} \right) \geq \alpha_j,\ j=1,...,m, \tag{8}$$

where the calculation of $I_{n_\theta,j,l}$ is conducted according to (5). In the problem $mN_j^{(k)}$ of equality constraints of the form (7).

Note that in problem (6)-(8) it is assumed that for getting value $\overline{\varphi}_{j,l}^{(k)}$ is used the dependence $\theta_{n_\theta} = \varphi_j(d,z,\theta_1,...,\theta_{n_\theta-1})$ in the subregion $R_{j,l}$. However, it is not always convenient and rational to use the same undefined parameter for getting the value for various constraints $g_j(d,z,\theta) \leq 0$, $j=1,...,m$ when we solve the process design problems. Obviously, it can be used different undefined parameters for different constraints.

Let suppose that for getting a value $\overline{\varphi}_{j,l}^{(k)}$ for a constraint with a number j, we will use an undefined parameter with the number i_j, and can be executed $i_{j_1} = i_{j_2}$. In this case, the problem (6)-(8) takes the form

$$F^{(k)} = \min_{d,z\in H,\overline{\varphi}_{j,l}} E_{ap}[f(d,z,\theta)], \tag{9}$$

$$g_j(d,z,\Theta_j,\overline{\varphi}_{j,l}) = 0,\ j=1,...,m,\ l=1,...,N_j^{(k)}, \tag{10}$$

$$\sum_{l=1}^{N_j^{(k)}} \left(\prod_{i=1}^{n_\theta-1} [\Phi(\widetilde{\theta}_r^{(k)U,j,l}) - \Phi(\widetilde{\theta}_r^{(k)L,j,l})] \cdot I_{n_\theta,j,l} \right) \geq \alpha_j,\ j=1,...,m, \tag{11}$$

where $\Theta_j = \{\overline{\theta}_i^{j,l}, i \in I_j\}$, $I_j = \{i : i=1,...,n_\theta\}/\{i = i_j\}$, $\dim I_j = n_\theta$.

The problem (9)-(11) is the problem of non-linear deterministic programming. To solve this problem, it is not necessary to conduct multidimensional integration in the process of implementing the optimization procedure. It is also not necessary to separately solve the equations $g_j(d,z,\overline{\theta}_1^{j,l},...,\overline{\theta}_{n_\theta-1}^{j,l},\overline{\varphi}_{j,l}) = 0$ for each region to get a value. It should be noted that the derivation of the equations for the optimization level will allow us to get a faster solution of problems (9)-(11).

3. Improving chance constraints regions approximation

To improve the getting evaluation, we can use the partitioning rules for the regions T_q, $q=1,...,Q^{(k)}$, $R_{j,l}$, $j=1,...,m$, $l=1,...,N_j^{(k)}$ that proposed in [2, 7]. Let $d^{(k)}, z^{(k)}$ is the problem (9)-(11) solution. We should partition the subregion T_{q*} with the worst quality of the approximation of the function $f(d,z,\theta)$ by the function $\bar{f}(d,z,\theta,\theta^q)$. To find the q^* we will solve the problem

$$g^* = \arg\max_q \max_{\theta \in T_q} (f(d^{(k)}, z^{(k)}, \theta) - \bar{f}(d^{(k)}, z^{(k)}, \theta, \theta^q))^2 .$$

We should partition subregion R_{r*} the numbered $r^* = \{j, l_j^*\}$ with the worst quality of the approximation of the function $\varphi_j(d, z, \theta_1, ..., \theta_{n_\theta - 1})$ by the hyperplanes $\overline{\varphi}_{r*}^{(k)} = \varphi_{r*}(d, z, \overline{\theta}_1^{r*}, \overline{\theta}_2^{r*}, ..., \overline{\theta}_{n_\theta - 1}^{r*})$, $\overline{\theta}_i^{r*} = 0.5(\theta_i^{(k)L, r*} + \theta_i^{(k)U, r*})$, $i = 1, ..., n_\theta - 1$. To find the l_j^* we will solve the problems

$$l_j^* = \arg\max_l \max_{\theta \in T_l} (\varphi(d^{(k)}, z^{(k)}, \theta_1, ..., \theta_{n_\theta - 1}) - \overline{\varphi}_{j,l}^{(k)})^2 .$$

The effectiveness of the proposed approach was demonstrated on the solution of the problem of synthesis of the optimal workable one-stage of heat exchangers network (HEN). To reduce the dimension of the solving problem was used an approach to the synthesis of optimal HENs, proposed in [8].

The using of the approach became possible due to the decomposition of the multidimensional region of uncertainty into a set of two-dimensional regions. As a result, a set of problems of optimal workable HENs design on two-dimensional regions of uncertainty was obtained. By solving each of the problems of optimal workable HENs design, the level of the HEN heat and mass balance is realized in the modeling program UNISIM (Honeywell International Inc.).

The obtained optimal values of the criteria of effectiveness work of each of the operational networks were summarized in the matrix of effectiveness evaluations of networks [8]. The optimal topology of the workable HEN was obtained as a result of the solution of the assignment problem, and the problem did not contain uncertainty, it was exhausted at the level of solving separate problems of optimal workable HENs design.

Conclusions

In this paper we propose the development of the approach that we proposed earlier to solve the optimal workable CP design problems based on reducing the problem of a one-stage optimization problem with separate chance constraints to a sequence of deterministic nonlinear programming problems.

The new approach makes it possible to get rid of the procedure of the analytical solution of nonlinear equations describing the boundary of the region of satisfaction of constraints, which made it possible to approximate the constraint functions when reducing chance constraints to deterministic form. The elimination of this procedure was made possible by including these equations in the list of constraints of the solving optimization problem. This made it possible to extend the scope of the approach to cases where the analytical solution of the equations is very difficult or impossible, for example, when modeling programs are used to reduce the heat and mass balances of CP.

The efficiency of the approach was demonstrated on the solution of the problem of synthesis of an optimal workable one-stage of heat exchangers network, when the heat and mass balance of the network was calculated in the simulating program, which did not allow to obtain analytical descriptions of the boundaries of the regions for satisfaction of the chance constraints of the solving problem.

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