Optimization of chemical processes under uncertainty

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Introduction. In chemical process (CP) design, some design specifications must always be met. Examples of these specifications are (a) safety, (b) ecological, and (c) performance. The satisfaction of design specifications is complicated by the presence of the uncertainties in mathematical models. This uncertainty is the consequence of original inexactness of the mathematical models and a change of internal and external factors during the CP operation. We consider here the problem of optimal design of CP under uncertainty.

One can give the following general formulation of CP optimization under design: using the inexact mathematical models it is necessarily to find optimal equipment sizes and regimes of CP that guarantee flexibility of CP i.e. its ability to satisfy all the constraints during the operation stage. The constraints are of the form

$$g_j\left(d,z,\theta\right)\le 0 \qquad j=1,\ldots,m, \tag{1}$$

where d is a vector of the design variables, z is a vector of the control variables and θ is a vector of uncertain parameters with an uncertainty region T: $\theta\in T$. They can be "hard" or "soft". Hard constraints must never be violated during the operation stage. On the other hand, if occasional violations are allowed, then the constraints are said to be soft. Safety and ecological environmental specifications can often be considered as hard constraints. Process performance is often considered to be a soft constraint. We consider here two-stage optimization problem with hard constraints and one-stage optimization problem with soft constraints.

Two-stage optimization problem with hard constraints. This problem is formulated under the following supposition: At each time instant during the operation stage, one carries out CP optimization with process models in which at least one uncertain parameter is estimated more accurately using available process data. In [1] flexibility condition and two-step optimization problem (TSOP) for solving the optimization problem under uncertainty were formulated. Flexibility condition is of the form [1]:

$$\chi_1(d)\equiv\max_{\theta\in T}\min_{z}\max_{j\in J} g_j(d,z,\theta)\le 0 \tag{2}$$

It is clear that F

flexibility condition (2) must be used as the constraint in optimization problem under uncertainty. Therefore the optimization problem under uncertainty has the following form

$$f_1^*=\min_d E_\theta\{f^*(d,\theta)\} \tag{3}$$

$$\chi_1(d)\le 0, \tag{4}$$

where $E\{f^*\left(d,\theta\right)\}$ is the mathematical expectation of the $f^*\left(d,\theta\right)$ where

$$
\begin{aligned}
& f^*(d,\theta) = \min_z f(d,z,\theta) \\
& g_j(d,z,\theta) \le 0, \qquad j = 1,\ldots,m.
\end{aligned} \tag{5}
$$

This is the two-stage optimization problem (TSOP1). However, this formulation of the TSOP1 is based on the implicit supposition that during an operation stage we can determine exact values of the uncertain parameters. This supposition is very restrictive and it is often not satisfied in practice. In connection with this we will develop a new formulation of TSOP based on real assumptions about a level of uncertainty of the parameters of the mathematical models at the operation stage. Namely we consider here the important case when the vector θ of the uncertain parameters consists of two sets θ^1 and θ^2 of the parameters, $[\theta = (\theta^1, \theta^2)]$. Let $\theta^1 \in T^1$ and $\theta^2 \in T^2$, $(T = T^1 \cup T^2)$ where T^1 and T^2 are uncertainty regions of the parameters θ^1 and θ^2 respectively. The first set θ^1 consists of the parameters that can be determined during the operation stage with sufficient precision, and the second set θ^2 consists of the parameters for which available experimental information at the operation stage does not permit to correct their values.
We showed that in this case the flexibility condition is of the form

$$
\chi_2(d) \equiv \max_{\theta^1 \in T_1} \min_z \max_{\theta^2 \in T_2} \max_{j \in J} g_j(d,z,\theta^1,\theta^2) \le 0 \tag{6}
$$

and optimization problem under uncertainty (TSOP2) is of the form

$$
\begin{aligned}
& f_2 = \min_d E_{\theta^1} \{f^*(d,\theta^1)\} \\
& \chi_2(d) \le 0.
\end{aligned} \tag{7}
$$

where $f^*(d,\theta^1)$ given by

$$
\begin{aligned}
& f^*(d,\theta^1) = \min_z E_{\theta^2} \{f(d,z,\theta^1,\theta^2) \\
& \max_{\theta^2 \in T^2} g_j(d,z,\theta^1,\theta^2) \le 0, \qquad j = 1,\ldots,m
\end{aligned} \tag{8}
$$

and $E_{\theta^2}\{f(d,z,\theta^1,\theta^2)$ is the mathematical expectation of $f(d,z,\theta^1,\theta^2)$ with respect to θ^2

$$
E_{\theta^2}\{f(d,z,\theta^1,\theta^2) = \int_{T^2} f(d,z,\theta^1,\theta^2)\rho_2(\theta^2)d\theta^2 .
$$

The peculiarity of TSOP1 and TSOP2 is that it is necessary to solve a maxminmax problem for calculation of constraints. We developed the method of solving TSOP2 which is an extension of the *split and bound* (SB) method developed by us for solving TSOP1 [2].The method is a two-level iterative procedure that employs a partitioning of *T*. The lower level is used to calculate the upper and lower bounds of the objective function of TSOP2. The upper level serves to partition *T* using information obtained from the lower level.

One-stage optimization problem with soft constraints. A characteristic property of one stage optimization problems is the constancy of the control variables at the operation stage. We consider the case when the constraints must be satisfied with some probability (the case of chance constraints). The problem has the following form

$$\min_{d,z} E_\theta \left\{ f\left(d,z,\theta\right) \right\} \tag{8}$$

$$\Pr\left\{g_j\left(d,z,\theta\right) \le 0\right\} = \int_{\Omega_j} \rho(\theta) d\theta \ge \alpha_j \qquad j = 1,\ldots,m \tag{9}$$

where $\Omega_j = \left\{\theta : g_j\left(d,z,\theta\right) \le 0, \theta \in T\right\}$, $\Pr\left\{g_j\left(d,z,\theta\right) \le 0\right\}$ is the probability of satisfaction of constraint (1), α_j is a probability level. The main issue in solving one-stage optimization problems is the calculation of multiple integrals that give mathematical expectation of the objective function and probability of constraints satisfaction. The use of known methods of nonlinear programming (for example SQP) requires the calculation of multiple integrals at each iteration. This operation is very intensive computationally even for small dimensionality of vector θ of the uncertain parameters. So many authors developed methods of efficient calculation of multiple integrals (see, for example, [3], [4]).Here we will develop a method based on the transformation of the chance constraints into deterministic ones. This method will use calculation of an upper and lower bounds of the objective function of problem (8).

Conclusion. In this paper we give the formulations of some optimization problems of chemical processes with hard and soft constraints under uncertainty and the approaches for their solving.

References: 1.K.P. Halemane and I.E. Grossmann, Optimal Process Design under Uncertainty, AIChE Journal, 29 (1983) 425-433

2. Ostrovsky G. M.; L.E.K. Achenie and Volin Yu, Optimization of chemical processes under uncertainty209-228, In: System Modelling and Optimization, Methods, Theory and Applications, Ed. by M.J.D. Powell and S. Sholtes, Kluwer Academic Publisher (2000)

3. Wendt, M., P. Li, K. Wozny., Nonlinear chance constrained process optimization under uncertainty, Ind. & Eng. Chem. Res., 41(2002), 3621-3629.

4. Diwaker U.M., Kalagnanam J.R. An efficient sampling technique for optimization under uncertainty. AIChE Journal 1997; 43; 440-447.