DEVELOPMENT OF THE ALGORITHM OF TWO-STAGE OPTIMIZATION OF INDUSTRIAL CHEMICAL PROCESS APPARATUS

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Abstract: A two-stage problem of optimal design of industrial chemical process apparatus under the uncertainty of physical, chemical, technological and economic initial data has been formulated. A characteristic feature of two-stage optimization problems is a possibility to tune up regime (control) variables of a chemical process system depending on the refinement of uncertain parameters during the running stage. An algorithm of two-stage optimization of technical systems has been developed and its efficiency is demonstrated on the example of optimal design of the following chemical process apparatus: turbulent tube reactor of thin organic synthesis, adsorption oxygen concentrator, and a mold for the high-temperature synthesis of hard-alloyed materials.

Symbols

A – a set of variants of unit setting of industrial chemical process apparatus;

d – design parameters vector;

F – optimization criterion;

g – constraint function;

$I^{(k)}$ – a set of indices i for points ξ, where constraints can be violated;

k – algorithm iteration counter;

J_1 – a set of indices j for "soft" constraints;

J_2 – a set of indices j for "hard" constraints;

m – total number of problem constraints;

m_1 – a number of "soft" constraints;

n_ξ – length of vector ξ;

$\Pr\{\cdot\}$ – probability of $\{\cdot\}$ constraint fulfillment, %;

r – a function of approximation procedure;

$S^{(k)}$ – a set of points where constraints are violated;

u – scalar variable;

y – vector of mathematical model output variables;

z – vector of control variables;

Ξ – domain of uncertain parameter change;

Ψ – operator of a chemical process system mathematical model;

ξ – vector of uncertain parameters;

ρ – a preset value of constraint fulfillment probability, %;

$\chi(d)$ – flexibility function;

TC – total costs.

Introduction

When designing industrial chemical process apparatus, two kinds of uncertainties are always present. Some of them, such as raw materials parameters and external environment temperature, may change during the process running, keeping up to a certain size of changing. It is in essence impossible to set a single value for them. Others may actually be constant uncertainties for a specific industrial apparatus, but their values are known up to a certain interval, for example, some coefficients in kinetic

equations and heat- and mass-transfer equations. To consider the uncertainties in the mathematical description of industrial apparatus, it suffices to include them into dependencies involving criterion F and constraint function g_j of optimization problem, meaning that $F = F(d, z, \xi), g_j = g_j(d, z, \xi), j = 1, ..., m,$ where ξ is a vector of uncertain parameters that take on any value from a given domain Ξ, generally considered to be rectangular: $\Xi = \left\{ \xi : \xi^L \leq \xi \leq \xi^U \right\}.$

In such case a solution of the problem of optimization by criterion $F = F(d, z, \xi)$ and with constraints $g_j = g_j(d, z, \xi), j = 1, ..., m,$ is uncertain and depends on the value of vector ξ. A traditional way of overcoming this complication is the following.

A vector of uncertain parameters is assigned a certain "nominal" value, $\xi = \xi^N$, and an optimization problem for nominal ξ^N is solved obtaining the nominal value of d^N vector of design parameters for a given unit setting. Afterwards, using the available data on the object of design, the so-called overdesign coefficients $k_i(k_i > 1)$ are introduced, and it is considered that $d_i = k_i d_i^N$, where d_i is i-numbered component of the vector $d, i = 1, ..., n$ (length and diameter of reactor, heat-exchange area in heat exchanger, number of trays in a rectification column, etc.).

The drawbacks of such an approach are obvious, as it does not guarantee neither obtaining optimal solution, nor fulfillment of all constraints during apparatus running. If overdesign coefficients result to be insufficient, the constraints will be violated, and in case of excessive overdesign coefficients, the costs will be excessive too.

An approach which considers uncertainty in the coefficients of mathematical description and technological parameters in the optimization problem statement itself is significantly more scientifically grounded and correct.

Statement of the two-stage problem of chemical process system optimization

It is common to formulate a problem of chemical process unit setting as a non-linear programming problem:

$$\min_{d,z} F(d, z, \xi) ; \tag{1}$$

$$y = \Psi(d, z, \xi) ; \tag{2}$$

$$g_j(d, z, \xi) \leq 0 , j = 1, ..., m , \tag{3}$$

where $F(\cdot)$ is optimization criterion; $y = \Psi(d, z, \xi)$ is an operator of chemical process system mathematical model; and y, d, z, ξ are vectors of output, design, control variables and chemical process system uncertain parameters, accordingly.

Let ξ belong to domain Ξ, that is $\xi \in \Xi$. We shall reduce problem (1) – (3) the following way:

$$\min_{d,z,u} u ; \tag{4}$$

$$F(d, z, \xi) \leq u ; \tag{5}$$

$$g_j(d, z(\xi), \xi) = y_{j,\text{giv}} - y_j \leq 0; \tag{6}$$

$$j = 1, ..., m,$$

where $y_{j,giv}$ is allowed limited value of j-numbered output variable of a chemical process system. For fixed values of ξ these two statements are equivalent. However, when considering uncertain parameters, the statement (4) – (6) has advantages over the initial problem (1) – (3) as it considers the optimization criterion $F(d, z, \xi)$ along with other constraints.

When formulating an optimization problem under the uncertainty of initial data, a form of goal function (optimization criterion) and constraints should be determined. A concept of two stages of a unit 'life cycle' is taken as a basis: the stage of design and running stage. During the running stage the following cases are possible:

a) all uncertain parameters can be determined exactly at any moment of time (either by direct measurement, or through the solution of a reverse problem using the information obtained by measurements);

b) the domains of uncertain parameters at the running stage and at the design stage are the same;

c) some parameters ξ_i can be determined exactly at the running stage, while others have the same interval as at the design stage;

d) during the running stage all parameters ξ_i include uncertainty, but their intervals of uncertainty are smaller than the corresponding intervals at the design stage.

An optimization problem may have "hard" (unconditional) and "soft" (probable) constraints. "Hard" constraints may not be violated under any circumstances. "Soft" constraints should be fulfilled with a given probability. In reality most problems include a number of "hard" constraints and a certain number of "soft" constraints. For example, apparatus safety constraints are "hard" constraints, while productivity and selectivity constraints can be regarded as "soft" ones.

Let us consider a two-stage problem of chemical process apparatus optimization under the uncertainty of intervals. Let there be a simulation model of an apparatus performance in static $y = \Psi(d, z, \xi)$, where y – is a vector of output system variables, constraints with indices $j = 0, j \in J_1 = (1, 2,..., m_1)$ are "soft", and constraints with indices $j \in J_2 = (m_1 + 1, m_1 + 2, ..., m)$ are "hard".

A two-stage problem of industrial apparatus optimization in static is formulated the following way: it is necessary to determine vectors d^* and z^*, which provide for the extremum of goal function $F(d, z)$ and fulfillment of "soft" and "hard" constraints disregarding changes in uncertain parameters vector ξ in a given domain Ξ. Mathematically this problem is formulated as follows:

$$F^* = \min_{d,u,z(\xi)} u; \tag{7}$$

$$y = \Psi(d, z, \xi); \tag{8}$$

$$\Pr\{g_0(d, z(\xi), \xi) = F(d, z(\xi), \xi) \le u\} \ge \rho_0; \tag{9}$$

$$\Pr\{g_j(d, z(\xi), \xi) \le 0\} \ge \rho_j, \ j \in J_1; \tag{10}$$

$$\chi_1(d) = \max_{\xi \in \Xi} \min_z \max_{j \in J_2} g_j(d, z, \xi) \le 0. \tag{11}$$

In the problem (7) – (11) u is a scalar variable (analog to design variables); $\Pr\{\cdot\}$ – probability of constraint $\{\cdot\}$ fulfillment; g_0, g_j – are constraint functions; ρ_0, ρ_j – given values of constraint fulfillment probability; $\chi_1(d)$ – is apparatus flexibility function.

A characteristic feature of two-stage apparatus optimization problems is a possibility to tune up regime (control) variables z depending on the refinement of uncertain parameters vector ξ during the running stage, i.e. control variables z are multidimensional functions $z = z(\xi)$.

Algorithm of two-stage optimization on chemical process systems

We shall introduce symbols

$$\overline{g}_j(d, u, z, \xi) = \begin{cases} g_j(d, z, \xi) - u, & j = 0; \\ g_j(d, z, \xi), & j \in J_1, \end{cases}$$

and a set $S^{(k)} = \left\{ \xi^i : i \in I^{(k)} \right\}$ of accumulation of points ξ with indices $i \in I^{(k)}$, in which constraints (9) – (11) are violated, and a set $S_1^{(k)}$ will accumulate points of "hard" constraint violation and a set $S_2^{(k)}$ will accumulated points of "soft" constraint violation. In addition, we shall use an auxiliary non-linear programming problem (A)

$$F^* = \min_{d, u, z^i} u$$

$$\overline{g}_j(d, u, z^i, \xi^i) \le 0, \ j = 0, \ j \in J_1, \ i \in I^{(k)};$$

$$g_j(d, z^i, \xi^i) \le 0, \quad j \in J_2, \ i \in I^{(k)}. \tag{A}$$

The problem (A) is solved when a minimal value of the scalar variable u is found and all problem constraints in the given set of points $\xi^i, i \in I^{(k)}$ are fulfilled.

Algorithm.

Step 1. Let $k = 1$. Select initial set $S^{(k-1)}$ on the condition of optimal approximation of functions $z(\xi)$. Set initial approximations $d^{(k-1)}, u^{(k-1)}, z^{i,(k-1)}$.

Step 2. Solve auxiliary problem (A) and let $d^{(k)}, u^{(k)}, z^{(k)}$ be a solution of this problem.

Step 3. Compute

$$\chi_1(d^{(k)}) = \max_{\xi \in \Xi} \min_z \max_{j \in J_2} g_j\left(d^{(k)}, z, \xi\right), \tag{12}$$

using an algorithm of external approximation [1]. We shall consider $\overline{\xi}^{(k)}$ to be a solution of problem (12) and verify if the following condition is fulfilled

$$\chi_1(d^{(k)}, \overline{\xi}^{(k)}) \le 0. \tag{13}$$

If the condition (13) is not fulfilled, go to step 4, otherwise, go to step 5.

Step 4. Extend a set of points $S_1^{(k)}$ where constraints (13) are violated, that is

$$S_1^{(k)} = S_1^{(k-1)} \bigcup \overline{\xi}^{(k)}; \ \overline{\xi}^{(k)} : \chi_1(d^{(k)}) > 0;$$

$$I_1^{(k)} = I_1^{(k-1)} \bigcup (n+1); \ n := n + 1.$$

Step 5. Check the fulfillment of "soft" constraints

$$\Pr\left\{\overline{g}_j(d^{(k)}, z(\xi), \xi) \le 0\right\} \ge \rho_j, \quad j = 0, j \in J_1. \tag{14}$$

At this point we have not obtained functions $z = z(\xi)$, we only know the values of these functions in discrete points ξ^i, $i \in I^{(k)}$. Thus, we shall use these points for the approximation of functions $z = z(\xi)$.

If the condition (13) is fulfilled and the condition (14) is not fulfilled, then go to step 6.

If both conditions (13) and (14) are fulfilled, a solution is obtained $d^* = d^{(k)}$, $z^* = z^{i,(k)}$.

Step 6. Compute

$$\chi_2(d^{(k)}) = \max_{\xi \in \Xi} \min_z \max_{j \in \overline{J}_1} \overline{g}_j\left(d^{(k)}, u^{(k)}, z, \xi\right), \tag{15}$$

where $\overline{J}_1 = (0,1,2, \ldots, m_1)$, using an algorithm of external approximation [1]. We shall identify a solution of the problem (15) as $\overline{\overline{\xi}}^{(k)}$ and extend the set of points $S_2^{(k)}$, where "soft" constraints are violated, that is

$$S_2^{(k)} = S_2^{(k-1)} \bigcup \overline{\overline{\xi}}^{(k)}; \quad \overline{\overline{\xi}}^{(k)} : \chi_2\ (d^{(k)}) > 0;$$
$$I_2^{(k)} = I_2^{(k-1)} \bigcup (n+1); \quad n := n+1.$$

Step 7. Form sets $S^{(k)} = S_1^{(k)} \bigcup S_2^{(k)}$, $I^{(k)} = I_1^{(k)} \bigcup I_2^{(k)}$, let $k := k+1$ and go to step 2.

Let us comment on the algorithm.

At step 5 multivariate interpolation is carried out with the help of functions $z = z(\xi)$ at the known discrete points ξ^i, z^i, $i \in I^{(k)}$. It can be achieved through the use of multivariate cubic splines or using approximation procedure as follows. When implementing the simulation model, for every random value ξ we shall accept value $z^l(\xi^l)$, $l \in I^{(k)}$ as a respective $z(\xi)$, which corresponds to point ξ^i, the closest to point ξ, that is:

$$r^i(\xi, \xi^i) = \sqrt{\sum_{j=1}^{n_\xi} (\xi_j - \xi_j^i)^2}, \ i \in I^{(k)} = I_1^{(k)} \bigcup I_2^{(k)}, \ n_\xi = \dim \xi,$$

$$\widehat{\xi} = \min_{i \in I^{(k)}} r^i(\xi, \xi^{(l)}) \ \Rightarrow \ \hat{i} = \arg \min_{i \in I^{(k)}} r^i(\xi, \xi^{(i)}) \ \Rightarrow \ \hat{z} = z^{(\hat{i})}.$$

In fact, the described procedure uses piecewise constant approximation of functions $z = z(\xi)$.

At step 6 the inequality $\chi_2(d^{(k)}) \le 0$ implies that "soft" constraints are fulfilled with probability 1. Thus, if the condition (14) is not fulfilled, then knowingly $\chi_2(d^{(k)}) > 0$, and we shall obtain point $\overline{\overline{\xi}}^{(k)}$ where "soft" constraints are violated.
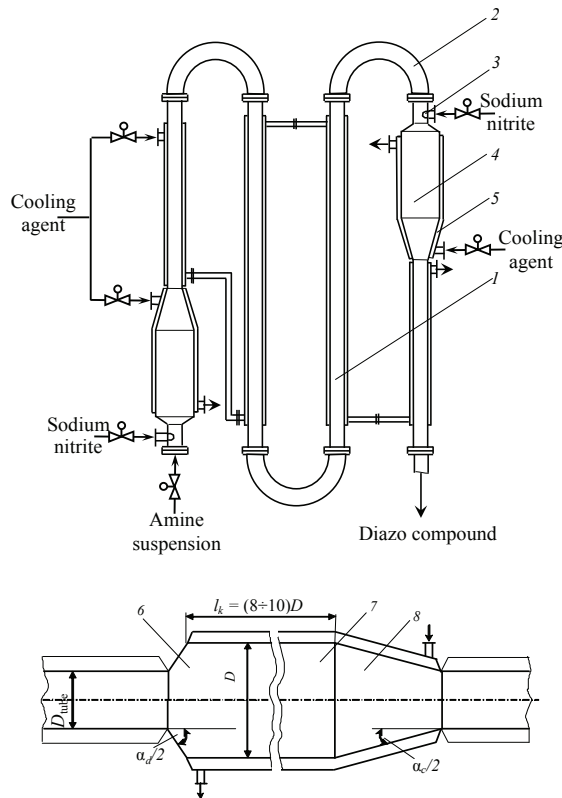
When implementing additional variable u it is suggested to conduct the ranging of search variables in order to make the ranges of variables more or less equal.

Examples of optimal design of industrial chemical process apparatus

We shall demonstrate the effectiveness of the suggested algorithm on the examples of optimal design of several industrial chemical process apparatus: turbulent tube reactor of thin organic synthesis, short-cycled adsorption unit, and a mold for the high-temperature synthesis of hard-alloyed materials.

The simulation model $y = \Psi(d, z, \xi)$ of the static of non-linear process of thin organic synthesis – diazotization of aromatic amines in the turbulent tube diazotization reactor – allows calculating output variables y of diazotization reactor: productivity Q; concentrations $c^{(\text{out})} = (c_D, c_{NA}, c_\chi, c_\sigma)$ of diazo compound, nitrous acid, diazo rosins and nitrose gases; flow rates $G^{(\text{out})} = (G_l^{(\text{out})}, G_s^{(\text{out})})$ of liquid and solid phases of diazo solution suspension, amount of solid phase of amine Π_η, diazo rosins Π_χ, nitrose gases Π_σ in diazo solution at the output of diazotization reactor [2]; where d, z, ξ are vectors of design, control variables and diazotization reactor uncertain parameters correspondingly.

We shall formulate specifications for the design of turbulent tube reactor of aromatic amine diazotization with diffuser-contractor devices of flow turbulization (Figure).

Turbulent tube reactor with diffuser-contractor type mixing chambers:
1 – tube module; *2* – bend; *3* – nozzles for sodium nitrite spray; *4* – diffuser-contractor device; *5* – heat exchange jacket; *6* – diffuser; *7* – straight part; *8* – contractor; d_{tube} – diameter of reactor tube part; D – mixing chamber diameter; l_k – mixing chamber length; α_d – angle of diffuser expansion; α_c – angle of contractor narrowing

For the set (diazo compound) reactor productivity $Q = 1000$ tons per year, it is necessary to ensure that the values of

− aromatic amine unreacted particles $\Pi_\eta = \dfrac{G_S^{(\text{out})}}{G_S^{(0)}} 100\%$;

− diazo rosin content $\Pi_\chi = \dfrac{c_\chi^{(\text{out})} \times G_l^{(\text{out})}}{[c_A^{(0)}]_s \times G_l^{(\text{out})}} 100\%$;

− nitrose gas content $\Pi_\sigma = \dfrac{c_{NA}^{(\text{out})} \times G_l^{(\text{out})}}{c_N^{(0)} \times G_N^{(0)}} / 100\%$,

do not exceed the maximum values $\hat{\Pi}_\eta = 0{,}25\ \%$, $\hat{\Pi}_\chi = 0{,}9\ \%$, $\Pi_\sigma = 0{,}5\ \%$, that is $\Pi_\eta \le \hat{\Pi}_\eta$, $\Pi_\chi \le \hat{\Pi}_\chi$ and $\Pi_\sigma \le \hat{\Pi}_\sigma$, where $[c_A^{(0)}]_S, c_\chi^{(\text{out})}$ − concentration of aromatic amine solid phase at the reactor input and concentration of diazo compound at the reactor output; and $c_N^{(0)}, G_N^{(0)}$ − concentration of sodium nitrite and sodium nitrite flow rate at the reactor input. These requirement should be fulfilled under interval uncertainty of certain technological parameters and coefficients of mathematical model of diazotization process, namely: concentration of amine solid phase $[c_A^{(0)}]_S = 370{,}0\ (\pm\ 4\ \%)$ mole/m^3 at the reactor input and kinetic coefficient in the equation of aromatic amine solid phase dissolution $A = 5{,}4 \cdot 10^5 (\pm\ 5\ \%)$.

The task of optimal design is to determine such design parameters d (diameter D and length of tube reactor L, number m and place of installation $l_j, j = 1, 2, \ldots$ of diffuser-contractor devices) and control variables z (temperature $T^{(0)}$ of aromatic amine suspension at the reactor input, and sodium nitrite flow distribution $G_N^{(i)}, i = 1, 2, \ldots, p$ over the reactor length) that the total costs $\text{TC}(d, z, \xi)$ of reactor development are minimal and its efficiency does not depend on random changes of uncertain parameters vector ξ in a given domain Ξ. The constraints can be "hard" and/or "soft". "Hard" constraints usually include the requirements for product quality and explosion, inflammation and environmental safety. Let us formulate the two-stage problem of optimal design of turbulent tube reactor of aromatic amine diazotization with mixed constraints: such vectors d^* and z^* must be determined that the total costs are minimal, i.e.

$$\text{TC}^* = \min_{d, u, z(\xi)} u ; \tag{16}$$

$$y = \Psi(d, z, \xi) ; \tag{17}$$

$$\Pr\{g_0(d, z(\xi), \xi) = \text{TC}(d, z(\xi), \xi) \le u\} \ge \rho_0 ; \tag{18}$$

$$\Pr\{g_1(d, z(\xi), \xi) = Q_{\text{init}} - Q(d, z(\xi), \xi) \le 0\} \ge \rho_1 ; \tag{19}$$

$$\chi_1(d) = \max_{\xi \in \Xi} \min_z \max_{j \in J_2} g_j(d, z, \xi) \le 0 ; \tag{20}$$

where $g_2(d, z(\xi), \xi) = \Pi_\eta(d, z(\xi), \xi) - \hat{\Pi}_\eta$; $g_3(d, z(\xi), \xi) = \Pi_\chi(d, z(\xi), \xi) - \hat{\Pi}_\chi$; $g_4(d, z(\xi), \xi) = \Pi_\sigma(d, z(\xi), \xi) - \hat{\Pi}_\sigma$.

In problem (16) – (20) u – a scalar variable (analogous to design parameters); $\Pr\{\cdot\}$ – probability of constraint $\{\cdot\}$ fulfillment; $g_0, g_j, y_{j,\text{init}}$ – constraint functions and maximum values of output variables; ρ_0, ρ_j – given values of constraint fulfillment probability; $\chi_1(d)$ – flexibility function of diazotization reactor; the constraints with indices $j \in J_1 = \{0, 1\}$ are "soft", and the ones with indices $j \in J_2 = \{2, 3, 4\}$ are "hard".

The results of the two-stage optimal design problem solution for industrial diazotization turbulent reactor at each iteration are presented in Table.

The problem of optimal design (by total costs criterion) of short-cycled adsorption unit for oxygen-enrichment is formulated as follows: for a given unit setting $a \in A$ of adsorption unit and given productivity rates Q_{init} and oxygen concentration $c_{O_2}^{\text{out}}$ at the unite output, such design parameters (type of adsorber $b \in B$, height of adsorbent layer H, diameter of adsorber D_{inner}) and regime variables (pressure P_{ad}, P_{des}, duration of cycle τ_c, backwashing coefficient θ) should be determined that the total costs of unit development are minimal. Some input data are uncertain, for example, oxygen concentration in the air fed into adsorber $c_{O_2}^{\text{in}}$ can fluctuate between 18 to 23 % vol.,

Results of optimal design problem solution

Iteration No., k	Design variables, d	Regime (control) variables, z	Total costs u, USD	Flexibility function, χ	Values of "soft" constraints fulfillment probability $\Pr\{\cdot\}$, %
1	$D = 0{,}04$ m; $L = 115$ m; $m = 3$ pcs; $l_1 = 40$ m; $l_2 = 80$ m	$T^{(0)} = 296$ °C; $p = 3$; $G_N^{(1)} = 5{,}1 \cdot 10^{-5}$ m³/s; $G_N^{(2)} = 2{,}55 \cdot 10^{-5}$ m³/s; $G_N^{(3)} = 2{,}55 \cdot 10^{-5}$ m³/s	2225	0,326	$\Pr\{g_0 \le u\} = 92{,}1$; $\Pr\{g_1 \le 0\} = 95$
2	$D = 0{,}04$ m; $L = 120$ m; $m = 3$ pcs; $l_1 = 42{,}5$ m; $l_2 = 82{,}5$ m	$T^{(0)} = 300$ °C; $p = 3$; $G_N^{(1)} = 6{,}3 \cdot 10^{-5}$ m³/s; $G_N^{(2)} = 1{,}95 \cdot 10^{-5}$ m³/s; $G_N^{(3)} = 1{,}95 \cdot 10^{-5}$ m³/s	2230	0,00075	$\Pr\{g_0 \le u\} = 94{,}1$; $\Pr\{g_1 \le 0\} = 97{,}7$
3	$D = 0{,}04$ m; $L = 123$ m; $m = 3$ pcs; $l_1 = 43$ m; $l_2 = 84$ m	$T^{(0)} = 300$ °C; $p = 3$; $G_N^{(1)} = 6{,}1 \cdot 10^{-5}$ m³/s; $G_N^{(2)} = 2{,}05 \cdot 10^{-5}$ m³/s; $G_N^{(3)} = 2{,}05 \cdot 10^{-5}$ m³/s	2232	–0,036	$\Pr\{g_0 \le u\} = 100$; $\Pr\{g_1 \le 0\} = 98{,}8$

maximum adsorption volume of zeolite adsorbent W_0 – from 0,160 to 0,230 cm^3/g, and mass delivery coefficient value β – from 1,2 to 1,8 $\times 10^{-5}$ s^{-1}. Mathematically the problem is stated as follows

$$I^* = \min_{a,b,H,D_{\text{inner}},u,P_{\text{ad}},P_{\text{des}},\tau_{\text{c}},\theta} u \qquad (21)$$

for variables' connections with the mathematical model of unsteady process of the oxygen concentration process [3] under the constraints:
 – on goal function value

$$\Pr\{g_0(a,b,H,D_{\text{inner}},P_{\text{ad}},P_{\text{des}},\tau_{\text{c}},\theta,\xi) = \text{TC}(a,b,H,D_{\text{inner}},P_{\text{ad}},P_{\text{des}},\tau_{\text{c}},\theta) \le u\} \ge \rho_0 ; \quad (22)$$

 – on unit productivity

$$\Pr\{g_1(a,b,H,D_{\text{inner}},P_{\text{ad}},P_{\text{des}},\tau_{\text{c}},\theta,\xi) = (Q_{\text{inner}} - Q) \le 0\} \ge \rho_1 ; \qquad (23)$$

 – on oxygen concentration and unit dimensions

$$\chi_1(a,b,H,D_{\text{вн}}) = \max_{\xi \in \Xi} \min_{P_{\text{ad}},P_{\text{des}},\tau_{\text{c}},\theta} \max_{j=2,3} g_j(a,b,H,D_{\text{inner}},P_{\text{ad}},P_{\text{des}},\tau_{\text{c}},\theta,\xi) \le 0 , \quad (24)$$

where $g_2(a,b,H,D_{\text{inner}},P_{\text{ad}},P_{\text{des}},\tau_{\text{c}},\theta,\xi) = [c_{\text{O}_2}^{\text{out}}]_{\text{init}} - c_{\text{O}_2}^{\text{out}}$;

$g_3(a,b,H,D_{\text{inner}},P_{\text{ad}},P_{\text{des}},\tau_{\text{c}},\theta,\xi) = M - \hat{M}$;

$$k_p \le \hat{k}_p , \ H \le \hat{H} , \ D_{\text{inner}} \le \hat{D} , \qquad (25)$$

where u – scalar variable; $\Pr\{\cdot\}$ – constraint fulfillment probability; ρ_0, ρ_1 – given probability values; χ – unit flexibility function; $Q_{\text{inner}}, [c_{\text{O}_2}^{\text{out}}]_{\text{init}}$ – given values of unit productivity output oxygen concentration; $\hat{M}, \hat{k}_p, \hat{H}, \hat{D}_{\text{inner}}$ – maximum values of mass, pressure coefficient and adsorber dimensions of the unit.

We shall study the development of a portable medical oxygen concentrator as an example of optimal design of energy-saving short-cycled adsorption unit. The specifications for its design are the following: concentrator productivity is $Q_{\text{init}} = 0,05 \cdot 10^{-3}$ m^3/s, output oxygen concentration $[c_{\text{O}_2}^{\text{out}}]_{\text{init}} \ge 90$ %; $\rho_0, \rho_1 = 0,9$; maximum values of adsorber mass $\hat{M} = 0,6$ kg; adsorption P_{ad} and desorption P_{des} pressure ratio $\hat{k}_p = 3$; adsorbent layer height $\hat{H} = 0,4$, and adsorber diameter $\hat{D}_{\text{inner}} = 0,1$ m.

Alternate variants of unit setting included column adsorber, two-adsorber scheme without pressure leveling between adsorbers, two-adsorber scheme with pressure leveling, four-adsorber scheme with pressure leveling, and five-adsorber scheme with two pressure leveling operations. For each variant, different schemes of oxygen-enrichment process were analyzed (pressured, with vacuum desorption, vacuum-pressured), and various types of adsorbents were considered (granulated and block – NaX, LiLSX).

During the optimal design of two-adsorber unit with vacuum desorption under uncertainty, the following optimal values were determined: of design parameters $H^* = 0{,}22$ m; $D^*_{inner} = 0{,}035$ m; of regime variables $P^*_{ad} = 1{,}5 \times 10^5$ Pa; $P^*_{des} = 0{,}5 \times 10^5$ Pa; $\theta^* = 2{,}5$; $\tau^*_c = 1{,}6$ s; $Q^*_{out} = 2{,}93 \times 10^{-4}$ m^3/s; and technical and economic characteristics of the portable medical oxygen concentrator: total costs – 45250 rub.; $M^* = 0{,}5$ kg; $N^* = 76$ W.

For the design of medical oxygen concentrators with productivity range up to $0{,}08 \times 10^{-3}$ m^3/s we would recommend implementing adsorbers with dimensions $4 \leq H/D_{inner} \leq 6$ for pressured scheme with vacuum desorption ($k_p = P_{ad}/P_{des} \leq 3$) and block zeolite adsorbents LiLSX with $d_{eq} \leq 0{,}5 \cdot 10^{-3}$ m. This ensures the increase of energy-saving characteristics of medical oxygen concentrators by 20 % average as compared with international analogues.

Traditionally when calculating strength properties of thermoloaded cylindrical cowlings (apparatus or mold shell and others), it is assumed that the temperature profile of an installation's wall is linear, which results in unnecessarily thick and heavy installation shells. Self-propagating high-temperature synthesis of hard-alloyed materials using press molding combines high temperature and power loadings: the temperatures inside the mold are ~2000–3000 °C, and excess pressure within the material during press molding reaches ~200 MPa. High power and temperature loadings applied at different time intervals, non-stationarity, and qualitative diversity of temperature gradients in installation shell walls require a detailed study.

To calculate strength properties of the mold, a mathematical model with non-linear equations of thermal conductivity and flame front motion with edge conditions were used [4]. Press molding time lag t_{init} (a time period between the end of material's combustion and the beginning of internal pressure loading) and pressing pressure P are the model's input variables. While calculating temperature fields, speed U_{com} and temperature T_{com} of material sample's combustion were taken into account. The mathematical model allows calculating output variables: temperature at the internal wall T_1^w, thickness of the boundary layer δ_1 of the wall, and equivalent loading σ_{eq} that develops in the wall because of thermal and mechanical influences. The value δ_1 is set by admissible temperature difference in the wall, by which the mechanical properties of the wall's material are sustained and the changes in the material of the wall are reversible.

We have considered speed U_{com} and temperature T_{com} of the pressed material's combustion as uncertain parameters ξ. The uncertainty of U_{com} and T_{com} data results from different factors related to the properties of initial charge (bulk density, humidity, etc.). The problem of strength properties calculation of a mold for self-propagating high-temperature synthesis of hard-alloyed materials is formulated as follows. Such time lag t_{init} and pressure P must be determined that the thickness of the mold wall δ is minimal, that is

$$\min_{\delta, t_{init}, P} \delta, \tag{26}$$

for variables' connections with the mathematical model of thermal conductivity [1] and under constraints: temperature at the mold's internal wall

$$g_1(\delta, t_{init}, P, \xi) = \max_{\xi \in \Xi} \ \min_{t_{init}, P} (T_1^w(\delta, t_{init}, P, \xi) - T^{lim}) \leq 0, \tag{27}$$

thickness of the mold's boundary layer

$$g_2(\delta, t_{\text{init}}, P, \xi) = \max_{\xi \in T} \min_{t_{\text{init}}, P} (10\delta_1(\delta, t_{\text{init}}, P, \xi) - \delta) \leq 0 , \qquad (28)$$

equivalent stress in the wall

$$g_3(t_{\text{init}}, P, \xi) = \max_{\xi \in T} \min_{t_{\text{init}}, P} (\sigma_{\text{eq}}(t_{\text{init}}, P, \xi) - [\sigma]) \leq 0 . \qquad (29)$$

As an example, the problem of optimization of a mold's wall thickness was solved under the experimentally determined intervals of combustion speed changes $U_{\text{com}} \in [5\ldots25]$ mm/s and charge combustion temperature $T_{\text{com}} \in [1950\ldots2050]$ ºC. This problem was solved in three iterations. Its solution allowed determining optimal values of the mold's wall thickness $\delta^* = 48,3$ mm, time lag $t_{\text{init}}^* = 4,3$ s, pressing pressure $P^* = 100$ MPa, and $\chi_0(\delta^*) = -0,00019$. In our earlier works we have calculated the thickness of a mold with nominal values of $U_{\text{com}} = 15$ mm/s and $T_{\text{com}} = 2000$ ºC: $\delta^* = 42$ mm, $t_{\text{init}}^* = 4,7$ s, $P^* = 100$ MPa.

Comparative analysis proves that implementation of the mold 48,3 mm thick is fail-safe, disregarding any random changes of uncertain parameters ξ. The scientifically grounded overdesign coefficient for the mold's thickness is 15 % and is based on real temperature profile.

Conclusion

The article describes an algorithm of two-stage optimization of chemical process systems, based on a scientific approach which considers the uncertainty of mathematical description and technological parameters coefficients in the statement of the optimization problem. As the examples of the algorithm's efficiency, its implementation for the optimal design of the following industrial chemical process apparatus is discussed: turbulent tube reactor of thin organic synthesis, adsorption oxygen concentrator, and a mold for the high-temperature synthesis of hard-alloyed materials

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Разработка алгоритма двухэтапной оптимизации промышленных аппаратов химической технологии

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Ключевые слова и фразы: двухэтапная оптимизация; конструктивные параметры; управляющие переменные; химико-технологические аппараты.

Аннотация: Сформулирована двухэтапная задача оптимального проектирования промышленных аппаратов химической технологии в условиях неопределенности физико-химических, технологических и экономических исходных данных. Характерной особенностью двухэтапных задач оптимизации является возможность подстройки режимных (управляющих) переменных химико-технологической системы в зависимости от уточнения (измерения) неопределенных параметров на этапе ее эксплуатации. Разработан алгоритм двухэтапной оптимизации технических систем, эффективность которого демонстрируется на примерах оптимального проектирования ряда химико-технологических аппаратов: турбулентного трубчатого реактора тонкого органического синтеза, адсорбционного концентратора кислорода и пресс-формы высокотемпературного синтеза твердосплавных материалов.

Erarbeitung des Algorithmus der zweietappischen Optimisierung der industriellen Apparate der chemischen Technologie

Zusammenfassung: Es wird die zweietappische Aufgabe der optimalen Projektierung der industriellen Apparate der chemischen Technologie in den Bedingungen der Unbestimmtheit der physikalisch-chemischen, technologischen und ökonomischen Ausgangsangaben formuliert. Die charakteristische Besonderheit der zweieteppischen Aufgabe der Optimisierung ist die Möglichkeit der Abstimmkorrektur der Regimevariablen des chemietechnologischen Systems je nach der Präzisierung (der Messung) der unbestimmten Parameter während seiner Explutuation. Es ist das Algorithmus der zweietappischen Optimisierung der technischen Systeme erarbeitet. Seine Effektivität wird an den Beispielen der optimalen Projektierung der einigen chemie-technologischen Apparate: des turbulenten Rohrreaktors der dünnen organischen Synthese, des Adsorbtionskonzentrators des Sauerstoffes und der Pressforme der hochtemperaturischen Synthese der Hartmetallstoffe demonstriert.

Élaboration de l'algorithme de l'optimisation à deux étapes des appareils industriels de la technologie chimique

Résumé: Est formulée une tâche à deux étapes de la conception optimale des appareils industriels de la technologie chimique dans les conditions de l'indétemineté des données initales physico-chimiques, tecnologiques et économiques. La particularité

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caractéristique des tâches à deux étapes de l'optimisation est la possibilité de la construction des variables de régime (commandées) du système chimico-technologique en fonction de la précision (mesure) des paramètres indéterminés à l'étape de son exploitation. Est élaboré l'algorithme de l'optimisation à deux étapes des systèmes techniques dont l'efficacité est montrée aux exemples de la conception optimale d'une série des appareils chimico-technologiques: réacteur turbulent tubulaire de la fine synthèse organique, concentrateur absorbant de l'oxygène et moule de la synthèse des matéraux d'une solide alliage à haute température.

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