New problem statements, algorithms and problems of integrated design of flexible chemical processes and automatic control systems

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Abstract

A multi-stage strategy for the integrated design of energy- and resource-saving chemical processes and regime control systems under uncertainty of physical, chemical, technological and economic initial data has been developed. Depending on the changes of uncertainties at the stages of design and exploitation of chemical processes (CP), two-stage stochastic optimization problems with “hard” and “soft” (probable) constraints are formulated (Halemane and Grossmann, 1983; Ostrovsky et al., 1993). Modified methods and algorithms of their solution are suggested.

Keywords: integrated design, optimization under uncertainty, azo-dyes

1. Introduction

While carrying out integrated design, it must be strived to fulfill technological “hard” and/or “soft” constraints set by production procedure – “hard” constraints must never be violated, “soft” constraints should be fulfilled with the given probability. The problem of constraints fulfillment is largely complicated by inexactness of physical and chemical phenomena underlying CP and control systems mathematical models, by model coefficients’ drift during exploitation of a process (for example, chemical reaction speed constants, diffusion, mass and heat transfer coefficients, etc.), and by accidental changes of technological variables (temperature, speed and composition of raw material flows, etc.). In such case the necessity to create flexible/workable CPs arises. A CP shall be flexible if, during its exploitation, the conditions for carrying out the process, set by technological procedure, are fulfilled disregarding accidental changes of uncertain parameters in a given area by a suitable choice of vectors of design parameters and controlling influences at design stage (when solving one-stage optimization problem (Ostrovsky et al., 1993) or by necessary adjustment of controlling influences at exploitation stage (during the solution of two-stage optimization problem (Halemane and Grossmann, 1983). Thus, flexibility of CP in static and dynamics is determined by CP design and regime variables and is secured by a suitable choice of controlling influences realized by an automatic control system (ACS).

Therefore, during integrated design optimal design parameters of CP equipment framework and its functioning regimes must be chosen on the basis of a reasonable compromise between the efficiency of a chemical process in terms of energy- and resource-saving and "good" dynamic characteristics of the process in terms of control/regulation channels.

2. Strategy of Integrated Design

In accordance with the developed methodology of integrated design three problems are solved iteratively:

1. generating alternative CP variants meeting "soft" or "hard" flexibility requirements;
2. selecting alternative classes and structures of CP ACS, fulfilling the requirements of structural observability and controllability of CP with given dynamic characteristics in terms of control channels;
3. solving one- or two-stage problem of optimization of design and regime variables of CP-control system (CS) complex under uncertainty of vector criteria, which include product quality indexes, energy- and resource-saving indexes, and technical and economic production indexes.

The selection of control system class and structure is done with the use of an array of regulated (observable) variables and controlling influences, obtained through analyzing the structural matrix of CP dynamics equations. In this process, observability of CP output variables, estimation of sensor and equipment development costs, possibility and accuracy of output variables forecast on the basis of indirect indexes, as well as controllability of a CP with various combinations of controlling influences, are taken into account. Alternative ACS classes and structures are studied through imitational modeling in the order of their economic efficiency rating. For admissible ACS structures a research of CP dynamic indexes (regulability, inertness, etc.) in control channels is conducted. In the case controlled in static CPs have unsatisfactory dynamic characteristics, design and regime parameters chosen at the first stage are correlated, or new types of CP equipment are selected.

At the final stage of integrated design a multi-criteria optimization problem for alternative CP-ACS complexes is solved. During imitational research, energy- and resource-saving and economic efficiency index values are calculated, as well as specifications for accuracy and capacity of information measurement subsystem, optimal control algorithms, executive mechanisms and control devices, control algorithm and model adaptation subsystems, are defined. Basing on the results of imitational research, attainability of the set CP functioning goals and fulfillment of specification requirements is assessed. Should the requirements be not met, transition to new forms of CP equipment or to selecting a new CP structure is made.

3. Methods of CP Optimization under Uncertainty

To formulate the problem of optimization under uncertainty it is necessary to set the form of the goal function and define constraints. Underlying this definition is the concept of two stages of CP: the design stage (which is practically always uncertain), and the exploitation stage. At the second stage the following cases are possible.

3.1 Case 1

At the CP exploitation stage the area of uncertain parameters is the same as at the design stage. This case brings us to a class of one-stage stochastic optimization problems, the formulations and solution methods of which have been considered in our earlier works.

3.2 Case 2

At the exploitation stage uncertain parameters ξ may be determined at any moment of time and control variables z may be used to provide for the fulfillment of these constraints. In this case, CP flexibility condition will be formulated as $\forall \xi \in \Xi \; \exists \, z \; \forall j \in J \quad \varphi_j(d,z,\xi) \le 0$ or $F_2 = \max\limits_{\xi \in \Xi} \min\limits_{z} \max\limits_{j \in J} \varphi_j(d,z,\xi) \le 0,$ and the problem of stochastic optimization with “hard” constraints will read as following:

$$I_2^* = \min_d E_\xi \left\{ \min_z I(d,z,\xi) \middle| \; \varphi_j(d,z,\xi) \le 0, \; j \in J \right\} = \min_d \int_\Xi I^\oplus(d,\xi) P(\xi) d\xi,$$

where $I^\oplus = \min\limits_z I(d,z,\xi) \big| \; \varphi_j(d,z,\xi) \le 0, \; j \in J.$

Let $d^* -$ be a solution of the problem, then if $d = d^*$ CP flexibility and workability can be guaranteed. In fact, calculation of $E_\xi \{ I^\oplus(d,\xi) \}$ presupposes the possibility of solving the problem $\min\limits_z I(d,z,\xi) \big| \; \varphi_j(d,z,\xi) \le 0, \; j \in J$ for all $\xi \in \Xi$, and therefore, the existence of vector z for each ξ, when all the constraints are fulfilled. However, when solving the problem of I_2^* definition with a certain calculation method, it may occur so that with certain d and ξ the constraints cannot be fulfilled. Normally in such situation the calculations stop. That is why it is important to include flexibility constraints explicitly in the problem formulation. Then the optimization problem will be formulated as following:

$$I_2^* = \min_d E_\xi \left\{ I^\oplus(d,\xi) \right\}, \quad F_2(d) \le 0.$$

This is the so-called two-stage problem of stochastic optimization with “hard” constraints.

If “soft” constraints are used, the flexibility condition can be expressed in the following form: $\rho_{init} - \Pr\text{ob}\left\{ \xi \in \Xi^\otimes \right\} \le 0,$ where $\Xi^\otimes(d) = \left\{ \xi : \min\limits_z \max\limits_{j \in J} \varphi_j(d,z,\xi) \le 0, \; \xi \in \Xi \right\}$, and the value of the goal function $I^\oplus(d,\xi)$ is found from the solution of the problem

$$I^\oplus(d,\xi) = \begin{cases} \displaystyle\int_{\Xi^\otimes} \left(\min_z I(d,z,\xi) \middle| \; \varphi_j(d,z,\xi) \le 0, \; j \in J \right) P(\xi) d\xi \;\; if \;\; \xi \in \Xi^\otimes; \\ \displaystyle\int_{\Xi \setminus \Xi^\otimes} \left(\min_z \left[I(d,z,\xi) + A \cdot \max\left(\max_{j \in J^\otimes} \varphi_j(d,z,\xi), 0 \right) \right] \right) P(\xi) d\xi \;\; if \;\; \xi \notin \Xi^\otimes, \end{cases}$$

where $A-$ is a penalty coefficient, and $J^{\otimes}-$ is an array of constraint indexes, the violation of which incurs penalty.

It must be mentioned that if there exists such d that $F_2(d) \le 0,$, then if $\rho_{init} = 1$ the optimization problem with “soft” constraints transforms into a problem with “hard” constraints.

3.3 Case 3

The vector ξ of uncertain parameters consists of two subvectors ξ^1 and ξ^2, i.e. $\xi = (\xi^1, \xi^2)$. Subvector ξ^1 includes parameters which can be identified at the CP exploitation stage, and subvector ξ^2- parameters with the same uncertainties at exploitation and design stages. In this case let $\xi^1 \in \Xi^1$ and $\xi^2 \in \Xi^2$. Then the two-stage stochastic programming problem is formulated as following:

$$I_3^* = \min_{d \in D} E_{\xi^1}\left\{I^{\oplus}(d, \xi^1)\right\}, \text{ when CP flexibility requirement is fulfilled}$$

$$F_3(d) = \max_{\xi^1 \in \Xi^1} \min_{z} \max_{\xi^2 \in \Xi^2} \max_{j \in J} \varphi(d, z, \xi^1, \xi^2) \le 0,$$

$$\text{where } I^{\oplus} = \min_{z} E_{\xi^2}\left\{ I(d, z, \xi^1, \xi^2) \,\middle|\, \max_{\xi^2 \in \Xi} \varphi_j(d, z, \xi^1, \xi^2) \le 0,\ j \in J \right\}, \text{ or}$$

$$I^{\oplus} = \min_{z} E_{\xi^2}\left\{ I(d, z, \xi^1, \xi^2) \middle| \Pr\text{ob}_{\xi^2}\left[\varphi_j(d, z, \xi^1, \xi^2) \le 0\right] \ge \rho_{init},\ j \in J \right\}.$$

Thus, the optimization problem in design of chemical processes can be formulated with account to various levels of information on CP available at the stage of its exploitation. Each solution offers an optimal variant of CP for a given level of information. However, designers must consider that obtaining the information may itself involve certain expenses. The development of more precise models, installation of new measurement devices and automatic control systems to stabilize uncertain parameters increase the level of available information about CP but require additional expenses. And this sets an important problem of choosing optimal (or reasonable) level of experimental information as input data for designing a CP.

We have developed modified algorithms of calculating flexibility functions $F_2(d)$ and solving two-stage stochastic optimization problem for cases 2 and 3 (Dvoretsky and Dvoretsky, 2003).

4. Examples of Integrated Design of Thin Organic Synthesis Reactor Systems with Automatic Control

Diazotization and combination processes carried out in a turbulent tube reactor with capacity 1000 tons per year have been investigated.

Design specifications include fulfillment of “hard” and/or “soft” constraints for coloristic characteristics of output dyes (pigments), for organic semi-products and dyes’ output, for norms of nitrose gases’ emission in diazotization reactor, for energy- and resource saving indexes of continuous technologies and equipment, for quality indexes of transition processes in temperature regulation automatic systems, as well as for nitrous acid concentration in diazosolution and pH environment concentration in azocombination reaction zone.

The fulfillment of the above-mentioned specification requirements for designing diazotization and azocombination turbulent tube reactors must be secured under the uncertainty of mathematical model coefficients, input variables and external factors at the design stage, particularly, of amine solid phase concentration and average particle radius in the feed of the reactor, and kinetic coefficients of diazotization and azocombination reaction, accompanied by mass exchange processes of amine solid phase dissolution and pigment crystallization.

Modified algorithms (Dvoretsky and Dvoretsky, 2003) have been used to solve one and two-stage problems of design and regime parameters optimization in diazotization and azocombination turbulent tube reactors under the mentioned uncertainties.

Comparative analysis of the obtained solutions proves that optimal values of design parameters may differ depending on the problem formulation.

Thus, having optimized a combined diazotization turbulent tube reactor under uncertainty, the following results have been obtained:

- when one-stage problem with “hard” constraints is solved, the number of the fixed length tube sections and reaction mass intermediate mixing chambers equals $N = 13,$ and capital and maintenance costs total $C^* = 2011.4$ USD/ton;
- when two-stage problem with “soft” constraints is solved, $N = 12, C^* = 1979.5$ USD/ton;
- when two-stage problem with “hard” constraints is solved, $N = 10, C^* =$ 1898.8 USD /ton.

If we compare these design results with the ones without consideration of uncertainty, we can see that extra technical resources are expressed in the increased number of tube sections and mixing chambers of combined turbulent tube reactor. For one-stage problem this extra resource is 85% of the initial variant; for two-stage problem it equals 66%.

Capital and maintenance costs of producing one ton of pigment were the lowest with the realization of the two-stage optimization problem solution results; however, calculations of the C criterion components did not include θ identification system development costs and the costs of controlling the functioning regimes of diazotization reactor unit. That is why the final decision on the selection of design techniques and functioning regimes was taken at the stage of designing “diazotization reactor unit – control system” automated complex.

The optimization of the turbulent tube reactor allowed obtaining the following results:

- with the solution of one-stage problem with “hard” constraints, the reactor length is $l_{tube} = 19{,}9\ m,$ and total costs are $C^* =$ 2419.1 USD/ton;
- with the solution of two-stage problem with “soft” constraints, $l_{tube} = 18{,}34\ m, C^* = 2384.0$ USD/ton;
- with the solution of two-stage problem with “hard” constraints, $l_{tube} = 14{,}6\ m, C^* =$ 2316.0 USD/ton.

As it can be concluded from the analysis of the obtained data, when designing a reactor unit for the synthesis of azopigments under uncertainty, extra technical resources expressed in the increase of reactor length are needed (as compared to designing without considering uncertainties). From the physical point of view, it can be explained by the possibility to vary the time pigment suspension is in the reactor in order to grow pigment crystals of certain size; this provides for pigment coloristic characteristics’ corresponding to the set values of standard samples.

5. Conclusion

The direction of research on developing a strategy, methods and algorithms of integrated design of flexible automated CPs is determined on the basis of system analysis of modern technologies, equipment units and automation of multiple-range chemical productions. Two-stage problems for the stochastic optimization of design and regime variables of CPs and apparatus are formulated. Modified methods and algorithms, allowing solving the problem of integrated design of industrial CPs and automatic control systems under uncertainty of physical, chemical, technological and economic information in an appropriate period of time, are discussed.

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