Integrated Design of Power- and Resource-Saving Chemical Processes and Process Control Systems:
Strategy, Methods, and Application

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Abstract—A strategy for the integrated design of power- and resource-saving chemical processes and the systems controlling their operating conditions with uncertain input data on physicochemical and process parameters is formulated. A multistep iterative procedure for solving integrated design problems is developed. The procedure includes the generation of alternative chemical processes meeting the “rigid” and/or “soft” flexibility constraints and the choice of operating (control) actions, the synthesis of alternative systems for the automatic control of the operating conditions of the chemical process and the choice of the best control system, the pairwise comparison of feasible automated integrated systems consisting of the chemical engineering process and its control system and the choice of the best integrated system using the criterion based on the power and resource savings and control quality by solving one- and/or two-stage stochastic optimization problems with rigid and/or soft constraints. An example integrated design of the flexible continuous synthesis of azo pigments with an automatic-control system for stabilizing the optimal static conditions is discussed.

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Although the problem of integrated design of flexible chemical processes and the automated systems controlling their operating conditions was many times formulated and solved during several decades [1–10], this has not resulted yet in developing a completed theory and rather simple computational algorithms for the complex solution of this difficult multicriterial problem.

The goal of the integrated design of engineering processes, equipment, and automatic control systems (ACS) is to provide a stable and safe production of high-quality competitive products. In this case, it is necessary to meet the chemical process flowsheet specifications and the environmental protection and life safety regulations, which are involved in the problem of optimal design as constraints. These constraints can be rigid or soft. The rigid constraint includes, as a rule, the process flowsheet specifications related to the process explosion, fire, and environmental safety, product quality, and the like. To prevent high factors of safety, the soft constraint includes the requirements that are not related to the process explosion and fire safety, such as specified production rates, some process variables and product quality indices, and the like. In this case, it is necessary to meet the constraint with a given probability.

It is much more difficult to solve the problem of meeting the constraint when the input information is somewhat uncertain, which includes incomplete data about the physical and chemical relationships and coefficients (chemical reaction rate constants, diffusion, heat, and mass transfer coefficients, and the like) on which the mathematical models of the chemical process and its control system are based and unpredictable (random) variations of process variables (temperature, feed flow rate and composition, and the like) during the operation of the process.

The goal of the integrated design can be achieved only if flexible chemical processes are designed. The flexibility of a chemical process is understood as its ability to control and retain its designed operating conditions when the internal and external uncertain parameters are randomly varied. When the flexible process is operated, the operating conditions specified by the process flowsheet specifications should be provided by an appropriate choice of control actions produced by the process automatic control system when the values of randomly varying uncertain process parameters remain within specified ranges.

Analysis of conventional design approaches shows that the attempt to achieve the maximum performance efficiency of a chemical process on the power- and resource-saving basis, as a rule, leads to the choice of equipment (plant) design parameters that reduce the dynamic characteristics of the process. In this case, the process flexibility can be provided only by using com-
plex (and therefore expensive) automatic control systems. At the same time, there is often a way to improve the dynamic properties of the process and reduce the total cost of the project by making small changes in the design of the process equipment or in the designed operating parameters.

Consequently, in the integrated design the optimal design parameters of the equipment of a chemical process, its operating conditions, and the manipulated parameters of its automatic control system should be chosen as a reasonable compromise between the efficient performance of the process on the power- and resource-saving basis and the quality of controlling (regulating) its operating conditions.

**SUBJECT OF STUDY**

The object of design is the continuous diazotization of aromatic amines by sodium nitrite in hydrochloric acid; that is, the process of fine organic synthesis in the production of azo dyes and pigments.

In the optimal design of the equipment and operating conditions of a continuous diazotization process, it is necessary to determine the design and operating variables of a multimodular reactor (Fig. 1), and the class, design, and vector of manipulated parameters of its automatic control system that will allow the process to meet the project design specifications with some uncertainty in the values of several process and kinetic parameters.

A multimodular reactor is a vertical continuous-flow column composed of modules $l$ with the same volume connected in series. The bottom module is continuously fed with a hydrochloric suspension of amine (feed). The supply of an aqueous solution of sodium nitrite (diazotizing agent) is distributed over the modules. The diazotization reaction is accompanied by the release of high amounts of heat, which is withdrawn by cooling jacket $2$. The produced diazo solution is withdrawn from the top module of the reactor. To prevent the deposition of amine particles in the reacting zone, the reactor is equipped with a multilevel mechanical stirrer $3$. The simulation of the reactor is based on the assumption that the solid particles of amine entering the module are perfectly distributed throughout the reactor whole volume.

In our analysis, the vector of design parameters $d$ includes the number of modules $N$ in the reactor and module volume $V$. The vector of operating (process control) variables $z$ includes the temperature $T$ and the distribution of the sodium nitrite feed rate over reactor modules $\gamma(i)$.

The uncertain parameters $\xi$ include the concentration of the amine solid phase $[C_A^{(0)}]_{\text{sol}} = 370.0 (\pm 4\%) \text{ mol/m}^3$, kinetic constant for the dissolution of the amine solid phase $K = 5.4 \times 10^5 (\pm 5\%)$, kinetic constants for diazo compound decomposition such as activation energies $E_{\text{a}4} = 87150 (\pm 0.2\%) \text{ J/mol}$ and $E_{\text{a}5} = 63690 (\pm 0.2\%) \text{ J/mol}$. 

![Fig. 1. Automated multimodular diazotization reactor: 1, module; 2, cooling jacket; 3, multilevel stirrer; 4, tray; 5, electric drive; QE, device for measuring the concentrations of diazo solution, amine suspension, sodium nitrite solution.](image-url)