Optimization of Catalytic Processes and Reactors

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Abstract—Efficient methods and algorithms have been developed for the optimization of catalytic processes and reactors. In mathematical terms, these problems reduce to finding the extremum of a functional of a large number of variables whose domain of variation is subject to various constraints as sets of partial differential equations and algebraic inequalities. This implies solving problems in which the domain of extremals is closed. Applying Pontryagin's maximum principle to catalytic processes described by sets of differential equations with constrained phase and control variables allows the necessary set of optimal conditions to be found. A numerical algorithm has been developed for solving nonlinear boundary-value problems that arise when the maximum principle is employed. The efficiency of this algorithm is demonstrated by the example of the catalytic oligomerization of α-methylstyrene, a typical process requiring various kinds of optimization problems to be solved. The theoretical optimization of the process has served as the basis for the engineering optimization of an industrial reactor. Optimal controls were determined in both the theoretical and engineering optimization steps.

The ultimate goal of mathematical modeling is the optimization of apparatuses and processes. These problems arise both when designing new processes and when intensifying existing processes, including the development of automated process control systems. The development of process optimization methods was begun simultaneously with research into the mathematical modeling of processes. Pioneering works in this field were carried out by Boreskov and Slin'ko [1] at the Institute of Catalysis, Siberian Division, Russian Academy of Sciences. Pontryagin's maximum principle [2] was used as the mathematical basis for process optimization. The application of this principle has stimulated the development of optimization methods for catalytic processes [3–5].

The variables characterizing a catalytic process are divided into two groups. The first is made up of phase variables, which determine the state of a given process but cannot be directly varied. The second group consists of control variables (controls), which determine the operating regime and can be varied in order to modify the course of the process. In chemical processes, the phase variables are the component concentrations and the amounts of substances absorbed by the catalyst. The amount of catalyst, reactor dimensions, feed rate, inlet temperature, and the composition of the reaction mixture are often regarded as controls.

There are two trends in process optimization. The first is that an increasingly large number of variable process parameters are taken into account, including the number of apparatuses in the flowsheet and the number of controls involved in the models of separate apparatuses. The other trend is that progressively more

exact and, accordingly, more complicated mathematical models are used, implying an increasing amount of calculations.

The first trend signifies a marked increase in the dimensionality of the optimization problems to be solved, and the second makes it more difficult to calculate objective functions. Therefore, it is necessary to improve optimization methods and to select the quickest, the most reliable, and the least laborious ones. Another essential characteristic of an optimization method is universality, which means applicability to various types of problems.

The experience gained by solving numerous problems suggests that processes should be optimized in two steps [6, 7].

The first step is theoretical optimization based on a kinetic model. Solving this problem is followed by choosing a contact assembly design so as to approach the theoretical optimum regime (in particular, the optimum temperature regime (OTR)) as close as possible. It was to these problems that primary importance was assigned in early studies on the optimization of catalytic processes. A typical result of those studies was the determination of kinetic model parameters and their numerical values for the chemical reaction underlying the process. In some situations, small errors in kinetic data and, accordingly, in model parameters may lead to an ambiguous or even qualitatively opposite technological interpretation. For example, even if a set of activation energy data from a given confidence interval suggests that the optimal process is isothermal, another set may offer a nonisothermal process. Therefore, in the case of uncertain kinetic constants, it is necessary to
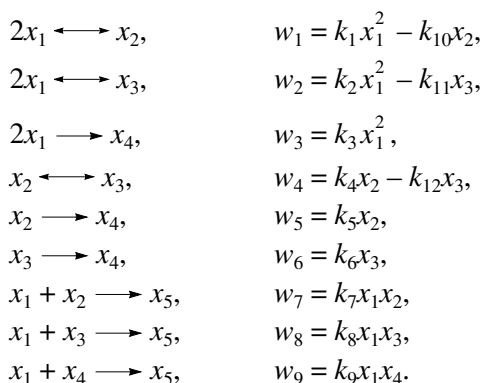
evaluate the reliability of theoretical optimization results and to estimate the limits within which the optimal solution can vary [8, 9].

Note that most theoretical optimization studies have been qualitative. If a process is described by a simple kinetic network, its mathematical model consists of two or three ordinary differential equations and it is possible to obtain an explicit expression for the Pontryagin function and for the optimal solution. However, almost without exception, real systems have a much higher dimensionality and can be investigated only by numerical experiments. Therefore, it is necessary to develop efficient numerical methods and adequate, high-service mathematical tools.

The second step is engineering optimization, which means calculating optimal controls for the type of reactor chosen. The purpose of this step is to optimize the design and operation parameters of the reactor: isometric dimensions, shape, assemblies, temperature variation rate, pressure, concentrations, etc. The second most important task is to find the optima of the objective functions under the constraints imposed on phase variables. The mathematical aspect of such systems has been studied to a much lesser extent, so considerable difficulties in computational experimentation are anticipated.

The theoretical step of optimization will be considered for a kinetic model of α-methylstyrene oligomerization in the presence of a zeolite catalyst [10]. Necessary experimental data were obtained under the guidance of Doctor Kutepov at the Laboratory of Catalyst Preparation, Institute of Petrochemistry and Catalysis, Academy of Sciences of Bashkortostan and the Ufa Scientific Center of the Russian Academy of Sciences. The products of this reaction (linear and cyclic dimers) have found application as plasticizers, polymer modifiers, rubber, reagents in the manufacture of synthetic oils, etc.

Here, we introduce the following designations: x_1, α-methylstyrene; x_2, 4-methyl-2,4-diphenylpentene-1 (α-dimer); x_3, 4-methyl-2,4-diphenylpentene-2 (β-dimer); x_4, 1,1,3-trimethyl-3-phenylindan (cyclic dimer); and x_5, trimers. According to the law of mass action, the rate equations corresponding to the reaction network in α-methylstyrene oligomerization are written as

$$2x_1 \longleftrightarrow x_2, \qquad w_1 = k_1 x_1^2 - k_{10} x_2,$$
$$2x_1 \longleftrightarrow x_3, \qquad w_2 = k_2 x_1^2 - k_{11} x_3,$$
$$2x_1 \longrightarrow x_4, \qquad w_3 = k_3 x_1^2,$$
$$x_2 \longleftrightarrow x_3, \qquad w_4 = k_4 x_2 - k_{12} x_3,$$
$$x_2 \longrightarrow x_4, \qquad w_5 = k_5 x_2,$$
$$x_3 \longrightarrow x_4, \qquad w_6 = k_6 x_3,$$
$$x_1 + x_2 \longrightarrow x_5, \qquad w_7 = k_7 x_1 x_2,$$
$$x_1 + x_3 \longrightarrow x_5, \qquad w_8 = k_8 x_1 x_3,$$
$$x_1 + x_4 \longrightarrow x_5, \qquad w_9 = k_9 x_1 x_4.$$

Here, w_j is the rate of the jth step (m³ (kg Cat)⁻¹ h⁻¹), $j = 1$–9; x_i is the mole fraction of the ith component, $i = 1$–5; k_s is the rate constant of the sth reaction (m³ (kg Cat)⁻¹ h⁻¹), $s = 1$–12, which depends on temperature T according to the Arrhenius equation

$$k_s(T) = k_s^0 e^{-\frac{E_s}{RT}},$$

in which k_s^0 is the preexponential factor and E_s is the activation energy of the sth reaction (cal/mol); and R is the universal gas constant (cal mol⁻¹ K⁻¹).

When developing a mathematical model for a process, the variation of the number of moles N (reaction volume) during the reaction is taken into account. The material balance equations for α-methylstyrene oligomerization in the presence of zeolite are written as

$$\frac{d(Nx_i)}{dt} = F_i,$$
$$F_i = \frac{G_{Cat}}{V_r} \sum_{j=1}^{9} v_{ij} w_j \quad (i = 1 \dots 5), \tag{1}$$

where G_{Cat} is the catalyst weight, V_r is the reactor volume, and v_{ij} are stoichiometric coefficients. The initial ($t = 0$) conditions appear as $x_i = x_i^0$.

The set of equations (1) is closed by the following normalization condition for the liquid-phase components:

$$\sum_{i=1}^{5} x_i = 1. \tag{2}$$

By rearranging the set of equations (1), subject to condition (2), we obtain the following set of ordinary nonlinear differential equations:

$$\frac{dx_i}{dt} = \frac{F_i - x_i F_n}{N}, \quad i = 1 \dots 5,$$
$$\frac{dN}{dt} = \frac{G_{Cat}}{V_p} \sum_{j=1}^{9} w_j \sum_{i=1}^{5} v_{ij} \tag{3}$$

with the initial ($t = 0$) conditions

$$x_i = x_i^0, \quad N = 1. \tag{4}$$

This set of equations provides a mathematical description for α-methylstyrene oligomerization in the presence of a zeolite catalyst.

The theoretical optimization of this catalytic process is viewed as the problem of finding the optimal reactor regime $\bar{u}$ minimizing (maximizing) the optimality criterion defined by the functional

$$I = \int_{t^{(0)}}^{t^{(k)}} \psi_0(\bar{x}, \bar{u})\,dt. \tag{5}$$

Here, $\psi_0(\bar{x}, \bar{u})$ is the prescribed function of $\bar{x}$ (process state variables as functions of the independent variable t) and $\bar{u}$ (controls).

Depending on the problem to be solved, the optimality criterion (5) may take various forms, including the following:

(1) $t^{(k)} - t^{(0)} \longrightarrow \min$ (for the operation speed problem);

(2) $x_2(t^{(k)}) + x_3(t^{(k)}) + x_4(t^{(k)}) \longrightarrow \max$ (for the maximum product yield problem);

(3) $x_2(t^{(k)}) + x_3(t^{(k)}) - x_4(t^{(k)}) - x_5(t^{(k)}) \longrightarrow \max$ (for maximizing the yield of desired products while minimizing the yield of by-products, which are cyclic dimers and trimers);

(4) $\sum\limits_{i=1}^{5} c_j x_j(\tau_r) \longrightarrow \max$, where c_j is the estimated cost of the jth reaction product (for the economic optimality problem).

In the general case, it is possible that the initial ($t^{(0)}$) and final ($t^{(k)}$) values of t are not specified in the initial formulation of the optimization problem and their determination should be included in the solution procedure. The initial and final states of the process may be defined by an incomplete set of $x_i(t^{(0)})$ and $x_i(t^{(k)})$ values, or the final values of x_i may be subject to the constraint $\sum\limits_{i=1}^{5} d_j x_j(\tau_r) = d_0$, where d_j are positive or negative constant coefficients (some of them may be zero), τ_r stands for the reactor dimensions, and d_0 is the overall composition of the reaction mixture at the reactor outlet. This type of problem may arise when it is necessary to optimize a process at a fixed product yield or at a preset conversion of the starting reactant. The region of admissible controls may be defined as an aggregate of equalities or inequalities.

Let us consider the problem of optimizing the temperature regime $T(t)$ for α-methylstyrene oligomerization in order to maximize the product yield. Let the following constraint be imposed on the optimal temperature:

$$T_1 \leq T \leq T_2. \tag{6}$$

No initial assumptions are made as to reactor dimensions, and the specific features differentiating the cases of specified and unknown τ_r values will be discussed while presenting the solution.

This problem will be solved using Pontryagin's maximum principle [2]. An advantage of this mathematical tool is that it allows solutions in the form of discontinuous functions. This type of function appears in optimization problems for many other catalytic processes. The set of constraints involved in the maximum principle is always closed; that is, the number of equations is always equal to the number of variables. It is clear from physical considerations that an optimal regime does exist; therefore, the single equation derived from the constraints of the maximum principle will be optimum. Pontryagin's maximum principle can serve as the basis for efficient computational algorithms for finding optimal controls subject to various constraints and allows the optimal solution to be analyzed on the qualitative level. According to the maximum principle, the optimum temperature in each cross section of the reactor is derived from the maximum condition for the function

$$H(\bar{x}, T, \bar{\lambda}) = \sum_{i=1}^{5} \lambda_i \frac{F_i - x_i F_n}{x_6}$$
$$+ \lambda_6 \frac{G_{Cat}}{V_r} \sum_{j=1}^{9} w_j \sum_{i=1}^{5} v_{ij}, \tag{7}$$

where $x_6 = N$.

Here, the $\lambda_i(t)$ functions satisfy the following set of conjugate equations:

$$\frac{d\lambda_i}{dt} = -\frac{\partial H}{\partial x_i}, \quad i = 1\ldots 6. \tag{8}$$

The following boundary conditions at $t^{(k)}$ are derived from the transversality condition for the $\lambda_i(t)$ functions:

$$\lambda_1(t^{(k)}) = 0, \quad \lambda_2(t^{(k)}) = 1, \quad \lambda_3(t^{(k)}) = 1,$$
$$\lambda_4(t^{(k)}) = -1, \quad \lambda_5(t^{(k)}) = -1, \quad \lambda_6(t^{(k)}) = 0. \tag{9}$$

Thus, optimizing the temperature regime is reduced to the problem of integrating the sets of differential equations given by Eq. (3) and the conjugate set of equations for the auxiliary functions (Eq. (8)) subject to boundary conditions imposed on both ends of the integration interval. That is, this optimization problem implies solving a nonlinear boundary-value problem. This type of problem is difficult to solve because, if the set of equations has a large dimensionality (includes more than three equations), one can hardly hope to obtain an analytical solution. For this reason, it is impossible to find the general integrals of the above sets of equations and thus determine $x_i(t)$ and $\lambda_i(t)$ at any t. Therefore, numerical integration methods have to be used.

The algorithm for solving the problem is as follows. In the first step, all unknown functions are assigned some values. The missing values of variables are set in a somewhat random manner and are then refined based on the specified values of the $x_i(t)$ and $\lambda_i(t)$ functions at the end of the trajectory.
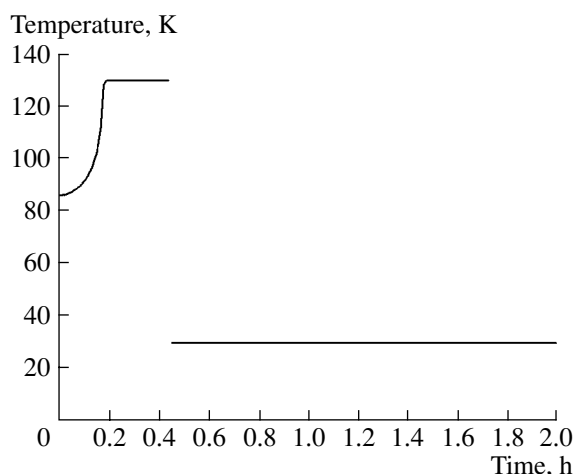
Fig. 1. Optimal temperature regime for α-methylstyrene oligomerization on a zeolite catalyst.

Fig. 2. Concentrations of the products of α-methylstyrene oligomerization on a zeolite catalyst as a function of time.

In the second step, it is possible to determine the optimal control corresponding to the initial value of the independent variable t:

$$H(\lambda_i(t^{(0)}), x_i(t^{(0)}), T_{\text{opt}}(t^{(0)}))$$
$$= \max_T H(\lambda_i(t^{(0)}), x_i(t^{(0)}), T). \qquad (10)$$

If there are no constraints imposed on the control variable, the determination of optimal control in terms of Eq. (10) can be carried out by any unconstrained minimization method. However, in view of Eq. (6), the optimal control is found by constrained minimization (using the penalty or barrier function method).

Once the optimal control at the initial time point, $T_{\text{opt}}(t^{(0)})$, is determined, it is possible to make a step forward by setting $t = t^{(0)} + \Delta t$ and, using any numerical method for the integration of sets of differential equations, determine $x_i(t)$ and $\lambda_i(t)$.

Next, the optimal control at $t = t^{(0)} + \Delta t$ is determined from the maximum condition (10). This yields a certain solution of the set of Eqs. (3) and (8). During numerical integration, it is necessary to see how close the resulting trajectory is to the specified final point. If the final point of intergration is preset, this can be done using the relationship

$$r = \sum_{i=1}^{5} [x_i(\tau_k) - x_i^{(k)}]^2 \longrightarrow \min, \qquad (11)$$

if $t^{(k)}$ is not preset,

$$r = \min_t \sum_{i=1}^{5} [x_i(t) - x_i^{(k)}]^2. \qquad (12)$$

In both cases, the value of r shows how good the initial approximations $\lambda_i(t^{(0)})$ are. The quantity r is viewed as
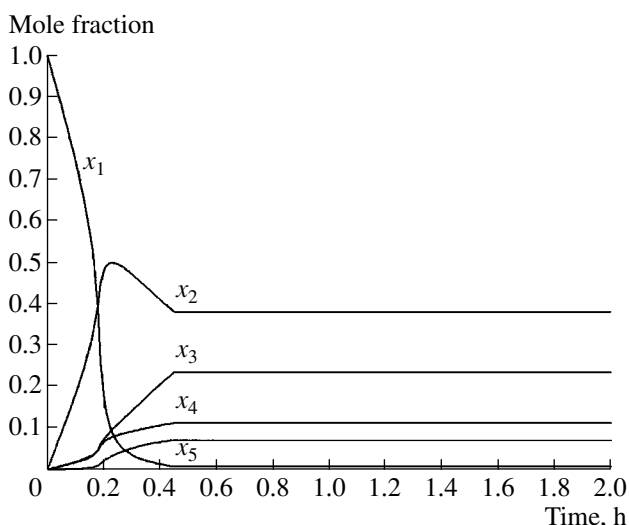
a function of $\lambda_i(t^{(0)})$ ($i = 1, ..., 6$). It should be minimized by choosing an appropriate set of $\lambda_i(t^{(0)})$. In other words, it is necessary to solve the minimization problem

$$\min_{\lambda(t^{(0)})} r(\lambda(t^{(0)})) = 0. \qquad (13)$$

This can be done by linear programming methods. The optimal solution is obtained as a result.

Based on available experimental data, the mathematical description of α-methylstyrene oligomerization, and the above algorithm, we developed software for solving the theoretical optimization problem in terms of criterion 3 with the initial data $x_1^0 = 1$, $x_2^0 = 0$, $x_3^0 = 0$, $x_4^0 = 0$, and $x_5^0 = 0$. The constraint $30°C \leq T \leq 130°C$ was imposed on temperature. The zeolite content was 10%, and the duration of the reaction was 2 h.

Consider the resulting time dependences of the optimal temperature (Fig. 1) and product concentrations (Fig. 2) corresponding to the optimal temperature regime. The optimal temperature is a sectionally continuous function consisting of three sections: in the first, the temperature grows from 86°C to the maximum; in the second and third, the temperature is constant and has the maximum and minimum values, respectively. For this temperature regime, the criterion chosen takes its maximum value and the dimer concentrations vary with time as shown in Fig. 2. The α isomer forms first. Its concentration reaches a maximum in a rather short time depending on the reaction temperature and then gradually decreases. The concentration of the β isomer increases much more slowly and reaches its maximum at the point at which the optimal control switches from one isothermal section to the other.

Thus, we have demonstrated the way of optimizing catalytic processes in terms of the generalized Pontryagin's maximum principle. A numerical algorithm has

been developed for solving nonlinear boundary-value problems that arise when Pontryagin's principle is employed. This principle is universal and enables one to solve problems with various input data and various optimality criteria.

The theoretical step is followed by the optimization of process design. Some engineering constraints are usually imposed on controls and phase variables. For example, the reactor temperature may be limited from above to rule out thermal damage to the catalyst or equipment. For very exothermic processes, particularly those accompanied by changes in volume, some limitations may be imposed on the feed flow rate and the feed temperature in order to prevent hydrodynamic shocks.

In mathematical terms, the process optimization problem with engineering constraints is formulated as follows: find the extremum of a functional of a large number of variables whose domain of variation is subject to various constraints as sets of partial differential equations and algebraic inequalities. These constraints complicate the optimization problem. It may turn out that the optimality criterion has no extremum in the analytical sense and takes the largest or smallest value when one or several variables are fixed at their limiting values.

Engineering optimization will be considered for α-pinene hydrogenation on a nickel silicate catalyst. This reaction includes an irreversible reaction between α-pinene and hydrogen and reversible α-pinene isomerization [11]:

$$\text{Pinene} + H_2 \longrightarrow \text{Pinane,}$$

$$\text{Pinene} \rightleftharpoons \text{Isomers.}$$
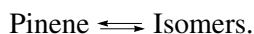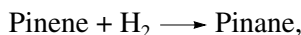
In the liquid phase,

$$W_1 = k_1 x_1 y_H, \quad \text{where} \quad k_1 = \bar{k}_1 P C_l,$$

$$W_2 = k_2 x_1 - k_3 x_3, \quad \text{where} \quad k_2 = \bar{k}_2 C_l, \ k_3 = \bar{k}_3 C_l.$$

In the gas phase,

$$w_1 = k_4 y_1 y_H, \quad \text{where} \quad k_4 = \bar{k}_4 C_g^2,$$

$$w_2 = k_5 y_1 - k_6 y_3, \quad \text{where} \quad k_5 = \bar{k}_5 C_g, \ k_6 = \bar{k}_6 C_g.$$

Here, C_g and C_l are the molar densities of the gas and liquid phases (kmol/m^3), $\bar{k}_i$ are reaction rate constants calculated by the Arrhenius equation, W_j and w_j are the reaction rates in the liquid and gas phases (kmol m^{-3} h^{-1}), and x_i and y_i are component concentrations in the liquid and gas phases ($i = 1$ for α-pinene, $i = 2$ for *cis*-pinane, and $i = 3$ for the α-pinene isomers).

Mathematically, the nonisothermal hydrogenation of α-pinene in a tubular reactor with a fixed catalyst bed is described by the following set of material- and heat-balance equations:

$$\frac{1}{S}(C_p^l L + C_p^g G)\frac{dT}{dl} = \sum_{j=1}^{2} Q_j[(1-\varphi)W_j + \varphi w_j]$$

$$- \frac{V_{\text{vap}}}{V_r}\sum_{i=1}^{3}\Delta H_i^{\text{vap}}Y_i + \alpha_x S_{x_1}(T_x - T),$$

$$\frac{G_x C_x dT_x}{S \ dl} = \alpha_x S_{x_2}(T - T_x),$$

$$\frac{1}{S}\frac{dL}{dl} = -\frac{V_{\text{vap}}}{V_r} = F_1,$$

$$\frac{1}{S}\frac{dx_i}{dl} = \frac{F_i - x_i F_1}{L},$$

$$F_i = \sum_{j=1}^{2}(1-\varphi)v_{ij}W_j - \frac{V_{\text{vap}}}{V_r}Y_i, \quad i = 1, 2, 3,$$

$$\frac{1}{S}\frac{dG}{dl} = -(1-\varphi)W_1 - \varphi w_1 + \frac{V_{\text{vap}}}{V_r} = \Phi_g,$$

$$\frac{1}{S}\frac{dy_i}{dl} = \frac{\Phi_i - y_i\Phi_g}{G},$$

$$\Phi_i = \sum_{j=1}^{2}\varphi v_{ij}w_j + \frac{V_{\text{vap}}}{V_r}Y_i, \quad i = 1, 2, 3,$$

$$\frac{1}{S}\frac{dy_H}{dl} = \frac{-(1-\varphi)W_1 - \varphi w_1 - y_H\Phi_g}{G},$$

(14)

with the initial conditions

$$x_i = x_i^0, \quad y_i = y_i^0,$$
$$L = L_0, \quad G = G_0, \quad (15)$$
$$T = T_0, \quad T_x = T_x^0,$$

where Q_j is the heat of the jth reaction (kcal/mol), ΔH_i^{vap} is the heat of evaporation of the ith component (kcal/mol), C_p^g and C_p^l are the molar heat capacities of the gas and liquid (kcal mol^{-1} K^{-1}), C_x is the mass heat capacity of the cooling agent (kcal kg^{-1} K^{-1}), G_x is the weight flow rate of the cooling agent (kg/h), S_{x_1} and S_{x_2} are the inner and outer specific heat-transfer areas (m^{-1}), α_x is the heat-transfer coefficient (kcal m^{-2} h^{-1} K^{-1}), L is the molar flow rate of the liquid (kmol/h), l is the reactor length (m), V_r is the reaction volume (m^3), S is the cross-sectional area of the tubes (m^2), V_{vap} is the molar evaporation rate (kmol/h), v_{ij} are stoichiometric coefficients, and φ is the mole fraction of the gas phase.

Using this mathematical formalism, it is possible to carry out process design calculations for nonadiabatic and adiabatic reactors (in the latter case, $\alpha_x = 0$ in the
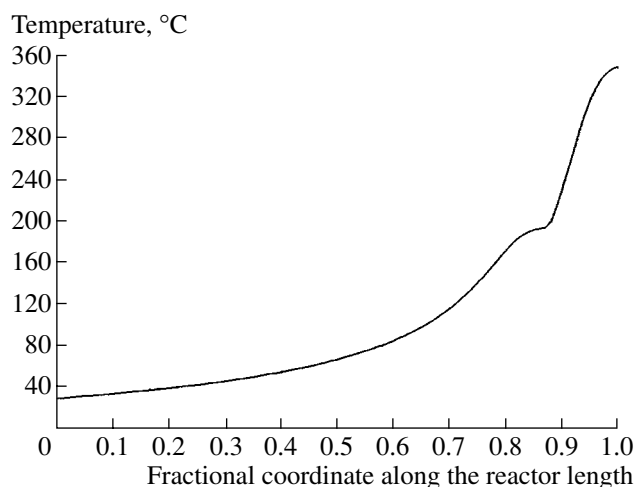
Fig. 3. Longitudinal profile of temperature for α-pinene hydrogenation on a nickel silicate catalyst in an adiabatic reactor.

heat-balance equation). The longitudinal profiles of temperature, component concentrations, and liquid and gas flow rates calculated using Eqs. (14) and (15) are plotted in Figs. 3–5.

The plots shown in Figs. 3–5 reflect all of the specific features of the chemical reaction, which is accompanied by phase transitions. Flowing from the reactor inlet to the reactor outlet, the reaction mixture is gradually heated owing to the heat of the reaction, which mainly takes place in the liquid phase (Fig. 3). At ~180°C and 4 atm, the draw-off fraction is equal to unity, so the evaporation rate of the liquid phase is the highest. As a consequence, the temperature rise rate decreases sharply and the molar gas flow rate increases (Fig. 4), although the reaction takes place in the gas phase. Once the rate at which the number of moles of

matter in the gas phase decreases as a result of the reaction exceeds the evaporation rate, the molar flow rate of the gas begins to fall again.

Heat evolution in the gas phase accelerates the reactions and causes a sharp temperature rise. As a consequence, there are kinks in the profiles of the reactor temperature (Fig. 3), of the molar flow rates of the liquid and gas (Fig. 4), and of the component concentrations (Fig. 5).

The highest pinane yield was taken to be the optimality criterion in the optimization of the operating regime of the fixed-bed tubular flow reactor. The control variables were reactor pressure (P), inlet temperature (T), inlet liquid (pinene) flow rate (L), and inlet gas (hydrogen) flow rate (G). In the computational experiment, we varied one of the controls at fixed values of the others. The starting set of controls was the following: $P = 3$ atm, $L = 350$ l/h, and $G = 55$ m^3/h.

For a tubular reactor with tubes 50 mm in diameter and 2 m in length, the *cis*-pinane yield and the maximum reactor temperature are plotted in Figs. 6 and 7, respectively.

As the pressure or α-pinene flow rate is increased, the *cis*-pinane yield tends to an asymptotic limit (Fig. 6). As the hydrogen flow rate is increased, the *cis*-pinane yield passes through a maximum because of the shortening contact time and the corresponding decrease in α-pinene conversion. The maximum temperature in the tubular reactor (Fig. 7) varies monotonically. Specifically, it rises as the pressure or α-pinene flow rate is increased and falls as the hydrogen flow rate is raised because of the decreasing α-pinene conversion.

Thus, we have demonstrated the way of optimizing catalytic processes in terms of the generalized Pontryagin's maximum principle. A numerical algorithm has been developed for solving nonlinear boundary-value problems that arise when Pontryagin's principle is
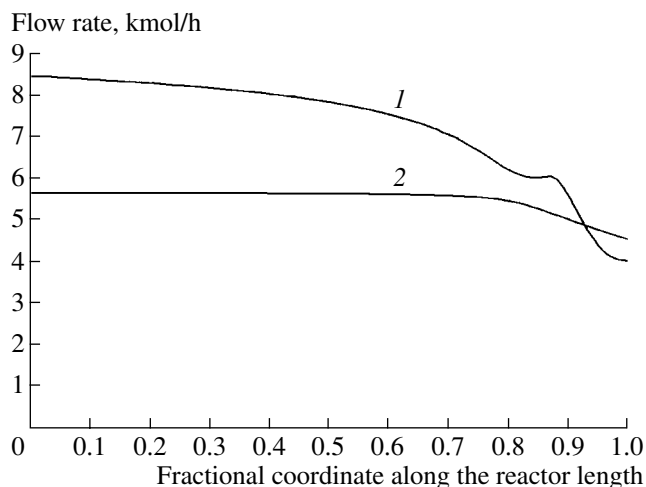

Fig. 4. Variation of (*1*) gas and (*2*) liquid flow rates along the adiabatic reactor for α-pinene hydrogenation on a nickel silicate catalyst.
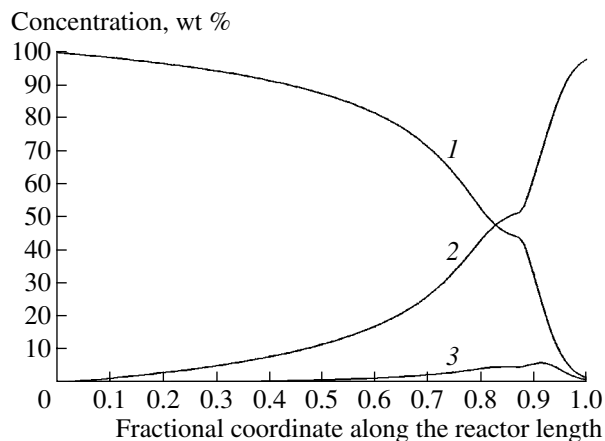

Fig. 5. Variation of component concentrations along the adiabatic reactor for α-pinene hydrogenation on a nickel silicate catalyst: (*1*) pinene, (*2*) pinane, and (*3*) isomers.
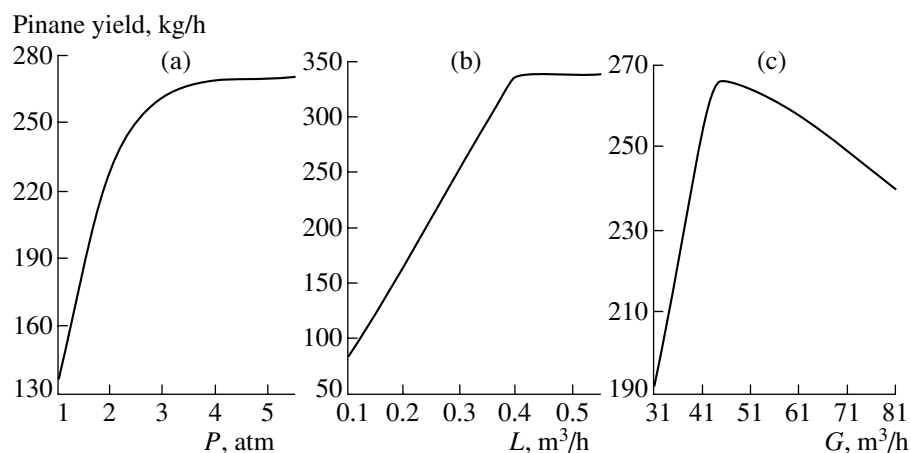
Pinane yield, kg/h

Fig. 6. Pinane yield in the tubular reactor as a function of (a) pressure, (b) pinene flow rate, and (c) hydrogen flow rate.
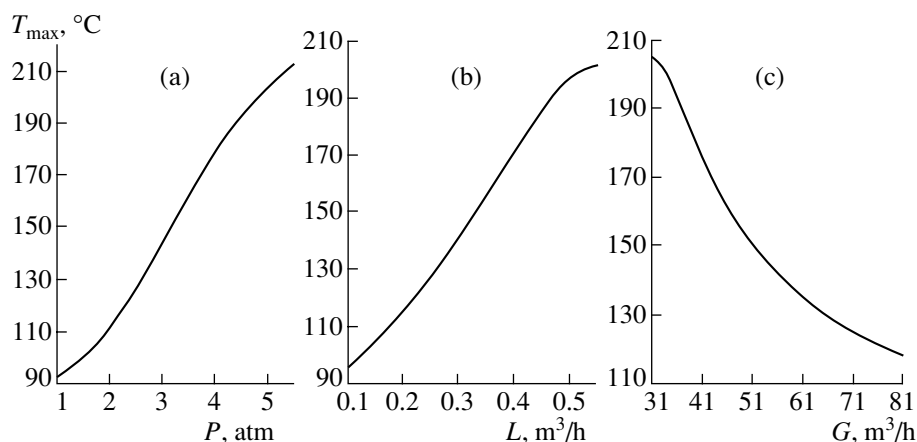
T_{max}, °C

Fig. 7. Maximum temperature in the tubular reactor for α-pinene hydrogenation as a function of (a) pressure, (b) pinene flow rate, and (c) hydrogen flow rate.

employed. The efficiency of this algorithm is demonstrated by the example of the catalytic oligomerization of α-methylstyrene, a typical process involving various kinds of optimization problems. The theoretical optimization of the process has served as the basis for the engineering optimization of an industrial reactor. Optimal controls were determined in both the theoretical and engineering optimization steps.

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