NUMERICAL OPTIMIZATION OF SEPARATION PROCESSES IN A DISTILLATION COLUMN

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Abstract

An optimal control problem when modeling the rectification process in the column is considered. The process is described by a system of first-order hyperbolic equations with dynamic boundary conditions. A specific peculiarity of the model under consideration is in the boundary conditions of a special type. At each of the boundaries, boundary conditions are determined from a system of ordinary differential equations, which also includes unknown values of functions on another boundary. Three variants of numerical methods for solving the considered problem are proposed. The first method is based on a linearized maximum principle. Structurally it coincides with a conditional gradient method in a corresponding functional space. The second method is a modification of a two-parameter maximum principle method. This method makes it possible to work effectively with internal admissible controls in contrast to standard iterative maximum principle methods. The third method is based on the procedure of discretization of the problem and the use of the standard *SciPy Python* library to solve the corresponding mathematical programming problem. The results of numerical experiments are illustrated by a series of tables and graphs. As a result, the conditional gradient method may be recommended for solving the problem under consideration.

Key words

Distillation column, hyperbolic systems, dynamic boundary conditions, optimal control, maximum principle, numerical methods.

1 Introduction

The paper considers an optimal control problem when modeling the rectification process in the column. The process is described by a system of first-order hyperbolic equations with dynamic boundary conditions.

Cascade systems of hyperbolic and ordinary differential equations are used when modeling a number of processes of chemical rectification [Demidenko, 2006a; Demidenko, 2006b; Gushchin, 2020], blood flow dynamics [Ruan, 2008], nanoparticles [Wang, 2022], etc.

This paper does not aim to analyze existing methods for solving problems of optimal control of systems with distributed parameters. We note the large number of reviews in this area, from the first works (see, e.g., [Butkovsky, 1968]) to modern books (see, e.g., [Fursikov, 2000]). Note that most methods for solving optimization problems in distributed parameter systems are based on the use of necessary optimality conditions (Pontryagin's maximum principle, gradient conditions), their generalizations (conditions of higher orders), sufficient optimality conditions (Hamilton-Jacobi methods, Krotov conditions), and discretizations of problems in one or another form.

A specific peculiarity of the model under consideration is in the boundary conditions of a special type. At each of the boundaries, boundary conditions are determined from a system of ordinary differential equations, which also includes unknown values of functions on another boundary. In [Arguchintsev, 2023] a modification of the numerical method of characteristics is proposed to solve this initial-boundary value problem. The method is based on constructing a characteristic difference grid obtained by linear transforming a classical rectangular grid.

In this paper, an optimal control problem with a quadratic cost functional is considered. It is important that a classic Pontryagin's maximum principle in the problem is not a sufficient optimality condition.

Three variants of numerical methods for solving the considered problem are proposed.

The first method is based on a linearized maximum principle. Structurally, it coincides with a conditional gradient method in a corresponding functional space.

The second method is a modification of a two-parameter maximum principle method [Vasiliev, 1990]. Using one-parameter maximum principle methods of Krylov-Chernous'ko type [Krylov, 1972; Vasiliev, 1990; Vasiliev, 1981] in the problem does not make sense. Due to the linearity of systems of hyperbolic and ordinary differential equations, Pontryagin function linearly depends on control functions in most problems of the considered type. Thus, these methods will search only for boundary values of admissible controls. Theoretically, the method is stronger than a conditional gradient method. The proposed method allows to work effectively with internal admissible controls in contrast to standard iterative maximum principle methods.

The third method is based on the procedure of discretization of the problem and the use of the standard *SciPy Python* library to solve the corresponding mathematical programming problem. The solver implements a modification of the quasi-Newton method BFGS (Broyden – Fletcher –Goldfarb – Shanno algorithm) [Nocedal, 2006]. The "minimize" function of the "Optimize" module of the *SciPy* library was used.

The results of numerical experiments are illustrated by a series of tables and graphs. Finally, the conditional gradient method may be recommended for solving the problem under consideration. It is possible that this is due to the linearity of hyperbolic and ordinary differential equations.

2 Problem statement

The mathematical model of two-component mixture separation is described by the following first-order system of hyperbolic equations with dynamic boundary conditions [Demidenko, 2006a]:

$$\frac{\partial x}{\partial t} - c_1 \frac{\partial x}{\partial s} = B_{11}(s,t)x + B_{12}(s,t)y + F_1(s,t), \quad (1)$$

$$\frac{\partial y}{\partial t} + c_2 \frac{\partial y}{\partial s} = B_{21}(s,t)x + B_{22}(s,t)y + F_2(s,t), \quad (2)$$

$$\frac{\partial x(s_1,t)}{\partial t} = G_1(u(t),t)(y(s_1,t) - x(s_1,t)), \quad (3)$$

$$\frac{\partial y(s_0,t)}{\partial t} = G_2(v(t),t)(x(s_0,t) - y(s_0,t)), \quad (4)$$

$$x(s,t_0) = x_0(s), \quad y(s,t_0) = y_0(s), \quad (5)$$

Here t is a time variable, $t \in T = [t_0, t_1]$; s is a spatial variable, $s \in S = [s_0, s_1]$; $(s,t) \in \Pi = S \times T$; $x(s,t)$ and $y(s,t)$ are component concentrations in liquid and steam phases; positive constants c_1, c_2 and functions $B_{11}(s,t)$, $B_{12}(s,t)$, $B_{21}(s,t)$, $B_{22}(s,t)$, $F_1(s,t)$, $F_2(s,t)$, $x_0(s)$, $y_0(s)$ are given.

The incoming mixture is subjected to evaporation and condensation procedures. The boundary conditions (3) and (4) are obtained from the corresponding material balance equations [Arguchintsev, 2023; Demidenko, 2006a]. Control functions $u(t)$ and $v(t)$ specify the shares of the final product extracted at the bottom ($s = s_0$) and at the top ($s = s_1$) of the distillation column. The admissible controls are assumed to be bounded and measurable scalar functions. They are determined on the interval T and satisfy, almost everywhere, inclusion-type constraints

$$u(t) \in U = [\underline{u}, \overline{u}], \; v(t) \in V = [\underline{v}, \overline{v}], \; t \in T. \quad (6)$$

The goal of the optimal control problem is to minimize the functional at the final time moment t_1.

$$J(u,v) = \int_S [(x(s,t_1) - \overline{x}(s))^2 + (y(s,t_1) - \overline{y}(s))^2] ds, \quad (7)$$

where $\overline{x}(s)$ and $\overline{y}(s)$ are given functions.

So, the optimal control problem (1) – (7) is the problem of minimizing the finite state norm.

The physical meaning of this functional is to control the system so that it arrives at a given state at the final time t_1. The problem (1) – (7) can also be interpreted as an inverse problem of mathematical physics. Based on the known observational data $\overline{x}$, $\overline{y}$ at a finite moment of time t_1, it is required to recover the parameters of the right-hand sides of boundary conditions (3) and (4).

The problem (1) – (7) is considered under the following assumptions.

1) Functions $B_{11}(s,t)$, $B_{12}(s,t)$, $B_{21}(s,t)$, $B_{22}(s,t)$, $F_1(s,t)$, $F_2(s,t)$ are continuous in Π.

2) Functions $G_1(u,t)$, $G_2(v,t)$ are continuous in aggregate of its arguments on $U \times T$, $V \times T$ respectively.

3) Admissible controls $u, v \in L_\infty(T)$.

For any admissible controls, there is a unique generalized solution of the initial-boundary value problem (1) – (5), which is continuous in Π function [Godunov, 1979]. Components x, y of the solution are continuously differentiable along the characteristics $s = -c_1 t + const$ and $s = c_2 t + const$ respectively. The continuity of the solution is guaranteed by above assumptions on the parameters of the problem. These conditions do not guarantee existence of a classical solution in the rectangle Π. This requires the fulfillment of higher-order matching conditions closely related to the hyperbolic system itself [Godunov, 1979].

3 Necessary optimality conditions

In [Arguchintsev, 2009] a necessary optimality condition for the problem (1) – (7) was proved in contrast for smooth admissible controls. An estimate of a state increment that depends on a measure of the control variation region was obtained. Application of the general technique of proving necessary optimality conditions together with this estimation makes it possible to derive in (1) – (7) a necessary optimality condition of the classical maximum principle type.

Consider the following constructions. Let's introduce a conjugate problem in Π

$$\begin{gathered}\frac{\partial\psi_1}{\partial t} - c_1\frac{\partial\psi_1}{\partial s} = -B_{11}\psi_1 - B_{21}\psi_2,\\ \frac{\partial\psi_2}{\partial t} + c_2\frac{\partial\psi_2}{\partial s} = -B_{12}\psi_1 - B_{22}\psi_2;\\ \psi_1(s,t_1) = -2(x(s,t_1) - \overline{x}(s)),\\ \psi_2(s,t_1) = -2(y(s,t_1) - \overline{y}(s)),\ s\in S;\\ \psi_1(s_0,t) = \frac{1}{c_1}G_2(v(t),t)p_2(t),\\ \psi_2(s_1,t) = \frac{1}{c_2}G_1(u(t),t)p_1(t),\ t\in T,\end{gathered} \tag{8}$$

and an initial value problem in T

$$\begin{gathered}\frac{dp_1}{dt} = G_1(u(t),t)p_1(t) - c_1\psi_1(s_1,t),\\ \frac{dp_2}{dt} = G_2(v(t),t)p_2(t) - c_2\psi_2(s_0,t),\ t\in T;\\ p_1(t_1) = 0,\ p_2(t_1) = 0.\end{gathered} \tag{9}$$

Let's denote

$$\begin{gathered}h(p,x,y,u,v,t) = p_1G_1(u(t),t)[y(s_1,t) - x(s_1,t)]+\\ +p_2G_2(v(t),t)[x(s_0,t) - y(s_0,t)].\end{gathered}$$

Then the necessary optimality conditions can be formulated in the following forms (classical and linearized maximum principles).

Theorem. Let admissible bounded and measurable controls $(u^*(t),v^*(t))$ be optimal in (1) – (7); $(x^*(s,t),y^*(s,t))$ be solutions of the initial-boundary value problem (1) – (5) for controls (u^*,v^*); $(p_1^*(t),p_2^*(t))$ be solutions of the initial-boundary value problems (8) – (9) for (u^*,v^*) and (x^*,y^*).

Then almost everywhere on T the following conditions are satisfied.

$$h(p^*,x^*,y^*,u^*,v^*,t) = \max_{(u,v)\in U\times V} h(p^*,x^*,y^*,u,v,t) \tag{10}$$

and

$$\begin{gathered}\frac{\partial h(p^*,x^*,y^*,u^*,v^*,t)}{\partial u}u^*(t)+\\ +\frac{\partial h(p^*,x^*,y^*,u^*,v^*,t)}{\partial v}v^*(t) =\\ =\max_{(u,v)\in U\times V}[\frac{\partial h(p^*,x^*,y^*,u^*,v^*,t)}{\partial u}u(t)+\\ +\frac{\partial h(p^*,x^*,y^*,u^*,v^*,t)}{\partial v}v(t)].\end{gathered} \tag{11}$$

Note that the pointwise maximum principle (10) in this problem is not a sufficient optimality condition despite the linearity of the differential equations (1) – (4) and convexity of the cost functional (7). This is due to the presence in (3), (4) the bilinear summands of the form $G_1(u(t),t)(y(s_1,t) - x(s_1,t))$, $G_2(v(t),t)(x(s_0,t) - y(s_0,t))$.

The conditions (10), (11) are the theoretical basis for construction of numerical methods.

4 Numerical methods

To illustrate the methods of numerical solution of the problem, all calculations have been carried out for control function $v(t)$ only.

4.1 Solution of hyperbolic equations

A specific peculiarity of the model is in the boundary conditions of a special type. At each of the boundaries, boundary conditions are determined from a system of ordinary differential equations, which also includes unknown values of functions on another boundary. In [Arguchintsev, 2023] the authors proposed a method of constructing a characteristic difference grid based on a linear transformation of a classical rectangular grid. Implicit second-order difference schemes were used, taking into account the above-mentioned features at the boundaries. The advantage of this approach is in consideration of the specifics of the propagation of perturbations in hyperbolic equations. The solution of the conjugate problem (8) – (9) is symmetric to the solution of the original initial boundary value problem (1) – (5).

4.2 Two-parameter maximum principle method

Iterative processes of the maximum principle are based on the constructive use of the needle variation of controls. A rather detailed analysis of these methods for optimal control problems of ordinary differential equations is given in [Vasiliev, 1990], and for boundary control optimization problems in hyperbolic systems is in [Arguchintsev, 2007]. In this paper, a two-parameter version of the iterative maximum principle method is applied to the problem (1) – (7).

Let $V = [\underline{v},\overline{v}]$. Let us describe the k-th iteration of the method. Let the control $v^k(t)$, the solutions $x^k(s,t), y^k(s,t)$ of the initial boundary value problem (1) – (5) and the solutions $p_1^k(t), p_2^k(t)$ of the conjugate problem (8) – (9) corresponding to this control be computed at the previous iteration. Let's construct a function

$$\omega_k(v,t) = h(p^k,x^k,y^k,v(t),t) - h(p^k,x^k,y^k,v_k(t),t).$$

At the points $t \in T$ we find the control from the maximum condition

$$\overline{v}^k(t) : \overline{\omega}_k(t) = \omega_k(\overline{v}^k(t), t) = \max_{v \in V} \omega_k(v, t).$$

Let's calculate the value

$$\theta_k = \frac{1}{(t_1 - t_0)} \int_T \overline{\omega}_k(t)\, dt.$$

Obviously, if $\theta_k = 0$, then the control $v^k(t)$ satisfies the maximum principle and the iterative process ends.

If $\theta_k > 0$, then let us construct a two-parameter family of controls

$$v^k_{\varepsilon,\alpha}(t) = v^k(t) + \chi_{\varepsilon,\alpha}(t)(\overline{v}^k(t) - v^k(t)),\ t \in T,$$

where $\chi_{\varepsilon,\alpha}$ is a variation function

$$\chi_{\varepsilon,\alpha}(t) = \begin{cases} \alpha, & t \in T_k(\varepsilon), \\ 0, & t \in T \setminus T_k(\varepsilon). \end{cases}$$

Here $T_k(\varepsilon)$ is one-parameter family of sets from the segment T, whose measure depends linearly on $\varepsilon \in [0, 1]$, and $\alpha \in (0, 1]$ is a parameter. Specific methods for constructing sets $T_k(\varepsilon)$ are given in [Vasiliev, 1990]. In this paper, we choose as $T_k(\varepsilon)$ the union of segments satisfying the condition $\{t \in T : \overline{\omega}_k(t) \geq \theta_k\}$.

The next approximation is found as a solution of the two-parameter problem

$$J(v^k_{\varepsilon,\alpha}) \to \min_{\varepsilon,\alpha}.$$

When $\alpha = 1$, the convergence of this method to the fulfillment of the maximum principle in the sense of $\theta_k \to 0,\ k \to \infty$ is proved in [Vasiliev, 1990]. The introduction of the second parameter α complicates a solution of the problem, but allows to work constructively with inner control functions.

The method is theoretically more accurate than classical one-parameter maximum principle methods. However, the need to solve a two-parameter finite-dimensional optimization problem at each iteration significantly complicates the computational process. To calculate a value of the cost functional at each set of parameters we have to solve the initial-edge problem for the hyperbolic system every time. In the numerical solution, the method of coordinate descent for each of the parameters was applied. A dichotomy method was applied for descent on each variable. The stopping condition was non-improvement of the cost functional.

4.3 Conditional gradient method

The method is based on using the linearized maximum principle (11). In the example considered next, $G_2(v, t) = v$. For linear variants of the function G_2, the auxiliary control $\overline{v}^k(t)$ is the same as in subsection 4.2. The one-parameter family of controls is constructed by the rule

$$v^k_\alpha(t) = v^k(t) + \alpha(\overline{v}^k(t) - v^k(t)),\ t \in T,\ \alpha \in [0, 1].$$

The next approximation is found from the solution of the one-dimensional optimization problem

$$J(v^k_\alpha) \to \min_\alpha.$$

Since there is no need for an exact solution to this problem, the point of the local minimum a_1 close to 1 is selected. In the next step, the problem is already considered in the segment $[0, a_1]$, etc.

Structurally, in the example considered next the method coincides with a conditional gradient method in the functional space $L_2(T)$. This is due to the linearity of hyperbolic and ordinary differential equations. It should be noted that usually the conditional gradient method is applied under stronger conditions on the parameters of optimal control problems than the conditions of Pontryagin's maximum principle [Vasil'ev, 2002].

4.4 Method of mathematical programming

The corresponding mathematical programming problem is constructed on the characteristic difference grid. We solved the minimization problem using the *Python* library *SciPy* version 1.13.0. The solver implements a modification of the quasi-Newton method BFGS (Broyden – Fletcher –Goldfarb – Shanno algorithm) [Nocedal, 2006]. The "minimize" function of the "Optimize" module of this library was used to solve the problem. Discretization procedure is based on a characteristic implicit difference grid for the boundary value problem [Arguchintsev, 2023]. Piecewise linear controls were used.

5 Computational experiment

The following problem was chosen for the computational experiment:

$$\frac{\partial x}{\partial t} - \frac{\partial x}{\partial s} = -2s \cdot x + \frac{4}{3}s^2 \cdot y + 4s^3 \sin t + 2\cos t + \frac{4}{3}\frac{s^2 \cos t}{s+1},$$

$$\frac{\partial y}{\partial t} + 2\frac{\partial y}{\partial s} = -\frac{3s+1}{4(s^2+1)(s+1)}x + \frac{4}{(s+1)(3s+1)}y,$$

$$x(s, 0) = 0, \quad y(s, 0) = \frac{3s+1}{2(s+1)};$$

$$\frac{\partial x(s_1, t)}{\partial t} = \frac{4\cos t}{\cos t - 4\sin t}(y(s_1, t) - x(s_1, t)),$$

$$\frac{\partial y(s_0, t)}{\partial t} = v(t) \cdot (x(s_0, t) - y(s_0, t));$$

$$S = [0, 1],\ T = [0, 0.2].$$

For simplicity, it is assumed that the control $u(t)$ is fixed:

$$u(t) = \frac{4\cos t}{\cos t - 4\sin t}.$$

Thus, the cost functional depends on $v(t)$ only:

$$J(v) = \int_S [x(s, t_1) - x^*(s, t_1)]^2 ds + \\ + \int_S [y(s, t_1) - y^*(s, t_1)]^2 ds \to \min.$$

This functional is equal to 0 at

$$x^* = 2(s^2 + 1)\sin t, \quad y^* = \frac{3s + 1}{2(s + 1)}\cos t.$$

The corresponding optimal control is

$$v^*(t) = \frac{\sin t}{\cos t - 4\sin t}.$$

For the numerical solution, the segment S was divided into 100 nodes. A characteristic difference grid is constructed on the base of a linear transformation of a classical rectangular grid [Arguchintsev, 2023]. In total, the characteristic difference grid consists of 5763 nodes.

The calculations were carried out for the following initial controls $v^0(t)$:

a) $v^0(t) \equiv 0,\ t \in T$;

b) $v^0(t) = v^*(t) + 1,\ t \in T$;

c) $v^0(t) = v^*(t) \cdot \sin(50t),\ t \in T$;

d) $v^0(t) = \begin{cases} -1,\ 0 \le t < 0.1, \\ 1,\ 0.1 \le t \le 0.2. \end{cases}$

The stopping condition was non-improvement of the cost functional.

The corresponding results are shown in Figures 1–4 and Tables 1–4.

Table 1. Results for initial control a

method	MPM	CGM	IMPM
times (sec)	4.5	50.0	392.3
$\max\lvert\Delta_{t_1}x\rvert$	9.5e-06	7.8e-06	6.9e-06
$\max\lvert\Delta_{t_1}y\rvert$	1.0e-02	4.7e-03	2.0e-03
$\int_S(\Delta_{t_1}x)^2ds$	2.6e-11	1.4e-11	1.7e-11
$\int_S(\Delta_{t_1}y)^2ds$	1.0e-05	4.9e-06	2.1e-07
$\int_T(\Delta_{s_0}v)^2dt$	2.7e-02	4.8e-03	8.3e-03
J	1.0e-05	4.9e-06	2.1e-07

Here the following abbreviations and designations are used. The abbreviations “MMP”, “CGM”, and “IMPM” are used for the mathematical programming method, conditional gradient method, and iterative maximum principle method, correspondingly. $\max|\Delta_{t_1}x|$ and $\max|\Delta_{t_1}y|$ are the maximum modulo deviations of the calculated values $x^k(s, t_1), y^k(s, t_1)$ from the optimal values $x^*(s, t_1), y^*(s, t_1)$ on the segment T; $\int_S(\Delta_{t_1}x)^2ds$ and $\int_S(\Delta_{t_1}y)^2ds$ are squares of norm in $L_2(T)$ deviations of the calculated values $x^k(s, t_1), y^k(s, t_1)$ from the optimal values

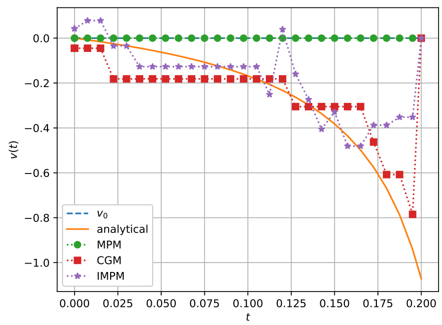

Figure 1. Results for initial control a.

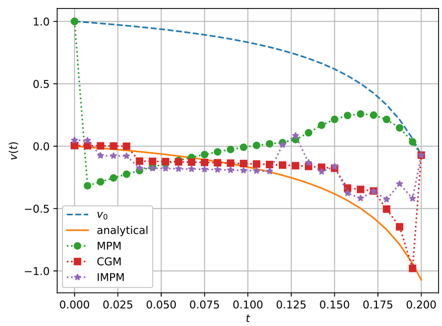

Figure 2. Results for initial control b.

Table 2. Results for initial control b

method	MPM	CGM	IMPM
times (sec)	43.6	51.4	395.4
$\max\lvert\Delta_{t_1}x\rvert$	6.0e-06	5.9e-06	4.9e-06
$\max\lvert\Delta_{t_1}y\rvert$	7.9e-03	1.8e-03	3.3e-03
$\int_S(\Delta_{t_1}x)^2ds$	1.1e-11	1.1e-11	8.0e-12
$\int_S(\Delta_{t_1}y)^2ds$	5.1e-06	2.7e-07	1.5e-06
$\int_T(\Delta_{s_0}v)^2dt$	4.8e-02	4.4e-03	9.5e-03
J	5.1e-06	2.7e-07	1.5e-06

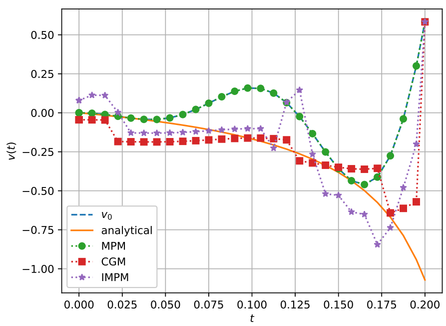

Figure 3. Results for initial control c.

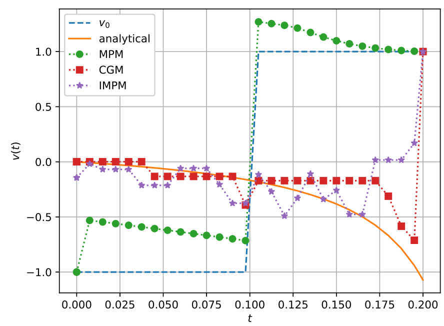

Figure 4. Results for initial control d.

Table 3. Results for initial control c

method	MPM	CGM	IMPM
times (sec)	4.5	50.4	391.2
$\max \lvert\Delta_{t_1} x\rvert$	9.3e-06	7.9e-06	7.8e-06
$\max \lvert\Delta_{t_1} y\rvert$	8.4e-03	4.6e-03	1.9e-03
$\int_S (\Delta_{t_1} x)^2 ds$	2.3e-11	1.5e-11	2.1e-11
$\int_S (\Delta_{t_1} y)^2 ds$	9.2e-06	4.8e-06	4.2e-07
$\int_T (\Delta_{s_0} v)^2 dt$	2.7e-02	9.5e-03	1.5e-02
J	9.2e-06	4.8e-06	4.2e-07

Table 4. Results for initial control d

method	MPM	CGM	IMPM
times (sec)	39.2	47.6	391.2
$\max \lvert\Delta_{t_1} x\rvert$	7.0e-05	6.0e-06	5.0e-06
$\max \lvert\Delta_{t_1} y\rvert$	2.9e-02	2.7e-03	4.6e-03
$\int_S (\Delta_{t_1} x)^2 ds$	8.2e-10	1.2e-11	9.7e-12
$\int_S (\Delta_{t_1} y)^2 ds$	1.1e-04	3.5e-07	3.8e-06
$\int_T (\Delta_{s_0} v)^2 dt$	2.8e-01	1.6e-02	3.2e-02
J	1.1e-04	3.5e-07	3.8e-06

$x^*(s,t_1), y^*(s,t_1)$; $\int_T (\Delta_{s_0} v)^2 dt$ are squares of norm in $L_2(T)$ deviations of the calculated values $v^k(t)$ from the optimal values $v^*(t)$. Computation times are for the home computer used (Intel(R) Core(TM) i3-10105F CPU @ 3.70GHz).

In all figures, the values of the time variable are given on the abscissa axis. The values of control functions are given on the ordinate axis. Each of the graphs contains four curves, namely, the curve corresponding to the optimal control and the controls found by the corresponding three methods.

Let's briefly characterize the results of the numerical experiment.

First, the conditional gradient and maximum principle methods give relatively similar results in terms of accuracy. However, the realization of the maximum principle method requires much more time. This is due to the need to solve a two-parameter optimization problem. In order to calculate the cost functional value at each set of parameters, it is necessary to solve the initial boundary value problem for the hyperbolic system. It was theoretically expected that the two-parameter maximum principle method should provide greater accuracy than all other methods. However, computational experiments have disproved this assumption. This is probably due to the linearity of the dynamical systems under consideration.

Second, the mathematical programming method is the most time efficient. This is probably due to the good debugging of the standard *Python* library. The final values are worse than the results calculated by the conditional gradient and maximum principle methods. However, these results are quite satisfactory. It should be noted that the structure of the control obtained by mathematical programming is often quite different from the optimal one.

Conclusively, the conditional gradient method may be recommended for solving the problem under consideration. It is possible that this is due to the linearity of the differential equations (1), (2) and (3), (4).

6 Conclusions

A quantitative comparison of numerical methods for solving the problem of optimal control of a distillation column has been carried out. The results show that the methods that use the necessary optimality conditions of pointwise and linearized maximum principles types give the result close to the structure of the true optimal control under different initial approximations. It turned out that the one-parameter conditional gradient method is not worse in accuracy than the method based on the iterative maximum principle, but at the same time it is much faster. It is possible that the maximum principle method can provide greater accuracy for non-linear dynamical systems.

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