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# Optimal Control in Chemical Fractionation Problem

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**Abstract**—We study a chemical fractionation process in a tower. This process is described by a system of first-order partial differential equations. We obtain necessary optimality conditions for the optimal control problem in a class of smooth boundary controls with pointwise restrictions and perform numerical tests.

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**1. The problem.** Chemical technological processes are described by rather awkward systems of partial differential equations. Mathematical models contain many intricately connected parameters. A great part of them is presented by functions with respect to time and space coordinates. The mathematical model of the fractionation process represents the following system of equations with respect to concentrations of components in liquid and vapor phases [1]:

$$\frac{\partial(G_x x_i)}{\partial t} - \frac{\partial(L x_i)}{\partial s} = k_{y_i}(y_i - y_i^*) + \Phi_{x_i}, \tag{1}$$
$$\frac{\partial(G_y y_i)}{\partial t} + \frac{\partial(V y_i)}{\partial s} = k_{y_i}(y_i^* - y_i) + \Phi_{y_i},$$

$$\sum_{i=1}^{N} x_i = 1, \ \sum_{i=1}^{N} y_i = 1, \ i = \overline{1, N}.$$

Here $N$ is the number of components in the mixture; $x_i$ and $y_i$ are, respectively, concentrations of the $i$th component in the liquid and vapor phases; $s$ is the coordinate along the tower; $t$ is the work time of the tower; $G_x$ and $G_y$ stand, respectively, for quantities of the liquid and the vapor in the tower; $L = L(t)$ and $V = V(t)$ denote, respectively, flows of the liquid and the vapor in the tower; $k_{y_i}$ is the mass transfer coefficient; $y_i^*$ is the equilibrium concentration of the component in the vapor; $\Phi_{x_i}$ and $\Phi_{y_i}$ stand, respectively, for liquid and vapor flows introduced to the tower. The concentration of components in the vaporizer is defined from the material balance equation

$$\frac{dy_i(s_0,t)}{dt} = \frac{V(t)+W(t)}{Q_y}(x_i(s_0,t) - y_i(s_0,t)), \ \ y_i(s_0,t_0) = y_{i0}(s_0). \tag{2}$$

Material balance equations for the condenser take the form

$$\frac{dx_i(s_1,t)}{dt} = \frac{L(t)+D(t)}{Q_x}(y_i(s_1,t) - x_i(s_1,t)), \ \ x_i(s_1,t_0) = x_{i0}(s_1). \tag{3}$$

Boundary conditions (2), (3) contain controllable flows $D(t)$ and $W(t)$. Here $Q_y$ and $Q_x$ stand, respectively, for quantities of the liquid in the vaporizer and the condenser.

We understand the solution to the boundary-value problem (1)–(3) in the classical sense.

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