NUMERICAL SOLUTION OF THE INITIAL-BOUNDARY VALUE PROBLEM DESCRIBING SEPARATION PROCESSES IN A DISTILLATION COLUMN

Alexander Arguchintsev
Institute of Mathematics
and Information Technologies
Irkutsk State University
Russia
arguch@math.isu.ru

Daniil Kopylov
Institute of Mathematics
and Information Technologies
Irkutsk State University
Russia
it-daniil@yandex.ru

Article history:
Received 24.10.2023, Accepted 26.11.2023

Abstract

A modification of the numerical method of characteristics is developed to solve the initial-boundary value problem that arises when modeling the rectification process in the column. The process is described by a system of first-order 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. A characteristic difference grid is constructed on the base of a linear transformation of a classical rectangular grid. Implicit second-order difference schemes are used, taking into account the features of the problem at the boundaries. The advantage of this approach is in consideration of the specifics of the propagation of perturbations in hyperbolic equations. Numerical implementation of the method was carried out. An illustrative example shows the effectiveness of the proposed modification of the characterization method. This method is a base for further solution of optimal control problems of flows in columns.

Key words

Distillation column, hyperbolic systems, dynamic boundary conditions, numerical method of characteristics.

1 Introduction

Compositions of hyperbolic and ordinary differential equations are used when modeling a number of processes of population dynamics [Alekseev, 1992], interaction of flows (liquid or gas) with solids [Vazquez, 2003], plasma dynamics [Faugeras, 2017], blood flow dynamics [Ruan, 2008], nanoparticles [Wang, 2022], thermal-engineering processes in tube furnaces [Demidenko, 2006b], etc. In particular, models of separation of mixtures in a distillation column are described by first-order hyperbolic systems with non-standard dynamic boundary conditions given in the form of ordinary differential equations. By now, quite efficient methods have been developed for solving optimal control problems of such problems [Arguchintsev, 2007; Demidenko, 2006a]. Some of these methods are based on solving optimization problems within the framework of simplified models described by ordinary differential equations [Gushchin, 2020]. However, in the transition to more complex models, the problem arises of multiple solving initial-boundary problems for combinations of hyperbolic and ordinary differential equations. Typically, each iteration of the optimization method requires solving similar problems for original and adjoint systems.

In this paper, a modification of the numerical method of characteristics is developed to solve the initial-boundary value problem that arises when modeling the rectification process in the column. A specific peculiarity of the model is in the boundary conditions of a special dynamic 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. Therefore, the initial-boundary value problem cannot be solved by solving the initial value problems first for ordinary differential equations, and then by integrating the hyperbolic system. A joint solution to the combination of hyperbolic and ordinary differential equations is needed.

The authors propose a method of constructing a characteristic difference grid based on a linear transfor-

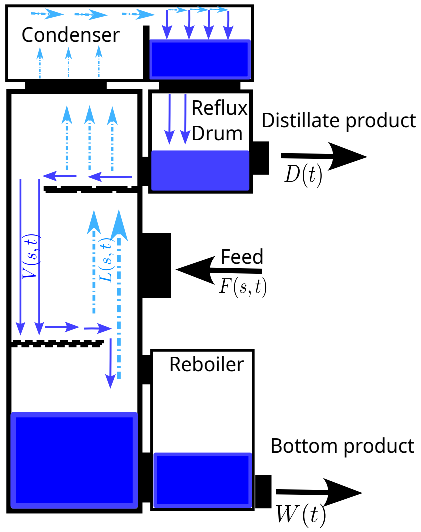

Figure 1. Scheme of operation of the distillation column.

mation of a classical rectangular grid. Next, implicit second-order difference schemes are 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. Numerical implementation of the method was carried out. An illustrative example shows the effectiveness of the proposed modification of the method.

2 Problem statement

The mathematical model of separation processes of mixtures can be described by the following first-order system of hyperbolic equations [Demidenko, 2006a]:

$$\frac{\partial(H_x x_i)}{\partial t} - \frac{\partial(L x_i)}{\partial s} = kV(y_i - p(s,t)x_i) + \Phi_{x_i}, \quad (1)$$

$$\frac{\partial(H_y y_i)}{\partial t} + \frac{\partial(V y_i)}{\partial s} = kV(p(s,t)x_i - y_i) + \Phi_{y_i}, \quad (2)$$

$$\sum_{i=1}^{N} x_i = 1, \ \sum_{i=1}^{N} y_i = 1, \ i = 1, \ldots, N. \quad (3)$$

Here t is a time variable, $t \in [t_0, t_1]$; s is a spatial variable, $s \in [s_0, s_1]$; $x_i(s,t)$ and $y_i(s,t)$ are i-th component concentrations in liquid and steam phases; functions $L(s,t), V(s,t)$ specify the flows of liquid and steam in the column; functions $H_k(s,t), H_y(s,t)$ determine the retention capacity of the column with respect to liquid and steam; $\Phi_{x_i}(s,t), \Phi_{y_i}(s,t)$ are the densities of input flows of i-th components of the initial mixture; constant k is a steam mass transfer coefficient. Functions $L(s,t), V(s,t), H_k(s,t), H_y(s,t), \Phi_{x_i}(s,t), \Phi_{y_i}(s,t)$ and constant k are given.

A general process scheme is shown in Figure 1.

The incoming mixture is subjected to evaporation and condensation procedures.

Initial conditions at $t = t_0$ are given:

$$x(s,t_0) = x_0(s), \quad y(s,t_0) = y_0(s). \quad (4)$$

At the bottom of the column ($s = s_0$), the inlet liquid flow ($L(s_0,t)$) enters the evaporator. Part of this stream evaporates and returns to the bottom of the column ($V(s_0,t)$), and the other part of liquid exits the system as the bottom liquid product ($W(t)$) of the bottom column. Boundary conditions at $s = s_0$ are defined by the following material balance equations:

$$\begin{aligned} \frac{d(H_x(s_0,t)y_i(s_0,t))}{dt} &= L(s_0,t)x_i(s_0,t) \\ &- V(s_0,t)y_i(s_0,t) - W(t)y_i(s_0,t), \\ \frac{dH_x(s_0,t)}{dt} &= L(s_0,t) - V(s_0,t) - W(t), \\ x_i(s_0,t_0) &= x_{i0}(s_0), H_x(s_0,t_0) = H_{xk0}, \\ & i = 1, \ldots, N. \quad (5) \end{aligned}$$

At the top of the column ($s = s_1$), the steam flow enters the condenser. Part of the flow of liquid leaving the condenser returns to the column as a reflux ($L(s_1,t)$), and the other part exits the system as the finished product ($W(t)$). The following material balance equations determine boundary conditions $s = s_1$:

$$\begin{aligned} \frac{dH_x(s_1,t)x_i(s_1,t)}{dt} &= V(s_1,t)y_i(s_1,t) \\ &- (L(s_1,t) + D(t))x_i(s_1,t), \\ \frac{dH_x(s_1,t)}{dt} &= V(s_1,t) - (L(s_1,t) + D(t)), \\ x_i(s_1,t_0) &= x_{i0}(s_1), H_x(s_1,t_0) = H_{xd0}, \\ & i = 1, \ldots, N. \quad (6) \end{aligned}$$

Next, let's make some simplifying assumptions.

1. The substance is a two-component mixture. The content of the second component is determined by the following formulas:

$$x_2 = 1 - x_1 \quad y_2 = 1 - y_2.$$

2. The retention capacities are directly proportional to flows:

$$H_x(s,t) = \frac{1}{c_1} L(s,t), \quad H_y(s,t) = \frac{1}{c_2} V(s,t).$$

3. Flows are independent of s:

$$L(s,t) = L(t), \quad V(s,t) = V(t).$$

4. Raw materials are supplied only in liquid phase only:

$$\Phi_x = \Phi_x(s,t), \quad \Phi_y = 0.$$

5. The incoming flow satisfies the following rule:

$$\Phi_x(s,t) = x_F F_x(t) \cdot \phi(s),$$

$$x_F = const, \quad F_x(t) = D(t) + W(t),$$

where x_F is a concentration, F_x describes an incoming liquid flow, $\phi(s)$ is a distribution of the flow depending on a spatial coordinate.

Then (1) – (6) can be written as the following initial-boundary problem.

$$\frac{\partial x}{\partial t} - c_1 \frac{\partial x}{\partial s} = B_{11}(s,t)x + B_{12}(s,t)y + b_1(s,t), \quad (7)$$

$$\frac{\partial y}{\partial t} + c_2 \frac{\partial y}{\partial s} = B_{21}(s,t)x + B_{22}(s,t)y + b_2(s,t), \quad (8)$$

$$\frac{\partial x(s_1,t)}{\partial t} = G_{11}(t)y(s_1,t) + G_{12}(t)x(s_1,t), \quad (9)$$

$$\frac{\partial y(s_0,t)}{\partial t} = G_{21}(t)x(s_0,t) + G_{22}(t)y(s_0,t), \quad (10)$$

$$x(s,t_0) = x_0(s), \quad y(s,t_0) = y_0(s), \quad (11)$$

where

$$B_{11}(s,t) = \frac{-c_1 k V(t)\tilde{p}(s,t) - L'(t)}{L(t)},$$

$$B_{22}(s,t) = -(kc_2 + \frac{V'(t)}{V(t)}),$$

$$B_{21}(s,t) = c_2 k \tilde{p}(s,t), \quad B_{12}(s,t) = \frac{c_1 k V(t)}{L(t)},$$

$$b_1(s,t) = \frac{c_1 x_F F_x(t)\phi_x(s)}{L(t)}, \quad b_2(s,t) = 0.$$

$$G_{11}(t) = -G_{12} = -\frac{L(t) + D(t)}{H_{xd0}},$$

$$G_{21}(t) = -G_{22}(t) = \frac{V(t) + F_x(t) - D(t)}{H_{xk0}}.$$

3 Method of characteristics

In the procedures of numerical solution of first-order hyperbolic systems, classical difference approximations of partial derivatives do not take into account the peculiarities of the problem under consideration. To build effective numerical methods, it is necessary to construct difference schemes with small steps and apply high-order approximations. The numerical method of characteristics is devoid of these deficiencies [Kulikovskii, 2001]. A traditional disadvantage of this method is the non-classical (often curvilinear) type of difference grid. In the problem under consideration, it is possible to construct an analogue of a classic rectangular difference grid. At the same time, standard second-order difference approximations gives a good computational effect.

Characteristics in (7), (8) are two families of curves

$$s^{(1)}(t) = -c_1 t + C_1, \quad C_1 = const$$

$$s^{(2)}(t) = c_2 t + C_2, \quad C_2 = const.$$

Let $s_0 = 0,\ t_0 = 0$. First, in $[0; s_1] \times [0, t_1]$ we enter a classical difference grid generated by the unit vectors $\vec{i} = (1,0)$, $\vec{j} = (0,1)$ (steps s and t are equal to 1). After that, we carry out a linear transformation of independent variables using a matrix

$$L = \begin{pmatrix} \Delta s & \Delta s \\ \Delta_1 t & \Delta_2 t \end{pmatrix} = (\vec{v}, \vec{w}).$$

Here $\Delta s = \frac{s_1 - s_0}{m}$, m is a parameter characterizing a grid size; $\Delta_1 t = -c_1 \cdot \Delta s$ and $\Delta_2 t = c_2 \cdot \Delta s$. So, $\vec{v}$ and $\vec{w}$ are collinear with characteristic curves.

Hyperbolic equations (7), (8) will be transformed into ordinary differential equations on the corresponding characteristic curves. They can be approximated using trapezoid formulas and be integrated together with the boundary conditions. In this case, a stage-by-stage solution of ordinary differential equations (9), (10) is carried out using previously calculated solutions on lower nodes.

Technically, the difference grid is generated as a graph. Each node of the graph stores information about the coordinate of the node of the grid, as well as the value of the desired functions at a point. Additionally, the node stores information about its type (central, left or right). An array of grid nodes consists of references to graph nodes, which represents the ability to work with the grid in two modes (with the grid as a whole or selected surfaces). This graph representation is convenient to navigate.

An implicit second-order difference scheme is used for inner points ($s_0 < s_{ij} < s_1$ and $t_0 < t_{ij} < t_1$):

$$\frac{x_{ij} - x_{i+1j}}{h_1} = \frac{B_{11}(s_{ij}, t_{ij})x_{ij} + B_{11}(s_{i+1j}, t_{i+1j})x_{i+1j}}{2} + \frac{B_{12}(s_{ij}, t_{ij})y_{ij} + B_{12}(s_{i+1j}, t_{i+1j})y_{i+1j}}{2} + \frac{b_1(s_{ij}, t_{ij}) + b_1(s_{i+1j}, t_{i+1j})}{2}, \quad (12)$$

$$\frac{y_{ij} - y_{ij-1}}{h_2} = \frac{B_{21}(s_{ij}, t_{ij})x_{ij} + B_{21}(s_{ij-1}, t_{ij-1})x_{ij-1}}{2} + \frac{B_{22}(s_{ij}, t_{ij})y_{ij} + B_{22}(s_{ij-1}, t_{ij-1})y_{ij-1}}{2} + \frac{b_2(s_{ij}, t_{ij}) + b_2(s_{ij-1}, t_{ij-1})}{2}, \quad (13)$$

$$h_1 = (s_{ij} - s_{i+1j})^2 + (t_{ij} - t_{i+1j})^2,$$
$$h_2 = (s_{ij} - s_{ij-1})^2 + (t_{ij} - t_{ij-1})^2,$$

$$j = r_{0i} + 1, r_{0i} + 2, ...r_{1i} - 1,$$
$$i = q_{0i} + 1, q_{0i} + 2, ..., q_{1i} - 1.$$

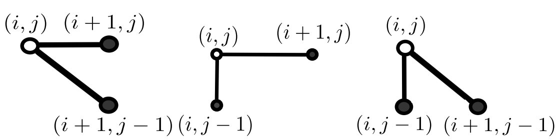

Figure 2. left, center, right templates.

On the left border we use (12):

$$\frac{y_{ij} - y_{i+1j-1}}{h_3} = \frac{G_{21}(s_{ij}, t_{ij})x_{ij} + G_{21}(s_{i+1j-1}, t_{i+1j-1})x_{i+1j-1}}{2} + \frac{G_{22}(s_{ij}, t_{ij})y_{ij} + G_{22}(s_{i+1j-1}, t_{i+1j-1})y_{i+1j-1}}{2}, \quad (14)$$

$$h_3 = (s_{ij} - s_{i+1j-1})^2 + (t_{ij} - t_{i+1j-1})^2$$
$$j = r_{0i}, i = q_{0j}.$$

On the right border we use (13):

$$\frac{x_{ij} - x_{i+1j-1}}{h_3} = \frac{G_{11}(s_{ij}, t_{ij})x_{ij} + G_{11}(s_{i+1j-1}, t_{i+1j-1})x_{i+1j-1}}{2} + \frac{G_{12}(s_{ij}, t_{ij})y_{ij} + G_{12}(s_{i+1j-1}, t_{i+1j-1})y_{i+1j-1}}{2}, \quad (15)$$

$$j = r_{1i}, i = q_{1j},$$

To calculate nodes $t_{ij} : t_{ij} - \Delta t < t_0 < t_{ij}$ we use nodes formed by the intersection of the characteristics with the line $t = t_0$.

The pattern of the difference scheme in the central and boundary regions is shown in Figure 2.

The difference scheme provides a second order of approximation and is absolutely stable [Rozhdestvensky, 1978; Ryabenky, 2010].

4 Numerical experiment

The programming language *Python 3.12* and its *NumPy* library were used for numerical experiments.

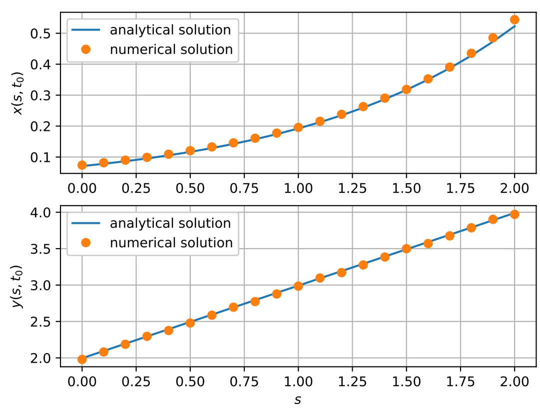

Figure 3. The state of a hyperbolic system at a finite time.

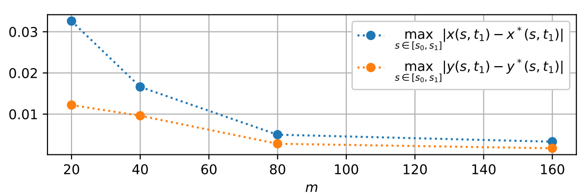

Figure 4. Solution discrepancy with different grid size.

The problem (7) – (11) is considered for the following parameters:

$$c_1 = 1, \quad c_2 = 3, \quad m = 20;$$
$$s_0 = 0, \quad s_1 = 2 \quad t_0 = 0, \quad t_1 = 1.5;$$
$$x_0(s) = e^s, \quad y_0(s) = 0;$$
$$B_{11}(s,t) = -c_1, \quad B_{12}(s,t) = -\frac{e^s}{s+2},$$
$$B_{21}(s,t) = \frac{s+2}{e^s}, \quad B_{22}(s,t) = \frac{c_2}{s+2},$$
$$G_{11}(t) = \frac{e^{s_1} \cdot \sin t}{(s_1+2) \cdot \sin t - e^{s_1} \cdot \cos t},$$
$$G_{21}(t) = \frac{2 \cdot \cos t)}{\cos t - 2 \sin t},$$
$$G_{22}(t) = -G_{21}(t), \quad G_{12}(t) = -G_{11}(t).$$

This problem has an analytical solution

$$x_a(s,t) = e^s \cos t, \quad y_a(s,t) = (s+2) \sin t.$$

The results of numerical calculations are shown in Figures 3 and 4.

Figure 3 shows graphs of solutions of the initial-boundary problem at t_1. Figure 4 illustrates the dependence of the maximum modulus of the difference between numerical and analytical solutions on the number of nodes of the difference grid. The best result is obtained for maximum parameter value $m = 160$:

$$\max_{s \in [s_0, s_1]} |x(s,t_1) - x_a(s,t_1)| = 0.0214,$$
$$\max_{s \in [s_0, s_1]} |y(s,t_1) - y_a(s,t_1)| = 0.0210.$$

A significant improvement in accuracy occurred when the parameter changed from $m = 20$ to $m = 80$.

In optimal control problems, we also have to deal with conjugate problems that are solved in reverse time. A modification of the proposed method for solving conjugate problems was constructed also. An additional step is to rotate the grid.

In general, the calculations confirm effectiveness of the proposed method.

5 Conclusions

We developed a numerical method of characteristics for solution of a specific initial-boundary value problem describing separation processes in a distillation column. The boundary conditions are determined from ordinary differential equations. The difference scheme provides a second order of approximation and is absolutely stable. Numerical experiments prove effectiveness of the method. This effective algorithm for solving the initial-boundary value problem allows to proceed to the implementation of methods for optimal control of flows in columns using variational optimality conditions for such problems [Arguchintsev, 2021].

Acknowledgements

The reported study was financially supported by the Russian Science Foundation, Project No 23-21-00296, https://rscf.ru/project/23-21-00296.

References

Alekseev, V. V., Kryshev, I. I., and Sazykina, T. G. (1992). *Physical and Mathematical Modeling of Ecosystems*. Hydrometeoizdat Publ., Saint Petersburg (in Russian).

Arguchintsev, A. V. (2007). *Optimal Control of Hyperbolic Systems*. FIZMATLIT, Moscow (in Russian).

Arguchintsev, A., and Poplevko, V. (2021). An optimal control problem by a hybrid system of hyperbolic and ordinary differential equations. *Games*, **12**, paper 23.

Demidenko, N. D., Potapov, V. I., and Shokin, Yu. I. (2006). *Modeling and Optimization of Systems with Distributed Parameters*. Nauka, Novosibirsk (in Russian).

Demidenko, N. (2006). Optimal control of thermal-engineering processes in tube furnace. *Chem. Petrol. Eng.*, **142**, pp. 128–130.

Faugeras, B., Blum, J., Heumann, H., and Boulbe, C. (2017). Optimal control of a coupled partial and ordinary differential equations system for the assimilation of polarimetry Stokes vector measurements in tokamak free-boundary equilibrium reconstruction with application to ITER. *Computer Physics Communications*, **217**, pp. 43–57.

Gushchin, P., Furtat, I., Nekhoroshikh, A., and et al. (2020). Control of distillation column under perturbations: a case study. *Cybernetics and Physics*, **9** (4), pp. 182–186.

Kulikovskii, A. G, Pogorelov, N. V., and Semenov, A. Yu. (2001). *Mathematical Aspects of Numerical Solution of Hyperbolic Systems*. Chapman and Hall/CRC, Boka Raton, Fl.

Rozhdestvenskiyi, B. L., and Yanenko, N. N. (1978). *Systems of Quasilinear Equations and their Applications to Gas Dynamics*. Nauka, Moscow (in Russian).

Ruan, W. (2008). A coupled system of ODEs and quasilinear hyperbolic PDEs arising in a multiscale blood flow model. *J. Mathematical Analysis and Applications*, **343**, (2) pp. 778–796.

Ryabenky, V. S. (2010). *The Method of Difference Potentials and its Applications. 3rd ed.* Fizmatlit, Moscow (in Russian).

Vazquez, J. L., and Zuazua, E. (2003). Large time behavior for a simplified 1D model of fluid-solid interaction. *Comm. Partial Differential Equations*, **28**, (9-10) pp. 1705–1738.

Wang, Q. F. (2022). Quantum control of nanoparticles at low temperature. *Cybernetics and Physics*, **11** (1), pp. 37–46.