

Optimal Control of the Membrane Module Start-Up Mode in the Membrane Distillation Process

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Abstract: The study considers the issue of optimal control of the start-up mode of the membrane distillation process. The aim of the work is to increase the efficiency of controlling the process of concentrating solutions in a contact membrane distillation unit, which will contribute to reducing the cost and increasing the level of energy saving of the process with prior uncertainty and changes in the permeability of the membrane over time. An analysis of various publications has shown that no single approach has been proposed to control the start-up mode of the membrane module of the process. For control purposes, a mathematical model of the dynamics of the membrane distillation process is proposed. The written mathematical model of the contact membrane distillation process is nonlinear with respect to the temperature of the solution at the outlet of the membrane module, which is also included in the equations that take into account the vapor flow through the membrane. With an increase in the temperature of the solution at the inlet of the membrane module, the temperatures of the solution and distillate at the outlet of the membrane module increase nonlinearly. The optimality criterion was the minimum process start-up time in the presence of restrictions on the final solution temperature. The penalty method and the gradient procedure on the second interval were used to change the control in order to reach the specified regime. The solution depends on the value of the weight coefficients of the penalty functions, which allowed reaching the specified regime in the minimum time.

Index Terms: Contact membrane distillation, Modeling, Optimal control, Minimum time problem, Numerical solution method

1. Introduction

The relevance of the search for optimal control of the contact membrane distillation process lies in the fact that to date, no single approach to controlling the start-up mode of the process has been proposed. Water is of crucial importance for human life and nature. The demand for fresh water is rapidly increasing due to population growth and urbanization, while clean water resources are being depleted. So far, desalination remains the most reliable and practical technology for supplying drinking water. However, all traditional desalination technologies are energy-intensive methods, regardless of their advantages. Therefore, the projected growth of water desalination technology should correspond to the reduction of energy consumption and environmental impact. Today, membrane distillation (MD) technology is trendy and is developing rapidly due to its attractive properties. There is a strong need to develop less

energy-intensive and environmentally friendly methods of water purification. One of the sources of replenishment of drinking resources can be desalination of mineralized water. Currently, reverse osmosis accounts for 60% of desalination plants worldwide. An alternative to reverse osmosis is contact membrane distillation (CMD). The process is characterized by internal disturbances, in particular due to concentration polarization. During the transport of solvent through the pores of the membrane, the concentration of the solute near its surface increases, which leads to a number of undesirable consequences. Over time, the control of the CMD process becomes more complicated due to changes in membrane characteristics, such as porosity and thermal resistance. The membrane must be hydrophobic, using common materials, including polypropylene (PP), polytetrafluoroethylene (PTFE) and polyvinylidene fluoride (PVDF). The task was to develop and study the optimal control of the start-up mode of the membrane module in the contact membrane distillation process.

2. Literature Review

Some researchers began to focus on transient modeling and time analysis of MD processes [1-4].

Analysis of various publications showed that the optimal control of the contact membrane distillation process has been fully investigated only with the use of solar energy. The paper proposes an optimal control of direct contact membrane distillation with renewable energy sources, which allows to maximize water desalination by dynamically adjusting the flow rate of the cold stream in response to fluctuations in the inlet temperature caused by solar energy [5]. Other works have solved the problem of real-time optimization for a solar-powered water desalination system and direct contact membrane distillation [6]. This approach is possible in the case of sufficient solar energy. In most cases, regulation occurs by changing the temperature of the solution at the inlet. A comprehensive optimal control system for solar thermal membrane distillation systems is presented, which allowed to increase productivity [7]. The disadvantage of using a “burst-burst” type regulator (or positional regulator) is the high amplitude of fluctuations of the controlled parameter, which does not allow to achieve stable operation of the system.

3. Mathematical model

For control purposes, a mathematical model of the CMD process with lumped parameters was developed, which takes into account the heat transfer through the polymer structure of the membrane and the flow of solvent vapor, which consists of heat capacities [8-11]:

- solution channel;
- distillate channel.

When creating the mathematical model, the following assumptions were made:

- 1) the membrane is ideal, i.e. hydrophobic with the same pore radius and an intact selective layer;
- 2) the effect of temperature and concentration polarization was not taken into account;
- 3) the change in temperature and concentration along the MM channels was not taken into account;
- 4) the membrane capacity was not considered, taking into account its thickness in comparison with the height of the solution and distillate channels.

The structural diagram of the membrane module (MM) is presented in Fig. 1.

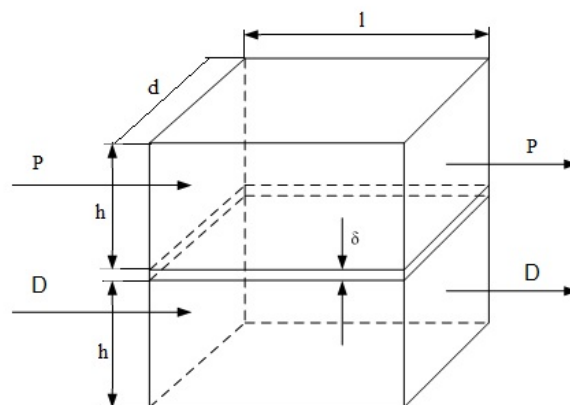


Fig. 1. Membrane module diagram.

The mathematical description of the MM is based on the material and energy flows of the process. The heat balance equation of the MM dynamics:

$$\begin{aligned} G_{pH}c_{pH}\theta_{pH} - kF(\theta_{pE} - \theta_{EK}) - F\varepsilon J_p r - G_{pK}c_{pK}\theta_{pE} &= V_p\rho_{pK}c_{pK}\frac{d\theta_{pE}}{dt}, \\ G_{DH}c_{DH}\theta_{DH} + kF(\theta_{pK} - \theta_{DK}) + F\varepsilon J_p r - G_{DK}c_{DK}\theta_{DK} &= V_D\rho_{DE}c_{DE}\frac{d\theta_{DE}}{dt}, \end{aligned} \quad (1)$$

where:

r is the specific heat of vaporization, J/kg; $VP=VD=Sl$ is the volume of the solution and distillate channel, m³;
 ρ_{PK} , ρ_{DK} is the density of the solution and distillate at the outlet of the MM, kg/m³;
 c_{PK} , c_{DK} is the heat capacity of the solution and distillate at the outlet of the MM, J/(kg·K); θ_{PH} , θ_{DH} is the temperature of the solution and distillate at the inlet of the MM, K.

The evaporated solvent is transferred in the pores of the membrane, condensing on the cold surface of the membrane. To calculate the specific mass flow of vapor, the relationship for the case of molecular diffusion was used

$$J_p = \frac{M\bar{D}_{BP}p_a}{\delta R\theta} \ln \frac{p_x - p_2(\theta_2)}{p_g - p_1(\theta_1)} \quad (2)$$

where

J_p is the specific mass flow of steam, kg/(m²·s);
 M is the molar mass of steam, mol;
 $\bar{D}_{BP}$ is the effective coefficient of mutual diffusion of steam in air, m²/s;
 p_a is the atmospheric pressure, Pa;
 p_g , p_x is the pressure of the steam-air mixture on the warm and cold surfaces of the membrane, Pa;
 p_1 , p_2 is the partial pressure of the solvent vapor on the warm and cold surfaces of the membrane, Pa;
 θ_1 , θ_2 is the temperature on the membrane surfaces in the solution and distillate channels, K;
 R is the universal gas constant, J/(mol·K); $\theta=(\theta_{PK}+\theta_{DK})/2$ is the average temperature of the membrane, K;
 θ_{PK} , θ_{DK} is the temperature of the solution and distillate at the outlet of the MM, K.

The ratio of pressure differences in (2) is represented by the ratio:

$$\frac{p_x - p_2(\theta_2)}{p_g - p_1(\theta_1)} = \exp \frac{D_{KP}(p_g - p_x)}{\bar{D}_{EP}p_a} \quad (3)$$

where D_{KP} is the Knudsen diffusion coefficient, m²/s;

The linearized energy conservation equations in increments on linear sections were presented in the form

$$\begin{aligned} a_{13}\theta_{PX} + a_{15}\theta_{PX} + a_{16}\theta_{DX} &= \frac{d\theta_{DX}}{dt}, \\ a_{25}\theta_{PK} + a_{26}\theta_{DK} &= \frac{d\theta_{DK}}{dt}, \end{aligned} \quad (4)$$

where the model coefficients are:
 solution channel heat balance equation

$$\begin{aligned} a_{13} &= \frac{G_{PH}c_{PH}}{V_p\rho_{PK}c_{PK}} \\ a_{15} &= \frac{1}{V_p\rho_{PK}c_{PK}} \left[-G_{PH}c_{PK} - kF + \frac{2MD_{KP}(p_g - p_x)\varepsilon F(r + c_{PK}\theta_{DK})}{\delta R(\theta_{PK} + \theta_{DK})^2} \right] \\ a_{16} &= \frac{1}{V_p\rho_{PK}c_{PK}} \left[kF - \frac{2MD_{KP}(p_g - p_x)\varepsilon F(r - c_{PK}\theta_{PK})}{\delta R(\theta_{PK} + \theta_{DK})^2} \right] \end{aligned}$$

distillate channel heat balance equation

$$a_{25} = \frac{1}{V_P \rho_{DK} c_{DK}} \left[kF - \frac{2MD_{KP}(p_g - p_x)\varepsilon F(r + c_{DK}\theta_{DK})}{\delta R(\theta_{PK} + \theta_{DK})^2} \right]$$

$$a_{26} = \frac{1}{V_P \rho_{DK} c_{DK}} \left[-G_{DH}c_{DK} - kF - \frac{2MD_{KP}(p_g - p_x)\varepsilon F(c_{DK}\theta_{PK} - r)}{\delta R(\theta_{PK} + \theta_{DK})^2} \right]$$

The initial membrane data during simulation are presented in Table 1, and the technological process data are presented in Table 2.

Table 1. Input data for membrane modeling.

Parameter	Parameter designation	Unit of measurement	Value
Membrane pore radius	r	m	$0,12 \cdot 10^{-6}$
Membrane module length	l	m	0,5
Membrane thickness	δ	m	$3,03 \cdot 10^{-4}$
Membrane porosity coefficient	ε	–	0,8
Membrane tortuosity coefficient	γ	–	0,2
Cross-sectional area	d	m ²	0,025

Table 2. Technological process data.

Parameter	Parameter designation	Unit of measurement	Value
Solution temperature	θ_H	K	333
Distillate temperature	θ_D	K	303
Concentration of salt solution	bH	kg/kg	0,1
Solution flow rate	wP	m/s	0,1
Distillate flow rate	wD	m/s	0,1
Diffusion coefficient	D_s	m ² /s	$3,24 \cdot 10^{-5}$
Vapor flow through membrane	J_w	kg/(m ² ·s)	$1,188 \cdot 10^{-5}$

4. Optimal Control

The task was set to optimally control the start-up mode of the membrane module. That is, to bring the device to a given temperature of the solution at the outlet of the membrane module in the shortest possible time, given the presence of restrictions on the temperature of the solution at the inlet.

The objective function of the task

$$I = t_f \rightarrow \min$$

under restrictions $\theta_{pk}(t_f) = \theta_{pk}^{GV}$ and $\theta_{PH \min} \leq \theta_{PH} \leq \theta_{PH \max}$

where t_f is the final moment of time, $\theta_{PH \min}$, $\theta_{PH \max}$ are the minimum and maximum values of the solution temperature at the inlet to the membrane module.

The penalty function method is applied in the gradient method of finding the extremum in the functional space to calculate the control and trajectory when translating the system (4), $\theta_{PH \min} \leq \theta_{PH} \leq \theta_{PH \max}$ from the state $\theta_{PH}(0) = \theta_{PH}$ and $\theta_{DH}(0) = \theta_{DH0}$ to the state $\theta_{PK}(t_f) = \theta_{PK}^{GV}$ for the minimum time.

This problem is solved as a minimum cost function problem [12]

$$I = t_f + \frac{1}{2} S_{11} [\theta_{PK}(t_f) - \theta_{PK}^{GV}(t_f)]^2 + \frac{1}{2} S_{22} [\theta_{DK}(t_f) - \theta_{DK}^{GV}]^2 \rightarrow \min$$

You can take into account restrictions on the control action by introducing a penalty function into the criterion

$$I = t_f + \frac{1}{2} S_{11} [\theta_{PK}(t_f) - \theta_{PK}^{GV}]^2 + \frac{1}{2} S_{22} [\theta_{DK}(t_f) - \theta_{DK}^{GV}]^2 + \int_0^{t_f} [Q(\theta_{PH \max} - \theta_{PK}(t))(\theta_{PH}(t) - \theta_{PH \min})] H(q_1, q_2) dt \quad (5)$$

where H is the Heaviside function,

$$q_1 = \theta_{PH \max} - \theta_{PH} \geq 0$$

$$q_1 = \theta_{PH}(t) - \theta_{PH \min} \geq 0$$

Then the Hamiltonian is equal to

$$H = (\theta_{PH \max} - \theta_{PH})(\theta_{PH} - \theta_{PH \min})H[q_1, q_2] + \lambda_1(a_{11}\theta_{PK} + a_{12}\theta_{DK} + b\theta_{PH})_2 + \lambda_2(a_{21}\theta_{PK} + a_{22}\theta_{DK}) \quad (6)$$

where $\lambda_1(t), \lambda_2(t)$ are Lagrange multipliers.

The conjugate system has the form

$$\begin{aligned} \lambda'_1 &= -\frac{\partial H}{\partial \theta_{PK}} = -a_{11}\lambda_1 - a_{21}\lambda_2 \\ \lambda'_2 &= -\frac{\partial H}{\partial \theta_{DK}} = -a_{12}\lambda_1 - a_{22}\lambda_2 \end{aligned} \quad (7)$$

Transversality conditions:

$$\begin{aligned} \lambda'_1(t_f) &= S_{11}(\theta_{PK}(t_f) - \theta_{PK}^{GV}) \\ \lambda'_2(t_f) &= S_{22}(\theta_{DK}(t_f) - \theta_{DK}^{GV}) \end{aligned} \quad (8)$$

We obtained an expression for $\frac{\partial H}{\partial \theta_{PH}}$

$$\frac{\partial H}{\partial \theta_{PH}} = Q(\theta_{PH \max} - 2\theta_{PH} + \theta_{PH \min})H(q_1, q_2) + b\lambda_1$$

To determine the final moment of time, the condition $\frac{\partial I}{\partial t_f} = 0$ was used as a criterion for stopping the iterative process.

$$\begin{aligned} \frac{\partial I}{\partial t_f} = 0 &= 1 + S_{11}(\theta_{PK}(t_f) - \theta_{PK}^{GV})\theta'_{PK}(t_f) + S_{22}(\theta_{DK \max}(t_f) - \theta_{DK}^{GV})\theta'_{DK}(t_f) + \\ &Q(\theta_{PH \max} - 2\theta_{PH} + \theta_{PH \min})H(q_1, q_2) + Q(\theta_{PH \max} - \theta_{PH})(\theta_{PH} - \theta_{PH \min})H(q_1, q_2) + b\lambda_1 \end{aligned}$$

Then the optimal control procedure can be described as follows [8].

We choose the initial control $\theta_{PH}(t)$, calculate the trajectory of the system state vector and the derivative $\frac{\partial I^0}{\partial t_r}$. From the condition $\frac{\partial I^0}{\partial t_r} = 0$ we determine the termination time for the first iteration. With this final time we solve the adjoint equations in reverse time, which are necessary for calculating the increment

$$\Delta \theta_{PH}^N(t_f) = -k \frac{\partial H}{\partial \theta_{PH}^N} \text{ and control } \theta_{PH}^N(t) = \theta_{PH}^N(t) + \Delta \theta_{PH}^N(t) \quad (9)$$

for the next iteration. These calculations continue until the increment $\Delta \theta_{PH}^N$ of the control from iteration to iteration becomes small.

Suppose that the control $\theta_{PH}^0 = \theta_{PH}^1$ is chosen as the initial one. We solve the mathematical model of the process in

direct time until $\frac{\partial I}{\partial t_j} = 0$.

Then the control changes and takes the value $\theta_{PH} = \theta_{PH}^2$. The mathematical model of the process is solved again until the condition $\frac{\partial I}{\partial t_j} = 0$ is met.

If the initial control does not coincide with the optimal one and the system does not reach the desired mode, then the conjugate system is solved in reverse time from t_f to 0 [13-16]. Then the next value of the control

$$\theta_{PH}^1(t) = \theta_{PH}^0(t) + \Delta\theta_{PH}(t) = \theta_{PH}^0(t) - k \frac{\partial H}{\partial \theta_{PH}}$$

This calculation process continues until the specified mode is achieved.

For the solved problem $\theta_{PH}^1 = 65^\circ\text{C}$, $\theta_{PH}^2 = 80^\circ\text{C}$.

5. Materials and Methods

First, we calculated the transition trajectory of the final solution temperature at the minimum input temperature $\theta_{PH}^1 = 65^\circ\text{C}$ according to this algorithm (Fig. 2.). The final temperature reaches the level $\theta_{PH} = 64,5^\circ\text{C}$. Then we change the input solution temperature to the maximum $\theta_{PH}^2 = 80^\circ\text{C}$ (Fig. 2.). The solution temperature value at the membrane module outlet goes beyond the permissible $\theta_{PH} = 78^\circ\text{C}$.

6. Results and Discussion

Since the external point method is used in the penalty method, this is permissible. For the second stage of control, we calculated the conjugate system (7) with transversality conditions (8). We found the control gain and for the new iteration the change in the inlet solution temperature in time. The iterative process of finding the optimal control continues until the outlet solution temperature becomes a given one.

The graph of the change in control and the temperature at the outlet of the membrane module is shown in Fig. 2. and Fig. 3.

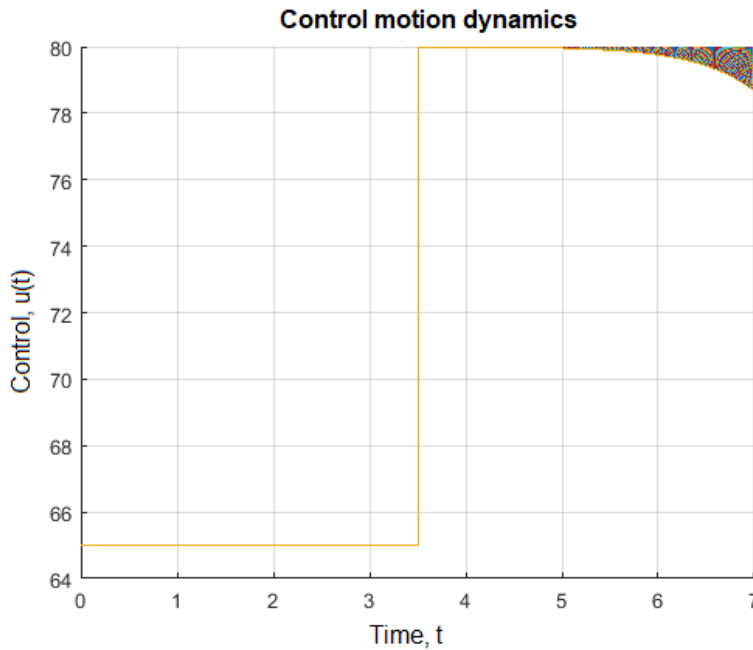


Fig. 2. Temperature control change schedule at intervals.

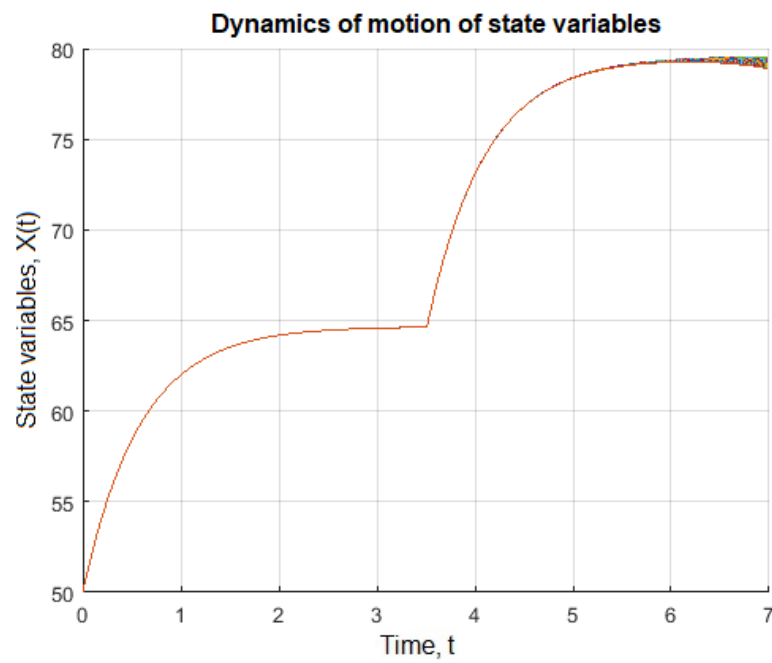


Fig. 3. Graph of change in solution at the module outlet during control stages.

Fig. 4. and Fig. 5. show the graph of the change in the optimality criterion and the graph of the change in the Lagrange multiplier over the control interval.

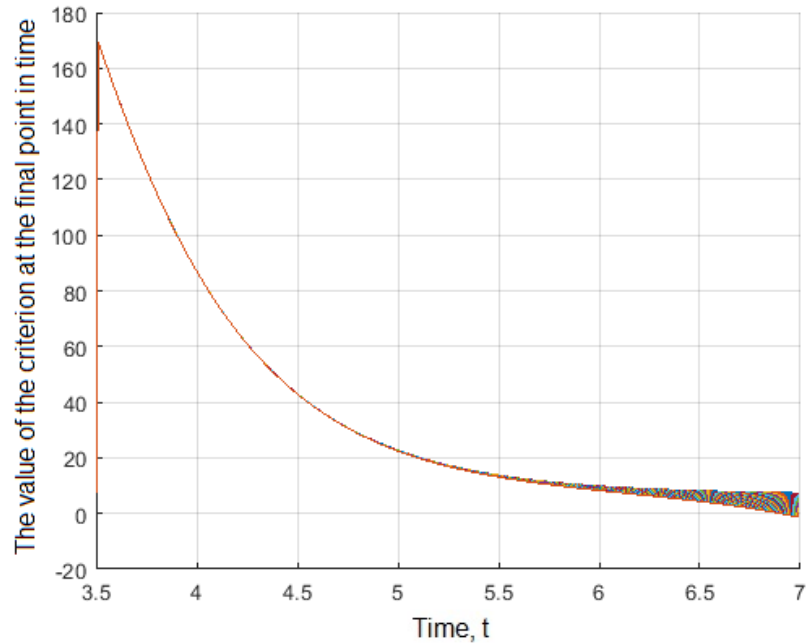


Fig. 4. Graph of changes in the optimality criterion.

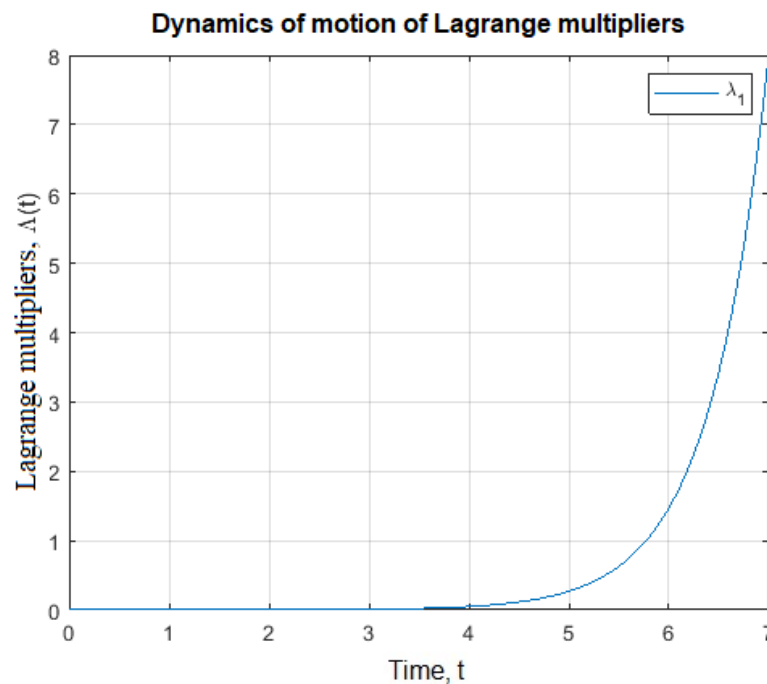


Fig. 5. Graph of the change in the Lagrange multiplier over the control interval.

We investigated the quality of the obtained control for a given system in the minimum time. The solution depends on s_{11} and s_{22} and k which are determined by trial and error. The problem was solved in 40 iterations, the minimum time for the system to reach the origin is 7.3 s.

7. Conclusion

An algorithm for optimal control of the membrane module start-up mode in the membrane distillation process is proposed. The minimum time for the membrane module to reach the specified mode with a limitation on the outlet solution temperature was chosen as the optimality criterion. The final start-up mode time was entered into the terminal component of the cost function. The penalty method and the gradient procedure were used to solve the problem. The applied algorithm allowed the membrane module to reach the specified technological mode.

All the Declarations and Statements

Author Contribution Statement

Lesya Ladieva – Conceptualization, Methodology, Supervision, Writing – original draft.

Roman Dubik – Investigation, Data curation, Formal analysis, Visualization, Writing – review and editing.

Bogdan Korniyenko – Writing – review and editing, Mathematical modeling.

All authors have read and agreed to the published version of the manuscript.

Conflict of Interest Statement

The Authors declared no conflicts of interest.

Funding Declaration

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Data Availability Statement

The data that support the findings of this study are from the corresponding author upon reasonable request.

Ethical Declarations

This study did not involve human participants or animals.

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Declaration of Generative AI in Scholarly Writing

During the preparation of the manuscript, the authors carefully reviewed the content and take full responsibility for the accuracy and integrity of the manuscript.

Abbreviations

Not applicable.

Appendix A/B/C..., with appendix title

Not applicable.

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