



Mathematical Model Desublimation Conditions

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

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ABSTRACT

The developed and software-implemented simplified three-dimensional mathematical model of the unsteady-state process of HFS desublimation is described. The study of regularities in the HFS desublimation process is performed by numerical modeling.

Keywords: Ammonium hexafluorsilicate; desublimation; mathematical modeling; heat transfer processes.

1. INTRODUCTION

This work is devoted to mathematical modeling of the process of desublimation of gaseous HFS

into vertical transport containers. The existing mathematical models of the HPS desublimation process [1-3] are, as a rule, stationary or quasi-stationary. Their common disadvantages are the

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lack of consideration of heat transfer by convection and friction of the gaseous HFS against the desublimator layer during its movement along the heat exchange walls; desublimation on the end elliptical walls of heat exchange tanks [4].

The study of gas mixture flows based on the solution of the complete system of Navier-Stokes equations has a long tradition. A very limited number of cases are known in the literature that allow analytical integration of the Navier-Stokes equations [5]. The Navier-Stokes equations have a number of specific features that significantly affect their numerical solution, regardless of their form of writing. One of the essential features is the non-linearity and paraboloelectric nature of these equations. Therefore, in order to correctly model the elliptic nature of the Navier-Stokes equations, it is necessary to use the elliptic Poisson equation for pressure. Therefore, progress in this area is possible only through the use of numerical methods. At present, for the numerical solution of the Navier-Stokes equations, several dozen varieties of difference schemes exist and are used [6].

At the present stage of the development of computational fluid mechanics, its further progress is associated with the improvement of flow models, mixing processes, and computer technologies for integrating the initial equations. The last of them are usually associated with the complication of computational algorithms through the use of approximation schemes of a higher order of accuracy and structured grids. However, this path is associated with the increasing complexity of computational algorithms and programs, which leads to great difficulties in their implementation, and therefore is available only to some professionals. This limits the possibility of their wide use in design and development activities. Therefore, the main goal of our work is to create and discuss a relatively simple numerical algorithm for solving the fundamental Navier-Stokes equations [7].

The determination of the aerodynamic regime in the volume of the apparatus was calculated out on the basis of axisymmetric averaged of the Navier-Stokes equations [8,9], written in variables of vorticity Ω , stream function Ψ :

$$u_r \frac{d\psi}{dr} + u_z \frac{d\psi}{dz} = \frac{1}{\text{Re}} \frac{1}{r} \left[\frac{\partial}{\partial r} \left(r v_t \frac{\partial \psi}{\partial r} \right) + \frac{\partial}{\partial z} \left(r v_t \frac{\partial \psi}{\partial z} \right) \right] + F_j. \quad (1)$$

$$\frac{\partial^2 \psi}{\partial r^2} + \frac{\partial^2 \psi}{\partial z^2} = \Omega r^2 + \frac{1}{r} \frac{\partial \psi}{\partial r}, \quad \Omega = \frac{1}{r} \left[\frac{\partial u_r}{\partial z} - \frac{\partial u_z}{\partial r} \right], \quad u_r = \frac{1}{r} \frac{\partial \psi}{\partial z}, \quad u_z = -\frac{1}{r} \frac{\partial \psi}{\partial r}. \quad (2)$$

Left side of eq. (1) describes the convective transfer of HFS due to the velocity of the vapor. The Poisson equation (2) for determining the stream function Ψ was obtained from the continuity equation [10]. Using the above equations, we have developed a program for calculating the processes of cooling and desublimation of HFS ammonia from a vapor-gas mixture.

2. THERMAL AND HYDRODYNAMIC CALCULATIONS

When calculating the desublimation, the HPS is successively determined for the flows shown in Fig. 1: 1) Parameters of the vapor at the inlet and outlet of the container; 2) heat transfer for an axisymmetric problem [11].

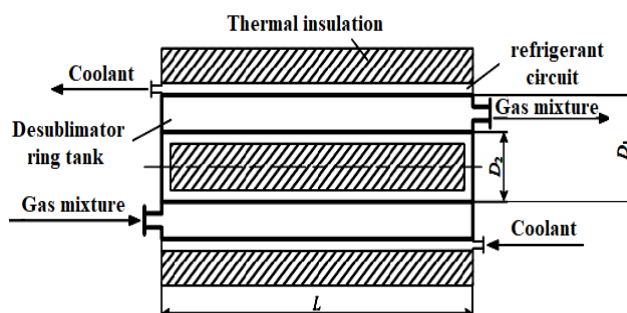


Fig. 1. Scheme of flows entering and leaving the desublimator

The speed of movement of the gas W , is determined by the formula $W = Q/S$, where S is the cross-sectional area of the apparatus, m^2 .

The criteria for similarity (Reynolds - Re , Prandtl - Pr and Peclet - Pe) are [5]:

$Re = \frac{W \rho_{mix} d_e}{\mu_{mix}}$; $Pr = \frac{c_{p,mix} \mu_{mix}}{\lambda_{mix}}$; $Pe = Re Pr$. Where d_e is the equivalent diameter of the annular section of the apparatus, m .

The heat transfer axially metric laminar flow has the form [12,13]:

$$\frac{\partial T}{\partial \tau} + W \frac{\partial T}{\partial x} = a \left(\frac{\partial^2 T}{\partial x^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} \right) \quad (3)$$

Then approximately, $\frac{\partial T}{\partial x} = \frac{T - T_0}{x}$, $\frac{\partial^2 T}{\partial x^2} = \frac{T - T_0}{x^2}$ and consider the relation

$$\left(W \frac{\partial T}{\partial x} \right) / \left(a \frac{\partial^2 T}{\partial x^2} \right) = \frac{Wx}{a} = \frac{W d_e}{\nu} \frac{\nu}{d_e} = Re Pr \frac{x}{d_e} = Pe \frac{x}{d_e} \gg 1$$

Where $W \frac{\partial T}{\partial x}$ is the convection heat transfer, $a \frac{\partial^2 T}{\partial x^2}$ is the diffusion heat transfer, $a = \frac{\lambda_{mix}}{c_{mix} \rho_{mix}}$ coefficient of thermal conductivity [14].

T_0 , T_1 , T_s , T_w are the temperatures of the gas at the inlet zone, the desublimation front, the desublimation surface and the cold wall of the desublimator; q_1 , q_2 are the heat fluxes removed from the gas flow to the desublimation surface and through the desublimator layer to the apparatus wall (Fig. 2).

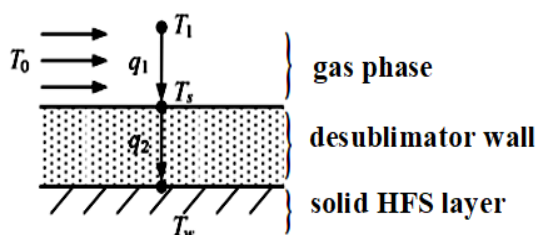


Fig. 2. Scheme of the process of desublimation of HFS

The length of the unsteady section of the flow l_i , one can use the equation [3-5]: $\frac{l_i}{d_e} = 0,055 Re$. Let us describe the heat balance in the system by the equation where ΔH is the HFS desublimation heat, kJ/mol ; dS is the area surface, V is the release rate of the HFS volume. Then $\beta = \frac{d\delta}{d\tau} \frac{\alpha dT}{\Delta H \rho_s}$ where β is the mass transfer coefficient from the gas to the cold surface [15]. By temperature: $\beta = \frac{\alpha(T_1 - T_s)}{\Delta H \rho_s}$.

From Newton's law for heat transfer, one can express the heat flux transferred by the gas to the desublimation surface: $q_2 = -\lambda_s \frac{T_s - T_w}{\delta} = -\frac{\lambda_s}{\delta} (T_s - T_w)$ and from the Fourier law for heat transfer:

$\alpha(T_s - T_w) = -\frac{\lambda_s}{\delta} (T_s - T_w)$. Based on the foregoing, we accept $q_1 = q_2$, then (6) desublimation surface temperature, we have: $T_s = \left(\alpha + \frac{\lambda_s}{\delta} \right) \alpha T_1 + \frac{\lambda_s}{\delta} T_w$.

$$T_s = \frac{\alpha T_1 + \frac{\lambda_s}{\delta} T_w}{\alpha + \frac{\lambda_s}{\delta}} = \frac{T_w}{1 + \frac{\alpha \delta}{\lambda_s}} + \frac{\frac{\alpha \delta}{\lambda_s} T_1}{1 + \frac{\alpha \delta}{\lambda_s}} \quad (4).$$

Since the Nusselt criterion is equal $Nu_s = \frac{\alpha \delta}{\lambda_s}$, you can get: $T_s = \frac{T_w}{1 + Nu_s} + \frac{Nu_s T_1}{1 + Nu_s}$ (5)

The physicochemical parameters Re, Pr, Nu are calculated, and coefficient α is determined [16].

Given that in the initial section of the cooling of the gas-vapor mixture, the process proceeds in a non-stationary mode, the calculation of the desublimating HFS mass is found taking into account the

proportion: $K = \frac{T_0 - T_i}{T_0 - T^*}$ where T_i is the current temperature, K; T^* is the desublimation temperature,

K. 4) after the end of the outer cycle, graphs of the function $\delta = f(x)$ are plotted. Figs. 3 and 4 show the change in the temperature of the gas depending on the transverse (y) and longitudinal (x) coordinates.

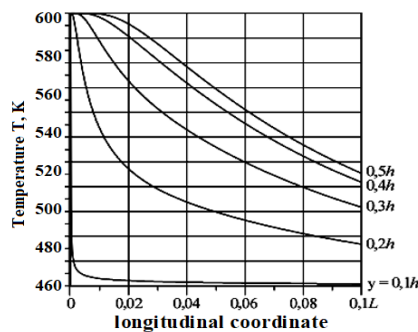


Fig. 3. Dependence of the temperature of the gas on the transverse coordinate at different values of x

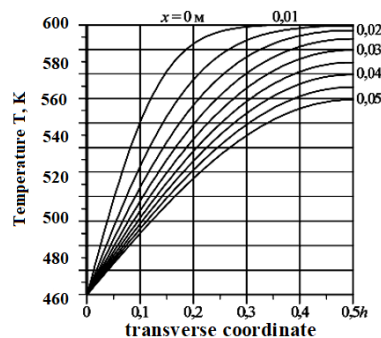


Fig. 4. Dependence of the temperature of the vapor-gas mixture on the longitudinal coordinate for various values of y

The length of the zone of the apparatus, in which the entire HPS determined at temperature of 243 K and a load of up to 0.5Gm according to HPS, is 0.5L in the absence of a region of non-stationary (Fig.5) and 0.8L in its presence (Fig.6), and cavity was 0.5h and 0.4h, respectively

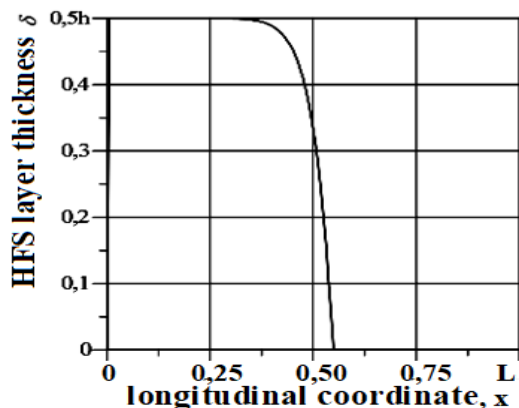


Fig. 5. Dependence of the layer thickness of the desublimated HPS

Graphs of desublimator zones in which the entire HPS is desublimated at apparatus wall temperatures of 245, 255, 265, and 275 K in the presence a non-stationary desublimation region of the vapor are shown in Fig. 6. From Fig. 6 it can be seen that the length of the zone of the apparatus, in which the entire HFS is desublimated when the desublimator is loaded up to 0.5Gmax according to the HFS in the presence of non-stationary region with the width of the annular gap h.

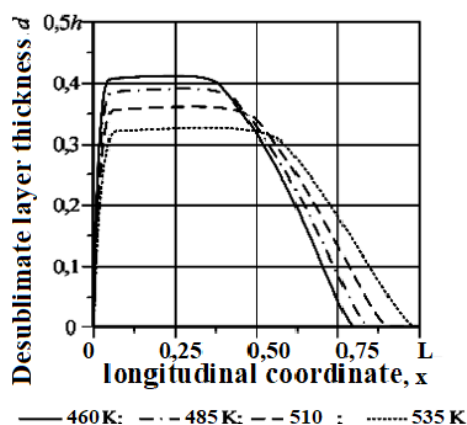


Fig. 6. Dependence of the thickness of the desublimated HFS layer on the longitudinal coordinate in the presence of a region of nonstationary cooling of the vapor–gas mixture at different temperatures of the apparatus wall

3. CONCLUSION

A mathematical model has been developed for the process of desublimation of HFSs a gas entering the desublimator, which makes it possible to determine the effect of heat transfer, aerodynamic parameters on the considered processes, optimizing the technological characteristics of the process and creating a system for control of the process.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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