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Research Article

Mathematical modelingof heat and mass transfer processes in the adsorbers of the air purification system

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Abstract:The present work is devoted to the study of the processes of heat and mass transfer in the adsorbers of the preliminary drying unit of the atmosphere purification system. A mathematical model has been developed that adequately reflects the physical processes at all stages of the adsorption cycle.Algorithms for solving problems and programs for calculating heat and mass transfer processes in an adsorption regenerated installation are obtained, results of parametric calculations of heat and mass transfer processes at each stage of the adsorption cycle and for the entire cycle as a whole are obtained.

Keywords:air purification, adsorption, heat and mass transfer, mathematical model

1 Introduction

In atmospheric purification systems, carbon dioxide is removed from the air by using the adsorption phenomenon. As a physical phenomenon, adsorption is widely used for directed formation of layers of various substances on a substrate surface [1-14]. A lot of coatings with modified properties can be attributed to the polymers, nanomaterials etc. [15-25]. Before the air is cleaned from carbon dioxide, it is dried in a preliminary drying unit also by passing through an adsorbent bed. The pre-drying unit consists of two alternately operating adsorbers covered with a granular absorber - silica gel. One of the adsorbers works to dry the air, and the second is regenerated at this time. The duration of each half-cycle is usually 1 hour, and it is determined by the appearance behind the adsorbent layer of the concentration of water vapor in the air at a level of -20 C according to the dew point temperature. Providing such a degree of air drying requires constant energy consumption (up to 240 W), which is used to heat the air to regenerate the adsorbent.

The solution of the set tasks requires a large amount of theoretical and experimental work. Due to the large number of parameters that determine the efficiency of the drying process, a complete analysis of the cycle is largely determined by the presence and implementation of reliable mathematical models and calculation algorithms in engineering practice [26-32]. On their basis, it is possible both to take into account the peculiarities of the flow of heat and mass transfer processes at each step of the cycle, and their interaction during the transition from the previous step to the next.

2 Systems of equations simulating the adsorption process

In accordance with the description of the physical processes of adsorption, it is necessary to write a system of equations describing the dynamics of sorption in the layer of the studied system [33-38]. Experimental studies have shown that the processes occurring in the sorbent layer are nonstationary and one-dimensional (we neglect the change in parameters along the layer height). In the general case, when the gas mixture is passed through the adsorption layer, the sought functions$\rho_i(x,t)$, $a_i\ (x,t)$and$T(x,t)$must satisfy the system of equations describing the balance of matter and energy in the layer, and also reflecting the kinetics and statics of adsorption.

The first equation reflecting the balance of matter in the layer can be written in the following form:

$$-\frac{\partial(U\rho_i)}{\partial x}+\frac{\partial}{\partial x}D_i(T,\rho_i)\frac{\partial\rho_i}{\partial x}=\frac{\partial a_i}{\partial t}+\varepsilon\frac{\partial\rho_i}{\partial t} \qquad (1)$$

$$i=1\div(N-1)$$

where N – number of gas mixture components. The first term expresses the transfer of matter due to the presence of flow velocity, the second longitudinal diffusion. The right side conveys the increase in concentration and the increase in the value of the sorbed substance, $\rho$and$a$here the average values of concentration and sorption, calculated per unit volume in a given place of the layer; D – is the diffusion

coefficient; ε - the porosity of the substance. The concentration and sorption values are averaged along the plane perpendicular to the *x* axis, since we assumed that ρdepends only on *x*. In this case, the values U, D_i n Eq. (1) are considered effective, not true, i.e. averaged over the length of the average distance between the granules. The convective transfer rate U , determined from the condition

$$U\sum_{i=1}^{N}\rho_i = \sum_{i=1}^{N}\rho_i U_i$$

.

Density of the diffusion flux of the *i*-th component $-D_i(T,\rho_i)\frac{\partial\rho_i}{\partial x} = j_i$ defined as $j_i = \rho_i U_i - \rho U$

The continuity equation as a whole is obtained by summing equations (1) over *i*.

$$\varepsilon\frac{\partial\rho}{\partial t} + \frac{\partial(U\rho)}{\partial x} = -\sum_{j=1}^{N}\frac{\partial a_j}{\partial t} \quad (2)$$

Instead of equation (2), the continuity equation for the *i*-th component can be used. Equation (2) corresponds to the law of conservation of matter and is not associated with any special hypotheses.

The equation reflecting the kinetics of the process is written in the following form:

$$\frac{\partial a_i}{\partial t} = \beta_i(a_i^* - a_i) i = 1 \div (N-1), \quad (3)$$

The following equation is the energy equation for the charge and filter gas, which can be written in the following form:

$$\frac{\partial}{\partial t}\left(\left[\rho_s C_s + \sum_{i=1}^{N} a_i C_i\right]T\right) + \frac{\partial(\rho U C_p T)}{\partial x} = \frac{\partial}{\partial x}\lambda_s\frac{\partial T}{\partial x} - \sum_{i=1}^{N}\Delta H_i\frac{\partial a_i}{\partial t} \quad (4)$$

where ρ_s – bulk density of dry charge; C_s – specific heat of dry charge; C_i - specific heat *i*-th component in the liquid phase; C_p - specific heat of gas at constant pressure; λ_s - heat conductivity coefficient of the charge; ΔH_i - specific enthalpy of condensation of the *i*-th component.

The change in the internal energy per unit volume is determined by convective heat transfer and thermal conductivity, as well as the release or absorption of heat in the layer during sorption or desorption, is described by the term in the equation (4):

$$-\sum_{i=1}^{N}\Delta H_i\frac{\partial a_i}{\partial t} .$$

To close the system of equations, it must be supplemented with equations fora_i^*, i.e. the previously considered sorption isotherms, as well as the equation of state:

$$a_i^* = \varphi(T,\rho_i) \quad i = 1 \div (N-1), \quad (5)$$

$$p = \rho RT. \quad (6)$$

The specific form of the function in the case of absorption of water vapor is determined from the experiment.

Thus, the following system of equations is obtained:

$$-\frac{\partial(U\rho_i)}{\partial x} + \frac{\partial}{\partial x}D_i(T,\rho_i)\frac{\partial\rho_i}{\partial x} = \frac{\partial a_i}{\partial t} + \varepsilon\frac{\partial\rho_i}{\partial t}$$

$$\varepsilon\frac{\partial\rho}{\partial t} + \frac{\partial(U\rho)}{\partial x} = -\sum_{i=1}^{N}\frac{\partial a_i}{\partial t}$$

$$\frac{\partial}{\partial t}\left(\left[\rho_s C_s + \sum_{i=1}^{N} a_i C_i\right]T\right) + \frac{\partial(\rho U C_p T)}{\partial x} = \frac{\partial}{\partial x}\lambda_s\frac{\partial T}{\partial x} - \sum_{i=1}^{N}\Delta H_i\frac{\partial a_i}{\partial t}$$

$$\frac{\partial a_i}{\partial t} = \beta_i(a_i^* - a_i) \quad i = 1 \div (N-1)$$

$$a^* = \varphi(T,\rho_i) \quad i = 1 \div (N-1)$$

$$p = \rho RT$$

Unknown quantities of the system of equations:

$\rho_i\ (i=1\div(N-1))$; T

$a_i\ (i=1\div(N-1))$; ρ

$a_i^*\ (i=1\div(N-1))$; U. Number of unknowns – 3*N*.

Number of equations:

(3.1) - $(N-1)$; (3.2) - 1; (3.3) - 1; (3.4) - (*N* – 1); (3.5) - (N-1); (3.6) - 1.

In total, the number of equations is 3*N*. The system is closed.

This system of differential equations must also be supplemented with initial and boundary conditions. The initial conditions specify the distributions of the functions*ρ, a*and*T*along the sorbent layer at the initial moment of time. The boundary conditions determine the required functions on the boundaries of the system.

3 Determination of essential physical factors and boundary conditions

Determination of essential physical factors for the equation of continuity of the i-th component. Let us compare the rates of diffusion and convection processes in the layer. Estimation of the characteristic times of diffusion and convection:

$\tau_{кон.} \sim \frac{l}{U}$ l –sorbent layer thickness.

$\tau_{кон}$ – the time during which the concentration front shifts by the layer length as a result of convective transfer. For diffusion, the characteristic time will be:

$\tau_{диф.} \sim \frac{l}{U_{диф.}}$.

$U_{диф.}$ – characteristic diffusion rate, defined as:

$U_{диф.} = U_i - U \sim \left|\frac{j_i}{\rho_i}\right|$;

ρ_i - layer-average density of the *i*-th component $|j_i| \approx D_i \frac{\Delta\rho_i}{l}$; $\Delta\rho_i$ - difference in concentration at the inlet and outlet from the layer; D_i - layer average longitudinal diffusion coefficient. Thus

$$\tau_{диф.} \sim \frac{l}{\left|\frac{j}{\rho_i}\right|} = \frac{l^2}{D\frac{\Delta\rho_i}{\rho_i}}, \quad (7)$$

Provided that

$$D_i \frac{\Delta\rho_i}{\rho_i} << lU \quad (7^1)$$

it turns out that $\tau_{кон.} / \tau_{диф.} << 1$, i.e. at low gradients of component densities and high average (convection) velocities, the convection process will be decisive.

Using the values of the parameters of the atmosphere regeneration plant on board the orbital station, the following numerical estimates are carried out. Total air consumption at the sorption stage is approximately 25 m^3/h, cross-sectional area of the bed F = 0,06158 m^2, l = 0,1 m, diffusion coefficient of water vapor in air (at atmospheric pressure and temperature 20 °C) $2\cdot10^{-5} m^2/c$. Then the characteristic times are: $\tau_{кон.} \approx 0{,}9c$, $\tau_{диф.} \sim 500c$. Thus, diffusion occurs three orders of magnitude slower than convection. Consequently, diffusion can be disregarded in the process of mass transfer and in equations (1) the term responsible for the diffusion flux can be discarded.

Other simpler equations are obtained: $\varepsilon\frac{\partial\rho_i}{\partial t} + \frac{\partial(U\rho_i)}{\partial x} = -\frac{\partial a_i}{\partial t}$.

2) A similar estimate is carried out for the energy conservation equation.

Members are compared $\frac{\partial(\rho U C_p T)}{\partial x}$ and $\frac{\partial}{\partial x}\lambda_s \frac{\partial T}{\partial x}$. The characteristic time of convective energy transfer, as well as for mass transfer, is $l/U = 0{,}9c$. The characteristic time of thermal conductivity will be $\tau_{T.П.} \sim \frac{l}{U_{T.П.}}$; где $U_{T.П.} \sim \left|\frac{S}{[\rho_s C_s + \sum a_i C_i]T}\right|$ $|S| \sim \lambda_s \frac{\Delta T}{l}$, where S – energy flux density.

We denote $g = \rho_s C_s + \sum_i^N a_i C_i$ – total heat capacity per unit volume of a layer. Then $U_{T.П.} \sim \left|\frac{S}{gT}\right| \sim \lambda_s \frac{\Delta T}{l} \cdot \frac{1}{gT} \sim \frac{\lambda_s}{\lg}$. After substitution of the corresponding values $\rho_s = 889$ kg/m^3; $C_s = 840$ J/kg·K. The specific heat of absorbed moisture can be neglected $a_{H_2O} C_{H_2O} \langle\langle \rho_s C_s$ at $a_{H_2O} \sim 5$ kg/m^3; $C_{H_2O} = 4200$ J/kg·K; $C_s \rho_s \sim 6 \cdot 10^5$ J/m^3·K; $a_{H_2O} C_{H_2O} \sim 2 \cdot 10^4$ J/m^3·K) we get $\tau_{T.П.} \sim 6 \cdot 10^4$ c. Thus, the transfer of heat within the layer by means of thermal conduction occurs 5 orders of magnitude slower than with convective heat transfer. Therefore, the thermal conductivity in the energy equation can be neglected.

After discarding the terms describing insignificant physical factors, we finally obtain the system of equations.

$$\varepsilon \frac{\partial \rho_i}{\partial t} + \frac{\partial(U\rho_i)}{\partial x} = -\frac{\partial a_i}{\partial t} \quad (8)$$

$$\varepsilon \frac{\partial \rho}{\partial t} + \frac{\partial(U\rho)}{\partial x} = -\sum_{j=1}^{N} \frac{\partial a_j}{\partial t} \quad (9)$$

$$\frac{\partial}{\partial t}\left(\left[\rho_s C_s + \sum_{i=1}^{N} a_i C_i\right]T\right) + \frac{\partial(\rho U C_p T)}{\partial x} = -\sum_{i=1}^{N} \Delta H_i \frac{\partial a_i}{\partial t} \quad (10)$$

$$p = \rho R T \quad (11)$$

$$\frac{\partial a_i}{\partial t} = \beta_i (a_i^* - a_i) \quad (12)$$

$$a_i^* = \varphi(T, \rho_i) \quad (13)$$

Let us write out the boundary conditions:

1) The continuity equations for the *i*-th component and the energy conservation equation before neglecting insignificant physical factors were equations of the second order, after dropping the terms describing diffusion and thermal conductivity, they became equations of the first order. The original equations (1), (2) are parabolic equations, which requires the setting of boundary conditions on both boundaries (at the input and output). Equations (8) and (10) of the 1st order, for which the boundary conditions are specified only on one boundary - the upper in the stream.

2) Boundary and initial conditions.

Border conditions.

When $x = x_1$ $\rho_i(x_1; t) = \rho_i^{(1)}(t)$ $\forall i = 1 \div (N-1)$ (14)

$$T(x_1; t) = T_1(t) \quad (15)$$

$$U(x_1; t) = \frac{G}{F} \quad (16)$$

Initial conditions:

When $t = 0$ $\rho_i(x, 0) = \rho_i^{(0)}(x)$ (17)

$$a_i(x, 0) = a_i^{(0)}(x) \quad (18)$$

$$T(x, 0) = T^{(0)}(x) \quad (19)$$

The equations obtained make it possible to simulate adsorption processes and carry out numerical experiments.

4 Conclusions

Onthebasisof the obtained expressions, it is possible both to take into account the peculiarities of the flow of heat and mass transfer processes at each of the steps of the adsorption-desorption cycle, and their interaction during the transition from the previous step to the next. Numerical experiments on predicting the behavior of an adsorption system with different organization of cycle steps make it possible not only to reasonably determine the technological parameters of the process, but in many cases also to reduce the amount of experimental research.

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