NUMERICAL MODELING OF HEAT AND MASS TRANSPORT PROCESSES IN AN EVAPORATIVE THERMAL PROTECTION SYSTEM

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We propose a mathematical model of heat and mass transport processes in a moist, porous material subject to capillary action. The material is in contact with a heated surface, and the processes take place while the liquid is evaporating in a cavity with a drainage hole. A sample calculation based on the model is presented.

Among the methods used by contemporary technology for heat protection of devices are those based on the absorption of heat flux incident on the structure by evaporation [1] or melting [2] of a coolant contained in the structure. Capillary-active, porous materials (CPM) are usually used as the coolant carrier. Modeling of heat and mass transport processes in such evaporative thermal protection systems can be based on the methods of the theory of drying [3-5]. The problems encountered in this case are, in general, nonlinear, and can only be solved by numerical methods [6, 7].

Heat and mass transport processes in CPM are described by the laws of conservation of mass, momentum, and energy [8]. Usually, however, to simplify the problem, instead of solving the momentum equations, which determine the transport velocities of each of the coupled materials, a connection is established between material fluxes and the gradients of the unknown functions [3, 7]. The transport coefficients entering into these expressions are determined experimentally, and in the calculations, they may be considered as known functions of the quantities to be determined [9]. This approach is also used in our work.

1. Statement of the Problem. We consider the following evaporative thermal protection scheme. A heat flux $q_e(t)$ is incident on one of the sides (outer) of a plane, thermally thin wall. The heat flux is in general a function of time t. The wall has area S, thickness h_w, and its material has density ρ_w and specific heat capacity c_w. A layer of moisture-saturated, capillary-porous material of thickness ℓ is in direct contact with the inner side of the wall, which is the opposite side that is exposed to the thermal action. The material is assumed to be homogeneous, to have porosity Π, density ρ_0, specific heat capacity c_0, and heat conduction coefficient λ_0 in the dry state. Liquid evaporates from the free CPM surface into a cavity having volume V and depth L = V/S. There is a hole of area s in the cavity, through which the vapor—air mixture flows out into the exterior medium with pressure $p_e(t)$. The cavity is thermally insulated. We neglect the heat capacity of the cavity walls.

In the case of uniform heat flux and when the condition $\ell \ll \sqrt{S}$ is satisfied, the problem can be treated in a one-dimensional formulation. We introduce a coordinate axis x perpendicular to the heated wall, with the origin in the plane of contact between the wall and the CPM layer.

It is assumed that liquid, vapor, and air can be found in the material pores at the initial instant of time. We introduce the volume concentration of the i-th coupled material in the pores (the degree of saturation of the pores by the i-th material) α_i [10]. For the gaseous phases $\alpha_v = \alpha_a = \alpha_g$, and there holds the obvious relation

$$\alpha_l + \alpha_g = 1. \tag{1}$$

Denoting by ω_i the derived density of the i-th material, we write the equation of mass conservation in the form

$$\frac{\partial \omega_i}{\partial t} + \nabla j_i = I_i, \tag{2}$$

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where $\omega_i = \Pi\rho_i\alpha_i$, and ρ_i, j_i, I_i are the loading density, the flux, and the source term for the i-th material, respectively, and $\nabla = \partial/\partial x$. Obviously $I_a = 0$, $I_v = -I_\ell$.

For a poly-capillary CPM structure, the liquid flux can be caused by gradients in the fluid concentration α_ℓ in the pores, temperature T gradients, and pressure p gradients of the vapor—air mixture [3]. The fluxes of vapor and air are caused by gradients in the pressure and mass concentration of the vapor in the mixture. Assuming that the percolation flow of the liquid and the gaseous phases are described by Darcy's law, we can write the flux of all three materials in the CPM in the form:

$$j_l = -a_l(\Pi\rho_l\nabla\alpha_l + \rho_0\delta\nabla T) - K\frac{\rho_l}{\mu_l}K_l\nabla p, \tag{3}$$

$$j_v = -K\frac{\rho_v}{\mu_g}K_g\nabla p - \Pi\alpha_g D_{\mathrm{eff}}\rho_g\nabla\left(\frac{\rho_v}{\rho_g}\right), \tag{4}$$

$$j_a = -K\frac{\rho_a}{\mu_g}K_g\nabla p + \Pi\alpha_g D_{\mathrm{eff}}\rho_g\nabla\left(\frac{\rho_v}{\rho_g}\right). \tag{5}$$

In (3)-(5), a_l and δ are the coefficient of fluid diffusion and the thermal gradient coefficient [9], K is the permeability coefficient of the material, μ the coefficient of dynamic viscosity, D_{eff} is the effective vapor diffusion coefficient in the CPM [7], $\rho_g = \rho_v + \rho_a$; K_ℓ and K_g are the relative permeabilities of the liquid and gaseous phases, which are characteristics of the specific material and which depend on α_ℓ in a manner that is quite complex [7, 9]. The simplest approximation which qualitatively reflects the dependence of the phase permeabilities on α_ℓ is that they are equal to the volume concentrations of the phases [10]. This is what we shall adopt in our work.

Henceforth, on the basis of (1), we will not consider pore saturation by the gaseous phases α_g, and we introduce the notation $\alpha \equiv \alpha_\ell$.

Summing (2) over $i = \ell$, v, we obtain the equation for conservation of moisture

$$\Pi\frac{\partial}{\partial t}[(\rho_l - \rho_v)\alpha + \rho_v] + \nabla j_m = 0, \quad j_m = j_l + j_v. \tag{6}$$

Equation (2) with $i = a$ serves to determine the density of the air:

$$\Pi\frac{\partial}{\partial t}[(1-\alpha)\rho_a] + \nabla j_a = 0. \tag{7}$$

The conservation of energy equation is represented as:

$$\frac{\partial}{\partial t}[c_{\mathrm{eff}}\rho_0 T + r_0\Pi(1-\alpha)\rho_v] = \nabla\left(\lambda\nabla T - r_0 j_v - \sum_i c_{pi}Tj_i\right), \tag{8}$$

where $c_{\mathrm{eff}} = c_0 + \Pi[c_{p\ell}\rho_\ell\alpha + (1-\alpha)(c_{pv}\rho_v + c_{pa}\rho_a)]/\rho_0$, c_{pi} ($i = \ell$, v, a) are the specific heat capacities at constant pressure; r_0 is the specific heat of evaporation at T = 0 K, which is determined on the basis of known values of the heats of evaporation r(T), according to $r_0 = r(T) + (c_{p\ell} - c_{pv})T$.

We assume that the vapor—air mixture is a mixture of ideal gases, and that its pressure is determined by

$$p = (\rho_v/M_v + \rho_a/M_a)RT, \tag{9}$$

where R is the universal gas constant, and M_i ($i = v$, a) are the molecular weights.

To close the system (6)-(9), we use the assumption that, in the region of a "moist" state of the CPM, that is, for $\alpha > 0$, the vapor is in a state of saturation. Consequently, its density is a function of temperature only:

$$\rho_v = \rho_{vs}(T) \quad \text{for} \quad \alpha > 0. \tag{10}$$

Condition (10) also denotes what is considered a typical capillary-porous material, for which it is possible to neglect the hygroscopic-state stage [11]. To determine the function $\rho_{vs}(T)$, we use the Filonenko formula [4], if water is used as the coolant.

The generally adopted equations of heat and mass transport in CPM are in the form of the system of equations of Lykov [3], or the equations of [7]. We note that, unlike these forms, representation (6)-(10) has the advantage that the vapor source term I_V can be eliminated from the number of unknowns (α, T, ρ_a). The source term I_V can be determined, after solution of the system, from (2) with i = v, taking (4) and (10) into account. This somewhat simplifies the numerical algorithm for solving the problem and reduces the computational time. In addition, the so-called criterion of phase transition enters into the Lykov equations. The dependence of this criterion on various parameters is very complicated [11], and in calculations it is prescribed quite arbitrarily [6].

Besides the particular ease of carrying out the algorithm of numerical solution, there is also the fact that (6), with the appropriate boundary conditions, remains valid even in the "dry" zone of the CPM, that is, during formation of a region without liquid. In such a material zone, α = 0 and I_V = 0, and (10) is no longer valid, while (6) becomes an equation for conservation of vapor mass and serves to determine the vapor density ρ_V. Thus, α is the unknown in (6) in the "moist" region, while ρ_V is the unknown in the "dry" region.

The boundary conditions for (6)-(10) are formulated in the following fashion. At initial time t = 0, the vapor–air mixture pressure in the CPM and in the cavity are equal to the external pressure $p_e(0) = p_0$. In this case, the vapor pressure is equal to the saturation pressure for the initial temperature of the entire system T_0. Thus, for $0 \leq x \leq \ell$:

$$T(x,\ 0)=T_0,\ \alpha(x,\ 0)=\alpha_0\leqslant 1,\ \rho_a(x,\ 0)=\frac{p_0-p_{vs}(T_0)}{RT_0}M_a. \tag{11}$$

The boundary conditions established on the inner surface of the heated, impermeable wall (x = 0) are obvious:

$$q_e=-\lambda\nabla T+\rho_u c_u h_u\frac{\partial T}{\partial t}+rj_v,\ j_m=0,\ j_a=0, \tag{12}$$

where $r = r_0 = (c_{p\ell} - c_{pv})T$.

The boundary conditions on the free surface of the CPM, which leads into the cavity ($x = \ell$), are:

$$\begin{gathered}
-\lambda\nabla T=rj_l+\frac{V}{S}(\rho_a c_{va}+\rho_v c_{vv})\frac{\partial T}{\partial t}+\\
+\frac{V}{S}\left(R_a\frac{\partial\rho_a}{\partial t}+R_v\frac{\partial\rho_v}{\partial t}\right)T,\\
Sj_m=Q_e\frac{\rho_v}{\rho_g}+V\frac{\partial\rho_v}{\partial t},\ Sj_a=Q_e\frac{\rho_a}{\rho_g}+V\frac{\partial\rho_a}{\partial t},\ \rho_v=\rho_{vs}(T_c),\\
Q_e=s\left[\gamma\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}}\right]^{1/2}Q(\varepsilon_p)\,p_c(R_gT_c)^{-1/2},\ \varepsilon_p=\frac{p_e}{p_c},\\
Q(\varepsilon_p)=\begin{cases}\left(\frac{\gamma+1}{2}\right)^{\frac{1}{\gamma-1}}\varepsilon_p^{\frac{1}{\gamma}}\left[\frac{\gamma+1}{\gamma-1}(1-\varepsilon_p)^{\frac{\gamma-1}{\gamma}}\right]^{1/2},\ \varepsilon_p>\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}},\\ 1,\ \varepsilon_p\leqslant\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}},\end{cases}
\end{gathered} \tag{13}$$

where T_c and p_c are the temperature and pressure in the cavity; Q_e is the gas discharge through the drainage hole, determined by the formulas of outflux from the cavity [12].

Boundary conditions (13) were obtained assuming that the gradients of temperature, pressure, and vapor concentration across the cavity are insignificant, and that the vapor pressure in the cavity is close to the saturation pressure at the cavity temperature. Below we give the conditions under which these assumptions are valid.

Clearly, the pressure gradient in the cavity will be small for the primarily subsonic velocities of outflow from the CPM, that is, for low evaporation rates. From this comes a bound on the external thermal flux:

$$\frac{q_e}{r\rho_v}\sqrt{\frac{\rho_g}{p_c}} \ll 1.$$

For low evaporation rates, after complete displacement of the air from the material and cavity, the Hertz–Knudsen formula can be used to estimate the evaporation rate:

$$j_m \sim \frac{p_{vs} - p_v}{(2\pi R_v T_c)^{1/2}}.$$

Since in this case $Sj_m \sim Q_e$, where $Q_e \lesssim s p_v/(R_v T_c)^{1/2}$ we obtain the condition of the proximity of the vapor state in the cavity to a saturated state:

$$\frac{p_{vs}}{p_v} - 1 \sim \frac{s}{S} \ll 1.$$

The condition that the temperature gradient be small can be obtained from the energy equation for the mixture of gases, neglecting convective transport. Clearly, in this case, we have an upper estimate:

$$\frac{\Delta T}{T_c} \lesssim \frac{c_{Vg}\rho_g L^2}{\lambda_g T_c}\frac{\partial T_c}{\partial t} \ll 1.$$

In the presence of air, the vapor concentration gradient along the cavity is estimated from the diffusion equation. Since close to the surface of the moist material, $\partial\rho_v/\partial t \sim d\rho_{vs}/dT \cdot \partial T/\partial t$, then by comparing the unsteady and diffusion terms, we obtain the condition:

$$\frac{\Delta\rho_v}{\rho_g} \sim \frac{L^2}{\rho_g D}\frac{d\rho_{vs}}{dT}\frac{\partial T_c}{\partial t} \ll 1.$$

It is evident that the presence of convective transport only weakens this condition.

Thus, the conditions have been formulated for which boundary conditions (13) can be applied to the free surface of the CPM.

2. Solution Method. A purely implicit, two-level, four-point conservative difference scheme is used to numerically solve the formulated boundary-value problem (6)-(13). The scheme uses constant step size in x, and is constructed on the basis of the integral-interpolation method [13]. The scheme is second-order accurate in space and first-order in time. The resultant system of nonlinear algebraic equations is solved using Newton's method.

When a "dry" zone occurs close to the heated surface x = 0, the method of trapping its boundary at the nodes of the difference mesh [14] is used. The required time step is found from the condition that the function α vanish at the boundary of the zone. To determine the time step, Newton's method with correction multipliers is applied. At the boundary of the "dry" zone, the following conditions must be satisfied:

$$\begin{gathered} T_- = T_+,\ q_- - q_+ = -rj_{l+},\ j_{l-} = 0,\ j_{v-} - j_{v+} = j_{l+}, \\ \rho_{v-} = \rho_{v+} = \rho_{vs}(T_-),\ j_{a-} = j_{a+},\ \rho_{a-} = \rho_{a+}. \end{gathered} \tag{14}$$

Here the subscripts + and − denote the limits of the corresponding function tending toward the boundary from the "moist" (α > 0) or the "dry" (α = 0) side of the zone, respectively. In (14), q is the heat flux. On the basis of the integral-interpolation method, it is easy to show that when the boundary is located at difference mesh nodes, the fine-differencing of the divergence terms in (6)-(8) does not change, and (14) is automatically satisfied. To approximate the unsteady terms in (6)-(8) at mesh nodes corresponding to boundary zones, the following formula is used to preserve second-order accuracy in x:

$$\int_{x_n-\Delta x/2}^{x_n+\Delta x/2} u(x, t)\,dx \cong \frac{\Delta x}{8}(u_{n-1} + 6u_n + u_{n+1}),$$

where n is a boundary node number and Δx is the mesh step size. This approximation is necessary because of discontinuities in the derivatives of the unknown functions at these boundary node points.

3. Sample Numerical Solution. To illustrate the use of this model, we carried out calculations for one set of parameters governing the problem. Water was used as the coolant. The calculations were done for constant heat flux $q_e = 10^4$ W/m² and constant external pressure $p_e = 10^4$ Pa. The initial temperature of the system is $T_0 = 290$ K. The heated wall

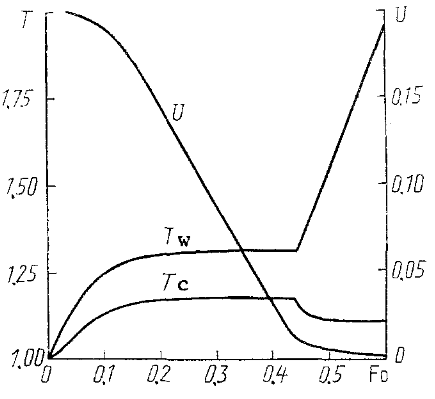

Fig. 1

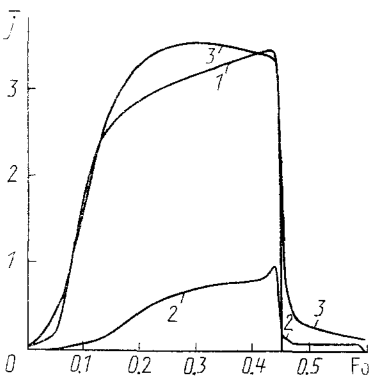

Fig. 2

Fig. 1. Dimensionless temperature of the heated wall T_w, cavity temperature T_c, and the integrated moisture saturation of the material U as functions of the Fourier number Fo.

Fig. 2. The dimensionless vapor flux at the impermeable surface (1), the dimensionless vapor flux from the free surface (2), and the total dimensionless moisture flux from the free surface of the material (3) as functions of the Fourier number Fo.

parameters are $h_w = 0.002$ m, $\rho_w = 2.7 \cdot 10^3$ kg/m³, $c_w = 0.9 \cdot 10^3$ J/(kg·K). The cavity parameters are $L = 0.03$ m and $s/S = 10^{-4}$.

The dependence of the transport coefficients on the unknown functions is prescribed using considerations of qualitative plausibility. The coefficients of thermal conductivity of the CPM and the liquid diffusion are defined in the form of continuously differentiable functions of α, which grow monotonically from 0 to some value with increasing α, and then remain constant with subsequent growth in α [9]:

$$\lambda(\alpha) = \begin{cases} \lambda_0 + (\lambda_l - \lambda_0)\sin(\pi\alpha/2\alpha_\lambda), & \alpha \leqslant \alpha_\lambda, \\ \lambda_l, & \alpha > \alpha_\lambda, \end{cases}$$

$$a_l(T, \alpha) = \begin{cases} [a_{l0} + (a_{ll} - a_{l0})\sin(\pi\alpha/2\alpha_a)](T/273)^{20}, & \alpha \leqslant \alpha_a, \\ a_{ll}(T/273)^{20}, & \alpha > \alpha_a. \end{cases}$$

According to [15], the dependence of the thermal gradient coefficient on moisture saturation, for the majority of CPMs, can be represented in the form of a parabola:

$$\delta(\alpha) = \delta_0[1 - 4(\alpha - 1/2)^2].$$

The numerical values of the CPM parameters are: $\ell = 0.005$ m, $\rho_0 = 150$ kg/m³, $c_0 = 10^3 \times$ J/(kg·K), $\lambda_0 = 0.06$ W/(m·K), $\lambda_\ell = 0.6$ W/(m·K), $\alpha_\ell = 0.1$, $a_{\ell 0} = 5 \cdot 10^{-9}$ m²/sec, $a_{\ell\ell} = 1.5 a_{\ell 0}$, $\alpha_a = 0.1$, $\delta_0 = 10^{-3}$ K⁻¹, $K = 10^{-14}$ m², $\Pi = 0.9$, and $\alpha_0 = 0.2$. The viscosity coefficients of water and gas, and the effective vapor diffusion coefficient as well are assumed to be constants: $\mu_\ell = 5 \cdot 10^{-4}$ kg/(m·sec), $\mu_g = 10^{-5}$ kg/(m·sec), $D_{eff} = 5 \cdot 10^{-5}$ m²/sec.

Figure 1 shows the dependence on $Fo = \lambda_0 t/(c_0 \rho_0 \ell^2)$ of the temperature of the heated surface $T_w = T(0, t)/T_0$, the cavity temperature $T_c = T(\ell, t)/T_0$, and the integrated moisture saturation of the material

$$U = \frac{1}{l}\int_0^l \alpha(x, t)\,dx.$$

From these curves it is obvious that after a period of heating, there follows a period of approximately constant temperatures. From the moment of formation of the "dry" zone at Fo = 0.438, the temperature of the heated wall grows almost linearly. At the same time, the cavity temperature drops sharply and then remains constant until the liquid has completely evaporated at Fo ≅ 0.65. Since the air leaves the system at Fo ≅ 0.1, then by the time

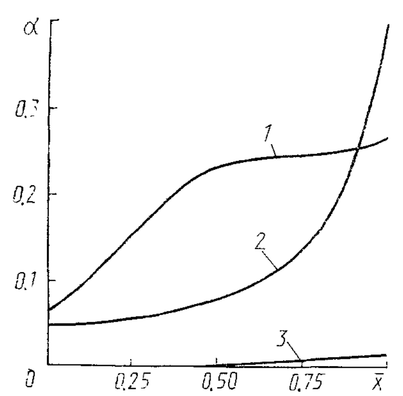

Fig. 3

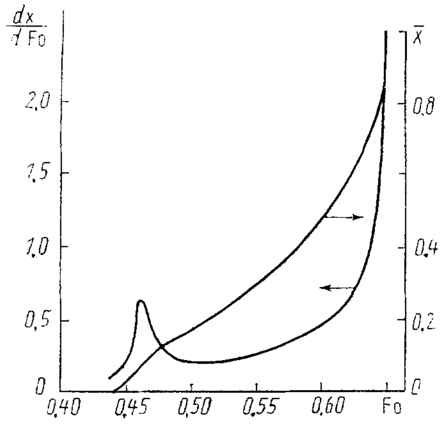

Fig. 4

Fig. 3. Distribution of moisture saturation with material thickness for three times: 1) Fo = 0.04; 2) Fo = 0.26; 3) Fo = 0.48.

Fig. 4. The dimensionless position and rate of motion of the "dry" zone boundary as functions of the Fourier number.

the "dry" zone appears, the cavity pressure is equal to the saturated vapor pressure, and it also decreases sharply and subsequently remains constant at a little above the external pressure.

The pattern of mass transport in the CPM is as follows. During heating of the system, a negative temperature gradient arises near the impermeable surface, which is accompanied by the appearance of a negative pressure gradient. In turn the latter, as a consequence of the final condition in (12), induces a negative vapor concentration gradient. A vapor flux arises at the impermeable surface, due to the action of the pressure and concentration gradients. This flux is directed into the material. As a result of the second condition in (12), the flux is compensated for by a liquid flux toward the heated surface. The time dependence of the vapor flux at the surface x = 0 is shown in Fig. 2 (curve 1). Vapor penetrating inside the CPM partly condenses (the vapor source term is negative for all material thicknesses), and partly reaches the CPM free surface. This vapor flux from the free surface is also shown in Fig. 2 (curve 2). The liquid flux changes sign at some distance from the impermeable surface. The liquid, flowing under the action of the pressure and temperature gradients to the CPM free surface, evaporates at this surface. The total flux of the evaporated moisture in the cavity is shown in Fig. 2, curve 3. Naturally, the moisture flux at x = 0 disappears with the formation of the "dry" zone. Then there is a sharp reduction in the vapor flux moving from the "dry" zone boundary to the CPM free surface, and in the total evaporation rate. Note that in Fig. 2, the dimensionless fluxes $\bar{j} = j\ell/(a_{\ell 0}\rho_0)$ are represented.

Figure 3 shows the distribution of moisture saturation α with material thickness $\bar{x} = x/\ell$ at three times, corresponding to the periods of heating, constant temperature, and the presence of the "dry" zone. Despite the increase in the liquid flux toward the impermeable surface with time (up to the formation of the "dry" zone), the gradient in α decreases in it. This is connected with the strong growth in the liquid diffusion coefficient with increasing temperature.

The profiles of temperature and pressure as a function of material thickness have the following features. In the heating period, both T(x, t) and p(x, t) have a positive second derivative in x, but in the constant temperature period, this derivative is negative. The pressure is almost constant in the "dry" zone, while the temperature decreases approximately linearly from x = 0 to the boundary zone. In the "moist" region, the second derivative in x changes sign for both functions from negative to positive with increasing x.

Figure 4 shows the time dependence of the position and the rate of motion of the "dry" zone boundary.

Conclusion. On the basis of this mathematical model, it is possible to study the effect of the properties of the coolant carrier, the heating regimes, and other parameters on the characteristics of the thermal protection system considered here.

NOTATION

q, the heat flux; t, time; S, wall area; ρ, density; c, specific heat capacity; λ, coefficient of thermal conductivity; h_w, wall thickness; ℓ, thickness of the capillary-active porous material; T, temperature; p, pressure; α, volume concentration of the coupled materials in the pores; V and L, volume and depth of the cavity; s, area of the drainage hole; j, material flux; I, material source term; Π, porosity; K, permeability; μ, coefficient of viscosity; D_{eff}, effective coefficient of vapor diffusion in the pores; a_l, liquid diffusion coefficient; δ, thermal gradient coefficient; R, gas constant; M, molecular weight; r, specific heat of evaporation; Q_e, gas outflux through the drainage hole; ε_p, pressure gradient; γ, adiabatic index; Fo, Fourier number. Indices: w, wall; ℓ, liquid; v, vapor; m, moisture; a, air; g, vapor—air mixture; s, saturation state; c, cavity; p, constant pressure quantity; 0, a characteristic value or the material in the dry state; v, a constant volume quantity.

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