ANALYSIS OF THE EFFECT OF THE DECOMPOSITION OF CHAR-FORMING HEAT-INSULATING MATERIALS ON THE FREE DISCHARGE OF A GAS MIXTURE

I. G. Borovskoi, A. B. Vorozhtsov, and E. A. Kozlov

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The article presents results of a numerical solution of a nonsteady problem on the free discharge of a mixture of gases from a hemispherical volume with allowance for thermal decomposition of heat-insulating materials.

The structural elements of certain heating and power plants have been provided with protective coatings which undergo thermal decomposition when they reach a certain temperature. The decomposition is accompanied by the formation of gaseous products which enter the through part of the equipment. The time required to empty the plant is one of the most important characteristics in the solution of practical problems, so it is interesting to determine the degree to which the decomposition of the insulating material affects the dynamics of free discharge.

We will examine a semiclosed volume V with its inside surface covered by a thermal insulating material (TIM). The working substance is comprised of a hot gas and volatile products of the decomposition of the TIM. The gas and products are located in the volume V at a constant pressure P_0 and T_0. They are discharged through an outlet orifice of area S_* into an environment with the pressure P_{en}, $P_{en} < P_0$. At the moment of time t_0, the supply of the high-enthalpy gas to the plant is shut off, and the period of nonsteady discharge of the two-component gas mixture begins.

The mathematical description of the problem is based on the following assumptions.

1. All of the chemical reactions accompanying the decomposition of the TIM are completed in an infinitely small region adjacent to the surface S, while the final products of the degradation of the thermal insulating material and the working gas are subject to the equation of state $P = \rho RT$. Here, it is assumed that both components of the mixture have equal gas constants R and adiabatic exponents γ.

Preliminary estimates based on the results of numerical calculations showed that during the period over which the pressure decreases from P_0 to the external pressure P_{en}, the kinetic energy of the gas flow is negligibly small compared to its internal energy. The second assumption follows from this statement.

2. In the time interval in question, convective heat transfer in the volume V can be ignored, and we can allow for heat losses by restricting ourselves to radiative heat transfer.

Following [1] and taking the above assumptions into consideration, we use the following equations to determine the change in the density of the gas mixture ρ and the pressure P in the volume V with mass transfer from the surface S and heat losses

$$V\frac{d\rho}{dt} = \rho_M uS - Ae\frac{PS_*}{\sqrt{RT}},$$

$$\frac{V}{\gamma-1}\frac{dP}{dt} = \frac{\gamma}{\gamma-1}RT_s\rho_M uS - QS - \frac{\gamma}{\gamma-1}RTAe\frac{PS_*}{\sqrt{RT}},$$

$$Q = \varepsilon\sigma(T^4 - T_s^4),\quad A = \sqrt{\gamma}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma-1}{2(\gamma+1)}}.$$

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Here, the initial conditions are $\rho - P_0/(RT_0)$, $P = P_0$. The coefficient e accounts for the effect of the counterpressure P_{en} on the discharge of the gas and, in accordance with [2], is calculated from the relation

$$e = \begin{cases} 1, \quad \text{if} \quad \dfrac{P_{en}}{P} \leqslant \left(\dfrac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}}, \\ \dfrac{1}{A}\left(\dfrac{P_{in}}{P}\right)^{1/\gamma} \sqrt{\dfrac{2\gamma}{\gamma-1}\left[1-\left(\dfrac{P_{en}}{P}\right)^{\frac{\gamma-1}{\gamma}}\right]}, \\ \qquad\qquad \text{if} \quad 1 \geqslant \dfrac{P_{en}}{P} > \left(\dfrac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}}. \end{cases}$$

Introducing the dimensionless variables $\tau = t/t_0$, $p = P/P_0$, $\theta = T/T_0$, $\theta_S = T_ST_0$, $v = u/u_0$, $q = Q/Q_0$ — where we take the corresponding values at the moment of time t = 0 as the scale values of pressure P_0, temperature T_0, decomposition rate u_0, and radiative heat transfer Q_0 and we take the relaxation time of the semiclosed volume $t_0 = V/(A\sqrt{RT_0}S_*)$ as the time scale t_0 — and using the equation of state to exclude the density of the gas mixture, we obtain a system of equations in dimensionless form to determine the change in pressure and temperature:

$$\frac{dp}{d\tau} = \gamma(\alpha v\theta_s - \alpha\beta q - p\sqrt{\theta}e), \tag{1}$$

$$\frac{d\theta}{d\tau} = \frac{\theta}{p}[(\gamma\theta_s - \theta)\alpha v - \gamma\alpha\beta q - (\gamma-1)p\sqrt{\theta}e], \tag{2}$$

$$q = \frac{\theta^4 - \theta_s^4}{1 - \theta_s^4}$$

with the initial conditions p = 1, θ = 1.

The parameter $\alpha = \rho_M u_0 S/G_0$ characterizes the ratio of the mass yield of TIM decomposition products to the steady-state discharge of the gas mixture $G_0 = AP_0S_*/\sqrt{RT_0}$. Physically, this parameter reflects the percentage of TIM decomposition products in the total discharge G_0. It has a natural range $0 \leq \alpha \leq 1$.

The parameter $\beta = Q_0(\rho_M u_0)/H_0$ represents the specific energy $Q_0/\rho_M u_0$, due to heat losses, referred to the enthalpy of the gas $H_0 = \dfrac{\gamma}{\gamma-1}RT_0$. The complex β changes within the range $0 \leq \beta \leq 1$ and is a quantitative characteristic of that part of the energy of the gas mixture which is transferred to the surface S by thermal radiation.

A two-front model [3] is used to mathematically describe the degradation of a thermal insulating coating. In accordance with this model, the ablation front (external entrainment) and the pyrolysis front (internal decomposition) possess characteristic values of temperature T_A, T_P ($T_A > T_P$) and specific enthalpies. In the coordinate system connected with the pyrolysis front, the equations modeling heat transfer in a char-forming TIM have the following form:

for the coke layer of the thickness δ(t)

$$(\rho c)_\Pi \frac{\partial T_\Pi}{\partial t} = \lambda_\Pi \frac{\partial^2 T_\Pi}{\partial x^2} + [(\rho_M - \rho_\Pi)c_v + (\rho c)_\Pi]u_P \frac{\partial T_\Pi}{\partial x}, \quad -\delta < x < 0, \tag{3}$$

for the undecomposed material

$$(\rho c)_M \frac{\partial T_M}{\partial t} = \lambda_M \frac{\partial^2 T_M}{\partial x^2} + (\rho c)_M u_P \frac{\partial T_M}{\partial x}, \quad x > 0, \tag{4}$$

with the initial condition $T(x, 0) = T_H(x)$ and the boundary conditions:

on the ablation front $x = -\delta$

$$\eta Q = -\lambda_{\Pi} \frac{\partial T_{\Pi}}{\partial x} + \rho_{\Pi} u_A H_A, \tag{5}$$

on the pyrolysis front, $x = 0$,

$$-\lambda_{\Pi} \frac{\partial T_{\Pi}}{\partial x} = -\lambda_M \frac{\partial T_M}{\partial x} + \rho_M u_P H_P, \quad T_{\Pi}(0, t) = T_M(0, t), \tag{6}$$

away from the ablation surface, $x \to \infty$

$$T_M(x, t) = T_{\infty}. \tag{7}$$

The term $(\rho_M - \rho_{\Pi}) c_v u_P (\partial T_{\Pi}/\partial x)$ in Eq. (3) describes heat transfer between diffusing pyrolytic gases and the porous skeleton of the coke residue [4], while the parameter $\eta(u_A, u_P, T, T_s, \ldots) \le 1$ in boundary condition (5) considers the reduction in heat flux Q by products of the TIM degradation [4, 5].

Here, to find the rate of disintegration of the heat-insulating coating during the period of free discharge, we use the steady-state solution of system (3)-(4) with the boundary conditions (5)-(7), $u \equiv u_A = u_P$:

$$u = \eta Q/w,$$
$$w = \rho_{\Pi} H_A + \rho_M H_P + (\rho c)_{\Pi} (T_A - T_P) + (\rho c)_M (T_P - T_{\infty}) + (\rho_M - \rho_{\Pi}) c_v (T_A - T_P). \tag{8}$$

Here, it is assumed that the velocity u changes in a quasisteady manner over time in relation to the running value of the heat flux.

In accordance with the chosen model of TIM decomposition, the temperature of the surface of the material is constant and is equal to:

$$\theta_s = T_A/T_0. \tag{9}$$

The parameter θ_s is the relative temperature of the surface of the protective coating and, with allowance for the fact that $T_0 > T_A$, varies within the range $0 < \theta_s < 1$.

Equation (8) also gives the relationship between the scale factors u_0 and Q_0. At $\eta = 1$, it follows from this equation that

$$v = q. \tag{10}$$

Equations (9) and (10) close system (1)-(2). We solved the system by using a Runge–Kutta finite-difference scheme with fourth-order accuracy [6].

We searched for the numerical solution of the problem within the ranges of the parameters α, β, θ_s only, since – with allowance for heat losses and the mass yield of TIM decomposition products – we could ignore the effect of counterpressure P_{en} and the adiabatic exponent γ on the time of completion of discharge τ_c. Here, the quantity τ_c is examined in relation to the quantity τ_a – the same characteristic obtained under adiabatic conditions. The moment τ_c corresponds to satisfaction of the condition $p(\tau) \le 1.001\, p_{en}$, where $p_{en} = P_{en}/P_0$. This inequality is used to determine the time of emptying of the plant in an adiabatic calculation of τ_a. Meanwhile, to compare the general and adiabatic solutions in the last case, it is assumed that the pressure $p_a(\tau)$ in the volume V is equal to p_{en} for all $\tau \ge \tau_a$.

Given small values of mass transfer from the TIM ablation surface $\alpha \le 0.1$ and any level of heat loss $\beta \in [0; 1]$, the change in the parameters within the semiclosed volume differs little from adiabatic discharge. A characteristic feature of this case is that the decomposition of the insulating coating is accompanied by discharge of gas throughout nearly the entire time interval $0 \le \tau \le \tau_c$ and, for $\alpha = 0.1$, results in the time τ_c being 22% ($\theta_s = 0.2$) and 10% ($\theta_s = 0.6$) greater than the value of τ_a.

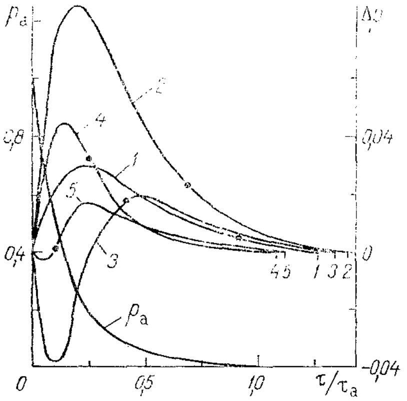

Fig. 1

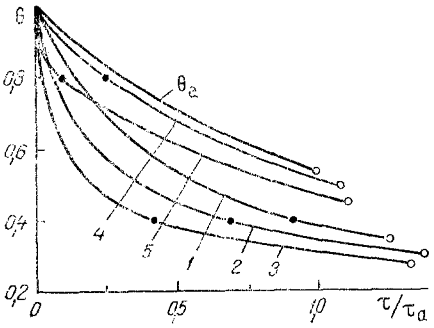

Fig. 2

Fig. 1. Change over time in the pressure in the semi-closed volume under adiabatic conditions P_a and with allowance for decomposition of the TIM $\Delta p = p - p_a$; $\theta_s = 0.4$: 1) $\alpha = 0.2$, $\beta = 0.2$; 2) 1.0 and 0.2; 3) 1.0 and 1.0; $\theta_s = 0.8$; 4) $\alpha = 0.2$, $\beta = 0.2$: 5) 1.0 and 1.0.

Fig. 2. Dependence of gas temperature on time; θ_a is the change in temperature under adiabatic conditions. The curves are numbered in the same manner as in Fig. 1.

The products of the TIM degradation have a greater effect at moderate and high values of the parameters α and β. An increase in the amount of gas removed from the surface S per second leads to a significant deviation of pressure p from the adiabatic value p_a (Fig. 1). The marks on the curves $\Delta p(\tau)$ correspond to the moments at which the TIM ceases to function τ_Π. The relation determining the time τ_Π is the inequality $v(\tau_\Pi) \leq 0$, which in turn corresponds to the condition $\theta(\tau_\Pi) \leq \theta_s$. At $\tau \geq \tau_\Pi$, it is assumed that $v = q = 0$.

It can be seen from the graph (curves 1 and 2, Fig. 1) that with $\alpha = 1$ and unchanged values of β and θ_s, the moment τ arrives earlier than with $\alpha = 0.2$. This can be explained as follows.

The entry of volatile products of TIM decomposition into the system reduces the enthalpy of the gas mixture, since the volatile products have a lower temperature than the gas occupying the system at $\tau = 0$. It is obvious that, other conditions being equal, the reduction in enthalpy will be greater, the more intensive the injection from the surface S. Thus, for $\alpha \to 1$ and β = idem, θ_s = idem, the gradient of the reduction in gas temperature in the volume V should be greater than the gradient of the function $\theta(\tau)$ at smaller values of α. As a result, the temperature of the gas $\theta(\tau)$ will more quickly reach the minimum value θ_s at which the TIM decomposition will continue, while the moment τ_Π is shifted in the direction of smaller values. This is confirmed by the results of calculations presented in Fig. 2 (curves 1 and 2). Here, the dark points denote the moments of time τ_Π, while the clear points represent the time of completion of discharge.

An increase in the level of heat losses (curves 2 and 3, Fig. 2) also leads to a reduction in the temperature of the gas mixture compared to adiabatic flow conditions. The change in pressure in the volume V is not as unambiguous and depends on which of two factors – mass delivery of TIM degradation products or heat loss – prevails in the given case. For example, an increase in the parameter α causes the pressure to increase substantially compared to the function $p_a(\tau)$ (curve 2, Fig. 1), while an increase in the parameter β causes pressure to decrease relative to $p_a(\tau)$ at the initial moments of time (curve 3, Fig. 1).

These tendencies are also manifest for higher values of the dimensionless temperature of the TIM (curves 4 and 5, Figs. 1 and 2). Meanwhile, as in the case of small α, these variants are characterized by slight deviation of pressure and temperature from the corresponding values $p_a(\tau)$ and $\theta_a(\tau)$. However, this is due to another reason – rapid cessation of the TIM decomposition process due to earlier satisfaction of the condition $\theta(\tau) \leq \theta_s$.

The completed analysis provides evidence of the very strong effect of the parameters α, β, and θ_s on the time τ_Π (Fig. 3), while the relation $\tau_c = \tau_c(\alpha, \beta, \theta_s)$ is more monotonic in character (Fig. 4). Here, the variants for which $\alpha > 0$, $\beta = 0$ correspond to flow of the

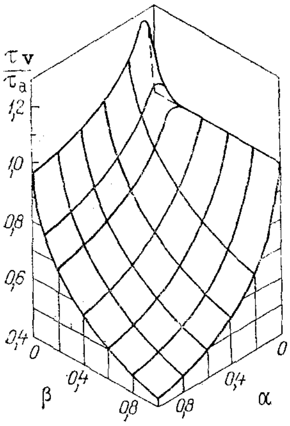

Fig. 3

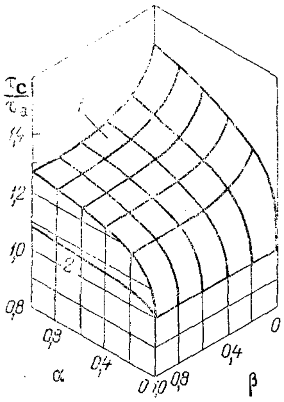

Fig. 4

Fig. 3. Time of cessation of TIM decomposition in relation to the parameters α and β at $\theta_s = 0.4$.

Fig. 4. Dependence of the time of completion of the discharge process on the parameters α, β, and θ_s: 1) $\theta_s = 0.4$; 2) 0.8.

gas without heat loss but with additional delivery of mass at the rate v proportional to θ^4. In the cases $\alpha = 0$, $\beta > 0$, the gas is freely discharged under adiabatic conditions.

It can be seen from Fig. 4 that the region in which the level of the relative heat loss β affects the time of completion of discharge τ_{II} is basically restricted to the range $0 \leq \beta \leq 0.2$. This allows us to approximate the surface τ_c with the simple expression

$$\frac{\tau_c}{\tau_a} = 1 + 0.6(1 - \theta_s)\alpha^{1/3} \tag{11}$$

for $\alpha \in [0;\ 1]$, $\beta \in [0,\ 2;\ 1]$, $\theta_s \in [0,\ 2;\ 1)$.

In order to use Eq. (11) to evaluate the dimensionless time of emptying of a semiclosed volume with allowance for thermal decomposition of the TIM, it is necessary to use relations presented above to determine the temperature of the surface of the material θ_s and the relative mass yield of degradation products α. The adiabatic time of discharge τ_a can be found from the expression

$$\tau_a = \frac{2}{\gamma - 1}\left(p_{\text{en}}^{-\frac{\gamma-1}{2\gamma}} - 1\right),$$

which follows from the solution of Eq. (1) under adiabatic conditions ($\alpha = 0$, $\theta = p^{(\gamma-1)/\gamma}$) and with a critical flow regime (e = 1).

To determine the reliability of our results, we performed a series of simultaneous calculations of Eqs. (1) and (2) with system (3)-(4). The latter equations model heat propagation for a char-forming material in a complete formulation considering nonsteady decomposition when the temperature of the TIM surface is below the threshold value T_A. In this case, the rate of decomposition is no longer determined by Eq. (8), and the temperature of the surface θ_s cannot be found from Eq. (9). These quantities can be determined only by numerical methods. In performing the calculations, we also considered both the convective component of heat flux and the reduction in heat flux by the decomposition products. The coefficient of convective heat transfer was calculated from relations presented in [7] in which it is dependent on the Reynolds number. The Reynolds number was evaluated from the running value of gas discharge.

These additional considerations, while not qualitatively changing the flow pattern, increase the time τ_c by 5-15% relative to the quasisteady solution. The exact increase in τ_c depends on the combination of values of the parameters α, β, and θ_s. Since Eq. (11) also gives a somewhat exaggerated (by an average of 6%) result, the accuracy of the proposed formula (11) can be considered acceptable for engineering calculations.

NOTATION

V, volume; S, area; t, τ; P, p; T, θ; u, v; Q, q, dimensional and dimensionless time, pressure, temperature, TIM decomposition rate, and heat flux; γ, adiabatic exponent; R, gas constant; ρ, density; H, specific enthalpy; c, specific heat; λ, thermal conductivity; α, β, θ_S, dimensionless complexes; ε, coefficient expressing the radiative properties of the gas medium and the heat-transfer surface; σ, Stefan–Boltzmann constant. Indices: 0, initial state and scale factors; s, surface; Π, coke; M, TIM material; P, pyrolysis front; A, ablation front; v, volatile degradation products; *a*, adiabatic conditions; c, completion of discharge.

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TEMPERATURE JUMP ACROSS A PLANE INTERFACE FOR A PHASE TRANSITION IN A PURE LIQUID

A. P. Osipov, M. G. Semena, and Yu. Yu. Sergeev

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We develop a theoretical model of the development of a temperature jump across the boundary between phases during a phase transition in pure liquids.

The temperature is the same across a plane boundary between the liquid and gas phases if there is no evaporation or condensation.

In order to maintain the stability of the processes of evaporation or condensation there must be a difference between the temperatures of the vapor and liquid at the boundary between the phases. This difference is usually referred to as a temperature jump in the literature. The temperature jump across the boundary between the phases is usually small: according to the data of [1, 2] it is of order of a tenth or a hundredth of a degree and hence it is neglected in engineering calculations of heat-exchange devices.

A theoretical calculation of the temperature jump has not been given in the literature, while the experimental data contradict one another [1-3]. However, general considerations and the experimental data both suggest that the temperature jump in the presence of a phase transition will increase as the vapor pressure drops, all other things being equal. This fact is important in the operation of heat-exchange devices such as a heat pipe operating at comparatively low pressure. Hence a theoretical calculation of the temperature jump in the presence of evaporation or condensation is a problem of current interest.

We consider the condensation of a pure vapor onto a liquid surface. A schematic diagram of the process is shown in Fig. 1.

For condensation the surface of the liquid must always be somewhat colder than the vapor. In this process some of the molecules of the liquid leave the surface and go into the vapor; we let G_2 be the corresponding mass flux. A mass flux G_V of vapor molecules approaches the interface 1—1, and there is a mass flux of molecules G_1 passing into the liquid.

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