CONDENSATION OF A CHEMICALLY REACTIVE GAS ON A HORIZONTAL TUBE

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A numerical solution is presented for a system of differential equations of heat and mass transfer in a boundary layer in the laminar condensation of a gas on a horizontal tube.

The promise held by the use of reactive nitrogen tetroxide as the coolant and working substance in nuclear power plants with fast reactors poses the problem of theoretically and empirically investigating the condensation of N_2O_4 on external surfaces [1]. In actual condensers in high-capacity power plants, condensation generally takes place on the outer surface of horizontal tubes. Condensation on an external surface has been studied for a chemically reactive gas only for the classical case of a vertical plate [2]. At the same time, the results of two experimental studies conducted to date on the condensation of nitrogen tetroxide of nonequilibrium composition on a horizontal tube [3, 4] are not in satisfactory agreement in their estimates of the effect of the most important factor — the kinetics of the chemical reaction.

The present work theoretically investigates the condensation of reactive nitrogen tetroxide on the outer surface of a horizontal tube in an infinite volume. In the region of parameters being studied here, the reactive N_2O_4 contains both condensing (N_2O_4, NO_2) and noncondensing (NO, O_2) components. The following chemical reactions take place between these components:

$$N_2O_4 \rightleftharpoons 2NO_2, \tag{1}$$

$$2NO_2 \rightleftharpoons 2NO + O_2. \tag{2}$$

Reaction (1) is nearly in equilibrium, but reaction (2) takes place at a measurable rate [5]. This makes it necessary to consider the kinetics of the latter.

The theoretical analysis will be based on the customary hypotheses of boundary-layer theory. They are examined in detail in [2] for the case of condensation.

The energy, motion, continuity, and mass conservation equations of the noncondensing components for the gas phase have the form:

$$\frac{\partial (\rho U)}{\partial x} + \frac{\partial (\rho V)}{\partial y} = 0, \tag{3}$$

$$\rho U \frac{\partial U}{\partial x} + \rho V \frac{\partial V}{\partial y} = g (\rho - \rho_\infty) \sin \left(\frac{x}{r} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial U}{\partial y} \right), \tag{4}$$

$$\rho U c_p \frac{\partial T}{\partial x} + \rho V c_p \frac{\partial T}{\partial y} = \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} \right), \tag{5}$$

$$U \frac{\partial C_{k0}}{\partial x} + V \frac{\partial C_{k0}}{\partial y} = \frac{\partial}{\partial y} \left(D \frac{\partial C_{k0}}{\partial y} \right) + \frac{I_k}{\rho}. \tag{6}$$

The corresponding equations for the liquid phase

$$\frac{\partial U_l}{\partial x} + \frac{\partial V_l}{\partial y} = 0, \tag{7}$$

$$\mu_l \frac{\partial^2 U_l}{\partial y^2} + g\rho_l \sin \frac{x}{r} = 0, \tag{8}$$

$$\frac{\partial^2 T_l}{\partial y^2} = 0. \tag{9}$$

The boundary conditions for systems (3)-(6) and (7)-(9) are formulated as follows: on the wall—liquid surface (y = 0)

$$T(x,\,0) = T_{wl}, \tag{10}$$

$$U_l = V_l = 0, \tag{11}$$

while the following conditions of continuity of temperatures, axial velocities, shear stresses, and mass and heat flows are assigned at the phase boundary (y = δ(x)):

$$T_{l\delta} = T_{h\delta} = T_s(C_{k0},\,P), \tag{12}$$

$$U_l(x) = U_h(x), \tag{13}$$

$$\mu_l \frac{\partial U_l}{\partial y} = \mu_h \frac{\partial U_h}{\partial y}, \tag{14}$$

$$\rho_l \left(U_l \frac{d\delta}{dx} - V_l \right) = \rho_h \left(U_h \frac{d\delta}{dx} - V_h \right), \tag{15}$$

$$\lambda_l \frac{\partial T_l}{\partial y} = \lambda_h \frac{\partial T_h}{\partial y} + \rho_h r_k \left(U_h \frac{d\delta}{dx} - V_h \right). \tag{16}$$

The conditions of nonpermeability of the noncondensing components through the phase boundary must also be satisfied

$$\rho_h C_{k0} \left(U_h \frac{d\delta}{dx} - V_h \right)_{y=\delta(x)} + \rho_h D_k \frac{\partial C_{k0}}{\partial y}\bigg|_{y=\delta(x)} = 0, \tag{17}$$

in the volume of the gas phase (at y → ∞)

$$U_{h(\infty)} = 0, \tag{18}$$

$$T_{(\infty)} = T_\infty, \tag{19}$$

$$C_{k0(\infty)} = C_{k0\infty}. \tag{20}$$

Using the "similitude" transforms proposed in [6], the above system of differential equations in partial derivatives may be reduced to ordinary differential equations in dimensionless form.

Let us introduce the dimensionless coordinate

$$\eta = \frac{y}{r} \left(\frac{gr}{v^2} \right)^{1/4} J(X) \tag{21}$$

and the dimensionless functions of current, temperature, and concentration of the k-th component

$$F(\eta) = -\frac{\Psi}{v \left(\frac{gr^3}{v^2} \right)^{1/4} \Phi(X)}, \tag{22}$$

$$\Theta(\eta) = \frac{T}{T_\infty}, \tag{23}$$

$$W(\eta) = \frac{C_{k0} - C_{k0\infty}}{C_{k0\delta} - C_{k0\infty}}, \tag{24}$$

where Ψ is the current function, satisfying the continuity equation

$$U = \frac{\partial \Psi}{\partial y}, \quad V = - \frac{\partial \Psi}{\partial x};$$ (25)

$X = x/r$ is a dimensionless coordinate; $J(X)$, $\Phi(X)$ are functions dependent on φ.

In the new variables, system (3)-(6) takes the form

$$F''' [\Phi(X) J^3(X)] + FF'' \left[\Phi(X) \frac{d\Phi(X)}{dX} J^2(X) \right] -$$
$$- [F']^2 \left[\Phi(X) \frac{d\Phi(X)}{dX} J^2(X) + \Phi^2(X) J(X) \frac{dJ(X)}{dX} \right] = - \frac{\rho - \rho_\infty}{\rho} \sin\left(\frac{x}{r} \right),$$ (26)

$$W'' + W'F \frac{v}{D_k} \left[\frac{1}{J(X)} \frac{d\Phi(X)}{dX} \right] + \frac{I_h r^2}{\rho D_k \left(\frac{gr^3}{v^2} \right)^{1/4} J(X)(C_{h0\delta} - C_{h0\infty})} = 0,$$ (27)

$$\Theta'' + \frac{v c_p \rho}{\lambda} \left[\frac{1}{J(X)} \frac{d\Phi(X)}{dX} \right] F\Theta' = 0.$$ (28)

Equations (8) and (9) for the liquid layer are transformed in a similar manner. In order to perform the formal transformations and reduce Eqs. (26)-(28) to ordinary differential equations, the terms dependent on X need to be excluded. For this, it is necessary that

$$\Phi(X) J^3(X) = a \sin X,$$ (29)

$$\Phi(X) \frac{d\Phi(X)}{dX} J^2(X) = b \sin X,$$ (30)

$$\Phi^2(X) \frac{dJ(X)}{dX} J(X) = c \sin X,$$ (31)

$$\frac{d\Phi(X)}{dX} = eJ(X),$$ (32)

where a, b, c, and e are constants.

Values of the functions $J(X)$ and $\Phi(X)$ were found in [7] from Eqs. (29)-(32) and were tabulated. Taking account of (29)-(32) and setting $d\eta/dx = 0$ [2], we convert Eqs. (4)-(6) and (8), (9) to the following form

$$F''' + 3FF'' - 2(F')^2 + \beta(\Theta - 1) = 0,$$ (33)

$$W''' + 3 \mathrm{Sc}\, FW' + \frac{I_h r}{\rho D_k \left(\frac{gr^3}{v^2} \right)^{1/4} J(X)(C_{h0\delta} - C_{h0\infty})} = 0,$$ (34)

$$\Theta''' + 3 \mathrm{Pr}\, F\Theta' = 0,$$ (35)

$$f''' + 1 = 0,$$ (36)

$$\Theta'' = 0.$$ (37)

In the new variables, boundary conditions (10)-(20) are written as follows: at $\eta = 0$

$$f(0) = 0, \quad f'(0) = 0, \quad \Theta(0) = \Theta_0;$$ (38)

at $\eta = \eta_\delta$ in the liquid and at $\eta = 0$ in the gas

$$F(0) = Rf(\eta_\delta), \quad F'(0) = f'(\eta_\delta), \quad F''(0) = f''(\eta_\delta) R,$$ (39)

$$\Theta' = \frac{\lambda_l c_l}{\lambda_h c_h} \Theta'(\eta_\delta) + 3\rho r_h v_h \frac{F(0)}{\lambda_h T_\infty J(X)},$$ (40)

$$W' = - 3 \mathrm{Sc}\, F \frac{C_{h0}}{(C_{h0\delta} - C_{h0\infty})},$$ (41)
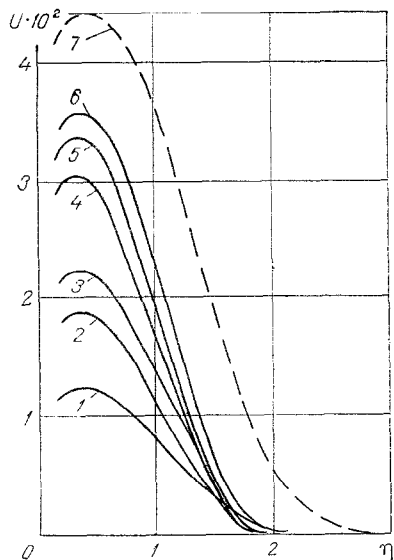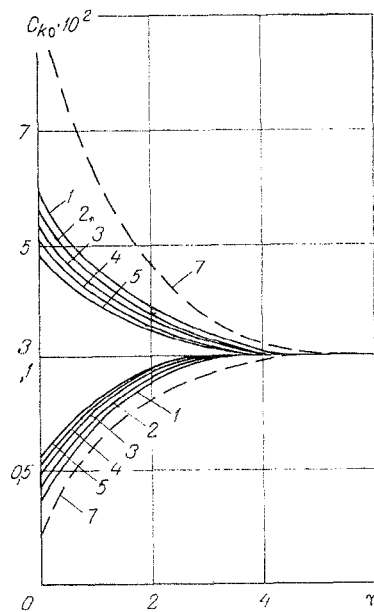
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Fig. 1   Fig. 2

Fig. 1. Distribution of tangential component of velocity in
the gaseous boundary layer for the angles: 1) 30°; 2) 170; 3)
60; 4) 151; 5) 90; 6) 120; 7) 120°. The dashed lines represent
the "frozen" case, while the solid lines depict the case where
allowance is made for reaction kinetics. $U \cdot 10^2$, m/sec.

Fig. 2. Profiles of temperatures and concentrations of non-
condensing components in the gaseous boundary layer for the
angle: 1) 30°; 2) 60; 3) 170; 4) 150; 5) 120; 7) 120°. The
curve notation is the same as in Fig. 1.

$$C_l = \left(\frac{gr}{v_l^2} \right)^{1/4}, \quad C_h = \left(\frac{gr}{v_h^2} \right)^{1/4}, \quad R = \sqrt{\frac{\mu_l \rho_l}{\mu_h \rho_h}}, \tag{42}$$

at $\eta \to \infty$

$$F'_{(\infty)} = 0, \tag{43}$$

$$\Theta'_{(\infty)} = 1, \tag{44}$$

$$C_{k0(\infty)} = C_{k0\infty}. \tag{45}$$

Equations (33)-(35) were solved numerically by the Runge–Kutta method with the use of
Gill's modification [8]. The overall computing scheme was similar to that used in [2]. The
convergence of the iteration processes in correcting the quantities f"(0), C_{k0}(0), and T_{wl}
was checked by Wegstein's method [9]. The inclusion of J(X), where X is dependent on the
angle φ in the dimensionless mass-conservation equation (34) for the noncondensing components
makes it impossible to obtain similitudinous solutions. The computations were performed for
each specified angle at a pressure P = 2 bar, T = 333°K, $C_{k0} = 0.3 \cdot 10^{-2}$. The thermophysical
properties of the system $N_2O_4 \rightleftarrows 2NO_2 \rightleftarrows 2NO + O_2$ were taken from [10], while the kinetic con-
stants were taken from [5].

In solving the above problem, we also examined the "frozen" case. Here, the rate of the
recombination reaction $2NO + O_2 \rightleftarrows 2NO_2$ is assumed to be zero. This corresponds to the normal
situation of condensation in the presence of inert noncondensing gases.

Of the greatest interest in terms of analysis are the processes occurring in the gaseous
boundary layer. Figures 1 and 2 show the distributions of the tangential velocity component,
temperature, and concentration of a noncondensing component (O_2). The maximums of the tangent-
ial component inside the boundary layer are evidence of the considerable effect of natural
convection on transport over nearly the entire volume of the gas. The maximum convection
(according to the calculated data) for the chosen parameters corresponds to an angle $\varphi \sim 120°$
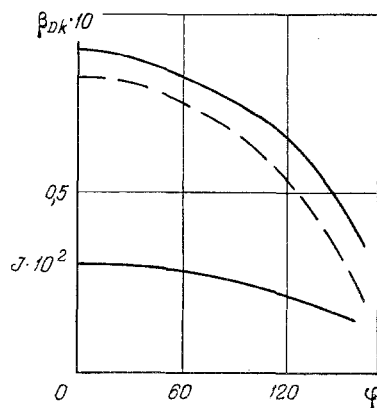from the vertical. It can be seen from Fig. 1 that the tangential velocity component is

Fig. 3. Distribution of diffusion coefficient
and unit mass flow in relation to angle. Nota-
tion is the same as in Fig. 1. φ , deg.

significantly greater in the "frozen" case than in the "kinetic" case, i.e., chemical reac-
tion promotes a certain reduction in natural convection. At the same time, the kinetics of
the chemical reaction significantly reduces the content of noncondensing components at the
phase boundary (Fig. 2), raises the saturation temperature, and smooths out the temperature
profile (Fig. 2).

A quantitative characteristic of transfer processes used in practical calculations for
the condensation of a chemically reactive gas is the diffusion coefficient. This coefficient
unambiguously characterizes the rate of the condensation process [1]. Figure 3 shows the
distribution of the diffusion coefficient

$$\beta_{D_h} \equiv \frac{\rho D_h \operatorname{grad} C_{h0\delta}}{C_{h0\delta} - C_{h0\infty}}$$

and the unit mass flow as a function of angle for the "frozen" and "kinetic" cases, other
conditions being equal. It is apparent from the data in Fig. 3 that the recombination
reaction between the noncondensing components weakens the adverse effect of convection and
promotes a substantial increase in the rate of the condensation process.

NOTATION

g, acceleration due to gravity; r, external radius of tube; r_k, latent heat of condensa-
tion; Pr, Prandtl number; Sc, Schmidt number; T, temperature; x, distance along circumference;
y, distance along radius beyond the cylindrical surface; μ, viscosity; ρ, density; ν, kinematic
viscosity. Indices: s, saturated; δ, liquid-gas interface; h, gas; q, liquid; wl, wall.

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