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MODELING OF THE FORMATION OF A VAPOR CLOUD IN A WIND FLOW WITH INTENSE EVAPORATION

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The stationary problem on formation of a vapor cloud as a result of evaporation above a liquefied-gas spillage under the action of the wind has been considered. It has been shown that the cloud parameters are influenced by the wind velocity, the degree of turbulence of the incident flow, and the geometric dimensions of the spillage. The results of numerical two-dimensional and three-dimensional calculations of the equation of convective diffusion with allowance for the wind-velocity profile have been presented. The effect of the Knudsen layer above the evaporating liquid on the cloud formation is discussed.

Keywords: *layer, turbulent diffusion coefficient, roughness size, atmospheric pressure, air temperature.*

Introduction. Studying the impurity propagation in the atmospheric boundary layer is a practically important and topical problem [1–3]. Here a special place is occupies by problems on the propagation, under the action of the wind, of a vapor cloud that is caused by the spillage of liquefied gases followed by their evaporation. Such situations occur in emergencies in industry (e.g., the meat, refrigeration, and semiconductor industries) as well as in transportation of such gases as ammonia and chlorine. The parameters of the cloud need to be known for its efficient localization. It should be noted that the problem on localization of an ammonia cloud due to its absorption by moving water droplets was considered in [4].

The spillage of certain technically important liquefied gases occurs when the pressure of their saturated vapors at air temperature is much higher than atmospheric pressure. Such cases, in particular, occur in spillages of liquefied ammonia or chlorine. In this case the formation of a cloud is substantially dependent on the distinctive features of the kinetics of evaporation of such gases [5, 6]. Importantly, qualitatively similar problems were studied when considering the interaction of high-power laser radiation with metals. This process also involves high-rate evaporation of a molten metal. Here the pressure of the saturated vapor of the metal is above atmospheric. It turned out that the decrease in the pressure (from the saturated-vapor pressure to the atmospheric one) occurs in a thin layer, the so-called Knudsen layer, above the metal surface. The Knudsen-layer thickness is no larger than ten molecular free paths [7, 8], i.e., at atmospheric pressure, it does not exceed several micrometers.

We illustrate subsequent discussion and calculations using as an example the formation of a chlorine cloud above the spillage of liquefied chlorine. Just as with evaporation of molten metals, the pressure in the evaporated chlorine cloud decreases to the atmospheric one in a thin Knudsen layer with a thickness of only several micrometers, and here all gas molecules entering into the air composition are displaced from the Knudsen layer. Above the Knudsen layer, the cloud is formed due to turbulent diffusion in the case of wind flow past the Knudsen layer.

In this case, for problems of the impurity (chlorine) transfer in the atmosphere, the number density of the impurity (chlorine) molecules above the spillage surface can be regarded as the pseudosaturated vapor density n_{ps} determined with the expression

$$n_{ps} = P/kT ,$$

where n_{ps} is the pseudosaturated number density of the impurity (chlorine), P is the atmospheric pressure, and T is the temperature of the atmospheric boundary layer. The pseudosaturated density acts as a boundary condition in solving

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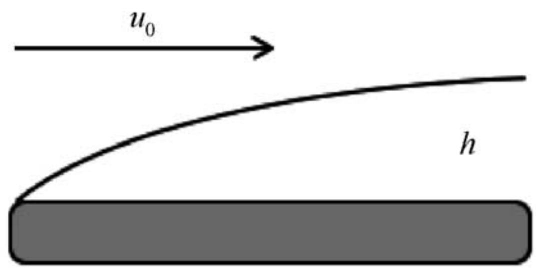


Fig. 1. Formation of an impurity cloud.

the problem on cloud formation. Modeling the cloud formation is the main aim of the present work. Initially the problem in a two-dimensional formulation is solved numerically, and afterwards the problem in a three-dimensional formulation is solved approximately.

Formation of the Chloride Cloud above the Spillage. A steady-state two-dimensional equation describing the formation of the chlorine cloud above the spillage has the form of the equation of convective diffusion

$$u(z)\frac{\partial n(x,z)}{\partial x} = D_t \frac{\partial^2 n(x,z)}{\partial z^2}, \tag{1}$$

where the x axis runs in the wind direction, the z axis runs vertically, $u(z)$ is the wind-velocity profile in the atmospheric boundary layer, D_t is the turbulent diffusion coefficient of chlorine, and n is the number density of chlorine molecules.

The wind-velocity profile is described using the following linear expression:

$$u(z) = u_0 z/2,$$

where u_0 is the wind velocity measured at a small height H above the spillage surface. In the present work, for experimental investigations this height is taken to be 2 m. We assume that above this mark up to 10 m the wind velocity is constant [1, 2].

The turbulent diffusion coefficient D_t of a scalar impurity in the atmospheric boundary layer is represented as

$$D_t = u_0 \delta, \tag{2}$$

where δ is the size of the characteristic roughness of the earth surface [2]. For a roadside area, the typical value is $\delta \sim 0.01$ m. According to expression (2), at u_0 = 1 m/s, is the turbulent diffusion coefficient is 0.01 m^2/s. Thus, the turbulent diffusion coefficient is three orders of magnitude higher than the molecular diffusion coefficient of chlorine [9]. Therefore, the contribution of the molecular diffusion of chlorine will be disregarded.

Boundary conditions to Eq. (1) are of the form

$$n(0,x) = n_{ps}(T). \tag{3}$$

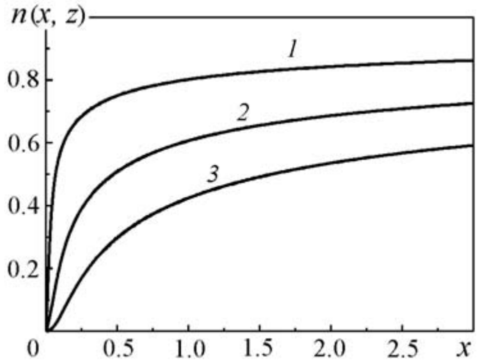
Taking into account the linear character of Eq. (1), we pass to dimensionless quantities

$$\hat{n} = n/n_{ps}(T)$$

and lower the "lid" above the new variable n. In this case boundary condition (3) for the dimensionless quantity n takes the form

$$n(0,x) = 1. \tag{4}$$

At the height H = 2 m, we set the condition



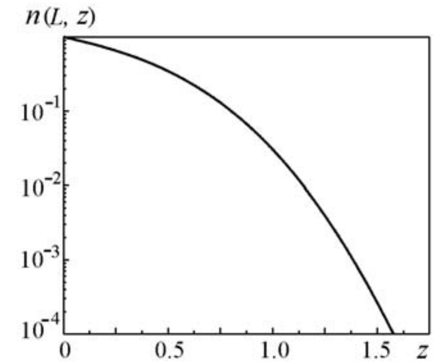


Fig. 2. Profiles of the normalized chlorine density at various heights: 1) 0.1 m, 2) 0.2 m, and 3) 0.3 m. $L = 3$ m, $n_0 = 5$ m/s, and $\delta = 0.01$ m.

Fig. 3. Profile of the normalized chlorine density in the flow at the end of the spillage. $L = 3$ m.

$$n(2, x) = 0 , \tag{5}$$

which is valid for small spillages with a characteristic dimension of the order of several meters. In certain problems, boundary condition (5) can be set at a larger height. We assume that the following initial condition (with no chlorine in the incident flow) is fulfilled:

$$n(z, 0) = 0 . \tag{6}$$

Before proceeding to numerical calculations, we make qualitative estimates of the solution of Eq. (1) [10]. As can be shown, after the wind passes over the spillage with dimension L in the wind direction, the cloud height h is approximately equal (see Fig. 1) to

$$h \sim \sqrt{D_t L/u_0} . \tag{7}$$

According to (2), h is independent of the wind velocity and is solely determined by the spillage dimension, such as $L^{0.5}$. Estimate (7) is obtained disregarding the wind-velocity profile, which, as indicated by the results of numerical modeling, somewhat complicates the picture.

The limits of applicability of steady-state equation (1) can be evaluated from the condition that the characteristic time of variation in the wind velocity is much larger than L/u_0. Thus, for the stationary approximation to be valid at $u_0 = 5$ m/s and $L = 3$ m, the characteristic time of variation in the wind velocity should be much longer than 0.5 s. The results of numerical modeling are presented in the next section.

Results of Numerical Modeling. In the Mathcad environment, two-dimensional equation (1) with boundary conditions (2)–(6) was solved by the method of straight lines [11]. This method enabled us to reduce Eq. (1) to a system of ordinary differential equations by using the explicit difference scheme for its right-hand side. The system of ordinary differential equations was solved by the Runge–Kutta method of 4th order. Some numerical results are given below.

Figure 2 shows the vapor-density distribution at small heights above the spillage. Clearly, at small heights on an about 0.5-m-long path along the spillage, the density distribution of the chlorine vapor reaches a practically constant value. Interestingly, even at a height of 0.3 m, the chlorine number density is already half as high as that immediately above the spillage surface.

For the same conditions, the final density distribution of chlorine (at the end of the spillage) over the height of the wind flow is shown in Fig. 3. First of all, it should be noted that setting the boundary condition $n = 0$ at a height of 2 m is quite justifiable for these conditions. The characteristic height of variation in the vapor density is 0.46 m, while qualitative estimate (7) disregarding the wind-velocity profile gives 0.17 m. Also, it is seen that the influence of the wind-velocity profile is fairly important.

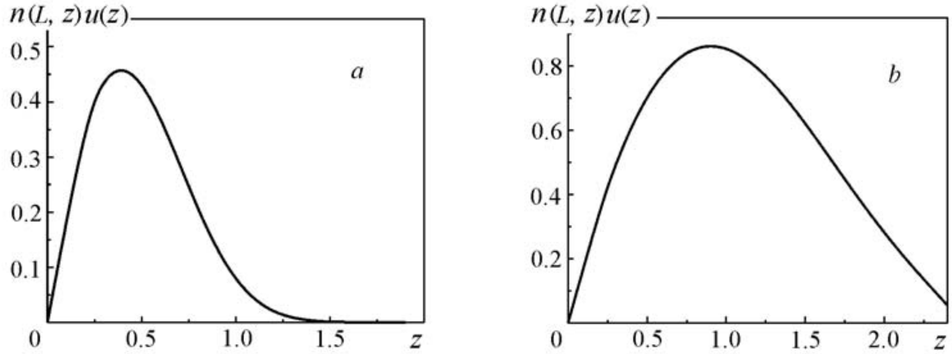


Fig. 4. Specific normalized chlorine discharge over the height above the spillage $L = 3$ m: a) $\delta = 0.01$ m and b) $\delta = 0.1$ m.

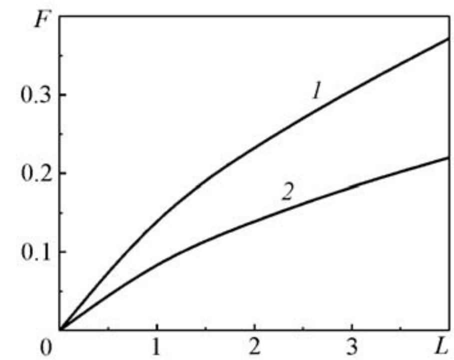


Fig. 5. Normalized chlorine discharge as a function of the spillage dimension L: 1) $u_0 = 5$ m/s and 2) 3 m/s. $\delta = 0.01$ m.

Let us introduce the concept of the average chlorine density n_{av} in the cloud at $x = L$:

$$n_{av} = \frac{\int_0^H n\,(L, z)\,u\,(z)\,dz}{\int_0^H u\,(z)\,dz}\,. \tag{8}$$

We are planning to use n_{av} for calculating the propagation of the chlorine cloud in the atmospheric boundary layer by the action of the wind. For conditions in Figs. 2 and 3, we have $n_{av} = 0.065$. Note that in Fig. 3 to this value there corresponds a height of 0.86 m.

Figure 4a gives the specific discharge of chlorine over the height $n(L, z)u(z)$ at the end of the spillage at $L = 3$ m. Clearly, the major specific discharge of chlorine is the case at a height of about 0.5 m where the wind velocity is already fairly high and at the same time the chlorine number density is still high.

Figure 4b shows the specific discharge of chlorine over the height at the end of the spillage for the roughness size $\delta = 0.1$ m where, according to expression (2), the turbulent diffusion coefficient is an order of magnitude larger compared to the conditions in Fig. 4a.

Results of the two-dimensional calculation of the effects of the spillage dimension and wind velocity on the total discharge of evaporated chlorine are presented in Fig. 5. Here, allowance for the wind-velocity profile above the spillage is important for correct calculation of the discharge of evaporated chlorine. With increase in the wind velocity the chlorine discharge will be less dependent on the wind-velocity profile.

Let us introduce the effective height of the chlorine cloud h_{eff} determined by the formula

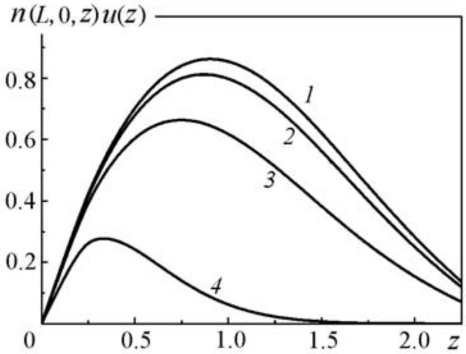


Fig. 6. Specific normalized chlorine discharge over the height above the spillage L = 3 m: 1) spillage width of 9 m, 2) 6 m; 3) 4 m, and 4) 1 m. δ = 0.1 m.

$$h_{\text{eff}} = F/(u_0 n_{\text{av}}) , \tag{9}$$

where F is the total discharge of chlorine evaporated from the spillage per unit of its width. Specifically, for a spillage with length 4 m and wind velocity 5 m/s, we have h_{eff} = 0.95 m, which is in good agreement with the data in Fig. 5.

Approximate Three-Dimensional Modeling. The equation for three-dimensional diffusion of chlorine in the wind flow is of the form

$$u(z) \frac{\partial n(x, y, z)}{\partial x} = D_{\text{t}} \frac{\partial^2 n(x, y, z)}{\partial z^2} + D_{\text{t}} \frac{\partial^2 n(x, y, z)}{\partial y^2} . \tag{10}$$

Allowance for the finite width of the spillage W leads to a change in the average chlorine number density in the cloud above the spillage as against the calculation based on two-dimensional equation (1). Physically, chlorine diffusion in directions different from the wind direction is insignificant if

$$W >> L .$$

An additional boundary condition to Eq. (10) has a simple physical meaning: far from the spillage, the number density of chlorine molecules tends to zero

$$n(x, \infty, z) = 0 . \tag{11}$$

The three-dimensional number density of chlorine molecules is approximately represented as

$$n(x, y, z) = n(x, z) \exp(-4y^2/W^2) . \tag{12}$$

In fact, $n(x, z)$ in expression (12) describes the normalized chlorine density along the line y = 0 above the spillage. It should be pointed out that expression (12) satisfies boundary condition (11). The method of decreasing the dimensions of a problem of the (12) type was widely used in problems of the impurity propagation, e.g., [2, 3]. Substituting expression (12) into Eq. (10) and using the Galerkin method [12], we obtain a steady-state two-dimensional equation with sink taking account of the chlorine diffusion in the direction normal to the wind velocity. Figure 6 shows results of the approximate three-dimensional calculation of the specific discharge of chlorine for the same conditions as in Fig. 4b. Clearly, the spillage width has a marked effect on certain integral cloud parameters. Near the edges of the spillage, the discharge density falls by 37% compared to the center, according to expression (12). Results of the three-dimensional modeling for the middle of the spillage approach those of the two-dimensional modeling for $W >> L$ (compare to Fig. 4b). It is seen that the solution for W = 4 mm and spillage length L = 3 m is still far from the results of the numerical two-dimensional solution. Thus, for a spillage of finite width, the position of the maximum specific discharge of chlorine lies at a smaller height than given by the calculation with a two-dimensional formulation of the problem.

Conclusions. A mathematical model is developed for calculating the formation of a vapor cloud in a turbulent wind flow with intense evaporation from the spillage. Programs are designed in the Mathcad environment for carrying out two- and three-dimensional numerical studies. The formation of a chlorine cloud is modeled numerically. It is shown that account for the effect of the Knudsen layer above the spillage of a liquefied gas (such as chlorine and ammonia) substantially simplifies the mathematical model of the problem.

It is found that the most important factors influencing parameters of the chlorine cloud formed above the spillage pool are dimensions of the spillage cloud, the wind velocity and its profile, the atmospheric temperature, and the degree of turbulence in the wind flow in the atmospheric boundary layer.

Using expression (7), we can show that if the dimensionless similarity parameter is

$$\frac{D_t L}{u_0 W^2} << 1\ ,$$

the cloud formation is of a two-dimensional character, and turbulent diffusion of the impurity (chlorine) in the vertical direction has a predominant effect on the formation of the vapor cloud by the action of the wind. Thus, for the conditions in Fig. 6 and the pool width W = 4 m, this similarity parameter is approximately 0.19.

Here with accuracy sufficient for engineering calculations, it can be assumed that the characteristic height of the chlorine cloud is h_{eff} (expression (9)), and the average chlorine number density in the cloud is equal to the pseudosaturated density n_{av}.

NOTATION

D, diffusion coefficient, m^2/s; F, chlorine discharge, particles/($m^2 \cdot s$); H, height of setting the boundary condition, m; h, height; k, Boltzmann constant; L, spillage dimension in the wind direction, m; x, axis of the coordinate system in the wind direction; y and z, axes of the coordinate system; δ, roughness size, m. Subscripts: av, average; eff, effective; ps, pseudosaturated; t, turbulent; 0, at the height H.

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