CALCULATION OF HEAVY GAS SPREADING
OVER THE EARTH SURFACE BY A THREE-DIMENSIONAL MODEL

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A mathematical model is constructed for motion of a heavy gas along the underlying terrain on the basis of equations of gas dynamics with allowance for the force of gravity, transfer by air masses, and turbulent diffusion. With the use of the method of coarse particles, the time dependences of the coordinates of the front, upper boundary, and volume of the cloud of a heavy gas in the presence and absence of wind are analyzed. It is shown that turbulent diffusion leads to a linear increase in cloud volume in time. Three-dimensional shapes of the heavy gas cloud are obtained for various ambient conditions. It is shown that, despite diffusion, the heavy gas spreads predominantly along the underlying terrain.

Key words: transfer of admixtures, turbulent diffusion, three-dimensional model, method of coarse particles.

Introduction. Significant amounts of industrial wastes into the surface zone of the atmospheric boundary layer are responsible for the arduous ecological situation in many regions. Such wastes are hazardous for nature and mankind, since they propagate along the underlying terrain. The description of this phenomenon requires a detailed study of the mechanism of this process and development of models of transfer of admixtures in the ambient space.

Industrial wastes are mixtures of gases, vapors, aerosols, and solid particles; propagation of these substances is studied on the basis of rather complicated mathematical models [1].

The characteristics of the heavy gas (mixture of wastes with atmospheric air) are determined by the Richardson number [2]

\[ \text{Ri} = \frac{(\rho - \rho_a)gh}{\rho_a v^2}, \]

which is the ratio of the acceleration of gravity of a turbulent particle \((\rho - \rho_a)g/\rho_a\) to inertial acceleration \(v^2/h\) caused by turbulent fluctuations of air with a velocity of the order of dynamic velocity \(u\) within a cloud of size \(h\).

The Richardson criterion \(\text{Ri} > 10\) imposes a condition on the mean density of the mixture of the heavy gas and atmospheric air \(\rho\) in the form

\[ \frac{\rho - \rho_a}{\rho_a} > 0.004 \]  \hspace{1cm} (1)

if we assume that the characteristic dynamic velocity for the neutral state of the atmosphere is \(v = 0.2\) m/sec and the cloud size is \(h = 10\) m [2].

In what follows, the heavy gas is understood as a mixture of air with a gas whose molar weight \(\mu_g\) (this gas will be called the heavy component) is greater than the mean molar weight of air \(\mu_a\) \((\mu_g > \mu_a)\).

1. Mathematical Model. The motion of the heavy gas is described by the Euler equations and diffusion equations [3–5]. Allowance for a large number of factors determining gas motion requires large computer resources; therefore, complicated models are usually calculated in a two-dimensional formulation [3]. A three-dimensional

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problem of spreading of a heavy gas in a spatial region of size 100–1000 m can be solved within the framework of a simplified model.

In our opinion, in most cases, the laws of propagation of heavy wastes in the atmosphere mainly depend on the action of the force of gravity, transfer by air masses (wind), and diffusion determined by small-scale turbulent fluctuations of wind velocity.

The present model describes the motion of air masses in the surface atmospheric layer up to 100 m thick, where the characteristics of vertical air flows remain almost unchanged with height [1]. Therefore, equilibrium stratification is observed if the temperature has a weak dependence on height.

We write the Euler equations with allowance for the force of gravity:

\[ \frac{\partial \rho}{\partial t} + \text{div} (\rho \mathbf{v}) = 0, \]

\[ \frac{\partial (\rho \mathbf{v})}{\partial t} + \text{div} (\rho (\mathbf{v}, \nabla) \mathbf{v}) + \text{grad} p = -\rho g. \] (2)

Here \( \mathbf{v} \) is the velocity of the mixture, \( p \) is the pressure in the mixture, \( g \) is the acceleration of gravity, and \( t \) is the time.

The dependence of pressure on density and concentration of the heavy component is written in the form of conservation laws in terms of physical processes.

Particles [8], which is one of the methods of splitting of the initial unsteady system of gas-dynamic equations written in the form of turbulent diffusion, and the equation of state for the heavy gas and atmosphere.

**2. Numerical Model.** The numerical model is based on solving system (2)–(4) by the method of coarse particles [8], which is one of the methods of splitting of the initial unsteady system of gas-dynamic equations written in the form of conservation laws in terms of physical processes.

The computational domain is divided by the computational grid into \( N = N_x N_y N_z \) cells, which are the so-called coarse particles. At the first stage, the grid moves together with the substance, and there are no mass fluxes through cell boundaries. The coarse particles move due to a pressure gradient. The substance density remains unchanged. At this stage, intermediate values of velocity and concentration are calculated:

\[ \tilde{v}_x^{n+1, j, k} - \tilde{v}_x^n = \frac{\Delta t}{\Delta x_i + \Delta x_{i-1}} p_{i+1, j, k} - p_{i-1, j, k}, \]

\[ \Delta t \]

\[ \tilde{v}_y^{n+1, j, k} - \tilde{v}_y^n = \frac{\Delta t}{\Delta y_j + \Delta y_{j-1}} p_{i, j+1, k} - p_{i, j-1, k}, \]

\[ \tilde{v}_z^{n+1, j, k} - \tilde{v}_z^n = \frac{\Delta t}{\Delta z_k + \Delta z_{k-1}} p_{i, j, k+1} - p_{i, j, k-1}, \]

\[ \tilde{C}_i^{n+1, j, k} - \tilde{C}_i^n = A \frac{\Delta t}{\rho_{i, j, k}}, \]

\[ A = A_1 + A_2 + A_3, \]

Here \( \rho_{i, j, k} \) is the roughness coefficient of the underlying terrain, and \( k_1 \) is the coefficient of vertical turbulent diffusion at the height \( z_1 \) \((z_1 \) is the scale height). This distribution of turbulent diffusion coefficients is valid for the surface atmospheric layer \((z \leq 100 \text{ m})\).

Thus, system (2)–(4) that describes gas motion includes the continuity equation, the Euler equations, the equation of turbulent diffusion, and the equation of state for the heavy gas and atmosphere.