# COMPUTATIONAL MODELING OF THE EMISSION AND DISTRIBUTION OF GASEOUS TOXIC MATTERS IN THE ATMOSPHERE

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During modern technological operations there can be different failures which are accompanied by the emission and distribution in the atmosphere of gaseous toxic matters. Rapid predicting of the given processes is needed for providing of enterprises personnel and population vital functions safety. The effective computational modeling of gases mixing in an environment allows you to expose the areas of dangerous concentrations of harmful admixtures.

Physical, mathematical models and numerical calculation algorithm of gaseous toxic matters dispersion in an atmosphere were developed. They take into account air motion, gravity, complex relief, gases thermo dynamics properties and presence of toxic matters variable source. In reality such task may arise up after liquefied gas spill. As a result of such a failure there are the instantaneous boiling up of liquid, formation of toxic matter cloud of known sizes in an environment and subsequent evaporation of cold liquid remains, that is the source of variable productivity. It is necessary to define the change of toxic matter concentration in the atmosphere under enumerated factors.

The computation domain is a parallelepiped. It is broken up on spatial cells. The dimensions of cells are chosen in accordance with the character dimension of toxic matter cloud.

The complete system of equations, describing the time-dependent three-dimensional two-component gas mixture flow, is written down in the Cartesian co-ordinates. These equations are the conservation laws of gas mixture mass, impulse and energy and of gas admixture mass. The system of equations is complemented by equations determining heat-transfer properties of the gas mixture components.

Entrance boundary conditions were set on the facets of those sells, joining the computation domain surfaces, through which atmospheric air enters. On impenetrable areas limiting the computation domain, the no-flow boundary conditions were determined. Exit boundary conditions were set on the facets of those sells, joining the computation domain surface, through which gas mixture flow out.

Set of the flow gas-dynamic parameters in all domain cells are calculated by means of explicit difference approximations for correlations within the framework of the integral-interpolation Godunov’s method.

To prove the use of the developed method and computer system of engineering analysis the following tasks were considered: gas outflow from a tank through its upper edge at a supposition of the unchanging gas discharge (fig. 1); atmospheric diffusion of various weight gaseous admixtures (fig. 2).

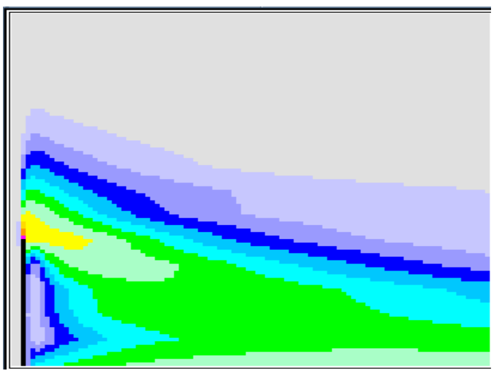


Fig. 1. Chlorine concentration field in the longitudinal section (side view)

The study to assess how the parameters of mathematical model and algorithm affect the computation accuracy was conducted in comparison with known theoretical methods and experimental data.

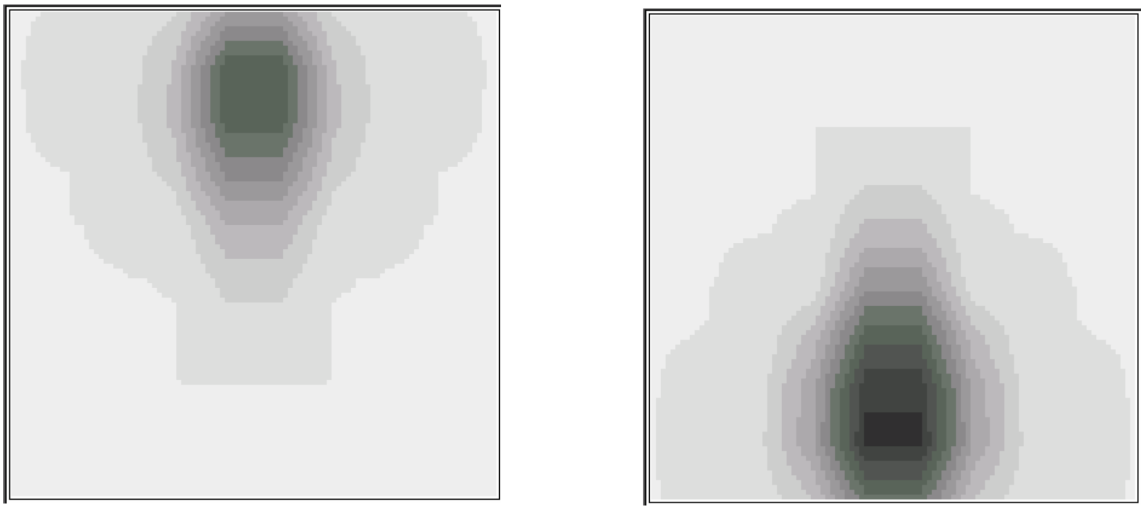
Verification of the mathematical model of gaseous admixture cloud dispersion in an environment was carried out in comparison with known analytical computation mathematical models: instantaneous emission of gaseous admixture (dispersion model of Gauss); stationary dispersion of gas admixture in to atmosphere on the assumption of constant admixture source discharge.

Three-model comparison results show:

- in a difference from the model of Gauss, three-dimensional model is taking into account such factors as a field of mass forces, non-isothermal character of expansion process, radial irregularities of speed and pressure of the approach flow; it allows to describe a physical process more precisely;
- use of turbulent diffusion allows to take into account an admixture dispersion in a computation domain;
- modification of the algorithm has caused little change of CPU time.

The developed software product is a computer interactive engineering analysis application modeling two nonreactive gases mixing three-dimensional processes. The friendly integrated user environment of the application includes all components of CA E (Computer-Aided Engineering) system: basic data generation, editing of data files, viewing of data files, execution management and data visualization.

In order to develop this computer system Visual C++ 6.0 programming language was used. It ideally befits for Windows-programming. The object-oriented approach allows to incapsulate the programmatic code and data in independent objects, that reduces the program's volume and facilitates it's debugging, maintenance and use.



a) b)

Fig. 2. Admixture concentration distribution in the plane of symmetry along the stream axis in the case of “light” (a) and “heavy” (b) gas admixture

Developed computer system allows carry out effectively the engineering three-dimensional analysis of gas-dynamic mixing processes, to predict further distribution of gas mixture in open air or apartment with ventilation, and also to forecast the concentration of toxic gas across space.