Proc. of Int. Conf. "Organized Vortical Motion As a Basis for Boundary Layer Control ", Kiev,2000. –p.32.

Numerical simulation of the dense gas plume effects on the atmospheric boundary layer structure

I. Kovalets, V. Maderich

Institute of Mathematical Machine and System Problems NASU, Kiev, Ukraine
e-mail: ik@env.immsp.kiev.ua

An increased public concern has expressed over past few decades for the hazards associated with the manufacture, storage, transport and use of large amount of chemicals in gaseous or liquefied form. In many accidents the releases produced dense gas plumes. Their dispersion is strongly affected by buoyancy forces and coupled with the dynamics of the near-surface atmospheric turbulent layer. To help understand and simulate the dispersion processes the comprehensive three-dimensional models are necessary. These models should describe main physical factors that govern dispersion of dense gas plumes.

In this paper we present the numerical model of dense gas cloud dispersion. The system of equations of mass, momentum, energy and state coupled with turbulence sub-model is used. The distinctive properties of model are:

(i) Use of Favre-Reynolds averaging procedure that results in the less complicated form than the Reynolds procedure;
(ii) The energy equation was rewritten in terms of pressure that has advantage for numerical solution of problem;
(iii) The modified for stratified compressible flow standard $k-\varepsilon$ model with algebraic relations for turbulent stresses and fluxes;
(iv) The heat conduction problem in the ground is solved to determine the heat transfer at the surface.

The eight differential equations in particular derivatives (three components of mean velocity, density, pressure, concentration, turbulent kinetic energy and dissipation) together with appropriate initial and boundary conditions are discretized by the finite-difference method in space and time. They are fully implicit in time. The splitting method upon the space directions and physical processes is used. The two-stage procedure is used for $n+1$ step. At first stage the velocity and pressure are calculated. At second stage density, concentration and turbulence are calculated using values of velocity at $n+1$ step. This approach allows using of larger time steps at second stage and improves mass conservation comparatively with use of enthalpy equation (Kovalets and Maderich, 1999).

The results of calculations are compared with the results of laboratory field experiments It was shown that in initial stage of dense gas plume collapse the "anelastic approximation" failed. In the calm atmosphere the plume formed vortex ring that spread in self-similar manner. The analysis of the energetics of the dense gas dispersion processes showed that at first stage the potential energy passed to mean kinetic and in the turbulence. The turbulent energy decays faster than the potential energy and mean kinetic energy at the cost of dissipation and mixing that increase the potential energy. In accordance with experiments of Zhu et al. (1998) model predicts strong inhibition of turbulence, changing mean velocity profile and concentration profiles inside of plume. The vertical turbulence intensity is reduced by more then 20% and local Richardson number attained the maximum value in the same place where turbulence intensities are most reduced (Fig.1).

References

Kovalets I., Maderich V. (1999) Dynamics and energetics of dense gas dispersion in near-surface atmospheric layer. Applied Hydromechanics, **1** (**73)**, p.12-20.

Kovalets I., Maderich V. (2000) Numerical modelling of heavy gas dispersion in the near-surface layer of atmosphere. Applied Hydromechanics, (accepted).

Zhu G., Arya S.P., Snyder W. (1998) An experimental study of the flow structure within a dense gas plume, J. Hazardous Materials, **62**, 161-186.

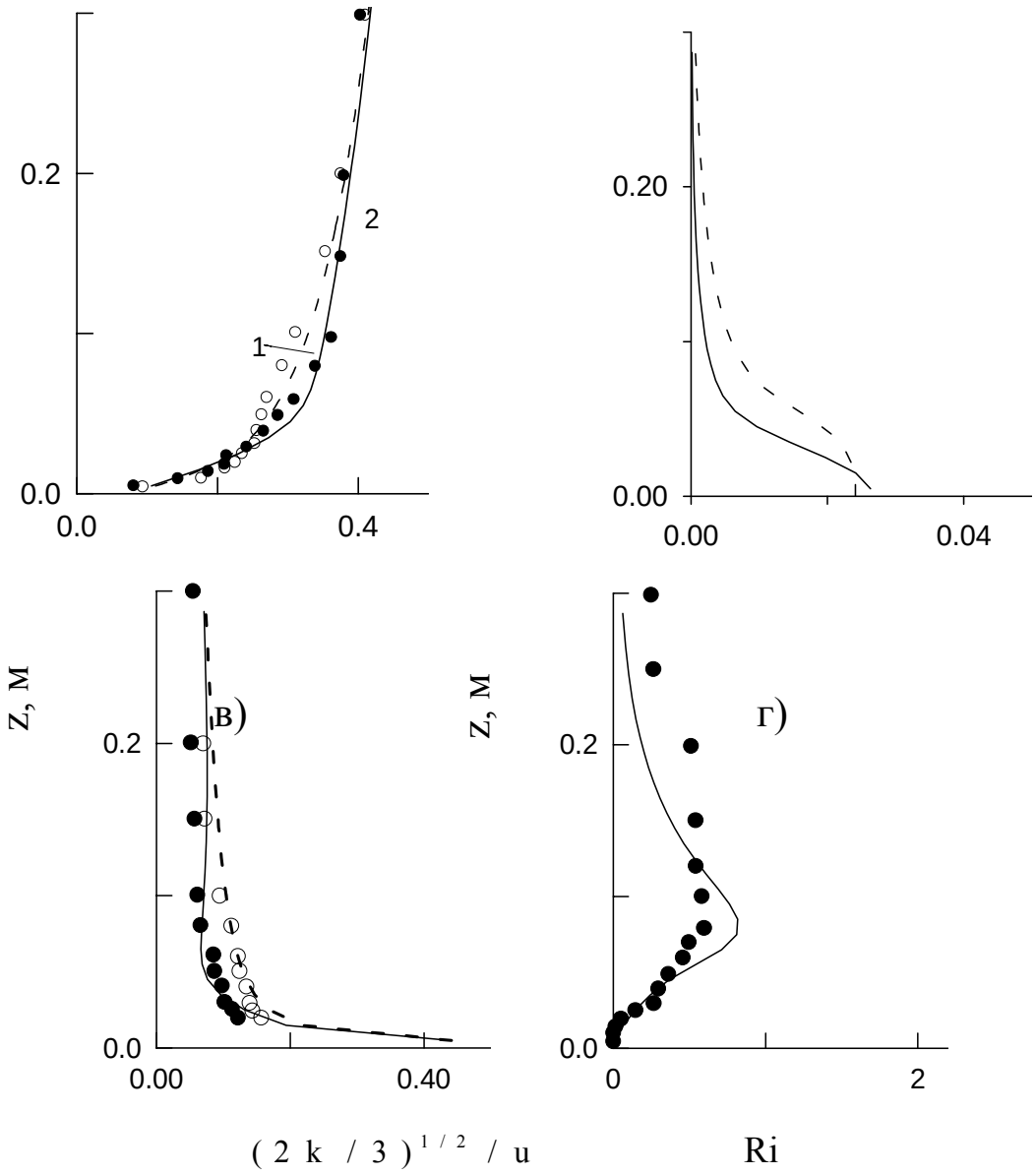

Figure 1 Computed (lines)and measured (circles) vertical profiles of mean velocity (a), concentration (b), energy of turbulence (c) and Richardson number (d) at the distance 2.1 m from source. Solid line and black circle correspond to the heavy gas and dashed line and open circles correspond to the passive scalar.