PARAMETERIZATION OF HEAT EXCHANGE WITH SURFACE IN THE DENSE GAS DISPERSION MODELING

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INTRODUCTION

A heat exchange of the cloud with the underlying surface is essential for the dispersion of the cold heavy gas clouds. Under the influence of the heating from the underlying surface the buoyancy forces in the cold cloud are reduced by convective turbulent mixing and or even change sign and initially heavy cloud lifts off the ground (*Meroney and Neff*, 1986).

The heat exchange with the underlying surface is occurring due to the presence of the mixed convection, which includes of the two main mechanisms: forced and free convection. When the temperature differences of the gas and surface are large enough the weight of the free convection in the heat exchange may be essential (*Neff and Meroney*., 1982). However, in the known 3D models the free convection is not taken into account explicitly in the parameterisation of the heat exchange.

The objective of the present paper is consideration of different parameterisation of the heat fluxes on the Earth surface in the 3D model of cold heavy gas. The comprehensive description of the model and results, presented here can be found in *Kovalets and Maderich,* (2005).

MODEL

The model of *Kovalets and Maderich,* (2003) is based on the unfiltered system of gas-dynamic equations, averaged by the Favre-Reynolds. The system of model equations was used in the form of equations for density-velocity-pressure-concentration. The turbulence was parameterized using the k-ε model. Computational domain was oriented in the direction of the main wind vector near the surface. The initial undisturbed conditions for all meteorological parameters were calculated from the Monin Obukhov similarity theory (MOST). On the upper boundary of the computational domain the distribution of all variables corresponds to the undisturbed atmospheric conditions. On the inflow boundary, the undisturbed distributions of all variables were used as a boundary condition. On the other lateral boundaries the condition $\partial\varphi/\partial\mathbf{n}=0$ for all variables were used, where $\mathbf{n}$ is normal vector to the lateral boundary. Near the Earth surface the absence of the gas flow through the solid boundary was assumed apart from the source of gas. Below the first computational level $z<z_1$ all variables were assumed to satisfy the MOST. The boundary conditions for the turbulent kinetic energy and dissipation rate at the bottom boundary were defined from the assumption of the local equilibrium of the developed turbulence near the Earth surface.

Heat exchange with the underlying surface was described by the boundary condition: $\left(\nu_T/\sigma_T\right)\partial T/\partial z\big|_{z=z_1/2}=-q_s$. Here ν_T,σ_T are turbulent viscosity and Prandtl number, T is the averaged gas temperature, q_s is the turbulent flux of temperature through the surface.

The parameterization of the heat exchange with the Earth surface was performed with the three different ways. In the first approach (parameterization A) the heat flux from the surface was represented as:

$$q_s=\lambda\left(T_s-T\left(z_1\right)\right) \qquad (1),$$

where T_s is the temperature of the underlying surface, and heat transfer coefficient λ was defined by relationships of *Yaglom and Kader,* (1974) for the forced convection.

In the second approach (parameterization B) the heat flux from the surface was also represented using (1), however the heat transfer coefficient was calculated using the simple interpolation formula:

$$\lambda = \lambda_1 + \lambda_2 = \lambda_1 + C_0\left((T_S - T(z_1))(\beta\nu / \mathrm{Pr})\right)^{1/3} \qquad (2)$$

Here λ_1 accounts for the forced convection and it is defined as in parameterization A, λ_2 accounts for the free turbulent convection, $\beta = g / T_s$, g is gravity acceleration, ν, Pr are kinematic viscosity and Prandtl number, $C_0 = 0.21$ (*Zilitinkevich*, 1991).

In the third approach (parameterization C) the vertical profiles of temperature and wind velocity near the wall were represented in the similarity form (*Monin and Yaglom*, 1971):

$$U(z_1) = \frac{u_*}{\kappa}\left[\ln\left(\frac{z_1}{z_0}\right) - \Psi_m\left(\frac{z_1}{L}\right) + \Psi_m\left(\frac{z_0}{L}\right)\right],$$

$$T_s - T(z_1) = \frac{q_s}{\kappa u_*}\left[\ln\left(\frac{z_1}{z_{0T}}\right) - \Psi_T\left(\frac{z_1}{L}\right) + \Psi_T\left(\frac{z_{0T}}{L}\right)\right], \qquad (4)$$

where z_0, z_T are the are the roughness lengths for momentum and temperature, u_* is the friction velocity, κ is von Karman constant, L is the Monin Obukhov length scale. The functions Ψ_m, Ψ_T are defined as in *Brutsaert,* (1999), on the basis of the scaling laws established by *Kader and Yaglom*, (1990), for the mixed convection. The temperature roughness length z_{0T} was determined as in *Yaglom and Kader* , (1974). With the given values of $T(z_1), U(z_1)$ the system of nonlinear equations (4), was solved by iterations for the unknown values of u_*, q_s. To determine the value of the temperature of the surface T_s the coupled problem of the heat transfer in the surface layer of the Earth was solved.

The numerical solution of the governing equations was performed with the use of implicit finite-difference splitting schemes upon spatial directions and physical processes following the approach of *Kovalets and Maderich*, (2003)**.**

RESULTS AND DISCUSSION

The study of the cold heavy gas dispersion in the atmosphere was carried out for the conditions of the field experiment BURRO 8 in which the dispersion of the liquefied natural gas (LNG) was studied (*Koopman et al.* , 1982). The dense gas dispersion in this experiment was modeled under the assumptions of the flat terrain, circular source with constant diameter 58 m and release rate 117 kg/s, lasting 107 seconds with the gas temperature $T_{exit} \approx 110\,^\circ K$. The wind speed was approximately 1.8 m/s and atmosphere was considered as neutral. The horizontal grid size near the source was approximately 17 m increasing in downwind and crosswind directions from the source and the vertical grid size was approximately 0.1 m near the ground, increasing vertically.

In the Fig. 1 the maximum centerline volume concentrations observed in the BURRO 8 experiment are shown together with the predictions of the model at the height 1 m, where gas sensors were placed. Four variants of the predictions are given to show the role of the different parameterizations of the heat exchange. In the worst case the heat exchange is not taken into account at all. It results in the underestimation by the factor of 1/4 of the maximum

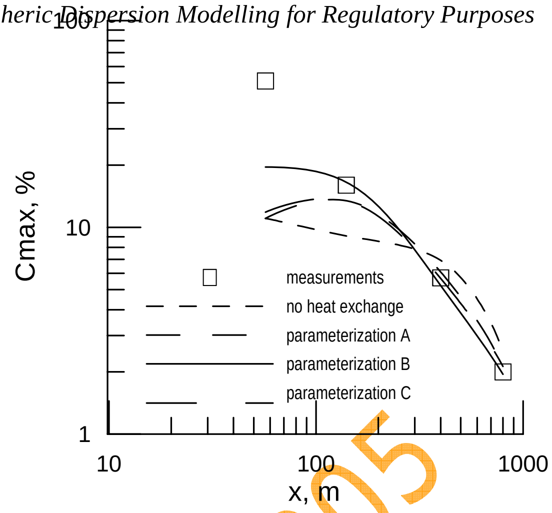

Fig. 1; Comparison of measured and simulated maximum centerline volume concentrations along wind in the BURRO 8 case study

concentration close to the source because of the relatively small height of the cloud was predicted at the sensor level. Far from the source the values of concentration were overestimated because the dilution was reduced by the stable stratification in the cloud. When the heat exchange was parameterized with the relationships that account for the forced convection (parameterization A) the agreement was good far from the source. However, near the source, where velocities in the plume are relatively small, this approach also fails to predict the observed concentration. Using the parameterization C to account for the mixed convection again did not improve the results. The best agreement for all distances from the source was achieved using the simple interpolation formula for the heat exchange coefficient (parameterization B) when in the relationship (2) forced and free convection mechanisms were taken into account. As follows from the Fig. 1 the free convection mostly affects the cold dense gas dispersion sufficiently close to the source, where temperature differences are large and the forced convection is damped due to the effect of the boundary layer displacement (*Kovalets and Maderich*, 2005).

Fig. 2 shows the measured and simulated crosswind volume concentration distributions at the distance 140 m from the source at the time $t = 180\,s$ from the release start. Three cases of calculations are shown: using parameterizations A, B and C. The characteristic maximum in the measured and calculated concentration distributions in Fig. 2 shows the beginning of the process of the cloud lift up, caused by the cloud heating from the ground.

The parameterization B results in the significantly higher height of the cloud (≈ 1.5 times) comparatively with the other parameterizations that is close to experiment in Fig. 2a. As follows from the Fig. 2 the root mean square and bias errors σ_H and ε_H for the prediction of the cloud height (defined by the position of the isoline of the concentration $C = 1\%$) are the following: for the parameterization B, $\sigma_H \approx 30\%$, $\varepsilon_H = -10\%$, while for A and C both errors were almost the same: $\sigma_H \approx 80\%$, $\varepsilon_H \approx -65\%$.

Thus, as in the case of the maximum centerline concentrations in Fig. 1 the comprehensive parameterization C did not bring the improvement of results of simulation. This fact can be considered as the general failure of MOST to adequately describe the nearly shear–free convective boundary layer due to existence of large-scale coherent structures (buoyancy driven convective cells), that are not taken into account by MOST (see *Zilitinkevich et al.*, 1998). Therefore, simple parameterization B for the mixed convection can be recommended for the use in the models of dense gas dispersion.

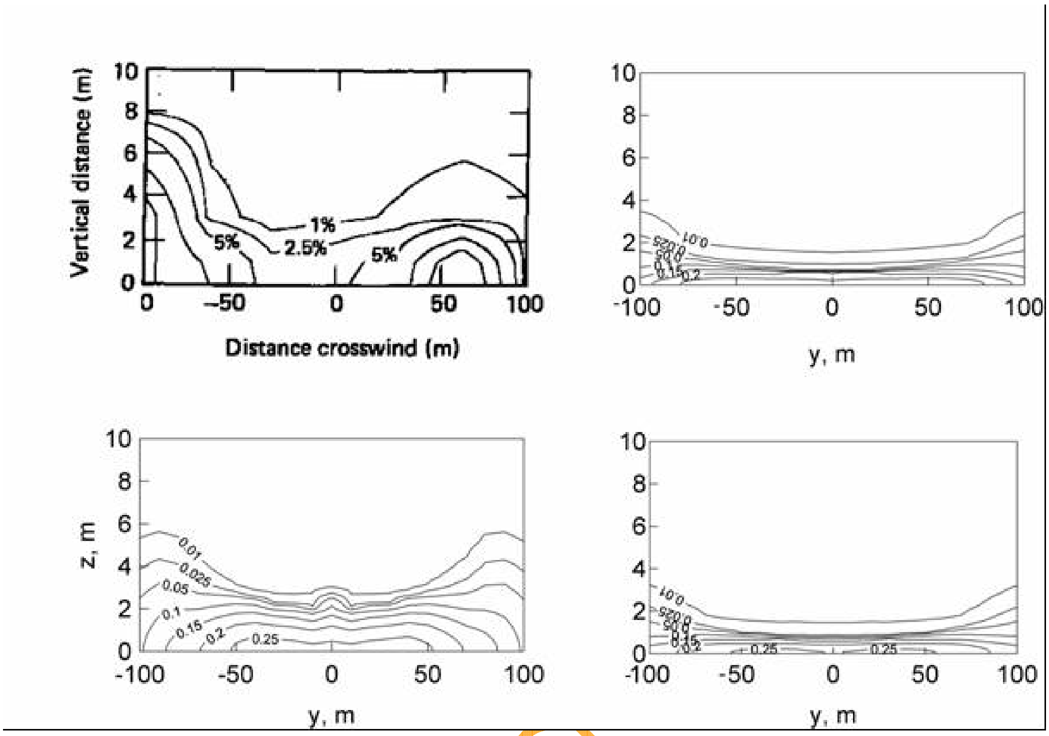

Fig. 2; Crosswind distribution of volume concentration in the BURRO 8 case study at the distance 140 m at t=180 s: (a) measurements (Koopman et al, 1982); (b) calculations with parameterization A; (c) calculations with parameterization B; (d) calculations with parameterization C

CONCLUSIONS

The presented work concerned improvement of the 3D model of Kovalets and Maderich, 2003, with the emphasis on the parameterisation of the heat fluxes on the Earth surface. Three parameterizations of heat exchange with the Earth surface were considered: (A) formula of *Yaglom and Kader,* (1974) for forced convection, (B) interpolation formula for mixed convection and (C) approach of *Brutsaert* , (1999), based on the scaling relationships of *Kader and Yaglom* , (1990).

The simulation of cold heavy gas dispersion and comparison with the field experiment BURRO 8 showed significant influence of the both components of the mixed convection: forced and free convection under the moderate wind speeds. It was shown that parameterization B for the mixed convection significantly improved results of simulation in comparison with the case of the calculations with the forced convection only. The comprehensive parameterization C, however, did not bring the significant improvement of results of simulation. It is therefore advised to use the simple parameterization B in the models of dense gas dispersion.

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