ON THE INFLUENCE OF PBL CONVENTIONAL AND NONLOCAL TURBULENT FACTORS ON POLLUTION CHARACTERISTICS IN LOCAL TO MESO SCALE

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INTRODUCTION

In many short-distance regulators dispersion Gaussian models the dispersions are often given a priory with the well known expressions, for example with these of Pasquill-Gifford, Smith-Hosker, Briggs, corresponding to the stability classes of Pasquill-Turner. On the other side as it is shown in the pioneer works of Safman and Smith F., the consideration of shear generated effect exerts significant influence on the dispersions. If we add to this and other PBL- factors: wind turning with height, stratification, roughness, baroclinicity, inversion, terrain slope and etc., it must expect that the corresponding effects will increase and simultaneously highly vary, particularly with increasing the pollutant transport range from short (=10 km) to meso (~10^2 km) scale. To study these processes we will use comparatively simple diffusion models allowing considering at same time the counted above factors, which are parameterized with PBL model in similarity format.

DIFFUSION MODELS COORDINATED WITH METHOD OF MOMENTS.

We will use two diffusion models.

Air pollution "puff" model (Syrakov, E. (1990), Syrakov, E. and K. Ganev (2004))

The air pollution model of instantaneous cloud takes into account the well-known statistically-based construction, which divides the vertical c_{00} and horizontal c_{hor} diffusion:

$$c(x,y,z,t) = c_{00}(z,t)c_{hor},\ c_{hor} = \frac{1}{2p\, s_x s_y}\exp\left(-\frac{(x-X)^2}{2s_x^2} - \frac{(y-Y)^2}{2s_y^2}\right) \qquad (1)$$

The Lagrangian cloud characteristics $X = c_{10}/c_{00}$, $Y = c_{01}/c_{00}$, $s_x = \sqrt{c_{20}/c_{00} - X^2}$, $s_y = \sqrt{c_{02}/c_{00} - Y^2}$ in (1) are calculated as numerical solution of the system of equations describing the moments c_{01}, c_{10}, c_{02}, c_{20} (see *Syrakov, E. et al*, 2007) and the vertical diffusion component c_{00} (zero moment) is determined according to the k_z equation

$$\frac{\partial c_{00}}{\partial t} + (w - w_0)\frac{\partial c_{00}}{\partial z} + a c_{00} = \frac{\partial}{\partial z} k_z \frac{\partial c_{00}}{\partial z} \qquad (2)$$

at respective initial and boundary conditions according to the type of the solved problem. Here w and w_0 are correspondingly the vertical velocity and the gravity deposition velocity, a is chemical transformation parameter, k_z is coefficient of vertical turbulent diffusion. With the principle of superposition the model allow to study continuous and more complex source too.

Plume model with taking into account of the wind rotation in PBL

The model is based on the following construction:

$$c(x,y,z,t) = \frac{c_0(x,z,t)}{\sqrt{2\pi\sigma_y}} \exp\left(-\frac{(y-Y)^2}{2\sigma_y^2}\right) \quad (3),$$

where the considering wind rotation effect - mean displacement Y (along y) and the dispersion σ_y are calculated by the definition formulae:

$$Y(x,z,t) = c_1/c_0\ ,\ \sigma_y^2 = c_2/c_0 - Y^2 \quad (4),$$

where the first and second moments $c_1(x,z,t)$ and $c_2(x,z,t)$ are calculated numerically.

The vertical diffusion (zero moment c_0) is determined from the equation:

$$\frac{\partial c_0}{\partial t} + u\frac{\partial c_0}{\partial x} + (w - w_0)\frac{\partial c_0}{\partial z} + \alpha c_0 = \frac{\partial}{\partial x}k_x\frac{\partial c_0}{\partial x} + \frac{\partial}{\partial z}k_z\frac{\partial c_0}{\partial z} \quad (5)$$

at traditional boundary and initial conditions.

It can be seen that the above diffusion models a) and b) are based on splitting the diffusion to horizontal and vertical parts, and are coordinated with the statistical moment's method, which allows determination of the trajectory–dispersion parameters in the process of decision of the problem, i.e. without to give them a priori. We will note that the presented models have medium position between the simple short distance regulator dispersion Gaussian and the more complex PDF Lagrangian or 3D Eulerian models. From one side they are comparably simple for operative use and from the other they take into account a wide range of PBL effects into local to meso scale.

TURBULENT REGIMES AND PBL MODEL

The dynamic parameters (profiles of the meteo elements) which are in (1)-(5) are determined by a model of nonstationary (z,t) PBL model over slopping terrain *Syrakov, E. and K. Ganev* (2003). The problem is generally enough parameterized on the basis of the similarity theory, considering a wide range of PBL-turbulent regimes, characterized by the following dimensionless parameters:

- external PBL aerologic–synoptic parameters (see *Syrakov,E.*, 1990, 2005, *Zilitinkevich, S. and P. Calanca*, 2000):

$$R_0\ ,\ S\ ,\ R_{0I}\ ,\ \Lambda_x\ ,\ \Lambda_y\ ;\ \varphi\ ,\ \psi\ ,\ X_a\ ,\ Y_a\ ,\ H_a\ ;\ \mu_N\ ,\ \mu_{cap} \quad (6)$$

- surface (standard + non-local) R_b - bulk parameters (see Syrakov and Cholakov, 2005):

$$R_b\ ,\ \lambda_u = \ln z_1/z_{0u}\ ,\ \lambda_q = \ln z_1/z_{0q}\ ;\ F_{i0} \quad (7)$$

- the relatively subjective but often used Pasquill–Turner stability parameters:

$$A, B, C, D, E, F \quad (8),$$

where $R_0 = G_0/fz_0$ and $R_{0I} = G_0/fh$ are geostrophic and inversion Rosby number, h – diagnostic or prognostic (actual or inversion) height of PBL, $S = \beta\delta\theta_{PBL}/fG_0$ –external parameter of the stratification in PBL, Λ_x, Λ_y (or equivalent parameters $M = \left(\Lambda_x^2 + \Lambda_y^2\right)^{1/2}$, $\phi = arctg(\Lambda_x/\Lambda_y)$) are baroclinic and φ ,ψ are terrain slope parameters, X_a, Y_a, H_a are entrainment convective PBL parameters (connected with momentum and heat flux on the top of PBL,) μ_N, μ_{cap} are non-local stable long–lived PBL parameters, connected with free atmosphere stability (*Zilitinkevich, S. and P. Calanca*, 2000) and capping inversion (*Syrakov, E.*, 2005), R_b is bulk Richardson number in layer (0– z_1) in BL, $F_{i0} = Nz_1/U_1$ is non-local parameter, accounting the effect of the free–flow Brunt–Väisälä frequency N in long-lived PBL condition, the rest symbols are traditional.

The used PBL model has different options for realization according to the used as input parameters each group (6)-(8) or mixed their variant. In the last case the necessary relations between the parameters (6)-(8) are determined on the basis of the developed in *Syrakov, E.* (2005), *Syrakov, E. and E. Cholakov* (2005) ($R_B - R_L$) parameterization approach (based on the joint and coordinated use of the bulk Richardson and resistance law methods). The model includes possibilities for closing with modified mixed length Blackadar approach, and also with k_z-model coincided with the PBL local similarity. In the last case, which we will use in the present work, the coefficient of vertical turbulent heat exchange has the form:

$$k_H = \begin{cases} \dfrac{k u_\bullet z}{j_q}(1 - z/h)^m + (z/h)^n k_h & at \quad z \le h \\ k_E = k_h \exp\left\{-\left[(z-h)/Dh\right]^2\right\} & at \quad h \le z \le h + Dh \\ k_T = k_h \exp\left\{-\left[(h_T - h)/Dh\right]^2\right\} & at \quad z \ge h + Dh \equiv h_T \end{cases} \qquad (9),$$

where $u_\bullet$ is dynamical velocity, j_q is universal function in M-O similarity theory (with asymptote "-1/3"), $k = 0.4$, Dh is entrainment layer depth given by the formulae of Deardorff, h is mixed layer height, $k_h = -\overline{w'q'_h}/(\partial q/\partial z)_h$, $n = 1$, $m = 2$ at unstable condition (according to LES data – (see Noh et al, 2003)), $m = 1$ at stable and neutral condition. At stable stratification k_H is given by (9) at $z \le h$ ($k_h = 0$) as j_q is respective universal function at these conditions. In similar way it is given the exchange coefficient of momentum k_M.

SOME EXAMPLES

By numerical realization of the diffusion "puff" (1), (4) and plume (3)-(5) models and PBL model with k_z-closure (9) it is calculated some cloud and plume pollutant characteristics at different PBL turbulent regimes characterizing: at $F_{i0} = 0$ with input parameters (6): for all cases in order for juxtaposition: $\log R_o = 0$, $G_0 = 8\, m.s^{-1}$ and $S = -500$ (unstable cases – un); $S = 0$ (neutral – n); $S = 500$ (stable – st); $S = -500$, $M = 10$, $f = 270^\circ$ (unstable baroclinic – unbc); $S = -500$, $R_{oI} = 200$ (unstable with inversion ($h_i = 200\, m$) – unin) and $S = -500$, $j = 0, y = 0.1$ (unstable with slope along Ox axis – unsl). At $F_{i0} \neq 0$ it is used the following input parameters (7): for all cases $u_1 = u_{10} = 3 m.s^{-1}$ and $F_{i0} = 0$, $R_b = 0.1$ (case without nonlocal effects); $F_{i0} = 0.4$, $R_b = 0.2$ and $F_{i0} = 0.8$, $R_b = 0.3$ (in these cases the input parameters for the PBL model are obtained by the $(R_B - R_L)$ method, which gives the necessary relations between parameters (7) and (6). On Fig. 1 it is demonstrated the influence of the stratification, baroclinicity and inversion on cloud characteristics: surface horizontal trajectory $Y(x)$, dispersion parameter $s_y(t)$ and vertical skewness Sk_z, and on Fig. 2 the influence of the nonlocal parameter F_{i0} on these cloud characteristics. On Fig. 3 it is shown the influence of the same regimes from Fig. 1 on the plume characteristics $Y(x)$ and $s_y(x)$.

Figures 1-3 results demonstrate the various and significant influence of the PBL turbulent regimes on the explored diffusion characteristics, i.e. their multiple parametric dependence on the input parameters (6)-(8). This influence increase with the increase of the transport scale and it can lead to significant errors at models which work with some mean dispersion parameters given a priory and not taking into account the wind rotation in PBL.

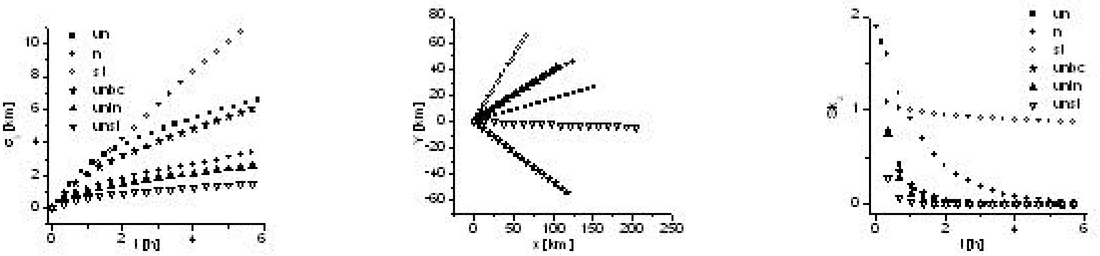

Fig. 1; Influence of different PBL turbulent regimes on cloud characteristics $\sigma_y(t)$, $Y(x)$, $Sk_z(t)$ *for surface source with height* $h = 5m$.

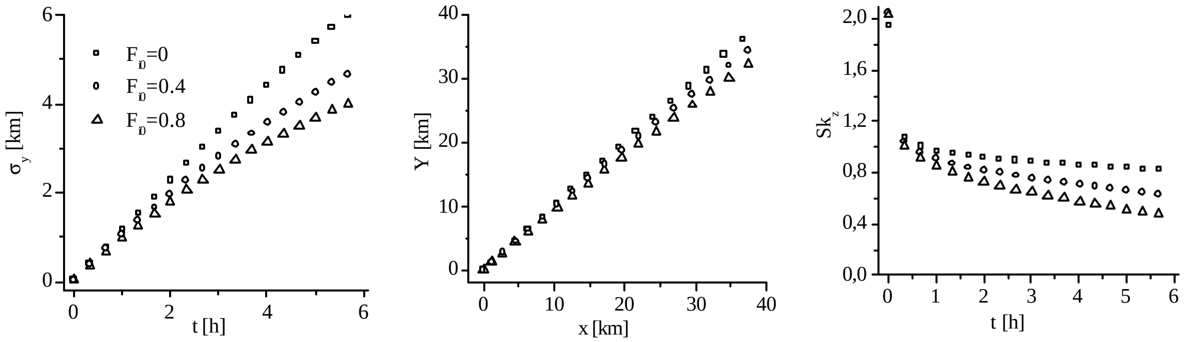

Fig. 2; Influence of the nonlocal parameter F_{i0} *on cloud characteristics* $\sigma_y(t)$, $Y(x)$, $Sk_z(t)$ *at long-lived stable PBL condition for surface source with height* $h = 5m$.

The influence of the wind rotation effect in horizontal direction can be relatively estimated with the parameter R, which is the ratio of the surface ($z = 0$) concentration c given with (3) respectively to $Y = Y(x)$ and $Y \equiv 0$ (at equality of the other parameters in (3)):

$$R = \frac{c(x,y,0,t)_{at\ Y=Y(x)}}{c(x,y,0,t)_{at\ Y\equiv 0}} = \frac{\exp\left(-(y-Y)^2/2\sigma_y^2\right)}{\exp\left(-y^2/2\sigma_y^2\right)}.$$

At $y = 0$ the quantity $R = R(x)$ is presented on Fig. 3. As it can be seen from this figure the considered effect is least expressed at unstable PBL (un) and strongest at stable (st) and unstable with inversion (unin) cases. At this two cases from definite range from Ox (several km) practically it is realized a zero surface concentration (because of the significant deviation of the plume about the axis Ox.

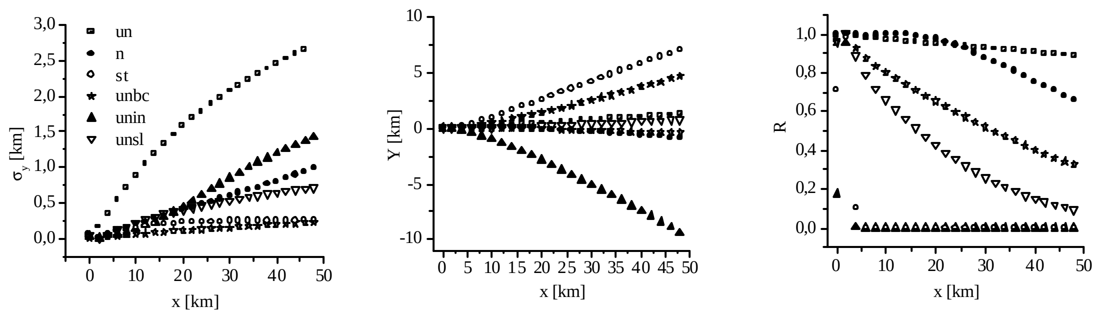

Fig. 3; Influence of PBL turbulent regimes corresponding to that from Fig. 1 on plume characteristics $\sigma_y(x)$, $Y(x)$, *and the dimensionless parameter* $R(x)$ *characterizing the horizontal wind rotation effect on the surface concentration for surface source with height* $h = 5m$.

CONCLUSION

PBL is complex turbulent medium characterizing with roughness, wind sheer, stratification, inversion, baroclinicity, terrain slope and other parameters. At these conditions the basic pollutant characteristics (trajectories, dispersions, concentrations and its distribution - skewness, kurtosis) have non standard behaviour and significantly depend on the PBL turbulent regimes and scales of transport. The suggested in the work approach based on the parameterization of these effects in similarity format respective PBL and diffusion models coordinated with the method of moments allow determining basic relations between the pollutant characteristics and the convenient for practical use input parameters (6)-(8). The approach can be used as for solving a series of independent tasks (including and estimation of extreme and critical parameters of pollution around the source, specifying of regulatory procedures and etc.), as for subgriding parameterization of complex diffusion processes at proper decrease (optimization) of the numerical step.

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