ON THE DIFFUSION TENSOR AND EFFECTS ON SOME LAGRANGIAN AND POLLUTION CHARACTERISTICS IN PBL

Evgeni Syrakov[1], Kostadin Ganev[2], Milen Tsankov[1], Emil Cholakov[1]
[1]University of Sofia, Faculty of Physics, Sofia, Bulgaria
[2]Institute of Geophysics, Bulgarian Academy of Sciences, Sofia, Bulgaria

INTRODUCTION

In the majority of the diffusion models, the coefficient of turbulent diffusion is given approximately with its diagonal components k_{ii}. The problem for determination of the nondiagonal components k_{ij} $(i \neq j)$ is comparatively less studied. In the present work it is developed an approach for calculating of the k_{ij} tensor of turbulent diffusion and taking into account the stratification, baroclinicity and inversion in horizontally homogeneous PBL. It is considered and some case for its influence on some Lagrangian pollutant characteristics. The tensor model is based on approach of *Freeman, B.* (1977) with weak modification of the remake of the equation of the turbulent kinetic energy (TKE) and using an PBL model taking into account the counted above factors in similarity format.

BACKGROUND

On the basis of Hellor-Yamada equations of covariances in *Freeman, B.* (1977) it is suggested the following relationships for k_{ij} tensor components:

$$k_{xx} = d\left[k'' + \left(2d'k_M - k'\right)\left(\frac{\partial u}{\partial z}\right)^2\right];\ k_{yx} = k_{xy};\ k_{xy} = d\left(2d'k_M - k'\right)\frac{\partial u}{\partial z}\frac{\partial v}{\partial z};$$

$$k_{yy} = d\left[k'' + \left(2d'k_M - k'\right)\left(\frac{\partial v}{\partial z}\right)^2\right];\ k_{zy} = k'\frac{\partial v}{\partial z};\ k_{yz} = -d\left(k_M + k_H\right)\frac{\partial v}{\partial z} \qquad (1)$$

$$k_{xz} = -d\left(k_M + k_H\right)\frac{\partial u}{\partial z};\ k_{zx} = k'\frac{\partial u}{\partial z};\ k_{zz} \equiv k_H;$$

$$k' = \frac{2}{2 + 3D_5\,Ri/Y}\,d\left[\frac{3D_5 Ri}{2Y}\left(k_M + k_H\right) - k_M\right] \qquad (2),$$

$$k'' = \frac{D_4 Ys^2 l^2}{3} - \frac{2C_2 A_1 Ri\, sk_H}{\sqrt{Y}}\quad d = \frac{3A_2}{\sqrt{Y}s};\ d' = \frac{3A_1}{\sqrt{Y}s} \qquad (3).$$

The dimensionless TKE and the gradient number of Richardson have the form:

$$Y = \frac{q^2}{l^2 s^2},\ Ri = \frac{b\, \mathrm{d}q/\mathrm{dz}}{s^2} \quad (4),$$

where $s = \sqrt{(\partial u/\partial z)^2 + (\partial v/\partial z)^2}$, $q^2 = \overline{u'^2} + \overline{v'^2} + \overline{w'^2}$ is TKE, l is mixing length, q, u, v are potential temperature and horizontal velocity components, k_M and k_H are respectively the coefficients of vertical turbulent exchange of momentum and heat, the rest notations are traditional. All constants in (1)-(3) are the same as in *Freeman, B.* (1977). Here we will use the equation for TKE in the form:

$$s^2 k_M - bbk_H\frac{\partial q}{\partial z} - \frac{q^3}{B_1 l} = 0 \qquad (5),$$

where b is empirical constant (taking into account approximately the proportionality of the diffusion and boyant force terms in the equation of TKE) and is given as $b = 1/R_{fcr}$ (R_{fcr} - critical value of flux Richardson number R_f) at stable and $b = 8$ at unstable stratification *Monin, A. and A. Yaglom* (1973). At $b = 1$, (5) coincide with the equation for TKE used in Freeman (1977). In our work using the semi-empirical relationship $k_M = l^2 s$, after some transformation we present (3) and (5) in the form:

$$Y = B_1^{2/3}\left(1 - bR_f\right)^{2/3},\ k'' = k_M s\left(\frac{D_4}{3}Y - 2C_2 A_1 \frac{R_f}{\sqrt{Y}}\right) \qquad (6),$$

where $R_f = a_H Ri$, $a = k_M / k_H$. The diffusion tensor k_{ij} can be determined on the basis of the quantities (1), (2), (6) at given profiles of the elements in ABL:

$$u(z),\ v(z),\ q(z),\ k_M(z),\ k_H(z),\ a_H = k_H / k_M,\ Ri(z) \qquad (7).$$

These parameters are determined with numerical one dimensional (z, t) PBL model over sloping terrain *Syrakov, E. and K. Ganev* (2003), (see also *Syrakov, E.* et al, 2007). The model describes a wide range of turbulent regimes in agreement with the similarity theory and has some options for closure. Here we will use the k_z-closure approach (see *Syrakov, E.* et al, 2007), formula (9) at $z \geq h$):

$$k_H = \frac{k u_\bullet z}{j_q}\left(1 - z/h\right)^m \qquad (8),$$

where j_q is universal function of temperature in MO similarity theory, h is mixed layer height at unstable and height of PBL at stable stratification, $m = 2$ at unstable, $m = 1$ at stable and neutral stratification. The dependence of parameters (7) on stratification, baroclinicity and inversions is determined by numerical realization of the PBL model using as input the following dimensionless external parameters

$$R_o,\ S,\ \Lambda_x,\ \Lambda_x,\ R_{oI} \qquad (9),$$

where $R_o = G_0 / fz_0$ $R_{oI} = G_0 / fh_i$ are geostrophic and inversion number of Rosby, h_i is inversion height, $S = bdq / fG_0$ is integral parameter of stratification in PBL Λ_x and Λ_y (or equivalent parameters $M = \left(\Lambda_x^2 + \Lambda_y^2\right)^{1/2}$, $f = arctg\left(\Lambda_x / \Lambda_y\right)$) are baroclinic parameters. For exploration of pollution in PBL it is used diffusion model of instantaneous cloud: which follows the well known statistically based construction for concentration c, which divides the vertical c_{00} and horizontal c_{hor} diffusion components (*Syrakov, E. and K. Ganev*, 2004):

$$c(x, y, z, t) = c_{00}(z, t) c_{hor},\ c_{hor} = \frac{1}{2p\, s_x s_y}\exp\left[-\frac{(x - \bar{x})^2}{2s_x^2} - \frac{(y - \bar{y})}{2s_y^2}\right] \qquad (10),$$

where the Lagrangian cloud characteristics $\bar{x} = c_{10}/c_{00}$, $\bar{y} = c_{01}/c_{00}$, $s_x = \sqrt{c_{20}/c_{00} - \bar{x}^2}$, $s_y = \sqrt{c_{02}/c_{00} - \bar{y}^2}$ in (10) are calculated as numerical decision of the system for the first c_{10}, c_{01} and the second c_{20}, c_{02} statistical moments in x and y axis:

$$\frac{\partial c_{10}}{\partial t} + (w - w_0)\frac{\partial c_{10}}{\partial z} + a c_{10} = \frac{\partial}{\partial z} k_H \frac{\partial c_{10}}{\partial z} + u c_{00} - \left(k_{xz} + k_{zx}\right)\frac{\partial c_{00}}{\partial z} - c_{00}\frac{\partial k_{zx}}{\partial z} \qquad (11)$$

$$\frac{\partial c_{01}}{\partial t} + (w - w_0)\frac{\partial c_{01}}{\partial z} + a c_{01} = \frac{\partial}{\partial z} k_H \frac{\partial c_{01}}{\partial z} + v c_{00} - \left(k_{yz} + k_{zy}\right)\frac{\partial c_{00}}{\partial z} - c_{00}\frac{\partial k_{zy}}{\partial z} \qquad (12)$$

$$\frac{\partial c_{20}}{\partial t} + (w - w_0)\frac{\partial c_{20}}{\partial z} + a c_{20} = \frac{\partial}{\partial z} k_H \frac{\partial c_{20}}{\partial z} + 2k_x c_{00} + 2u c_{10} - \left(k_{xz} + k_{zx}\right)\frac{\partial c_{10}}{\partial z} - 2c_{10}\frac{\partial k_{zx}}{\partial z} \qquad (13)$$

$$\frac{\partial c_{02}}{\partial t}+(w-w_0)\frac{\partial c_{02}}{\partial z}+ac_{02}=\frac{\partial}{\partial z}k_H\frac{\partial c_{02}}{\partial z}+2k_y c_{00}+2vc_{01}-\left(k_{yz}+k_{zy}\right)\frac{\partial c_{01}}{\partial z}-2c_{01}\frac{\partial k_{zy}}{\partial z} \quad (14)$$

and the vertical diffusion - zero moment $c_{00}(z,t)$ is determined according to the equation (which do not depend on the nondiagonal components k_{ij} $i \neq j$)

$$\frac{\partial c_{00}}{\partial t}+(w-w_0)\frac{\partial c_{00}}{\partial z}=\frac{\partial}{\partial z}k_M\frac{\partial c_{00}}{\partial z} \quad (15)$$

at corresponding initial and boundary condition. Here w and w_0 correspondingly the vertical and gravity deposition velocity, $\tilde{a}$ - chemical transformation parameter. The last two terms in (11)-(14) describe the effects connected with the nondiagonal terms k_{ij} ($i \neq j$).

RESULTS AND DISCUSSION

With numerical realization of the model (1) (2), (6) for k_{ij} (at $a = w = w_0 = 0$) at determination of the quantities (7) from the PBL model (the axis Ox is along the surface wind) at k_z - closing (8), on Fig. 1-5 it is shown the dependence of the vertical profiles of the diffusion tensor k_{ij} ($i, j = 1,2,3$ corresponding wth x, y, z) on stratification, baroclinicity and inversion in PBL, characterized with the external dimensionless parameters (9): $G_0 = 8$ m.s^{-1}, $R_o = 10^7$, $S = -500$.

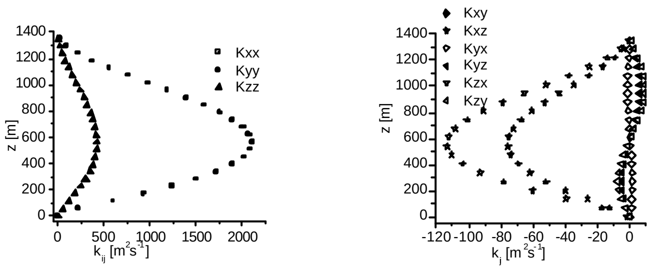

Fig. 1; Vertical profiles of $k_{ij}(z)$ at unstable PBL ($G_0 = 8m.s^{-1}$, $R_o = 10^7$, $S = -500$).

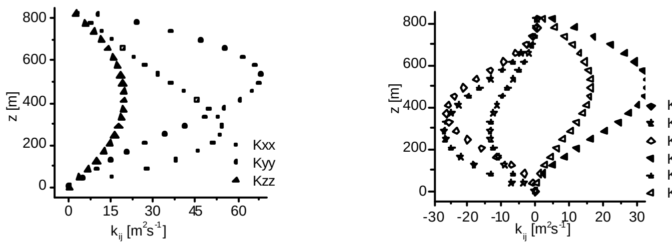

Fig. 2; Vertical profiles of $k_{ij}(z)$ at neutral PBL ($G_0 = 8m.s^{-1}$, $R_o = 10^7$, $S = 0$).

The comparison of the vertical profiles of $k_{ij}(z)$ at significantly unstable (Fig. 1) and neutral (Fig. 2) PBL show that in both cases there is a well expressed negative components k_{xz} and k_{zx}, but for the neutral cases this is and for $k_{xy} = k_{yx}$. The main difference is that, for unstable PBL, the components $k_{xy} = k_{yx}$, k_{xz} and k_{zx} are small and near to zero. The condition $k_{xy} = k_{yx} = k_{zy} = k_{yz} = 0$ is strictly fulfilled in the surface layer. As it can be seen from Fig. 3 the rest components of k_{ij} in the surface layer vary linearly with the height z at neutral case and reach approximately constant values (z - less regime) for the stable case above 10 m, which is in full accordance with the theoretical considerations. The influence of the inversion and baroclinicity can be seen from the juxtaposition of the results from Fig.4-5 with that from Fig. 1, these cases are all for unstable conditions at $S = -500$. At the baroclinic case on Fig. 4 the components $k_{xy} = k_{yx}$ are again near to zero, but in contrast to the unstable case without baroclinicity (Fig. 1) k_{zy} and k_{yz} are significant and positive. At the inversion case (Fig. 5) the values of k_{ij} in principle are significantly smaller (because of the not so big depth of the inversion layer ($h_i = 200m$)). The behaviour of the k_{ij} components is qualitatively like that from Fig. 1 with the difference that here k_{zy} and k_{yz} are entirely positive. Verification of the k_{ij} model is done on the basis of relative experimental data for the dependence of the quantity $p = k_{xz}/k_H$ on Ri in the surface layer presented in *Zilitinkevich, S.* (1970), (see also *Yordanov, D. and A. Alloyan,* 1980). The coincidence is well as in particular at very strong unstability $p \to 0$, at $Ri = -0.4$ $p = -1.5$, at $Ri \to 0$ $p = 2.1$ and at $Ri = 0.15$ $p = -5$. We will note that in limit case of free convection ($s = 0$) the diagonal diffusive components become proportional to $(bq)^{1/3} z^{4/3}$ (q is surface cinematic heat flux) and the off-diagonal components are zero.

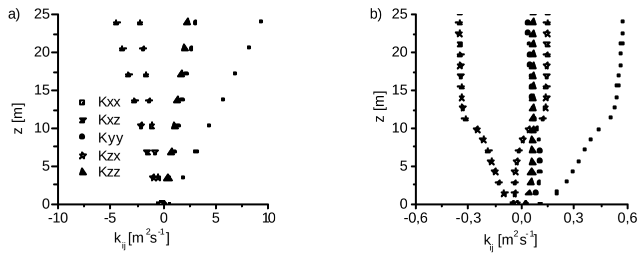

Fig. 3; Vertical profiles of $k_{ij}(z)$ in the surface layer at neutral ($G_0 = 8m.s^{-1}$, $R_o = 10^7$, $S = 0$) - a) and at stable ($G_0 = 8m.s^{-1}$, $R_o = 10^7$, $S = 500$) - b) conditions.

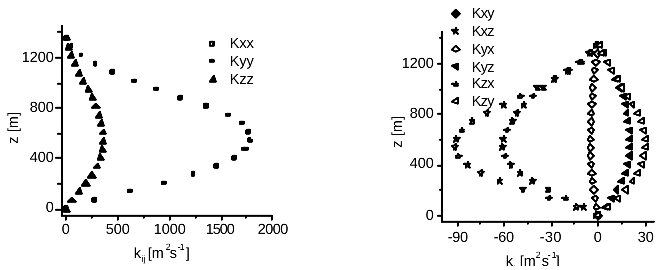

Fig. 4; Vertical profiles of $k_{ij}(z)$ at unstable and baroclinic PBL ($G_0 = 8m.s^{-1}$, $R_o = 10^7$, $S = -500$, $M = 10$, $f = 270^\circ$).

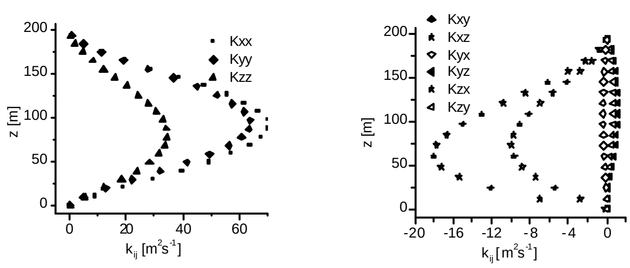

Fig. 5; Vertical profiles of $k_{ij}(z)$ at unstable PBL with inversion ($G_0 = 8m.s^{-1}$, $R_o = 10^7$, $S = -500$, $R_{oI} = 400$).

Finally, we will estimate the influence of the nondiagonal components k_{ij} $(i \neq j)$ on some diffusion characteristics in PBL. Because of the limited place this is done only for the cloud horizontal centroid coordinates $X(t)$ and $Y(t)$. On the basis of numerical integration of the system for the moments (11)-(15) it is calculated the ratio $P_x = X'(t)/X(t)$ and $P_y = Y'(t)/Y(t)$, where $X'(t)$ and $Y'(t)$ are calculated with taking into account, and $X(t)$ and $Y(t)$ without taking into account the nondiagonal components k_{ij} $(i \neq j)$ Fig. 6.

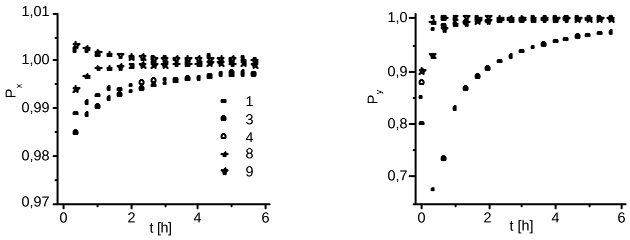

Fig. 6; Quantities P_x and P_y at conditions in PBL respective to that of Fig. 1 (case. 1), Fig. 2 (case. 2), Fig. 3 (case 3), Fig. 4 (case 4), Fig. 5 (case 5).

CONCLUSION

In the present work is studied the dependences of the diffusive tensor k_{ij} (z) on stratification baroclinicity and inversion. This allows in particular to give quantitative estimation for the horizontal coefficients k_{xx} and k_{yy} (which traditionally are given empirically) as well as and for the nondiagonal components k_{ij} $(i \neq j)$, which very often are neglected in the diffusion tasks. A further development of the study includes expanding the number of the PBL turbulent regimes, including and limit cases as free convection strong stability, still conditions and more detailed study of the influence of the k_{ij} tensor on pollutant characteristics in PBL at the mentioned conditions.

ACKNOWLEDGEMENTS

Milen Tsankov is scholar of WFS.

REFERENCE

Freeman, B., 1977: Tensor diffusivity of a trace constituent in a stratified boundary layer. J. Atmos. Sci., 34,№ 1, 397-412.

Monin, A. and A. Yaglom, 1973: Statistical fluid mechanics, part 1, Cambridge MA.

Syrakov, E. and K. Ganev, 2003: Accounting for effects of wind rotation in the PBL on the plume characteristics I. Journ. Environ. and Pollution, 20,154-164.

Syrakov, E. and K. Ganev, 2004: Stratification, baroclinicity and inversion effects on the lagrangian and diffusion characteristics of instanteously released cloud in the PBL. Proc. Nine Intern. Conf. on Harm. w Atm. Disp. Modell. for Reg. Purp,. 1, 272-276, Garm. Part. Kirch., Germany, 01-04 June.

Syrakov, E., E. Cholakov, M. Tsankov and K. Ganev, 2007: On the influence of PBL conventional and nonlocal turbulent factors on pollution characteristics in local to mesoscale (in the present proceedings).

Yordanov, D. and A. Alloyan, 1981: Surface layer parameterization when recording tensor diffusivity. Compt. Rand. Acad. Bulg, Sci.,№ 4, 509-512.

Zilitinkevich, S., 1970: Dynamics of the atmospheric boundary layer, Hydrometeoizdat, Leningrad.