#### P4.1 On Parameterization of Turbulence Diffusion in Stratified Atmosphere

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# 1 Introduction

The concentration concept of air pollutant, which is defined by pollutant content in unity volume of air, have been used for a long time by atmospheric environment community. Meanwhile the mixing ratio concentration which is defined by pollutant mass content in unit mass air should be used when the air density is no longer a constant because in this condition the volume concentration is not conservative with the motion of parcel. The mesosacle transport model for predicting air pollution level in the deep convection system the mixing ratio concentration is also applied due to air density changes with height on the one hand. The concentration of scalar properties such as pollutants and in the turbulent fluid environment such as atmospheric boundary layer (ABL) and upper mixing layer of ocean (UMLO) is described by the turbulent diffusion Equation, and the turbulent flux of property is parameterized by flux-gradient relation. In strict the both of diffusion equation and flux-gradient relation widely used now are just only available for shallow and idealized turbulent fluid system within which flow density is constant and the system is incompressible. In real atmosphere,

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however, the density obviously varies with height, which leads to the non mass conservative for mass concentration. This future can be clearly shown in the inversion layer in ABL and in the density saltation layer in ocean. Based on the equation of continuity some density correction and modification on the turbulent flux is made.

#### 2. Turbulent diffusion equation

On the study of turbulent diffusion for scalar property the general conservation of mass can be written as the follows

$$\frac{\partial \rho q}{\partial t} = \rho S_q - \frac{\partial \rho u_i q}{\partial x_i} \tag{1}$$

The term on the left hand presents the rate of mass changes within the unity volume at fixed location. The first term on the right hand stands for internal production rate for the scalar property q. The second term is the divergence of mass flux for the quantity of q. Accordingly, the mass concentration change rate can be written after introducing Reynolds postulates and using the equation of continuity for the incompressible fluid

$$\frac{\partial \overline{c}}{\partial t} + u_i \frac{\partial \overline{c}}{\partial x_i} = \overline{\rho} \overline{S_q} + \frac{\partial}{\partial x_i} (\overline{\rho} K_i \frac{\partial \overline{q}}{\partial x_i}) (2)$$

if no source term here

$$\frac{\partial \overline{c}}{\partial t} + \frac{\overline{u}}{u_i} \frac{\partial \overline{c}}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ K_i \left( \frac{\partial \overline{c}}{\partial x_i} - \frac{\overline{c}}{\overline{\rho}} \frac{\partial \overline{\rho}}{\partial x_i} \right) \right] (3)$$

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Absolutely the turbulent flux of concentration can be related

$$-\overline{u_ic} = K_i \left(\frac{\partial \overline{c}}{\partial x_i} - \frac{\overline{c}}{\overline{\rho}}\frac{\partial \overline{\rho}}{\partial x_i}\right)$$
(4)

Eq.(4) is just correct closure scheme for turbulent diffusion in non-constant density fluid. The second term on the right hand can be termed as density correction. The following relation is available only under the condition that

the density of fluid  $\overline{\rho}$  is constant

 $-\overline{u_ic} = K_i \frac{\partial \overline{c}}{\partial x_i}$  according to above

derivation the turbulent flux is dependent on not only the eddy diffusivity and gradient of concentration but also density gradient as described by Eq.(4) with respect to stratified fluid, therefore the turbulent flux becomes smaller or bigger in stratified fluid than that in non-stratified fluid, which is quite in with the laboratory agreement experiment on turbulent diffusion in stratified fluid conducted by Stillinger et al (1997).

**3. Numerical testing and discussion** Under the condition of homogeneous velocity field and constant source the concentration rate can rewritten

$$\frac{\partial \overline{c}}{\partial t} = \frac{\partial}{\partial x_i} (\overline{\rho} K_i \frac{\partial \overline{q}}{\partial x_i})$$
(5)

The efficient turbulent mixing leads to uniform distribution of mixing ratio concentration and finally there is no change for concentration at fixed location. This is why we almost have the constant mixing ratio of  $N_2$ ,  $O_2$  in background atmosphere though the air density is varies with height significantly.

The parameterization by Eq.(4) is correct with density gradient according to above analysis. Namely, the rate of mass concentration should be related to the divergence of mass mixing ratio. The local change rate of mass concentration is dependent on not only the spatial distribution of mass mixing ratio but also that of density as well as eddy diffusivity. The proposed flux-gradient relation which is more accurate parameterization in real world implies that exchange theory cannot be applied directly because the mass concentration is not conservative for vertical motions.

In order to investigate the effects of vertical density gradient on mass concentration, a simple numerical experiment is carried out with assumption of horizontal homogenous and without systemic vertical motion. After manipulating Eq.(3) the dimensionless presentation of Eq.(6) is obtained

$$\frac{\partial c}{\partial t} = \frac{1}{Ts} \left( \frac{\partial^2 c}{\partial z^2} - \frac{1}{\rho} \frac{\partial \rho}{\partial z} \frac{\partial c}{\partial z} \right)$$
(6)

where Ts is the Townsend Number

which is defined by 
$$Ts = \frac{W^* H^*}{K}$$
.

For the sake of simple, the density profile of circumstance fluid is presented as decreasing with height linearly. With this density profile Figure 1-a shows the concentration distribution only dependent on the diffusion term, the first term on the right hands of the Eq.(6). Solid line the initial concentration presents distribution in Gaussian pattern.

dashed line and solid dashed line stands for episodes of concentration distribution with different integration time steps. The figure 1-b shows the concentration distribution resulted only from density correction, the second term on the right hand of Eq.(6). The Figure 1-c is the differences between the concentration with the density correction and that without density It is clear correction. that the concentration at lower level from axes line tends to be greater than that at upper level when density correction is made. Maximum concentration axes becomes slantwise down comparing with that without density correction. The results are highly in agreement with Stohl and Thomson's (1999) study with Lagrangian method to estimate the influence of density profile on concentration distribution in ABL.

The density profile is more complicated other than simple linear relations with height in real ABL on the one hand. The density is not a routine observation term on the other. In order to make density correction easier to practice we can replace the density gradient in Eq.(6) with temperature gradient which is belong to a routine observation factor. In order this to be true we can rewrite density correction term as following by utilizing state equation of gas and hydraulic stationary assumption.

$$\frac{\partial \overline{c}}{\partial t} = K \frac{\partial^2 \overline{c}}{\partial z^2} - K \cdot \frac{1}{\overline{\rho}} \frac{\partial \overline{\rho}}{\partial z} \cdot \frac{\partial \overline{c}}{\partial z} = K \frac{\partial^2 \overline{c}}{\partial z^2} + \frac{K}{\overline{T}} (\gamma)$$
(7)

where  $\gamma_n$  and  $\gamma$  is the lapse rate of homogeneous atmosphere and the change of temperature with height. Absolutely the classic diffusion  $\frac{\partial \overline{c}}{\partial t} = K \frac{\partial^2 \overline{c}}{\partial z^2}$  is only available for homogeneous atmosphere with  $\gamma = \gamma_n$ , however, for general real atmosphere we have  $\gamma < \gamma_n$ . Let  $\frac{K}{\overline{T}}(\gamma_n - \gamma) = \dot{\omega}(z)$  then we have

$$\frac{\partial \overline{c}}{\partial t} - \dot{\omega}(z) \frac{\partial \overline{c}}{\partial z} = K \frac{\partial^2 \overline{c}}{\partial z^2}$$

The resulting equation implies that the constrained layer with the effects of downward transport and decreasing upward flux, which is in agreement with Stillinger et al (1983) laboratory results. Especially under the condition inversion that is available  $\gamma = -\frac{\partial T}{\partial z} < 0$  the density correction effect is significant. In order to validate above argument we can manipulate Eq.(7) into dimensionless form on which the simple numerical test is carried out. The results can clearly be shown in Figure 2.

## 4. Conclusion

Based on above discussion distribution scalar property in stratified ABL is highly dependent on density profile which is more significant in the condition of stratification. The leads higher stratification to -eqn equivalent the equivalent term of ABL duo to the downward transport effects caused by density profile. The resulting distribution non Gaussian with declined center line can be found. The derived density correction in this paper is likely reasonable when the turbulent diffusion and transport processes of pollutants in ABL and UMLO are taken account into properly. In order to investigate the density influences on mass concentration distribution the simplified constant eddy diffusivity is assumed in the paper, however, eddy diffusivity is highly dependent on stability and wind shear in ABL which results in very different turbulent exchange processes. As the further study of density correction on turbulent diffusion in ABL the extensive experimentally and theoretically study with a valid eddy diffusivity and real wind shear should be carried out.

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Fig.1 The variations of dimensionless concentration distribution with integration time (a)contribution of diffusion; (b)density correction (c) summation of (a) and (b)



Fig. 5 Variations of dimensionless concentration at heights below the top of inversion layer. (a) contribution of diffusion (b) density correction (c) summation of (a) and (b)