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# Nonlocal-closure schemes for use in air quality and environmental models

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## 1. Introduction

The description of the atmospheric boundary layer (ABL) processes, understanding of complex boundary layer interactions, and their proper parameterization are important for air quality as well as many other environmental models. In that sense single-column vertical mixing models are comprehensive enough to describe processes in ABL. Therefore, they can be employed to illustrate the basic concepts on boundary layer processes and represent serviceable tools in boundary layer investigation. When coupled to 3D models, single-column models can provide detailed and accurate simulations of the ABL structure as well as mixing processes.

Description of the ABL during convective conditions has long been a major source of uncertainty in the air quality models and chemical transport models. There exist two approaches, local and nonlocal, for solving the turbulence closure problem. While the local closure assumes that turbulence is analogous to molecular diffusion in the nonlocal-closure, the unknown quantity at one point is parameterized by values of known quantities at many points in space. The simplest, most popular local closure method in Eulerian air quality and chemical transport models is the K-Scheme used both in the boundary layer and the free troposphere. Since it uses local gradients in one point of model grid, K-Scheme can be used only when the scale of turbulent motion is much smaller than the scale of mean flow (Stull, 1988), such as in the case of stable and neutral conditions in the atmosphere in which this scheme is consistent. However, it can not: (a) describe the effects of large scale eddies that are dominant in the convective boundary layer (CBL) and (b) simulate counter-gradient flows where a turbulent flux flows up to the gradient. Thus, K-Scheme is not recommended in the CBL (Stull, 1988). Recently, in order to avoid the K-scheme drawbacks, Alapaty (Alapaty, 2003; Alapaty & Alapaty, 2001) suggested a “nonlocal” turbulent kinetic energy (TKE) scheme based on the K-Scheme that was intensively tested using the EMEP chemical transport model (Mihailovic & Jonson, 2005; Mihailovic & Alapaty, 2007). In order to quantify the transport of a passive tracer field in three-dimensional simulations of turbulent convection, the nonlocal and non-diffusive behavior can be described by a transilient matrix whose elements contain the fractional tracer concentrations moving from one subvolume to another as a function of time. The approach was originally developed for and applied to geophysical flows known as turbulent transilient theory (T3) (Stull, 1988; Stull & Driedonks,

1987; Alapaty et al., 1997), but this formalism was extended and applied in an astrophysical context to three-dimensional simulations of turbulent compressible convection with overshoot into convectively stable bounding regions (Miesch et al., 2000). The most frequently used nonlocal-closure method is the asymmetric convective model (ACM) suggested by Pleim & Chang (1992). The design of this model is based on the Blackadar's scheme (Blackadar, 1976), but takes into account the important fact that, in the CBL, the vertical transport is asymmetrical (Wyngaard & Brost, 1984). Namely, the buoyant plumbs are rather fast and narrow, while downward streams are wide and slow. Accordingly, transport by upward streams should be simulated as nonlocal and transport by downward streams as local. The concept of this model is that buoyant plumbs rise from the surface layer and transfer air and its properties directly into all layers above. Downward mixing occurs only between adjacent layers in the form of a slow subsidence. The ACM can be used only during convective conditions in the ABL, while stable or neutral regimes for the K-Scheme are considered. Although this approach results in a more realistic simulation of vertical transport within the CBL, it has some drawbacks that can be elaborated in condensed form: (i) since this method mixes the same amount of mass to every vertical layer in the boundary layer, it has the potential to remove mass much too quickly out of the surface layer and (ii) this method fails to account for the upward mixing in layers higher than the surface layer (Tonnesen et al., 1998). Wang (Wang, 1998) has compared three different vertical transport methods: a semi-implicit K-Scheme (SIK) with local closure and the ACM and T3 schemes with nonlocal-closure. Of the three schemes, the ACM scheme moved mass more rapidly out of surface layer into other layers than the other two schemes in terms of the rate at which mass was mixed between different layers. Recently, this scheme was modified with varying upward mixing rates (VUR), where the upward mixing rate changes with the height, providing slower mixing (Mihailović et al., 2008).

The aim of this chapter is to give a short overview of nonlocal-closure TKE and ABL mixing schemes developed to describe vertical mixing during convective conditions in the ABL. The overview is supported with simulations performed by the chemical EMEP Unified model (version UNI-ACID, rv2.0) where schemes were incorporated.

## 2. Description of nonlocal-closure schemes

### 2.1. Turbulent kinetic energy scheme (TKE)

As we mentioned above the well-known issues regarding local-closure ABL schemes is their inability to produce well-mixed layers in the ABL during convective conditions. Holtslag & Boville (1993) using the NCAR Community Climate Model (CCM2) studied a classic example of artifacts resulting from the deficiencies in the first-order closure schemes. To alleviate problems associated with the general first-order eddy-diffusivity  $K$ -schemes, they proposed a nonlocal  $K$ -scheme. Hong & Pan (1996) presented an enhanced version of the Holtslag & Boville (1993) scheme. In this scheme the friction velocity scale ( $u_*$ ) is used as a closure in their formulation. However, for moderate to strong convective conditions,  $u_*$  is not a representative scale (Alapaty & Alapaty, 2001). Rather, the convective velocity ( $w_*$ ) scale is suitable as used by Hass et al. (1991) in simulation of a wet deposition case in Europe by the European Acid Deposition Model (EURAD). Depending on the magnitude of the scaling parameter  $h/L$  ( $h$  is height of the ABL, and  $L$  is Monin-Obukhov length), either

$u_*$  or  $w_*$  is used in many other formulations. Notice that this approach may not guarantee continuity between the alternate usage of  $u_*$  and  $w_*$  in estimating  $K$  - eddy diffusivity. Also, in most of the local-closure schemes the coefficient of vertical eddy diffusivity for moisture is assumed to be equal to that for heat. Sometimes this assumption leads to vertical gradients in the simulated moisture fields, even during moderate to strong convective conditions in the ABL. Also, the nonlocal scheme considers the horizontal advection of turbulence that may be important over heterogeneous landscapes (Alapaty & Alapaty, 2001; Mihailovic et al. 2005).

The starting point of approach is to consider the general form of the vertical eddy diffusivity equation. For momentum, this equation can be written as

$$K_m = \frac{\bar{e}_* k z \left(1 - \frac{z}{h}\right)^p}{\Phi_m} \quad (1)$$

where  $K_m$  is the vertical eddy diffusivity,  $\bar{e}_*$  is the mean turbulent velocity scale within the ABL to be determined (closure problem),  $k$  is the von Karman constant ( $k = 0.41$ ),  $z$  is the vertical coordinate,  $p$  is the profile shape exponent coming from the similarity theory (Troen & Mahrt, 1986; usually taken as 2), and  $\Phi_m$  is the nondimensional function of momentum. According to Zhang et al. (1996), we use the square root of the vertically averaged turbulent kinetic energy in the ABL as a velocity scale, in place of the mean wind speed, the closure to Eq. (1). Instead of using a prognostic approach to determine TKE, we make use of a diagnostic method. It is then logical to consider the diagnostic TKE to be a function of both  $u_*$  and  $w_*$ . Thus, the square root of diagnosed TKE near the surface serves as a closure to this problem (Alapaty & Alapaty, 2001). However, it is more suitable to estimate  $\bar{e}_*$  from the profile of the TKE through the whole ABL.

According to Moeng & Sullivan (1994), a linear combination of the turbulent kinetic energy dissipation rates associated with shear and buoyancy can adequately approximate the vertical distribution of the turbulent kinetic energy,  $e(z)$ , in a variety of boundary layers ranging from near neutral to free convection conditions. Following Zhang et al. (1996) the TKE profile can be expressed as

$$e(z) = \frac{1}{2} \left( \frac{L_E}{h} \right)^{2/3} \left[ 0.4 w_*^3 + u_*^3 (h - z) \frac{\Phi_m}{kz} \right]^{2/3}, \quad (2)$$

where  $L_E$  characterizes the integral length scale of the dissipation rate. Here,  $\Phi_m = (1 - 15z/L)^{-1/4}$  is an empirical function for the unstable atmospheric surface layer (Businger et al., 1971), which is applied to both the surface and mixed layer. We used  $L_E = 2.6h$  which is in the range  $2.5h - 3.0h$  suggested by Moeng & Sullivan (1994). For the stable atmospheric boundary layer we modeled the TKE profile using an empirical function proposed by Lenschow et al. (1988), based on aircraft observations

$$\frac{e(z)}{u_*^2} = 6 \left( 1 - \frac{z}{h} \right)^{1.75}. \quad (3)$$

Following LES (Large Eddy Simulation) works of Zhang et al. (1996) and Moeng & Sullivan (1994), Alapaty (2003) suggested how to estimate the vertically integrated mean turbulent velocity scale  $\bar{e}_*$  that within the ABL can be written as

$$e_* = \frac{1}{h} \int_0^h \sqrt{e(z)} \Psi(z) dz, \quad (4)$$

where  $\Psi(z)$  is the vertical profile function for turbulent kinetic energy as obtained by Zhang et al. (1996) based on LES studies, later modified by Alapaty (personal communication), and  $dz$  is layer thickness.

The formulation of eddy-diffusivity by Eq. (1) depends on  $h$ . We follow Troen & Mahrt (1986) for determination of  $h$  using

$$h = \frac{Ri_c \left\{ u(h)^2 + v(h)^2 \right\}}{\frac{g}{\theta_0} \left\{ \theta_v(h) - \theta_s \right\}}, \quad (5)$$

where  $Ri_c$  is a critical bulk Richardson number for the ABL,  $u(h)$  and  $v(h)$  are the horizontal velocity components at  $h$ ,  $g / \theta_0$ , is the buoyancy parameter,  $\theta_0$  is the appropriate virtual potential temperature, and  $\theta_v(h)$  is the virtual potential temperature of air near the surface at  $h$ , respectively. For unstable conditions ( $L < 0$ ),  $\theta_s$  is given by (Troen & Mahrt (1986))

$$\theta_s = \theta_v(z_1) + C_0 \frac{\overline{w\theta_{v0}}}{w_s}, \quad (6)$$

where  $C_0 = 8.5$  (Holtslag et al., 1990),  $w_s$  is the velocity while  $\overline{w\theta_{v0}}$  is the kinematics surface heat flux. The velocity  $w_s$  is parameterized as

$$w_s = \left( u_*^3 + c_1 w_*^3 \right)^{1/3} \quad (7)$$

and

$$w_* = \left[ (g / \theta_0) w \theta_{v0} h \right]^{1/3}. \quad (8)$$

Using  $c_1 = 0.6$ . In Eq. (6),  $\theta_v(z_1)$  is the virtual temperature at the first model level. The second term on the right-hand side of Eq. (6) represents a temperature excess, which is a measure in the lower part of the ABL. For stable conditions we use  $\theta_s = \theta_v(z_1)$  with  $z_1 = 2$  m.

On the basis of Eq. (5) the height of the ABL can be calculated by iteration for all stability conditions, when the surface fluxes and profiles of  $\theta_v$ ,  $u$  and  $v$  are known. The computation starts with calculating the bulk Richardson number  $Ri$  between the level  $\theta_s$  and subsequent higher levels of the model. Once  $Ri$  exceeds the critical value, the value of  $h$  is derived with linear interpolation between the level with  $Ri > Ri_c$  and the level underneath. We use a minimum of 100 m for  $h$ . In Eq. (5),  $Ri_c$  is the value of the critical bulk Richardson number used to be 0.25 in this study.

In the free atmosphere, turbulent mixing is parameterized using the formulation suggested by Blackadar (1979) in which vertical eddy diffusivities are functions of the Richardson number and wind shear in the vertical. This formulation can be written as

$$K_m = K_0 + S(kl)^2 \frac{Rc - Ri}{Rc}, \quad (9)$$

where  $K_0$  is the background value ( $1 \text{ m}^2 \text{ s}^{-1}$ ),  $S$  is the vertical wind shear,  $l$  is the characteristic turbulent length scale (100 m),  $Rc$  is the critical Richardson number, and  $Ri$  is the Richardson number defined as

$$Ri = \frac{g}{\theta_v S^2} \frac{\partial \theta_v}{\partial z}. \quad (10)$$

The critical Richardson number in Eq. (9) is determined as

$$Rc = 0.257 (\Delta z)^{0.175}, \quad (11)$$

where  $\Delta z$  is the layer thickness (Zhang & Anthes, 1982).

## 2.2. Nonlocal vertical mixing schemes

The nonlocal vertical mixing schemes were designed to describe the effects of large scale eddies, that are dominant in the CBL and to simulate counter-gradient flows where a turbulent flux flows up to the gradient. During convective conditions in the atmosphere, both small-scale subgrid and large-scale super grid eddies are important for vertical transport. In this section, we will consider three different nonlocal mixing schemes: the Blackadar's scheme (Blackadar, 1976), the asymmetrical convective model (Pleim & Chang, 1992) and the scheme with varying upward mixing rates (Mihailovic et al., 2008).

Transilient turbulence theory (Stull, 1988) (the Latin word *transilient* means to jump over) is a general representation of the turbulent flux exchange processes. In transilient mixing schemes, elements of flux exchange are defined in an  $N \times N$  transilient matrix, where  $N$  is the number of vertical layers and mixing occurs not only between adjacent model layers, but also between layers not adjacent to each other. That means that all of the matrix elements are nonzero and that the turbulent mixing in the convective boundary layer can be written as



$$\frac{\partial c_i}{\partial t} = \sum_{j=1}^N M_{ij} c_j, \quad (12)$$

where  $c$  is the concentration of passive tracer, the elements in the mixing matrix  $M$  represent mass mixing rates, and  $i$  and  $j$  refer to two different grid cells in a column of atmosphere. Some models specify mixing concepts with the idea of reducing the number of nonzero elements because of the cost of computational time during integration.

The *Blackadar's scheme* (Blackadar, 1976) is a simple nonlocal-closure scheme, that is designed to describe convective vertical transport by eddies of varying sizes. The effect of convective plumes is simulated by mixing material directly from the surface layer with every other layer in the convective layer. The schematic representation of vertical mixing simulated by the Blackadar's scheme is given in Fig. 1. The mixing algorithm can be written for the surface and every other layer as

$$\frac{\partial c_1}{\partial t} = -Muc_1 \sum_{i=2}^N \frac{\Delta \xi_i}{\Delta \xi_1} + Mu \sum_{i=2}^N c_i \frac{\Delta \xi_1}{\Delta \xi_i}, \quad (13)$$

and

$$\frac{\partial c_k}{\partial t} = Muc_1 \frac{\Delta \xi_k}{\Delta \xi_1} + Muc_k \frac{\Delta \xi_1}{\Delta \xi_i} \quad (2 < k \leq N), \quad (14)$$

respectively, where  $Mu$  represents the mixing rate,  $\xi$  is the vertical coordinate, and  $\Delta \xi$  denotes the layer thickness. The mixing matrix which controls this model is nonzero only for the top row, the left most column, and the diagonal.

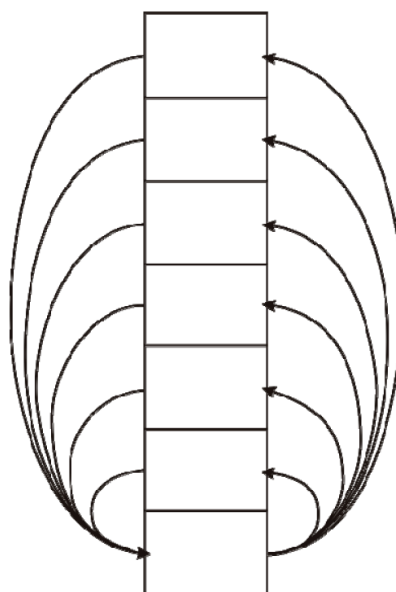


Fig. 1. A schematic representation of vertical mixing in a one dimensional column as simulated by the Blackadar's scheme.

The *asymmetrical convective model* (Pleim & Chang, 1992) is a nonlocal vertical mixing scheme based on the assumption of the vertical asymmetry of buoyancy-driven turbulence. The concept of this model is that buoyant plumes, according to the Blackadar's scheme, rise from the surface layer to all levels in the convective boundary layer, but downward mixing occurs between adjacent levels only in a cascading manner. The schematic representation of vertical mixing simulated by the ACM is presented in Fig. 2a. The mixing algorithm is driven by equations

$$\frac{\partial c_1}{\partial t} = Md_2 c_2 \frac{\Delta \xi_1}{\Delta \xi_2} - Muc_1 \sum_{i=2}^N \frac{\Delta \xi_i}{\Delta \xi_1}, \quad (15)$$

$$\frac{\partial c_k}{\partial t} = Muc_1 - Md_k c_2 + Md_{k+1} c_{k+1} \frac{\Delta \xi_{k+1}}{\Delta \xi_k} \quad (2 < k \leq N), \quad (16)$$

and

$$\frac{\partial c_N}{\partial t} = Muc_1 - Md_N c_N, \quad (17)$$

where  $Mu$  and  $Md$  are the upward and downward mixing rates, respectively. The downward mixing rate from level  $k$  to level  $k-1$  is calculated as

$$Md_k = \frac{\xi_N - \xi_k}{\Delta \xi_k} Mu. \quad (18)$$

The mixing matrix controlling this model is non-zero only for the leftmost column, the diagonal and superdiagonal.

The *scheme with varying upward mixing rates* (VUR scheme), suggested by Mihailović et al. (2008) is a modified version of the ACM, where the upward mixing rate changes with the height, providing slower mixing. The schematic representation of vertical mixing simulated by this scheme is shown in Fig. 2b. The upward mixing rates are scaled with the amount of turbulent kinetic energy in the layer as

$$Mu_k = Mu_1 \frac{e_k \Delta \xi_k}{\sum_{i=1}^N e_i \Delta \xi_i}, \quad (19)$$

where  $Mu_1$  is the upward mixing rate from surface layer to layer above and  $e_k$  denotes the turbulent kinetic energy in the considered layer. The upward mixing rate from surface



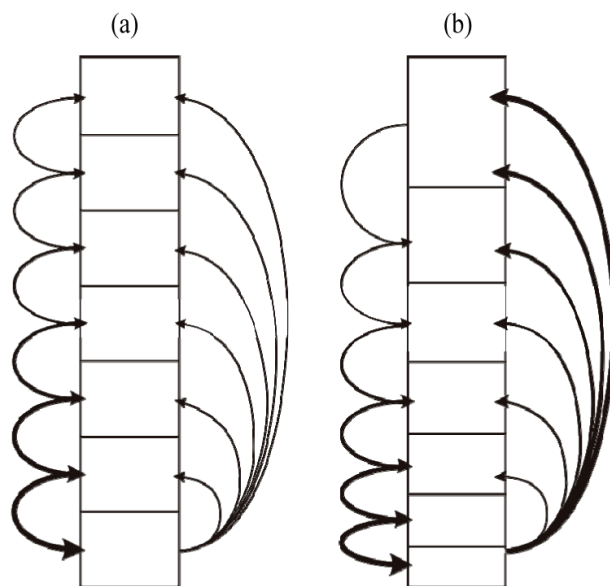


Fig. 2. Schematic representation of vertical mixing in a one-dimensional column as simulated by the (a) ACM and (b) VUR scheme.

layer to layer above is parameterized as

$$Mu_1 = \frac{\rho u_*^4 + H w_*}{h(\rho u_*^3 + H)}, \quad (20)$$

where  $\rho$  is the air density while  $H$  represents the sensible heat flux. Using the VUR scheme, the mixing algorithm for the lowest layer can be written in the form

$$\frac{\partial c_1}{\partial t} = Md_2 c_2 \frac{\Delta \xi_1}{\Delta \xi_2} - Mu_1 c_1 - \sum_{k=3}^N Mu_k c_k. \quad (21)$$

The algorithm for the other layers is very similar to the ACM algorithm [Eqs. (16) and (17)], with the upward mixing rate  $Mu$  substituted with varying upward mixing rates  $Mu_k$ .

### 3. Numerical simulations with nonlocal-closure schemes in the Unified EMEP chemical model

In the EMEP Unified model the diffusion scheme remarkably improved the vertical mixing in the ABL, particularly under stable conditions and conditions approaching free convection, compared with the scheme previously used in the EMEP Unified model. The improvement was particularly pronounced for  $\text{NO}_2$  (Fagerli & Eliassen, 2002). However, with reducing the horizontal grid size and increasing the heterogeneity of the underlying surface in the EMEP Unified model, there is a need for eddy-diffusivity scheme having a higher level of sophistication in the simulation of turbulence in the ABL. It seems that the nonlocal eddy-diffusivity schemes have good performance for that. Zhang et al. (2001) demonstrated some advantages of nonlocal over local eddy-diffusivity schemes. The vertical

sub grid turbulent transport in the EMEP Unified model is modeled as a diffusivity effect. The local eddy-diffusivity scheme is designed following O'Brien (1970). (In further text this scheme will be referred to the OLD one). In the unstable case,  $K_m$  is determined as

$$K_m(z) = K_m(h) + \left( \frac{h-z}{h-h_s} \right)^2 \left\{ [K_m(h_s) - K_m(h)] + (z-h_s) \cdot \left[ \frac{\delta}{\delta_z}(K_m(h_s)) + 2 \cdot \frac{K_m(h_s) - K_m(h)}{h-h_s} \right] \right\} \quad h_s \leq z < h \quad (22)$$

where  $h_s$  is the height of the surface boundary layer. In the model calculation  $h_s$  is set to 4% of height of the ABL.

To compare performances of the proposed nonlocal-closure schemes TKE scheme (Eqs.(1)-(4)) and local OLD scheme (Eq. (22)), both based on the vertical eddy diffusivity formulation, in reproducing the vertical transport of pollutants in the ABL, a test was performed with the Unified EMEP chemical model (UNIT-ACID, rv2\_0\_9).

### 3.1 Short model description and experimental set up

The basic physical formulation of the EMEP model is unchanged from that of Berge & Jacobsen (1998). A polar-stereographic projection, true at 60°N and with the grid size of 50×50 km<sup>2</sup> was used. The model domain used in simulation had (101, 91) points covering the area of whole Europe and North Africa. The  $\sigma$  terrain-following coordinate was used with 20 levels in the vertical- from the surface to 100 hPa and with the lowest level located nearly at 92 m. The horizontal grid of the model is the Arakawa C grid. All other details can be found in Simpson et al. (2003). The Unified EMEP model uses 3-hourly resolution meteorological data from the dedicated version of the HIRLAM (High Resolution Limited Area Model) numerical weather prediction model with a parallel architecture (Bjorge & Skalin, 1995). The horizontal and vertical wind components are given on a staggered grid. All other variables are given in the centre of the grid. Linear interpolation between the 3-hourly values is used to calculate values of the meteorological input data at each advection step. The time step used in the simulation was 600 s.

### 3.2 Comparison with the observations

The comparison of the TKE and VUR schemes with OLD eddy diffusion scheme has been performed, using simulated and measured concentrations of the pollutant NO<sub>2</sub> since it is one of the most affected ones by the processes in the ABL layer. The simulations were done for the years (i) 1999, 2001 and 2002 (TKE scheme) and (ii) 2002 (for VUR scheme) in the months when the convective processes are dominant in the ABL (April-September). The station recording NO<sub>2</sub> in air (μg(N) m<sup>-3</sup>) concentration was considered for comparison when measurements were available for at least 75% of days in a year [1999 (80 stations), 2001 (78) and 2002 (82)]. We have calculated the bias on the monthly basis as (M-O)/O\*100% where M and O denote the modeled and observed values, respectively. The comparison of the modeled and observed NO<sub>2</sub> in air (μg(N) m<sup>-3</sup>) concentrations and corresponding biases for

both schemes (TKE and OLD) are shown in Fig. 3. The values used in calculations were averaged over the whole domain of integration. It can be seen that both schemes underestimate the observations. However, for all considered months, NO<sub>2</sub> concentrations calculated with the TKE scheme are in general higher and closer to the observations than those obtained by the OLD scheme (of the order of 10%). Correspondingly, the bias of the TKE scheme is lower than the OLD scheme. The comparison of the modeled and observed NO<sub>2</sub> in air (μg(N) m<sup>-3</sup>) concentrations between VUR and OLD schemes is shown in Fig. 4. The values used in the calculations were also averaged over the whole domain of integration. It can be seen that both schemes underestimate the observations. However, for all considered months, NO<sub>2</sub> concentrations calculated with the VUR scheme are in general higher and closer to the observations than those obtained using the eddy diffusion scheme (of the order of 15-20%). Accordingly, the bias of the VUR scheme is lower than the OLD eddy diffusion scheme.

To quantify the simulated values of the both schemes we have performed an error analysis of the NO<sub>2</sub> concentration outputs NO<sub>2</sub> based on a method discussed in Pielke (2002). Following that study, we computed several statistical quantities as follows

$$\nu = \left[ \sum_{i=1}^N (\Gamma_i - \hat{\Gamma}_i)^2 / N \right]^{1/2}, \quad (23)$$

$$\nu_{BR} = \left\{ \sum_{i=1}^N [(\Gamma_i - \bar{\Gamma}) - (\hat{\Gamma}_i - \bar{\hat{\Gamma}})] / N \right\}^{1/2}, \quad (24)$$

$$\eta = \left[ \sum_{i=1}^N (\Gamma_i - \bar{\Gamma})^2 / N \right]^{1/2}, \quad (25)$$

$$\hat{\eta} = \left[ \sum_{i=1}^N (\hat{\Gamma}_i - \bar{\hat{\Gamma}})^2 / N \right]^{1/2}. \quad (26)$$

Here,  $\Gamma$  is the variable of interest (aforementioned variables in this study) while  $N$  is the total number of data. An overbar indicates the arithmetic average, while a caret refers to an observation. The absence of a caret indicates a simulated value;  $\nu$  is the rmse, while  $\nu_{BR}$  is rmse after a bias is removed. Root-mean-square errors (rmse) give a good overview of a dataset, with large errors weighted more than many small errors. The standard deviations in the simulations and the observations are given by  $\eta$  and  $\hat{\eta}$ . A rmse that is less than the standard deviation of the observed value indicates skill in the simulation. Moreover, the values of  $\eta$  and  $\hat{\eta}$  should be close if the prediction is to be considered realistic.

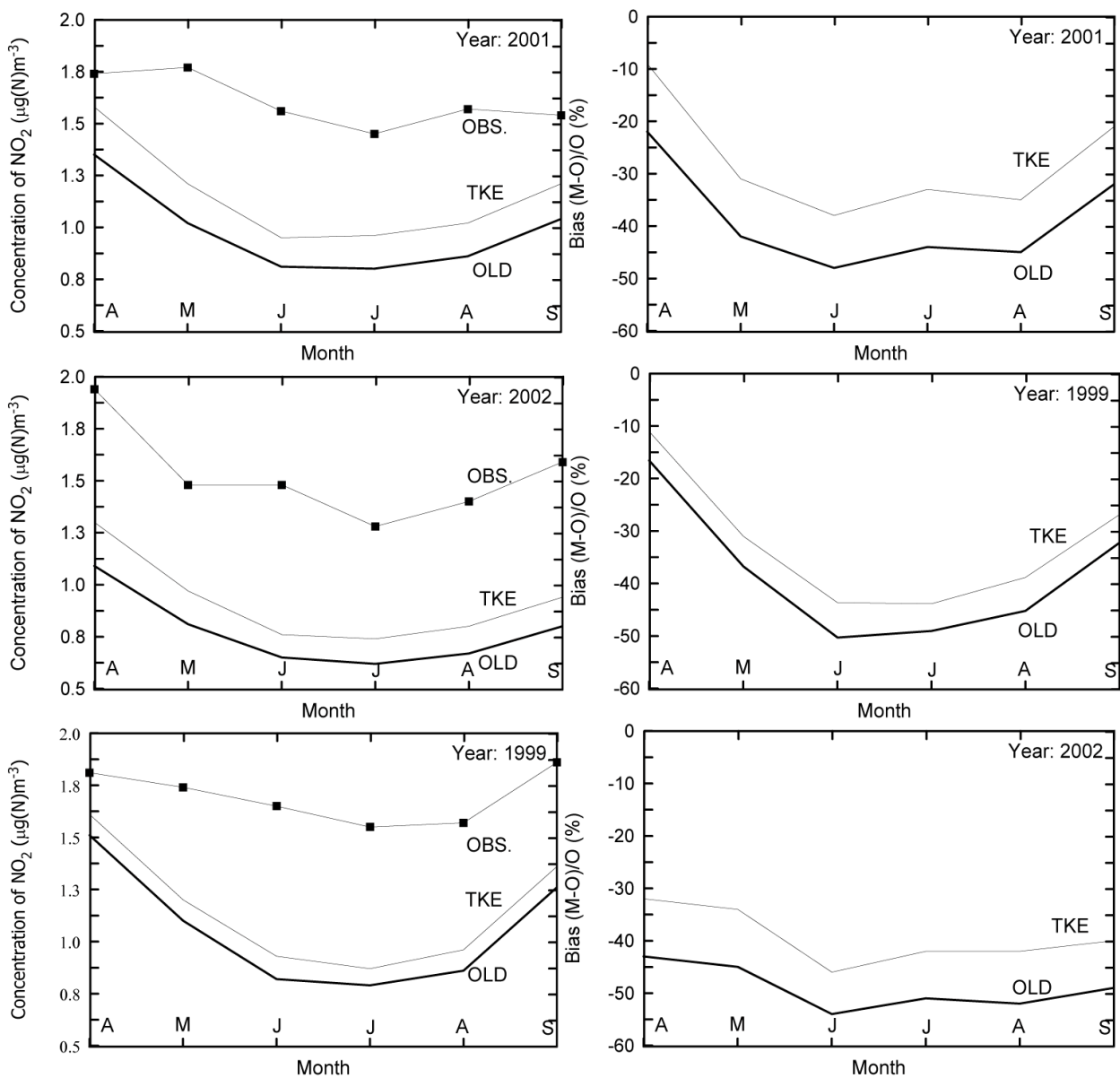


Fig. 3. The eddy diffusion (OLD) versus TKE scheme. Comparison of: the modeled and observed NO<sub>2</sub> in air (μg(N) m<sup>-3</sup>) concentrations (left panels) and their biases (right panels) in the period April-September for the years 1999, 2001 and 2002. M and O denotes modeled and observed value, respectively.

The statistics gave the following values: (1) TKE ( $\nu = 0.548, \nu_{BR} = 0.293, \eta = 0.211, \hat{\eta} = 0.147$ ) and OLD ( $\nu = 0.802, \nu_{BR} = 0.433, \eta = 0.303, \hat{\eta} = 0.147$ ) and (2) VUR ( $\nu = 0.571 \mu\text{g(N) m}^{-3}, \nu_{BR} = 0.056 \mu\text{g(N) m}^{-3}, \eta = 0.219 \mu\text{g(N) m}^{-3}, \hat{\eta} = 0.211 \mu\text{g(N) m}^{-3}$ ) and OLD ( $\nu = 0.802, \nu_{BR} = 0.159, \eta = 0.303, \hat{\eta} = 0.211$ ). A comparison of  $\eta$  and  $\hat{\eta}$ , for (1) and (2), shows that difference between them, is evidently smaller with the TKE and VUR scheme schemes versus the OLD one.

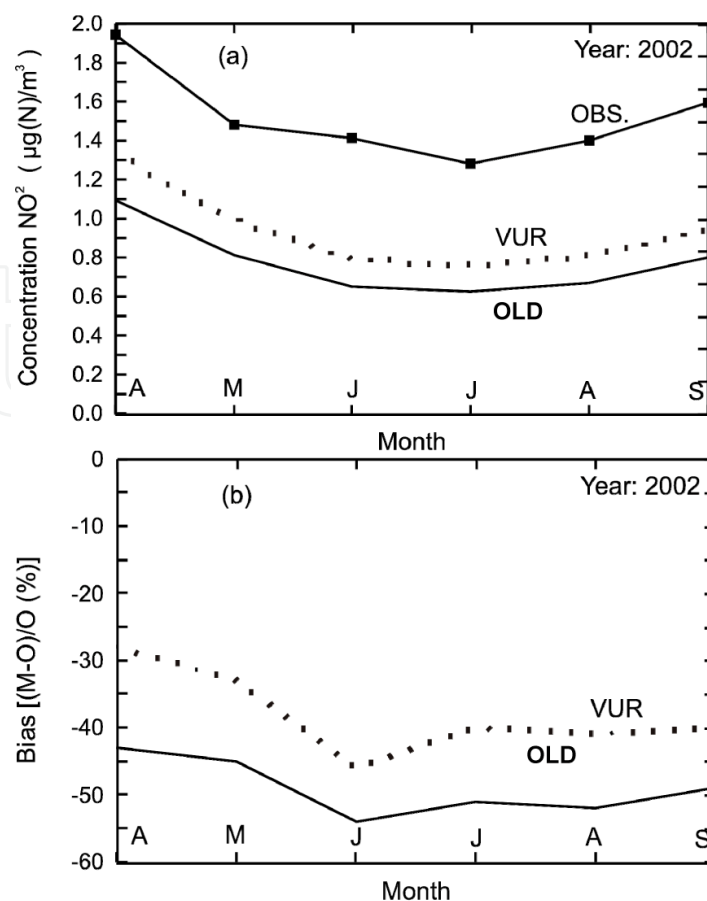


Fig. 4. The eddy diffusion (OLD) versus the VUR scheme. Comparison of: (a) the modelled and observed NO<sub>2</sub> in air ( $\mu\text{g(N) m}^{-3}$ ) concentrations and (b) their biases in the period April-September for the year 2002. M and O denotes modelled and observed value, respectively.

#### 4. Conclusions

In the ABL during convective conditions, when much of the vertical mixing is driven by buoyant plumes, we cannot properly describe mixing processes using local approach and eddy diffusion schemes. Nonlocal-closure schemes simulate much better vertical mixing than local ones. In this chapter, two nonlocal schemes (the TKE scheme and the VUR scheme) for applications in air quality and environmental models are described. The comparison of the TKE scheme and the VUR one with an eddy diffusion scheme (OLD) commonly used in chemical transport models was done. These comparisons were performed with the EMEP Unified chemical model using simulated and measured concentrations of the pollutant NO<sub>2</sub> since it is one of the most affected ones by the processes in the ABL layer. Nonlocal schemes gave better results than local one.

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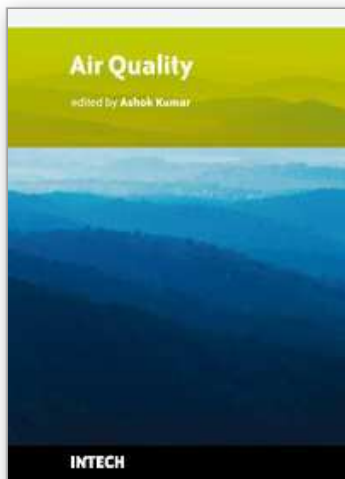
## 5. References

- Alapaty, K.; Pleim, J.E.; Raman, S.; Niyogi, D.S. & Byun, D.W. (1997). Simulation of atmospheric boundary layer processes using local- and nonlocal-closure schemes, *Journal of Applied Meteorology*, 36, 214–233 ISSN 0894-8763
- Alapaty, K. & Alapaty, M. (2001). Development of a diagnostic TKE schemes for applications in regional and climate models using MM5. *Research Note*, MCNC-North Carolina Supercomputing Center, Research Triangle Park, NC, pp. 5.
- Alapaty, K. (2003). Development of two CBL schemes using the turbulence velocity scale. *4th WRF Users' workshop*, Boulder, Colorado, June 25-27.
- Blackadar, A.K. (1976). Modeling the nocturnal boundary layer. *Proceedings of 4th Symposium of Atmospheric Turbulence, Diffusion and Air Quality*, pp. 46-49, Boston, American Meteorological Society
- Blackadar, A.K. (1979). Modeling pollutant transfer during daytime convection. *4th Symposium on Atmospheric Turbulence Diffusion and Air Quality*, Reno, NV, American Meteorological Society, pp. 443-447.
- Berge, E. & Jacobsen H.A. (1998). A regional scale multi-layer model for the calculation of long-term transport and deposition of air-pollution in Europe. *Tellus. Series B, Chemical and physical meteorology*, 50, 205-223, ISSN 0280-6509
- Bjorge, D. & Skalin, R. (1995). PARLAM – the parallel HIRLAM version of DNMI. Research Report No. 27, Norwegian Meteorological Institute, Oslo, Norway, ISSN 0332-9879
- Businger, J.A.; Izumi, Y. & Bradley, E.F. (1971). Flux profile relationships in the atmospheric surface layer. *Journal of the Atmospheric Sciences*, 28, 181-189.
- Fagerli, H. & Eliassen, A. (2002). Modified parameterization of the vertical diffusion. In: Transboundary acidification, eutrophication and ground level ozone in Europe. EMEP Summary Status Report, *Research Report No. 141*, Norwegian Meteorological Institute, Oslo, Norway, pp. 74.
- Hass, H.; Jacobs, H.J.; Memmesheimer, M.; Ebel, A. & Chang, J.S. (1991). Simulation a wet deposition case in Europe using European Acid Deposition Model (EURAD). In: *Air Pollution modeling and its Applications VIII*, pp. 205-213, Plenum Press, New York
- Holtstag, A.A.M.; de Bruin, E.I.F. & Pan, H.-L. (1990). A high resolution air mass transformation model for short-range weather forecasting. *Monthly Weather Review*, 118, 1561-1575, ISSN 0027-0644
- Holtstag, A.A.M. & Boville, B.A. (1993). Local versus nonlocal boundary layer diffusion in a global climate model. *Journal of Climate*, 6, 1825-1842, ISSN 0894-8755
- Hong, S.Y. & Pan, H.L., (1996). Nonlocal boundary layer vertical diffusion in a medium-range forecast model. *Monthly Weather Review*, 124, 2322-2339, ISSN 0027-0644
- Lenschow, D.H.; Li, X.S. & Zhu, C.J. (1988). Stably stratified boundary layer over the Great Plains. Part I: Mean and turbulent structure. *Boundary-Layer Meteorology*, 42, 95-121, ISSN 0006-8314
- Miesch, M.S.; Brandenburg, A.; Zweibel, A. & Zweibel, E.G. (2000). Nonlocal transport of passive scalars in turbulent penetrative convection. *Physical Review E*, 61, 457-467, ISSN 1539-3755
- Mihailovic D.T. & Jonson J.E. (2005). *Implementation of a TKE scheme in the Unified EMEP model. Air Pollution report 5/2005*, Norwegian Meteorological Institute, Oslo, ISSN 1503-8025.



- Mihailovic, D.T.; Rao, S.T.; Alapaty, K.; Ku, J.Y.; Arsenic, I. & Lalic, B. (2005). A study of the effects of subgrid-scale representation of land use on the boundary layer evolution using 1-D model. *Environmental Modelling and Software*, 20, 705-714, ISSN 1364-8152
- Mihailovic, D.T. & Alapaty, K. (2007). Intercomparison of two K-schemes: Local versus non-local in calculating concentrations of pollutants in chemical and air-quality models. *Environmental Modelling and Software*, 22, 1685-1689, ISSN 1364-8152
- Mihailović, D.T.; Alapaty, K. & Sakradžija, M. (2008). Development of a nonlocal convective mixing scheme with varying upward mixing rates for use in air quality and chemical transport models *Environmental Software and Pollution Research*, 15, 296-302, ISSN 0944-1344
- Moeng, C.-H. & Sullivan, P.P. (1994). A comparison of shear and buoyancy driven planetary-boundary-layer flows. *Journal of the Atmospheric Sciences*, 51, 999-1022, ISSN 0022-4928
- O'Brien, J.J. (1970). A note on the vertical structure of the eddy exchange coefficient in the planetary boundary layer. *Journal of the Atmospheric Sciences*, 27, 1213-1215, ISSN 0022-4928
- Pielke, R.A., Sr. (2002). *Mesoscale Meteorological Modeling*. 2<sup>nd</sup> ed. Academic Press, 676 pp. San Diego, CA.
- Pleim, J.E. & Chang, J. S. (1992). A non-local closure model for vertical mixing in the convective boundary layer. *Atmospheric Environment*, A26, 965-981, ISSN 1352-2310
- Simpson, D.; Fagerli, H.; Jonson, J.E.; Tsyro, S.; Wind, P. & Tuovinen, J.-P. (2003). Transboundary acidification, eutrophication and ground level ozone in Europe. Part I: Unified EMEP Model Description. *EMEP Status Report 2003*, pp. 74, The Norwegian Meteorological Institute, Norway
- Stull, R.B. & Driedonks A.G.M. (1987) Applications of the transilient turbulence parameterization to atmospheric boundary-layer simulations. *Boundary-Layer Meteorology*, 40, 209-239, ISSN 0006-8314
- Stull, R.B. (1988). *An Introduction to Boundary Layer Meteorology*, Dordrecht: Kluwer.
- Tonnesen, G.; Olaguer, J.; Bergin, M.; Russell, T.; Hanna, A.; Makar, P.; Derwent, D. & Wang, Z. (1998). *Air quality models*. Draft as of 11/26/98, pp. 55.
- Troen, I. & Mahrt, L. (1986). A simple model of the atmospheric boundary layer; sensitivity to surface evaporation. *Boundary-Layer Meteorology*, 37, 129-148 ISSN 0006-8314
- Wang, Z. (1998). Computing volatile organic compound reactivities with a 3-D AQM *Proceedings of the photochemical Reactivity Workshop*, U.S. Environmental protection Agency, Durham, NC.
- Wyngaard, J.C. & Brost, R.A. (1984). Top-down and bottom-up diffusion of a scalar in the convective boundary layer. *Journal of the Atmospheric Sciences*, 41, 102-112, ISSN 0022-4928
- Zhang, D. & Anthes, R.C. (1982). A high-resolution model of the planetary boundary-layer-sensitivity tests and comparisons with SESAME-79 data. *Journal of Applied Meteorology*, 21, 1594-1609, ISSN 0894-8763
- Zhang, C.; Randall, D.A.; Moeng, C.-H.; Branson, M.; Moyer, M. & Wang, Q. (1996). A surface parameterization based on vertically averaged turbulence kinetic energy. *Monthly Weather Review*, 124, 2521-2536, ISSN 0027-0644
- Zhang, K.; Mao, H.; Civerolo, K.; Berman, S., Ku, J.-Y.; Rao, S.T.; Doddridge, B.; Philbrick, C.R. & Clark, R. (2001). Numerical investigation of boundary layer evolution and nocturnal low-level jets: local versus non-local PBL schemes. *Environmental Fluid Mechanics*, 1, 171-208, ISSN 1567-7419





## **Air Quality**

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Air pollution is about five decades or so old field and continues to be a global concern. Therefore, the governments around the world are involved in managing air quality in their countries for the welfare of their citizens. The management of air pollution involves understanding air pollution sources, monitoring of contaminants, modeling air quality, performing laboratory experiments, the use of satellite images for quantifying air quality levels, indoor air pollution, and elimination of contaminants through control. Research activities are being performed on every aspect of air pollution throughout the world, in order to respond to public concerns. The book is grouped in five different sections. Some topics are more detailed than others. The readers should be aware that multi-authored books have difficulty maintaining consistency. A reader will find, however, that each chapter is intellectually stimulating. Our goal was to provide current information and present a reasonable analysis of air quality data compiled by knowledgeable professionals in the field of air pollution.

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