Impact of Local and Non-local Eddy-Diffusivity Schemes on Calculating the Concentration of Pollutants in Environmental Models

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Abstract: In this paper, we studied a local and a non-local scheme for vertical diffusion in the atmospheric boundary layer and their impact on the concentration of pollutants calculated with an environmental model. In the local diffusion scheme, the eddy-diffusivity is determined independently at each point in the vertical based on local vertical gradients of wind and potential temperature. The non-local scheme determines an eddy-diffusivity profile based on a diagnosed boundary layer height and a turbulent vertical scale. To compare these two approaches, we used a local (O'Brien [1970]) and a modified non-local (Alapaty [2003]) diffusivity scheme. Compared to the original, the modification introduced in the non-local scheme included different values of the parameter p in the equation for eddy-diffusivity depending on the stability regime. For the unstable conditions, the parameter p was set to 2, a value commonly used in parameterizations in regional climate modeling, while for stable conditions we used a value of 1.5 based on numerical experiments. To examine the performance of the schemes, simulated and measured concentrations of the pollutant believed to be one of the most affected ones by the processes in the atmospheric boundary layer (NO_2) were compared for the years 1999, 2001 and 2002. The comparison was made for the whole domain used in simulations performed by the chemical EMEP Unified model (version UNI-ACID, rv2.0).
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Keywords: Atmospheric boundary layer, Non-local closure model, Turbulent kinetic energy, Atmospheric chemistry, Environmental modeling.

1. INTRODUCTION

One of the well-known issues regarding local-closure atmospheric boundary layer (ABL) schemes is their inability to produce well-mixed layers in the ABL during convective conditions. Holtslag and 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 non-local K-scheme. Hong and Pan [1996] presented an enhanced version of the Holtslag and 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 and 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 depth of the atmospheric boundary layer (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, none of the first-order schemes consider the horizontal advection of turbulence that may be important over heterogeneous landscapes (Alapaty and Alapaty, [2001]; Mihailovic et al. [2004]; Mihailovic et al. [2005]).

In this paper, we propose a modified version of a first-order non-local K-scheme (Alapaty, [2003]),

addressing the deficiencies discussed above. The main feature of the scheme that has been used for tests in this study is shortly described in Section 2. The results of comparison with observations obtained by the Unified EMEP model (Simpson et al., [2003]), using local and non-local diffusivity schemes for the years 1999, 2001 and 2002, are presented in Section 3.

2. METHODOLOGY

2.1 Description of the TKE vertical diffusion scheme

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

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

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 and Mahrt, [1986]; usually taken as 2), and Φ_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 (TKE) 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 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 and Alapaty [2001]). However, it is more suitable to $\bar{e}_*$ from the profile of the TKE through the whole ABL.

According to Moeng and 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 (TKE), $e(z)$, in a variety of boundary layer ranging from near neutral to free convection conditions. Following Zhang et al. [1996] the TKE profile can be expressed as

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

where L_E characterizes the integral length scale oft he 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 and 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

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

Following LES (Large Eddy Simulation) works of Zhang et al. [1994] and Moeng and 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

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

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

The formulation of eddy-diffusivity by Eq. (1) depends on the boundary layer height h. We follow Troen and Mahrt [1986] for determination of h using

$$h = \frac{Ri_c\left\{u(h)^2 + v(h)^2\right\}}{\frac{g}{T_0}\left\{\theta_v(h) - \theta_s\right\}}, \qquad (5)$$

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/T_0 is the buoyancy parameter, $\theta_v(h)$ is the virtual temperature at h, and θ_s is the appropriate temperature of air near the surface. For unstable conditions $(L \prec 0)$, θ_s is given by (Troen and Mahrt [1986])

$$\theta_s = \theta_v(z_1) + C_0\frac{\overline{w\theta_0}}{w_s}, \qquad (6)$$

Where $C_0 = 8.5$ (Holtslag et al., [1990]), w_s is the

velocity while $\overline{w\theta_0}$ is the kinematic surface heat flux. The velocity w_s is parameterized as

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

$$w_* = \left((g/T)\overline{w\theta_0}h\right)^{1/3} \quad (8)$$

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 rhs 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 $z_1 = 2m$. On the basis of Eq. (5) the boundary layer height can be calculated by iteration for all stability conditions, when the surface fluxes and profiles of θ_v, u and v are known. The computation starts with calculating the bulk Richardson number Ri between the level θ_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 $Ri \succ Ri_c$ 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, which generally depends on the vertical resolution of the model. For coarse model resolution, $Ri_c = 0.5$ can be used (Troen and Mahrt, [1986]). In this study we use the theoretical value $Ri_c = 0.25$ that is suggested in the case of a higher vertical resolution.

The Monin-Obukhov length L is calculated as

$$L = -\frac{T_L u_*^3 \rho C_p}{kgH} \quad (9)$$

where T_L is the temperature at the lowest model level, C_p is the specific heat capacity of dry air, ρ is the air density (derived from the surface pressure and temperature) and g is the gravitational acceleration. The sign here is consistent with sensible heat flux H (its positive sign gives unstable conditions). 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

$$K_m = K_0 + S(kl)^2 \frac{Rc - Ri}{Rc} \quad (10)$$

where K_0 is the background value (1 $m^2\ s^{-1}$), 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

$$Ri = \frac{g}{\theta_v S^2}\frac{\partial \theta_v}{\partial z}. \quad (11)$$

The critical Richardson number in Eq. (10) is determined as (Zhang and Anthes [1982])

$$Rc = 0.257(\Delta z)^{0.175} \quad (12)$$

where Δz is the layer thickness.

2.2 Implementation in the EMEP Unified model

The vertical sub grid turbulent transport in the EMEP Unified model is modeled as a diffusivity effect. The turbulent transfer coefficient K_m is derived from basic meteorological parameters. The local diffusivity scheme is designed following O'Brien [1970], which is described in more detail in Fagerli and Eliassen [2002]. This 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. 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 K-schemes having a higher level of sophistication in the simulation of turbulence in the ABL. It seems that the non-local diffusion schemes have good performance for that. A lot of chemical models have already implemented this kind of scheme. Recently, Zhang et al. [2001] demonstrated some advantages of non-local over local diffusion schemes.

3. TESTS AND RESULTS

3.1 Experimental set up and tests description

To examine the success of the proposed non-local TKE scheme based on the vertical eddy diffusivity formulation in reproducing the vertical transport of pollutants in the ABL, a model sensitivity was performed with the Unified EMEP model (UNIT-ACID, rv2_0_9). This version of the model does not include photochemistry. The basic physical

formulation of the EMEP model is unchanged from that of Berge and Jacobsen [1998]. The model uses the same horizontal and vertical grid as the meteorological data (Simpson et al. [2003]) - a polar-stereographic projection, true at 60^0 N, is used. At 60^0 N the grid size is $50x50km^2$. The model domain used had 130x97 grid cells. The model is defined vertically with the terrain following σ coordinate with 20 from the surface to 100 hPa with the lowest level located nearly 92 m in depth. The horizontal grid of the model is the Arakawa C grid. All other details can be found in Simpson at al. [2003]. The Unified EMEP model uses 3-hourly resolution meteorological data from the dedicated version of the HIRAM (High Resolution Limited Area Model) Numerical Weather Prediction Model (NWPM) with a parallel architecture (Bjorge and Skaling [1995]). The horizontal winds are given on a staggered grid (this is also the case with the vertical wind component. All other variables are given in the center 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. We performed the runs for the following years: 1999, 2001 and 2002.

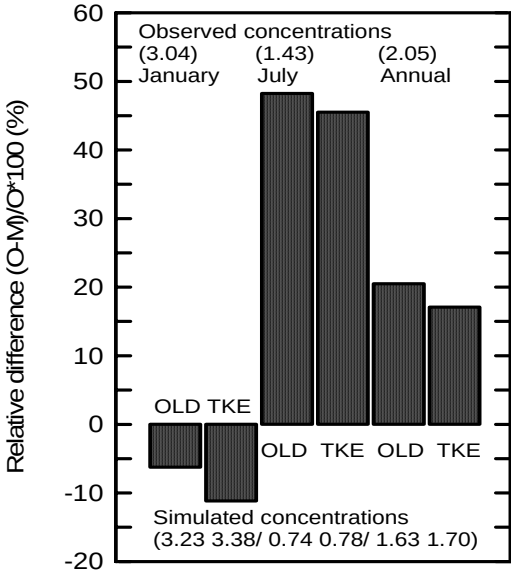

Figure 1. Comparison of simulated (OLD) versus observed (TKE) NO_2 in air ($\mu g(N)m^{-3}$) concentrations averaged over the period of three years. O and M denote the observed and measured values, respectively.

3.1 Comparison with the observations

To examine the performance of the proposed TKE scheme, simulated and measured concentrations of the pollutant believed to be one of the most affected ones by the processes in the ABL layer (NO_2) have been compared. For comparison, results obtained with the old scheme are also shown. The comparison was made for the whole domain used in the simulations. The calculated results obtained by both schemes (OLD and TKE) and the measured values of NO_2 for the years 1999, 2001 and 2002 (36 stations through the whole domain of integration) are shown in Figure 1. In general, the results obtained with the two schemes are similar. The NO_2 concentrations calculated with the TKE scheme are in general higher for all seasons (of the order of 10%) and thus on average closer to the observations for all three years. The other statistical parameters (bias, rmse) are mostly unchanged. The model, with both schemes, under-predicts NO_2 concentrations on an annual basis, particularly in summer (July). Concentrations with both schemes are over-predicted in winter (January), but they are less so with the OLD scheme. We realize that the results depend on the different interactions of the two diffusion schemes with the other part of the model. Since no attempt was made to calibrate the diffusion schemes to give the best possible simulations, the present comparisons can only serve as illustrations of the impact.

3.2 Conclusions and recommendation

In this study we have considered the impact of a local and a non-local scheme for vertical diffusion in the atmospheric boundary layer calculated with the EMEP Unified model (version UNI-ACID, rv2.0). In the local diffusion scheme the eddy diffusivity is determined independently at each point in the vertical based on local vertical gradients of wind and potential temperature following O'Brien [1970]. The non-local scheme determines an eddy-diffusivity profile based on a diagnosed boundary layer height and a turbulent vertical scale partly following Alapaty [2003].

Compared to the original scheme (Alapaty [2003]), we have slightly modified the TKE scheme. This modification includes different values of the parameter, p in this equation depending on the stability regime. For the unstable conditions, the parameter p is set to

2, a value commonly used in parameterizations in regional climate and air pollution modelling, while for stable conditions we used a value of 1.5 based on numerical experiments, i.e. comparison of the simulated and observed concentrations.

The outputs of the local and non-local diffusion schemes (obtained from numerical experiment using 3D simulation with both schemes for the years 1999, 2001, 2002) have been analyzed and compared with the model calculated concentrations (μgm^{-3}) of the pollutant most affected by the processes in the ABL layer (NO_2). The OLD scheme is used as a reference when assessing how well the TKE scheme simulates the mixing processes in the ABL.

Differences between them are seen with annual differences of the order of 10%. The comparison over single stations in some regions (coastal area and valley topography) indicates that the TKE scheme gives better results than the OLD one at these sites. Let us note that the TKE scheme is less time consumable then the OLD one.

Future studies with this non-local scheme may focus on the interaction of the scheme with the hydrological cycle, for example, deep and shallow convection, and the land-surface parameterization. Special consideration may be given to the entrainment process at the top of the boundary layer. Further improvements may consider the influence of entrainment on the scalar mixing and consistent treatment of cloud diffusion within the non-local scheme.

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REFERENCES

Alapaty, K., Development of two CBL schemes using the turbulence velocity scale, paper presented at 4th WRF Users' workshop, Boulder, Colorado, June 25-27, 2003.

Alapaty, K., and M. Alapaty, 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, 2001.

Blackadar, A.K., Modeling pollutant transfer during daytime convection. Paper presented at 4th Symposium on Atmospheric Turbulence Diffusion and Air Quality, Reno, NV, Amer. Meteor. Soc., 443-447, 1979.

Berge, E., and H.A. Jacobsen, A regional scale multi-layer for the calculation of long-term transport and deposition of air-pollution in Europe, *Tellus*, 50, 205-223, 1998.

Bjorge, D., and R. Skalin, PARLAM – the parallel HIRLAM version of DNMI. Research Report, No. 27, ISSN 0332-9879, Norwegian Meteorological Institute, Oslo, Norway, 1995.

Businger, J.A., Y. Izumi, and E.F. Bradley, Flux profile relationships in the atmospheric surface layer, *J. Atmos. Sci.*, 28, 181-189, 1971.

Fagerli, H., and A. Eliassen, 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, 2002.

Hass, H., H.J. Jacobs, M. Memmesheimer, A. Ebel, and J.S. Chang, Simulation a wet deposition case in Europe using European Acid Deposition Model (EURAD). In *Air Pllution modeling and its Applications* VIII, Plenum Press, New York, 205-213, 1991.

Holtslag, A.A.M., and B.A. Boville, Local versus nonlocal boundary layer diffusion in a global climate model*, J. Clim.*, 6, 1825-1842, 1993.

Holtslag, A.A.M., E.I.F. de Brujin, and H.-L. Pan, 1990, A high resolution air mass transformation model for short-range weather forecasting, *Mon. Wea. Rev.*, 118, 1561-1575, 1990.

Hong, S.Y., and H.L. Pan, Nonlocal boundary layer vertical diffusion in a medium-range forecast model, *Mon. Wea. Rev.*, 124, 2322-2339, 1996.

Lenschow, D.H., X.S. Li, and C.J. Zhu, Stably stratified boundary layer over the Great Plains. Part I: Mean and turbulent structure, *Bound.-Layer Meteor.*, 42, 95-121, 1988.

Mihailovic, D.T., K. Alapaty, B. Lalic, I. Arsenic, B.Rajkovic, and S. Malinovic, Turbulent transfer coefficient and calculation of air temperature inside tall grass canopies in land-atmosphere schemes for environmental modelling, *J. Appl. Meteor.*, 43, 1498-1512, 2004.

Mihailovic, D.T., S.T. Rao, K. Alapaty, J.Y. Ku, I. Arsenic, and B. Lalic, A study of the effects of subgrid-scale representation of land use on the boundary layer evolution using 1-D model. *Enivorn. Modelling and Software*, 20, 705-714, 2005.

Moeng., C.-H., and P.P. Sullivan, A comparison of shear and buoyancy driven planetary-boundary-layer flows. *J. Atmos. Sci.*, 51, 999-1022, 1994.

O'Brien, J.J., A note on the vertical structure of the eddy exchange coefficient in the planetary boundary layer, *J. Atmos. Sci.*, 27, 1213-1215, 1970.

Simpson, D., H. Fagerli, J.E. Jonson, S. Tsyro, P. Wind, J._P. Tuovinen, Transboundary acidification, eutrophication and ground level ozone in Europe. Part I: Unified EMEP Model Description. EMEP Status Report 2003, The Norwegian Meteorological Institute, Norway, pp. 74, 2003.

Troen, I., and L. Mahrt, A simple model of the atmospheric boundary layer; sensitivity to surface evaporation, *Boundary-Layer Meteorol.*, 37, 129-148, 1986.

Zhang, D., and R.C. Anthes, A high-resolution model of the planetary boundary-layer-sensitivity tests and comparisons with SESAME-79 data, *J. Appl. Meteor.*, 21, 1594-1609, 1982.

Zhang, C., D.A., Randall, C.-H., Moeng, M. Branson, M. Moyer, and Q. Wang, A surface parameterization based on vertically averaged turbulence kinetic energy, *Mon. Wea. Rev.*, 124, 2521-2536, 1996.

Zhang, K., H. Mao, K. Civerolo, S. Berman, J.-Y, Ku, S.T. Rao, B. Doddridge, B., C.R. Philbrick, and R. Clark, Numerical investigation of boundary layer evolution and nocturnal low-level jets: local versus non-local PBL schemes, *Environ. Fluid Mech.*, 1, 171-208, 2001.