A NON-LOCAL CLOSURE MODEL FOR VERTICAL MIXING IN THE CONVECTIVE BOUNDARY LAYER

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Abstract—A simple non-local closure model for vertical mixing in Convective Boundary Layers (CBL) has been developed specifically for application in regional or mesoscale atmospheric chemistry models. The model, named the Asymmetrical Convective Model (ACM), is based on the concept that vertical transport within the CBL is inherently asymmetrical. Upward transport by buoyant plumes originating in the surface layer is simulated by mixing from the lowest model layer directly to all other layers in the CBL. Downward transport, however, proceeds only to the next lower layer in order to emulate gradual compensatory subsidence. The ACM is similar to the model developed by Blackadar (1978, 4th Symp. on Atmospheric Turbulence, Diffusion and Air Quality, pp. 443-447, Reno, Am. Meteorol. Soc.) but differs in its treatment of downward transport. The realism of the ACM is tested through comparisons to large-eddy simulations of several idealized test cases. These tests show that while the ACM shares the Blackadar model's ability to simulate rapid transport upward from the surface layer to all levels in the CBL, it is clearly superior in its treatment of material emitted from elevated sources either within or above the CBL. The ACM is also tested in the context of the Regional Acid Deposition Model (RADM) both to determine sensitivity to different CBL mixing schemes and to compare to vertically resolved aircraft measurements. These tests demonstrate quicker upward transport of ground-level emissions by the ACM as compared to the eddy diffusion scheme currently used in RADM. The ACM also affects ozone photochemistry in the boundary layer resulting in lower ozone concentrations in areas of high NOx emissions.

Key word index: Convective boundary layer, non-local closure model, vertical mixing, regional atmospheric chemistry model, asymmetrical mixing.

1. INTRODUCTION

Comprehensive Eulerian grid models are increasingly becoming the preferred method for the study of a variety of issues over a wide range of spatial and temporal scales. Such models push the limits of computing speed as they try to include complex algorithms at ever increasing grid resolution. Therefore, the design of numerical algorithms for these models is governed by a trade-off between complexity and computing speed. Each process algorithm should be sufficiently complex to simulate realistically the features which are relevant to the model as a whole. As each component of the model gets more sophisticated the requirements on the other components also increases. The goal of the modeler is to bring continually the weaker links in the model system up to par with the rest of the model.

The simulation of subgrid vertical mixing is an important component of both chemical and meteorological Eulerian grid models. The key issue with regard to mesoscale Eulerian grid chemistry models is the realistic simulation of trace chemical transport, particularly during conditions of free convection, in a simple and economical manner. Note that the requirements of the vertical mixing algorithm are more stringent when applied to atmospheric chemistry models than when used in mesoscale meteorology models. In chemistry models more severe gradients are likely to occur in chemical concentrations than are common for heat, moisture or momentum. Also, chemical material can be emitted from sources at any point within, or above the PBL, so a much wider variety of dispersion situations must be simulated by a chemical model.

The most commonly used techniques for modeling vertical transport in Eulerian grid models are finite-difference applications of eddy diffusion. These models describe vertical fluxes as functions of local finite-difference gradients where eddy diffusion coefficients are parameterized either in terms of characteristics of the local flow (e.g. Louis, 1979; Blackadar, 1976) or boundary layer similarity theories (e.g. Brost and Wyngaard, 1978; Troen and Mahrt, 1986; Holtslag et al., 1990). The concept of eddy diffusion, or
local first-order closure, is that turbulent diffusion can be simulated in an analogous way to molecular diffusion. For this to be true the scale of the diffusion mechanism must be very small compared to the scale of the mean flow. In the case of molecular diffusion the scale of molecular motion is clearly microscopic. Therefore, eddy diffusion is a reasonable model only if the scale of turbulent motion is much smaller than the scale of mean motion. This necessitates the existence of a well-defined spectral gap between the scales of the turbulent and mean motion. During conditions of stable or neutral static stability this requirement is fairly well met. During convective conditions, however, the dominant eddy length scale is much longer, up to the depth of the Convective Boundary Layer (CBL). Unless the CBL is modeled as a single well-mixed layer, which is done for some atmospheric chemistry models, the turbulent motion cannot be considered entirely subgrid in the vertical direction. For models with finer vertical resolution, such as many meso and regional-scale atmospheric chemistry models, much of the mixing in the CBL is accomplished by vertical motions which are not subgrid in the vertical but are subgrid in the horizontal and therefore cannot be explicitly resolved. Neither are they well simulated as proportional to mean local gradients in the CBL which are very weak and are sometimes even counter to the flux. Therefore, the technique of integral or non-local closure is being increasingly applied to problems of vertical mixing in convective boundary layers (e.g. Stull and Driedonks, 1987). The theory and mathematical development of the ACM has been in the Regional Acid Deposition Model (RADM) (Chang et al., 1987; Fiedler and Moeng, 1985; Blackadar, 1978).

This paper describes the development and testing of a new non-local closure model named the Asymmetrical Convective Model (ACM). The ACM has been specifically developed to meet the needs of Eulerian grid atmospheric chemistry models, that it be computationally simple but capable of realistic transport of material from sources at any height. The concept of non-local closure along with a brief review of some existing non-local closure models are presented in Section 2. The theory and mathematical development of the ACM is outlined in Section 3. The realism of the model's simulation of vertical transport in the CBL is evaluated though comparisons to large-eddy simulations as described in Section 4. The initial application of the ACM has been in the Regional Acid Deposition Model (RADM) (Chang et al., 1987). The sensitivity of RADM results to the use of the ACM versus an eddy diffusion technique are discussed in Section 5. Simulations by the nested grid version of RADM (Pleim et al., 1991) using both the ACM and an eddy diffusion technique are compared to vertically resolved aircraft measurements in Section 6.

2. NON-LOCAL CLOSURE

Integral or non-local closure is designed to address the shortcomings of eddy diffusion without adjusting significantly to complexity and cost. Non-local closure means that turbulent fluxes are computed as functions of large-scale gradients rather than local gradients as in eddy diffusion. In a discrete non-local closure model, mixing occurs not only between adjacent model layers but also between layers not adjacent to each other. Such models are usually applied to convective boundary layers where local gradients are small and turbulent eddy length scales are often longer than the vertical grid increments of the model. Much of the mixing in the CBL is caused by buoyant plumes originating in the surface layer which rise to the top of the CBL and sometimes penetrate into the capping inversion. As discussed above, it is during these conditions that eddy diffusion is most inadequate.

The prognostic equation for a discrete model of integral mixing of any conserved parameter $C$ (e.g. potential temperature, momentum, specific humidity or trace species concentrations) is

$$\frac{\partial C_i}{\partial t} = M_{ij} C_j,$$

where $M_{ij}$ is a matrix of mixing coefficients between layer $i$ and layer $j$. More specifically, $M_{ij}$ is the rate of mass fractional mixing from level $j$ to level $i$. The dimension of $M_{ij}$ is $n \times n$, where $n$ is the number of vertical model layers. Stull (1988), who presents an extensive description of non-local closure models, refers to this matrix as a transilient matrix. In this framework, a simple eddy diffusion model can be viewed as a specific-form integral closure where only the tridiagonal elements of the transilient matrix are non-zero. Non-local closure, however, refers to models where at least some elements outside of the tridiagonals are non-zero.

The elements of the transilient matrix can be specified in a variety of ways. However, it should be noted that the more non-zero elements, the more complex and expensive the numerical solution will be. Stull and Driedonks (1987) suggest a responsive approach based on a simplified form of the Turbulent Kinetic Energy equation. Thus, the mixing acts to diminish static and dynamic instabilities in the flow. Their model was both calibrated and evaluated using data for several case studies taken at the Cabauw tower in the Netherlands. They found that the model was able to simulate realistically both convective and stable boundary layers. The main drawback of this approach, however, is that all of the matrix elements are non-zero resulting in relatively expensive numerical integration.

Another approach to integral closure is to specify the transilient matrix according to some conceptual model. For example, specific matrices may be constructed for simulating cumulus cloud mixing (e.g. Chatfield and Crutzen, 1984; Prather et al., 1987) or mixing in convective boundary layers. In this way, only a fraction of the elements in the transilient matrix...
need be non-zero thus reducing the cost of numerical integration considerably. The main limitation of this approach is that the model can only be used for the conditions which governed its design. For example, a model designed for convective boundary layers cannot then be used for stable boundary layers or for the free troposphere. Therefore, hybrid models are often used such that non-local closure is only used in convective boundary layers while eddy diffusion is used elsewhere. This is the approach used in the Mesoscale Meteorological Model Version 4 (MM4) (Anthes et al., 1987) as well as the method which we have recently developed for RADM.

An example of an integral closure model designed for the convective boundary layer is described by Fiedler and Moeng (1985). Their model has a $20 \times 20$ transilient matrix (the model has 20 equally spaced vertical levels in the CBL) which includes non-zero elements for the tridiagonal portion, as in simple eddy diffusion models. In addition, the matrix includes two non-zero columns down the left side of the matrix which are meant to represent buoyant plume transport from the lowest two layers (surface layer) to every other layer in the CBL. The values of these matrix elements were determined by specifying the non-diagonal elements in a physically reasonable manner and then adjusting the subdiagonal and superdiagonal elements to fit the results of large eddy simulations (LES). In this way they were able to reproduce nearly exactly the LES results. The conceptual framework of the ACM is very similar to this model but its numerical solution is considerably simpler and therefore more useful in comprehensive grid models.

Another, much simpler non-local closure model designed for the convective boundary layer was developed by Blackadar (1978). This model has been successfully applied in MM4 to simulate boundary layer processes during conditions of free convection (Zhang and Anthes, 1982). The concept of the Blackadar convective mixing scheme is similar to the Fiedler and Moeng scheme in that the effect of convective plumes is simulated by mixing material directly from the surface layer to every other layer in the CBL. Unlike the Fiedler and Moeng model, however, upward and downward mixing are symmetric in the sense that mixing goes from the surface layer to each level and symmetrically from each level back to the surface layer. Also, local mixing between adjacent layers, is not accommodated. Figure 1 shows the mixing scheme schematically. Another way of looking at this mixing scheme is that there are symmetrical eddies initiated in the surface layer of every size up to the depth of the CBL. The transilient matrix which controls this model is non-zero only for the top row, the left-most column and the diagonal. The main drawback of this model is that the downward mixing is identical to the upward mixing which leads to unrealistic transport of material from elevated sources. This deficiency is less important for meteorology models where the most critical task for the boundary-layer mixing algorithm is the simulation of heat and moisture fluxes upward from the surface.

3. MODEL THEORY AND DEVELOPMENT

It has been suggested, and confirmed through large eddy simulations, that there is a vertical asymmetry of buoyancy-driven turbulence which may be a fundamental property of convective boundary layers (Wynyard and Brost, 1984; Moeng and Wyngaard, 1984). Unlike Raleigh–Benard convection, which occurs between horizontal surfaces of differing temperatures, convection in the CBL is characterized by strongly buoyant rising plumes without similarly negatively buoyant sinking plumes. Because the rising plumes are buoyant, having been formed from super-adiabatic air in the surface layer, they accelerate as they rise through the mixed layer thereby causing their horizontal cross-sections to shrink with height due to mass continuity. Downdrafts, however, sink due to pressure forcing resulting from continuity of the updrafts and not because of negative buoyancy. In fact, since downdraft air primarily originates either in the entrainment zone above the mixed layer or from updrafts that have run into the inversion and spread laterally, downdrafts usually have slight positive buoyancy. Positive buoyancy causes deceleration and lateral growth of downdrafts as they descend. Therefore, the CBL is characterized by narrow fast-moving updrafts and fat slow-moving downdrafts. Large eddy simulations show that the horizontal fractional area of the updrafts decreases from about 50% at the surface to a minimum of about 33% near the top of the CBL with updraft velocities up to twice the downdraft velocities (Schumann, 1989).

![Fig. 1. Schematic representation of mixing in a 1-D column of air as simulated by the Blackadar convective boundary layer model.](image-url)
Since transport in the CBL seems to be inherently asymmetrical, CBL models should differ in their simulation of upward and downward mixing. Hence, eddy diffusion models fail to simulate realistically CBL mixing not only because of their inability to mix material rapidly between widely separated layers but also because no single $K_z$ profile can realistically simulate both upward and downward mixing. This is also why $K_z$ profiles derived from an LES for plume dispersion in the CBL have been found to depend on the source height (Lamb and Durran, 1978). While the Blackadar model is better than eddy diffusion because mixing is not controlled by local gradients, it is symmetric in that upward and downward transport occur between the same levels at the same rate (see Fig. 1). Therefore, the Asymmetrical Convective Model has been developed, which is just as computationally simple as the Blackadar model, with a modified scheme for downward mixing. The concept for this model is that strongly buoyant plumes rise from the surface layer to all levels in the CBL but that downward motion is primarily gradual compensating subsidence. Therefore, the upward mixing is identical to that of the Blackadar model but the downward mixing occurs between adjacent levels only in a cascading manner. Figure 2 shows the mixing scheme of the ACM schematically.

The governing equations for the ACM are derived from mass continuity within the framework of the mixing scheme shown in Fig. 2. The equations have been derived for a $\sigma$-coordinate system such that the vertical coordinate is proportional to mass, where $\sigma$ is defined as

$$\sigma = \frac{P - P_{\text{top}}}{P_{\text{surf}} - P_{\text{top}}} \quad \text{and} \quad P_{\text{top}} = 10 \text{ kPa}, \quad (2)$$

where $P$ is the pressure where $\sigma$ is evaluated, $P^* = P_{\text{surf}} - P_{\text{top}}$ and $P_{\text{surf}}$ is the surface pressure. The conserved form of tracer concentration in a $\sigma$-coordinate system is the product of mass mixing ratio and $P^*$.

The prognostic equation for concentration $C$ (mass mixing ratio $\times P^*$) in level $i > 1$ of the CBL is,

$$\frac{\partial C_i}{\partial t} = \frac{\partial}{\partial \sigma} \left( \frac{P^*}{\Delta \sigma_i} \frac{\partial C_i}{\partial \sigma} \right) = \frac{P^*}{\Delta \sigma_i} \left( \frac{\partial C_i}{\partial \sigma} + \frac{\partial}{\partial \sigma} \left( \frac{P^*}{\Delta \sigma_i} \frac{\partial C_i}{\partial \sigma} \right) \right),$$

(3)

where $\Delta \sigma_i$ is the thickness of level $i$. Note that the upward mixing rate ($Mu$) from level 1 to every other level in the CBL is constant with height. The downward mixing rate, however, increases from the top down in order to maintain mass continuity as described by Equation (4). For the surface layer ($i = 1$):

$$\frac{\partial C_1}{\partial t} = \frac{P^*}{\Delta \sigma_1} \left( F_S - F_1 \right),$$

(5)

where the fluxes through the bottom and top of level 1 for trace chemicals are,

$$F_S = -V_d C_1 \rho_1,$$

(6a)

and

$$F_1 = \frac{P^*}{g} \left[ Mu(\sigma_i - \sigma_{i-1}) C_i - Md_i \Delta \sigma_i C_2 \right],$$

(6b)

where $V_d$ is dry deposition velocity and $\rho_1$ is the air density in level 1, and $g$ is gravitational acceleration. Note that the minus sign in Equation (5) results from the fact that $\Delta \sigma$ is negative.

The upward mixing rate ($Mu$) between the surface layer and all other layers is determined by conservation of sensible heat energy as described by Blackadar (1978). When applied to the mixing of sensible heat energy the local change in temperature is equal to the divergence of sensible heat flux which is in turn caused by vertical mixing such that,

$$\frac{\partial \theta_i}{\partial t} = \frac{P^*}{c_p \rho} \frac{\partial H}{\partial \sigma} = Mu \theta_i - Md_i \theta_i + Md_{i+1} \frac{\Delta \sigma_{i+1}}{\Delta \sigma_i},$$

(7)

where $H$ is sensible heat flux and $c_p$ is the specific heat of air at constant pressure. By integrating Equation (7) from the top of the surface layer (layer 1) to the top of the CBL and by assuming zero heat flux though the
top of the CBL, the vertically averaged mixing rate can be determined as,

\[ M_u = H_1 \left\{ \frac{\rho^*}{\theta} \left( \sigma_1 - \sigma_2 \right) (\theta_1 - \theta_2) \right\}. \]  \hspace{1cm} (8)

The depth of the CBL is defined as the layer of positive buoyancy for a parcel of air with the potential temperature of the surface layer plus a small entrainment zone (see Zhang and Anthes, 1982). \( H_1 \) is the sensible heat flux at the top of the surface layer which is diagnosed from the potential temperature profile according to a relation derived by Priestly (1956):

\[ H_1 = c_p \rho^* B(\theta_1 - \theta_2)^{3/2} \]  \hspace{1cm} (9)

and

\[ B = \left( \frac{2g}{\theta_1} \right)^{1/2} \left[ \frac{1}{z_1(1/3)} - \left( \frac{2z_2}{3} \right)^{-1/3} \right]^{3/2}, \]

where \( z_1 \) is the top of level 1 and \( z_{3/2} \) is the middle of level 2.

For the RADM and nested RADM simulations discussed below, the meteorological simulations are provided by MM4 which uses the Blackadar model. In this case, the mixing rate is defined as:

\[ m = H_1 \left\{ \frac{\rho^*}{\theta} \int_{z_1}^{z_{3/2}} (\theta_1 - \theta) \, dz \right\} \]  \hspace{1cm} (10)

(Zhang and Anthes, 1982). If the ACM were used in the MM4 simulations, the mixing rate would be given by Equation (8) and the evolution of the temperature, humidity and momentum profiles would proceed somewhat differently than simulated by the Blackadar model. However, since it was beyond the scope of this study to modify MM4, \( M_u \) was defined according to the Blackadar model (Equation 10) for both the MM4 and RADM simulations since the potential temperature profile was produced by the Blackadar model in MM4.

**Numerical solutions**

The Asymmetrical Convective Model, as well as the eddy diffusion model used for conditions other than free convection, are solved using Crank-Nicholson semi-implicit finite differencing schemes. This technique has the advantage of being globally stable and accurate to a higher mathematical order than either explicit or fully implicit techniques. In practical terms, the semi-implicit technique is more accurate at time steps near the limit of stability of the explicit technique, thereby allowing the use of longer time steps which reduces computation time. A disadvantage of all implicit techniques is that they involve matrix inversion which can be computationally expensive. However, if the matrices are sufficiently sparse, as is the tridiagonal matrix which describes the eddy diffusion model, the computation is almost as efficient as the explicit solution.

Semi-implicit solutions to the set for differential equations describing the Asymmetrical Convective Model (Equations 3 and 5) have been derived for a \( \sigma \)-coordinate Eulerian grid with non-uniform vertical grid spacing. The numerical solution to Equation (5) for concentrations of trace chemicals in the surface layer is:

\[ C_i^{n+1} = C_i^n - \frac{\Delta t}{\Delta \sigma_i} \left[ \phi (F_{i+1} - F_i) + (1 - \phi) (F_i - F_{i-1}) \right]. \]  \hspace{1cm} (11)

where the superscripts \( n \) indicate the current time step and \( n + 1 \) is the next time step and the fluxes are given by Equation (6), \( \phi \) is the implicit parameter which is 1/2 for centered in time. For all other levels in the CBL the finite difference solution is:

\[ C_i^{n+1} = C_i^n - \frac{\Delta t}{\Delta \sigma_i} \left[ \phi (M_u C_i^{n+1} - M_d C_i^n) + M_d \frac{\Delta \sigma_{i+1}}{\Delta \sigma_i} C_{i+1}^{n+1} + (1 - \phi) (M_u C_i^n - M_d C_i^n) + M_d \frac{\Delta \sigma_{i+1}}{\Delta \sigma_i} C_{i+1}^{n+1} \right]. \]  \hspace{1cm} (12)

Together these equations can be expressed as the matrix equation

\[ A C^{n+1} = D(i), \]  \hspace{1cm} (13)

where \( A \) is the transient matrix containing the coefficients of the \( C^{n+1} \) terms and \( D \) is an array containing all the terms known at time step \( n \). Since the matrix is so sparse it is easily and efficiently inverted to solve for \( C^{n+1} \).

The accuracy of this scheme depends on the length of the time step compared to the time scale of the mixing. For the ACM the critical time scale is the turn-over time for air in the lowest model layer which can be computed as

\[ T_1 = \frac{1}{M_u (\sigma_1 - \sigma_2)}. \]  \hspace{1cm} (14)

Note that the turnover time for the other layers in the CBL increases with height until in the highest layer it is simply \( 1/M_u \). However, due to the design of the convective algorithm which requires that all upward mixing originate in the lowest layer, its turnover time is decreased by the ratio of the depth of the first layer to the depth of the CBL above layer 1. If the time step is greater than \( T_1 \) the algorithm can be significantly inaccurate. For example, the most extreme case would be a step function vertical profile where concentrations are zero in all but the lowest model level. For such a case, a time step longer than \( T_1 \) produces negative concentrations in the lowest level since more than 100% of the air in level 1 is replaced in a single time step. Such extreme concentration profiles are not only possible but also likely in an atmospheric chemistry model. For example, the model species known as OLT in RADM, which is a lumped group of olefins...
modeled as butene, often exhibits a step-function profile. OLT is emitted almost entirely into the lowest layer and reacts very rapidly with hydroxyl radical. Therefore, as soon as it is mixed out of the lowest layer much of it is destroyed by reactions leaving significant quantities in the first layer only. For these reasons the numerical requirements of the mixing algorithm are much more stringent for chemical modeling than for meteorological modeling where such extreme vertical profiles would be very rare.

The time-step constraints outlined above necessitate that during conditions of rapid convective mixing a shorter time step be used for the convective mixing algorithm than elsewhere in RADM (150s). Therefore, the time step used to solve the matrix equations for the ACM is determined individually for each grid cell as the greatest integer fraction of the model time step which is less than 0.5 \( T_i \), where the 0.5 factor is included for extra safety.

4. TESTING VERSUS LARGE-EDDY SIMULATIONS

Conceptual arguments for the greater realism of the newly developed Asymmetrical Convective Model for applications in atmospheric chemistry models such as RADM compared to previously used techniques have been outlined above. However, a more quantitative evaluation is necessary to determine if the ACM represents better simulations of transport in the convective boundary layer. For this purpose both the ACM and the Blackadar convective model are compared to large eddy simulations (LES) of vertical transport in the CBL for several idealized experiments.

A large-eddy model was used to study the characteristics of diffusion in the convective boundary layer by Wyngaard and Brost (1984). They argued that convective mixing can be viewed as the superposition of top-down diffusion and bottom-up diffusion. They show, through both simple similarity analysis and large-eddy simulation, that scalar gradients for top-down diffusion and bottom-up diffusion are not symmetric. Moeng and Wyngaard (1984), using a similar but independently developed large-eddy model, confirmed the results of Wyngaard and Brost (1984). The scalar gradient functions resulting from the LES can be vertically integrated to produce non-dimensional concentration profiles which can then be used to test boundary-layer mixing models.

Both LES models used a 1.5 order closure scheme with the same domain and grid structure. The domain was \( 5 \times 5 \times 2 \) km divided into 40 grid points in each dimension to give a vertical grid interval of 50 m and horizontal grid intervals of 125 m in both \( x \) and \( y \) directions.

Based on these studies, which demonstrated the asymmetrical nature of vertical transport in the CBL, several simple models have been recently developed. The results of the large-eddy simulations for idealized conditions were used to both tune and evaluate these models. For example, Fiedler and Moeng (1985) used LES results to derive elements of the transfer matrix in their non-local integral closure model. Chatfield and Brost (1987) similarly used LES results to determine parameters for their two-stream model. In both cases the tuning of certain parameters enable these simple models to nearly perfectly reproduce the LES results for top-down and bottom-up flux test cases.

Although greatly simplified with respect to large-eddy models, these models are significantly more complicated than either the Blackadar model or the Asymmetrical Convective Model. Therefore, they would be considerably more expensive for application in a 3-D atmospheric chemistry model like RADM. In addition, the greater detail afforded by these models would be lost in RADM where typically only 5 to 7 levels reside in the CBL.

Both the Blackadar model and the ACM were tested against the results of the LES for the bottom-up and top-down flux test cases. In addition, the Blackadar model and the ACM were tested for plume dispersion in CBL conditions.

4.1. Bottom-up

The bottom-up flux experiment has been used by several investigators as a test case for models of vertical transport in the CBL (Chatfield and Brost, 1987; Wyngaard and Brost, 1984; Moeng and Wyngaard, 1984; Fiedler and Moeng, 1985). A constant flux is emitted from the surface into the CBL at a rate such that if uniformly distributed through the depth of the CBL one non-dimensional unit of concentration would accumulate in one unit of non-dimensional time. Non-dimensional concentration is defined as \( C/C^* \), where \( C^* = F/w^* \) and non-dimensional time is defined as \( t/t^* \), where \( t^* = h/w^* \) (\( h \) is the depth of the CBL and \( w^* \) is convective velocity). Accordingly, the surface flux is given by \( F = C^*h/t^* = w^* \). The flux through the top of the CBL is held at zero. The mixing rate for the Blackadar model and the ACM is defined as \( m = w^*/h \).

Starting with an initial condition of zero concentration everywhere, vertical profiles of non-dimensional concentration at \( t=4t^* \) as simulated by the large-eddy model of Moeng and Wyngaard (1984) and by the Asymmetrical Convective Model are shown in Fig. 3a. Note that the Blackadar model and the ACM give the exact same results for the bottom-up flux experiment because they use identical algorithms for upward transport. The LES profile shows a steep negative gradient near the surface which lessens gradually through the lowest quarter of the CBL. Above 0.25 h, a slight and nearly constant negative gradient continues up to about 0.7 h where the gradient goes to zero until about 0.8 h. In the top fifth of the CBL the gradient becomes positive which shows that much of the transport to this region comes directly from the surface layer, where concentrations are the highest, as in convective plumes. Clearly, an eddy diffusion
model cannot reproduce this profile without negative eddy diffusivities.

For comparison, an eddy diffusion simulation which was fit to the LES results by Fiedler and Moeng (1985) is shown in Fig. 4. The eddy diffusivities for the upper portion of the CBL ($z>0.22\, h$) were fit to the top–down case while the eddy diffusivities near the bottom ($z<0.22\, h$) were fit to the bottom–up case. Presumably, an eddy diffusion model could do better for the bottom–up case if the eddy diffusivities were very large in the upper portion of the CBL which would result in a nearly constant profile. Of course, the model's ability to simulate accurately the top–down case would then be impaired.

The ACM produces a very simple profile for the bottom–up flux case where the concentrations are constant throughout the CBL with the exception of the lowest layer. Although the ACM cannot reproduce the upward gradient at the top of the CBL, the concentrations simulated by the ACM are quite close to the LES concentrations in this region. Furthermore, with the reduced resolution of RADM these differences would be even less significant. However, the smooth curve of the LES profile in the lowest quarter of the CBL is less well simulated by the ACM than by the eddy diffusion model. Therefore, while the eddy diffusion model performs quite well in the lowest portion of the CBL, the ACM is more realistic near the top of the CBL. Overall, the error in concentration as compared to the LES is smaller for the ACM than for the eddy diffusion model.

4.2. Top–down

In the top–down flux experiment a constant downward flux from above the CBL is specified at a rate equal to $w^*$ while the surface flux is held at zero. The initial condition is zero concentration throughout the CBL. The simulation is run for eight non-dimensional time units ($t=8\,w^*$). Vertical profiles of concentrations produced by the LES and both the Blackadar model and the Asymmetrical Convective Model are shown in Fig. 3b. Again, for comparison the eddy diffusion simulation of this case from Fiedler and Moeng (1985) is shown in Fig. 4.

The LES concentration profile shows very high concentrations in the topmost level (~$23\, C/C^*$), where the entrainment flux enters the CBL, decreasing rapidly in the layers below. The gradient of the concentration profile gradually decreases with descent down to around 0.6 h. Below 0.6 h the concentration profile is approximately linear with a very slight positive gradient at concentrations from 5 to $6\, C/C^*$. The precipitous gradients near the top of the mixed layer indicate that downward mixing is relatively slow in this region. The curved portion of the profile shows that mixing increases gradually lower down. The near uniform profiles in the lower portion of the mixed layer demonstrate that mixing is quite rapid below about 0.6 h. The monotonic increase of concentration with height suggests that downward mixing is more local and gradual than upward mixing.

In this case the simulations by the Blackadar model and the ACM differ considerably. The Blackadar model simulates a constant profile through all levels except the top layer, where material is entering the CBL, and the bottom layer. This profile deviates substantially from the LES profile, especially near the top of the CBL where the Blackadar model underestimates, and near the ground where it overestimates. The ACM profile, on the other hand, matches the LES nearly exactly, as does the eddy diffusion model. The ACM, therefore, combines the best features of both the Blackadar model and eddy diffusion. For upward transport where eddy diffusion is deficient, it uses non-local closure mixing like the Blackadar model, while downward transport, where the Blackadar model is lacking, is simulated by local closure like eddy diffusion. These experiments have supported the conceptual hypothesis which guided the development
of the ACM, that vertical transport in the CBL is characterized by rising buoyant plumes and gradual compensating subsidence.

4.3. Mid-level plume

The third test involves the release of material half way up in the CBL with no flux through either the top or bottom of the CBL. This case can be viewed either as a time simulation of one-dimensional dispersion of a puff release or a steady-state two-dimensional simulation of a plume in a constant uniform wind field. Simulations by the Blackadar model and the Asymmetrical Convective Model are compared to a large-eddy simulation reported by Lamb (1982), a laboratory simulation described by Willis and Dear dorff (1981) and the results of the two-stream model of Chatfield and Brost (1987). The results of the LES, the laboratory model and the two-stream model are presented in Fig. 5 which is reproduced from Chatfield and Brost (1987). The simulations by the ACM and the Blackadar model are shown in Fig. 6. Note that the x-axis in these plots is equivalently non-dimensional time \((t^*/h)\) for the 1-D puff or non-dimensional downwind distance \(((x^*/u))/hU)\) for the 2-D plume.

The most striking feature of all the simulations, except the Blackadar model, is the gradual descent of the axis of maximum concentration or plume centerline which intersects the ground somewhere between 0.5 and 1.5 non-dimensional time or distance units. This behavior is indicative of the asymmetrical character of vertical transport in the CBL. Specifically, material near the middle of the CBL is more likely to be affected by gradual subsidence than entrained into the much smaller, faster moving, buoyant plumes. In fact, in the ACM, gradual subsidence is the only possibility for a mid-level plume (see Fig. 2), which is probably why the ACM simulation shows the quickest transport of the plume centerline to the ground. The ACM results, shown in Fig. 6, are in fairly good agreement with the other models which demonstrates that the essential features of transport in the CBL can be simulated by a very simple model given the appropriate conceptual design.

Other simple first-order closure models such as eddy diffusion or the Blackadar model are not able to simulate the descending plume. Figure 6 shows that the descending plume is completely absent from the simulation by the Blackadar model. Also, dispersion in the Blackadar simulation is very un-plume-like. The plume centerline stays at the release height while the centerline concentration slowly decreases and concentrations outside the plume gradually increase. Concentrations at all levels are the same with the exception of the release level and the lowest level where concentrations are slightly higher. This lack of diffusive behavior is due to the absence of local mixing in the Blackadar algorithm. In terms of the transient matrix, the Blackadar mixing algorithm lacks non-zero values in the sub-diagonal and super-diagonal elements of the matrix. Therefore, for any type of transport other than bottom-up flux, the Blackadar model cannot even qualitatively approximate CBL mixing. This model may be sufficient for meteorological applications where the most important tasks are the simulation of upward heat and moisture fluxes.
Vertical mixing non-local closure model

Fig. 5. Comparison of several models in the simulation of material released half way up in the CBL ($z = 0.5 z_i$). (a) Results calculated from a large-eddy model (Lamb, 1982), (b) comparable results of a laboratory model (Willis and Dearsdorff, 1981), (c) results of the two-stream model of Chatfield and Brost (1987). (From Chatfield and Brost, 1987.)

and the evolution of the CBL. For atmospheric chemistry applications, however, a greater variety of situations need to be realistically simulated, including mid-level plumes.

5. SENSITIVITY IN RADM

In this section the effects of different boundary-layer vertical-mixing schemes with similar boundary-layer heights on simulated concentration fields are investigated. Specifically, RADM and Nested RADM simulations using a boundary-layer eddy-diffusion model are compared to simulations using the Asymmetrical Convective Model. In both cases the 15-layer version of RADM is used such that the vertical grid is the same as employed by MM4 (see fig. 4.3 of Anthes et al., 1987). The eddy-diffusion scheme used for comparison is based on boundary-layer scaling in a manner similar to Brost et al. (1988) and Holtslag and Nieuwstadt (1986). A brief description of this scheme is included in the Appendix. The coarse grid and nested simulations use meteorological data provided by simulations of MM4 and Nested MM4.

Vertical profiles of several chemical species as simulated by RADM and Nested RADM have been com-
pared for the study period of 30 August 1988 to 1 September 1988. The most pronounced difference caused by the different mixing models during daytime hours occurs for species which are primarily emitted at ground level. A good example is $NO_x(NO_2 + NO)$, which can be considered to be a good short-term tracer of atmospheric transport since most reactions involving NO$_2$ produce NO and vice versa. In an urban environment large quantities of NO$_x$ are emitted primarily by motor vehicles into the lowest model level. Therefore, NO$_x$ profiles over a large city should reveal the greatest differences between the two simulations.

Figure 7 shows vertical profiles of NO$_x$, O$_3$ and SO$_2$ concentrations as simulated by versions of RADM using both the ACM and eddy diffusion over the New York city grid cell at 2 pm EDT on 1 September 1988. 1 September was a clear day in the eastern U.S. with vigorous convective mixing as indicated by model-computed boundary-layer parameters such as convective velocity ($w^* = 1.6 \text{ m s}^{-1}$) and a boundary-layer height of about 1 km. Both simulations used the same algorithm for estimation of boundary-layer heights which produced nearly identical results as indicated by the similarity of the upper portions of the profiles. The lower portions, however, show marked differences. The model employing the eddy diffusion technique simulates a gradual decrease of NO$_x$ concentration with height with a nearly constant gradient throughout the CBL. The model using the ACM simulates a more well-mixed profile in the CBL with the steepest gradient near the ground caused by ground-level emissions. These profiles are characteristic of simulations by the two models during convective conditions in areas of strong ground level emissions. Where emissions are less important or from more elevated sources the two models exhibit much more similar profiles. For example, the vertical profiles of SO$_2$, which is largely emitted from elevated sources in the middle or even upper portions of the
CBL, are nearly identical. This is because the downward mixing portion of the ACM is very similar to eddy diffusion in that downward transport proceeds only to the next lower layer.

The ozone profiles simulated using the different mixing models are more difficult to interpret. Since ozone is not emitted, its daytime concentrations are primarily controlled by photochemistry and transport. The profiles presented in Fig. 7 show nearly identical concentrations above the boundary layer while in the mixed layer ozone concentrations simulated using the ACM are consistently lower. These results are intriguing since they suggest a nonlinear response of ozone photochemistry to vertical mixing. Although, the two models simulate similar quantities of NOx in the mixed layer, the ACM mixes NOx to the upper reaches of the mixed layer more quickly than the eddy-diffusion model. In particular, NO concentrations are much higher throughout the upper half of the mixed layer as shown in Fig. 8. Since roughly 90% of NOx is emitted as NO which rapidly reacts with O3, the effect of more rapid vertical mixing of ground level NO emissions is to reduce O3 concentrations in the upper part of the mixed layer. The lower O3 concentrations are then mixed throughout the mixed layer so that the ACM simulates lower O3 at all levels.

The eddy diffusivities used in the eddy diffusion model are shown for all model levels within the CBL in the bottom panel of Fig. 8. The eddy diffusivities for convective conditions are computed as functions of mixing height (h), height above ground (z) and convective velocity scale (w*) according to

\[ K_z = k w^* z (1 - z/h) \] (15)
as suggested by Brost et al. (1988), where \( k \) is the von Karman constant (see the Appendix for more description of the eddy-diffusion model). Note that \( K_z \) increases with height until it reaches a maximum at \( z = h/2 \) and then tends back toward zero at \( z = h \). The very large values of \( K_z \) represent an attempt to produce a well-mixed layer. The decreasing values at the top and bottom of the mixed layer, however, tend to inhibit rapid transport from the surface layer directly up to the top of the mixed layer. It is this large-scale upward mixing by buoyant plumes that the ACM is better able to simulate.

Figure 9 shows vertical profiles of \( \text{NO}_x \), \( \text{SO}_2 \) and \( \text{O}_3 \) over New York city as simulated by the nested model using the two different boundary-layer mixing schemes. The shape of the profiles of all three species is very similar to the coarse grid profiles. However, the magnitude of the differences is smaller for the nested simulations. The main difference is that the boundary layer is higher for the nested simulations (about 1.3 km) which leads to lower boundary-layer concentrations of \( \text{SO}_2 \) and \( \text{NO}_x \). Also, the higher mixing height in the nested simulations results in larger eddy diffusivities in the middle of the mixed layer. Therefore, the rate of mixing of the eddy-diffusion model is closer to the ACM.

Again, the ozone in the boundary layer is lower in the ACM simulation although the difference is not so pronounced. In fact, ozone concentrations in the lowest two layers are nearly the same. The smaller difference is related to the smaller difference in the \( \text{NO}_x \) profiles produced by the nested models. The fact that the ozone profiles increasingly diverge with height illustrates that the rate of transport of ground level emissions to the upper half of the mixed layer is an important influence on ozone concentration profiles.

The question remains as to which of these models is more realistic. The model comparisons over New York city show that the ACM mixes material upward from the ground more rapidly than the eddy-diffusion model. These results are very similar to comparisons of both mixing schemes to the large eddy simulation of the bottom-up experiment discussed in Section 4.1. Since \( \text{NO}_x \) over New York city is emitted primarily at the ground into a strongly convective boundary layer, the conditions were much like the bottom-up flux experiment. The large-eddy simulation of that experiment showed a rather constant profile through most of the CBL with increasing tails at both the bottom and the top. For both the LES comparisons and the RADM simulations over New York city the ACM was better able to simulate this rapid bottom-up mixing. To further address this question, nested RADM simulations using both boundary-layer mixing models are compared to aircraft observations of vertical distributions of chemical species.

6. COMPARISONS TO AIRCRAFT MEASUREMENTS

A series of aircraft measurement flights were made during August and September of 1988 as an integral part of the Acid MODES (Acid Models Operational and Diagnostic Evaluation Study) field study. Several different patterns were flown by three specially instrumented aircraft to diagnose various aspects of the performance of RADM and aid in the further development of RADM components. The aircraft were equipped to measure both meteorological parameters such as wind velocity, temperature and humidity, and chemical concentrations of \( \text{O}_3 \), \( \text{NO} \), \( \text{NO}_2 \), \( \text{H}_2\text{O}_2 \) and \( \text{SO}_2 \). Some preliminary results of these experiments and comparisons to RADM simulations are described by Laulainen (1990). Other papers concerning the Acid MODES study and analysis of RADM simulations were presented by Schaller et al. (1991) and Ching et al. (1991).
The data found to be most useful for evaluation of boundary-layer modeling techniques in RADM and particularly nested RADM were obtained during high-resolution box pattern flights over northeastern Pennsylvania on 1 September 1988. In this experiment, an aircraft flew an up and down saw-tooth pattern around the perimeter of a box, roughly 160 \times 160 km, resulting in 33 ramped soundings. Each ramp had a slope of about 25:1 (horizontal to vertical) between 500 and 3000 m above mean sea level. The result is a highly resolved, both vertically and horizontally, meteorological and chemical data base with diurnal representation. Schaller et al. (1991) describe an intercomparison study between the high resolution aircraft data and RADM simulations based on spatial and temporal average vertical profiles. Further comparisons of individual measured and modeled soundings are ongoing and will be presented in future papers.

For the purposes of this paper a sounding derived from a north–south flight segment of about 64 km in length, located over eastern Pennsylvania between Allentown and Scranton has been selected for comparison to model simulated profiles in order to assess the realism of vertical-mixing modeling techniques. The aircraft descended from 3156 m at the north end of the leg to 547 m AMSL at the south end from 11:39 to 11:48 a.m. EDT on 1 September 1988 with data recorded every 5 s. This particular portion of the flight data was chosen for its relative abundance of low altitude pollution (e.g. NOx) owing to its proximity to high emission areas in eastern Pennsylvania and New Jersey. Vertical profiles of NO, NO2 and O3 concentration measurements are shown in Fig. 10. The measurements show that NO and NO2 are largely confined to the boundary layer where the bulk of their emissions occur. Their profiles show considerable small-scale variance in the mixed layer extending up to about 90 kPa. The amount and variability of NOx suggests the influence of many small plumes from nearby sources along the flight path.

Figure 11 shows vertical profiles of the same chemical species as simulated by the nested RADM for a grid cell at the southern end (and lower end) of the flight segment. The results of simulations using the ACM and an eddy-diffusion model in the CBL are shown on each plot. Both simulations agree closely with the observations in terms of mixed-layer height and concentrations of NO and NO2 within the mixed...
layer. The biggest difference between the two simulations is in the gradients of NO and NO$_2$ in the CBL. The ACM simulation shows more well-mixed profiles for NO and NO$_2$, with NO increasing slightly with height and NO$_2$ decreasing slightly with height. The eddy-diffusion simulation shows negative gradients for both NO and NO$_2$ within the boundary layer with the NO$_2$ profile being more negative than the NO profile. The differences between the NO and NO$_2$ gradients in both simulations results from positive gradients in the photolysis rate of NO$_2$, due to decreasing attenuation of light with altitude, and negative gradients in the thermal reaction rate of NO and O$_3$, due to decreasing density and temperature with altitude. Therefore, the photostationary equilibrium between NO, NO$_2$ and O$_3$ shifts more towards NO with altitude.

Unlike NO and NO$_2$, NO$_x$ should be a nearly conserved quantity at time scales of boundary-layer mixing. Figure 12 shows NO$_x$ profiles for both simulations plotted in non-dimensional units in a manner similar to the LES comparisons discussed in Section 4. In this case the scaling concentration is defined as the emission flux into the mixed layer divided by the convective velocity ($C^* = F/w^*$). The ACM profile is nearly constant with height within the mixed layer with a very slight negative gradient while the eddy diffusion profile has a substantial negative gradient. These results bear resemblance to both the NYC profiles shown in Fig. 7 and the bottom-up flux test case shown in Fig. 3 which suggests that the bulk of the NO$_x$ emissions were near ground level. In fact about 58% of the emissions of NO$_2$ into the CBL were into the lowest model layer (0–77 m AGL). These results again demonstrate that the ACM transports material upward from ground level sources more rapidly than the eddy-diffusion model. Also, the similarity of the ACM profile to the LES of the bottom-up flux test case tends to support the realism of this approach. The reason that the non-dimensional concentrations for the bottom-up flux test case, shown in Fig. 3, are smaller than for the Nested RADM simulations is that the bottom-up flux test case simulation was carried out for only four non-dimensional time units from an initially zero profile. The non-dimensional NO$_2$ concentrations of about 16.5 for the nested RADM simulations means that under steady-state conditions it would take 16.5 times the convective mixing time scale, given by $h/w^*$, to accumulate this profile from a zero initial condition. Since the convective mixing time scale is about 560 s this translates into about 2.5 h. Of course a steady-state accumulation is not what happens in the real world and the initial condition is never zero. However, the above calculation is consistent with the time of day (local noon) since the bulk of the material in the upper part of the CBL would have only a couple of hours to accumulate.

The aircraft-measured NO$_x$ data have been made non-dimensional by the same scaling concentration used for the model simulations (namely, the model estimates of emission flux divided by $w^*$). Figure 13 shows non-dimensional observed NO$_x$ concentrations plotted vs $z/h$ using the same value of $h$ derived from the model. Note that this representation of the vertical profile differs considerably from the plots of concentration vs pressure shown above since there are substantial terrain gradients below the flight path. A major difference is in the vertical extent of the mixed layer. When plotted vs pressure the modeled and the measured profiles of NO and NO$_2$ were very similar in mixed layer height. When plotted vs $z/h$, however, the observed mixed layer for NO$_2$ seems to be lower than for the modeled profile. This is because the portion of the flight that was in the boundary layer traversed the edge of the Pocono Mountains. Therefore, although the altitude of the observed mixed-layer
top was similar to the model, the higher terrain to the north where the aircraft flew through the top of the mixed layer resulted in a lower height above ground.

The non-dimensional NO$_x$ concentrations within the mixed layer were observed to be slightly higher than modeled which is consistent with a shallower mixed layer. Although the measured concentrations showed considerable variability, there is little overall vertical gradient. This result tends to support the more well-mixed ACM simulation over the eddy-diffusion simulation. The usefulness of this data, however, for determining gradients within the mixed layer is questionable since the concentration gradients and variations may be more due to the horizontal distribution of NO$_x$ emissions along the flight path than the result of vertical mixing.

The aircraft measurements of ozone concentrations in the boundary layer range from about 60 ppb near the ground to about 52 ppb at the top of the mixed layer (see Fig. 10). Both simulations compare well to these observations with the ACM simulation resulting in concentrations of about 52 ppb and the eddy-diffusion simulation results ranging from 53 to almost 55 ppb (see Fig. 11). As with the New York city profiles, the ACM simulation produced a net smaller amount of ozone in the mixed layer. Again, the obvious explanation for this is that freshly emitted NO is transported up from near-ground sources more rapidly by the ACM. The vertical gradients of the simulated profiles also differ in that the eddy-diffusion profile increases with height while the ACM profile is essentially constant with height. Neither model agrees with the measurements in this respect since the observed ozone profile decreases with height in the mixed layer.

When plotted vs $z/h$, as shown in Fig. 14, the simulated and measured ozone profiles seem somewhat more similar. The negative gradient in the lower portion of the observed profile is less pronounced and therefore closer to the simulated profiles, particularly the ACM-simulated profile. Through the upper portion of the CBL, however, the measured ozone decreases steadily until about 1.4 $z/h$. This height corresponds to a strong wind-shear layer defining the limit of the boundary layer. The similarity of the negative ozone gradient to the negative observed NO$_x$ gradient in the upper portion of the CBL, see Fig. 13, suggests that the ozone is primarily of local photochemical origin within the boundary layer and probably of advective origin aloft.

7. CONCLUSIONS

The Asymmetrical Convective Model is a simple non-local closure algorithm for the simulation of vertical transport in the convective boundary layer. The ACM was specifically designed to meet the needs of regional and mesoscale Eulerian grid atmospheric chemistry models. Namely, that it be able to simulate realistically vertical transport of material from sources at any height within, or above the CBL while being computationally economical. The model is similar to the convective model developed by Blackadar (1978) which is currently used in MM4. The ACM differs from the Blackadar model in its treatment of downward transport in the CBL which is simulated as gradual compensatory subsidence rather than rapid descent to the surface layer. The superiority of this scheme is demonstrated by comparisons to large-eddy simulations for the top–down flux test case and the mid-level plume test case.

When applied to the Regional Acid Deposition Model, simulations using the ACM differ most from simulations using an eddy-diffusion scheme in regions of strong low-level emissions under free convective conditions. The ACM transports emitted material, such as NO and NO$_2$, to the upper reaches of the mixed layer more rapidly than the eddy-diffusion model. Consequently, under such conditions, as shown for the example over New York city during a
sunny summer afternoon, ozone concentrations in the mixed layer are lower for the ACM simulation.

Nested RADM simulations using both the ACM and eddy diffusion were compared to aircraft measurements made during ramped flight segments. While the vertical profiles derived from modeled and measured data showed many similarities, the relatively subtle distinctions in the modeled gradients produced by the two vertical mixing algorithms can not be reliably verified by these measurements. The horizontal extent of the aircraft-ramped flight segments makes it difficult to distinguish vertical gradients from horizontal gradients. On a qualitative level, however, the observations tend to support the more well-mixed profiles produced by the ACM simulation. Also, the fact that most of the NO$_x$ emissions were into the lowest layer suggests that the NO$_x$ profile should be similar to the results of the bottom-up flux test case. The ACM NO$_x$ profile is indeed closer to the LES result for the bottom-up case, particularly for the upper 80% of the CBL where both the ACM simulation and the LES showed nearly constant profiles.

The Asymmetrical Convective Model combines the advantages of eddy-diffusion techniques and the Blackadar convective model while avoiding some of their deficiencies. Upward transport in the CBL is simulated by non-local mixing, like the Blackadar model, in order to emulate the effects of rapidly rising buoyant plumes. Downward transport is simulated as local, layer by layer mixing, like eddy diffusion, emulating gradual compensatory subsidence. Therefore, a more realistic simulation of vertical transport within the CBL is obtained with very little increase in computational complexity.

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REFERENCES


APPENDIX

EDDY DIFFUSIVITIES BASED ON BOUNDARY-LAYER SCALING

In this Appendix the latest model for computing eddy diffusivities for RADM is described. This is the model used in the comparisons described in Sections 5 and 6 between RADM simulations using eddy diffusion and RADM simulations using the ACM.

In an attempt to provide more realistic eddy diffusivities in the planetary boundary layer, particularly for daytime conditions, a parameterization based directly on boundary-layer theory was applied to RADM Hass et al. (1991). Parameterizations of eddy diffusivities within the PBL are based on various length scales and velocity scales which characterize the turbulence in several distinct regimes. The various turbulent regimes are characterized by two dimensionless parameters, h/L, where h is the mixing height and L is the Monin–Obukov length, and z/h, where z is the height above ground (Holtslag and Nieuwstadt, 1986).

The surface layer is defined as the bottom 10% of the planetary boundary layer (PBL) where vertical fluxes are nearly constant with height and turbulence is mostly caused by eddy shear stress (Reynolds' stress) between the wind and the ground. The relevant length scales in the surface layer are the height above ground, which describes the size of the dominant eddies, the Monin–Obukov length (L), which defines the relationship between buoyant and shear production of TKE. The velocity scale in the surface layer is the friction velocity (u*), which is defined as u* = 1/2, where τw is the surface Reynolds' stress or momentum flux. Kz in the surface layer can be derived directly from the flux-profile relations of Monin–Obukov similarity theory as

\[ K_z = \frac{k u_* z}{\Phi(z/L)}, \]  

where

\[ L = \frac{u^2}{\partial w_0}, \]  

\[ \Phi = 0.74 z \left[ 1 - \Phi(z/L) \right]^{-1/2} \]  

for z/L < 0 (unstable) \hspace{1cm} (A3a)

\[ \Phi = 0.64 \]  

for z/L = 0 (neutral) \hspace{1cm} (A3b)

\[ \Phi = 0.74 + 4.7 (z/L) \]  

for 1 > z/L > 0 (stable) \hspace{1cm} (A3c)

\[ \Phi = 4.7 + 0.74 (z/L) \]  

for z/L > 1 (very stable). \hspace{1cm} (A3d)

Equation (A3d) has been added as recommended by Holtslag et al. (1990) in order to restrain \( \Phi \) from becoming too large, and \( K_z \) too small, in very stable conditions. Note that Equation (A3d) matches (A3c) for \( z/L = 1 \).

Above the surface layer, but within the PBL, an additional length scale becomes relevant, the mixing height (h). During stable or near neutral conditions (h/L ≥ 10), the surface layer formulation is extended by an empirical function of z/h as recommended by Troen and Mahrt (1986):

\[ K_z = k u_* z (1 - z/h)^2 \Phi(z/L). \]  

Note that when z/h < 1 Equation (A4) reverts to the surface layer expression (Equation A1). Also, Kz is constrained to go to zero at the top of the mixed layer.

In the mixed-layer portion of the convective boundary layer, buoyant production of TKE is much more important than shear production. Therefore, friction velocity (u*) as the scaling velocity during convectively unstable conditions (h/L < 10) in the mixed layer to give

\[ K_z = k u* (1 - z/h), \]  

where Kz is again constrained to equal zero at the top of the PBL. It is this dependence on the convective velocity, which is a function of surface heat flux rather than shear stress, which enables this model to produce more realistic Kz values for the mixed layer than the formulation of Louis (1979). A disadvantage of this model, however, is that both expressions for Kz in the PBL are very sensitive to the PBL height which may be poorly estimated.