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A New Mixing Length Formulation For The Eddy-Diffusivity Parameterization

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In this paper a new mixing length formulation for the eddy-diffusivity parameterization of turbulence is suggested. The new formulation relates directly the mixing length with the turbulent kinetic energy. The simulation of dry atmospheric convection and turbulence, with a 1D boundary layer model, shows that the model reproduces quite well the growth of the boundary layer. It is also shown that the eddy-diffusivity closure is not purely diffusive, since the diffusion coefficient changes with height, and that the "advective" term has a significant impact close to the surface and the boundary layer top. In general, it is shown that the new mixing length formulation is a promising alternative to fully close the turbulence problem in atmospheric models.

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1. Introduction

The eddy-diffusivity approach to represent turbulent motions can be easily traced back to Saint-Venant (1851) and Boussinesq (1870) (see Frish (1995) for details). The mixing length concept was introduced by Prandtl (1925) and has been used in the modelling of the atmospheric boundary layer turbulence and convection for a long time (e.g. Priestley 1959, Estoque 1960).

In one way or the other, virtually all climate, Numerical Weather Prediction (NWP) and mesoscale models use the eddy-diffusivity or k-diffusion (these two designations will be used interchangeably in this paper) approach to parameterize turbulent and convective motions in the atmospheric Planetary Boundary Layer (PBL). The physical parameterization "packages" of these global and mesoscale models are essentially one-dimensional in the vertical, making the development and validation of single-column (or 1D) models an essential step in the improvement of weather and climate simulations. These 1D versions of climate or NWP models, have been increasingly used to develop and validate turbulence and convection parameterizations for a variety of boundary layer situations (e.g. Bretherton et al. 1999).

For dry boundary layer atmospheric convection it has been argued for a long time that the eddy-diffusivity approach is not fully appropriate, since it fails to properly parameterize the large eddies that are responsible for counter-gradient fluxes and for a substantial amount of the entrainment at the top of the PBL. In order to represent counter-gradient fluxes in the dry boundary layer, corrections to the eddy-diffusivity parameterization have been suggested at least since Ertel (1942) (see Stevens (2000) for a review).

The idea of using a mass-flux approach to simulate convective fluxes has been suggested for moist convection by Arakawa (1969) and was used for the dry sub-cloud boundary layer convection by Betts (1976). Randall et al. (1992) suggested a framework in which to build a unified scheme for the convective PBL based on the mass-flux concept. In Siebesma and Teixeira (2000) a new approach using a combination of k-diffusion and mass-flux parameterizations is proposed and the results are quite realistic when compared with Large Eddy Simulation (LES) results for a dry convection case. This approach has been successfully tested in the ECMWF global model (Teixeira and Siebesma 2000).

In this paper, however, we will argue that it is possible to realistically simulate dry boundary layer convection in the atmosphere with an eddy-diffusivity closure. We will use a 1D Turbulent Kinetic Energy (TKE) boundary layer model with a new mixing length formulation.

In the surface layer, a linear relation between the mixing length and height has been established for a long time (e.g. Priestley 1959). But in general, in the eddy-diffusivity closure, the mixing length is usually introduced in a rather artificial way and constitutes one of the weakest points of this parameterization. In numerical models of the atmosphere, the expressions used for the mixing length have been rather simple (e.g. Blackadar 1962, Louis et al. 1981). Recently more complex algorithms have been used (e.g. Therry and Lacarrere 1983, Bougeault and Lacarrere 1989). Although formulations like Bougeault and Lacarrere (1989) are physically more realistic and flexible, there is no such thing as a "universal" diagnostic expression for the mixing length that is flexible (and simple) enough to allow a realistic simulation of all types of boundary layers that occur in the Earth's atmosphere (e.g. dry, stable, stratocumulus topped, cumulus topped). However, it must be noted that parameterizations with a prognostic equation involving the mixing length have been used with some success (e.g. Mellor and Yamada 1982).

In this paper we propose an alternative formulation to diagnose the mixing length. We link directly the value of the mixing length with the square root of TKE multiplied by a variable τ with time dimensions. The closure problem is now moved from determining a length-scale, to the determination of a time-scale τ. If we had to devise complex empirical formulations for this time-scale, then the new method suggested in here would not be of very much use and would definitely not simplify the issue. However, we will assume that the time-scale τ can be considered a constant. The basic idea behind this assumption is that the largest eddies are the most energetic ones and that their size is proportional to a turbulent velocity given by the square root of the TKE. There is some evidence from recent LES studies of the shallow convective PBL (Neggers et al. 2001), that support this assumption of a constant time-scale τ. In this way, and if we can actually have a constant value for τ, the problem is closed in a simple manner and there is no need for empirical formulations for the mixing length.

There are some similarities with an approach used to model the stable PBL (e.g. Deardorff 1976), which uses the inverse of the Brunt-Vaisala frequency as the time scale. However, the authors are not aware of the use of any similar approaches for the simulation of the convective PBL. But it should be noted that in the k-profile schemes (Troen and Mahrt 1986, Holtslag and Boville 1993) it is implicitly assumed that the turbulent velocity scale and length scale have the same vertical shape.

The direct coupling of the mixing length with the TKE, allows for a very general formulation of the mixing length. The main question for us is then: can this formulation provide realistic results when implemented in a boundary layer model?

This paper describes the testing of this mixing length formulation in the context of dry convection in the atmospheric boundary layer. In section 2, the model is described. The results are presented in section 3 followed by a discussion in section 4. A summary is in section 5.

2. Model Description

The 1D boundary layer model used in the present study has prognostic equations for the mean potential temperature and the turbulent kinetic energy. Under horizontally homogeneous conditions, assuming a zero mean vertical velocity and with no diabatic terms, the energy conservation equation is:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial}{\partial z}\left(\overline{w'\theta'}\right) \tag{1}$$

where the prime refers to the fluctuations and $(\overline{w'\theta'})$ is the turbulent flux of potential temperature. The prognostic equation for TKE, in the absence of wind and moisture, is (e.g. Stull 1989):

$$\frac{\partial e}{\partial t} = -\frac{\partial}{\partial z}\left(\overline{w'e'} + \frac{\overline{w'p'}}{\rho_0}\right) + \frac{g}{T_0}\overline{w'\theta'} - \varepsilon \tag{2}$$

where ε represents the TKE dissipation.

The parameterization of the turbulent terms uses the eddy-diffusivity approach:

$$\overline{w'\theta'} = -K_\theta \left(\frac{\partial \theta}{\partial z} \right) \tag{3}$$

$$\overline{w'e'} + \frac{\overline{w'p'}}{\rho_0} = -K_e \left(\frac{\partial e}{\partial z} \right) \tag{4}$$

where K_e and K_θ are the eddy-diffusivity coefficients for TKE and potential temperature, respectively. The closure scheme is completed by the introduction of a couple of length scales, namely a mixing length l and a dissipation length l_e, which relate the eddy-diffusivity coefficients and the TKE dissipation with the TKE, by means of the similarity relations:

$$K_\theta = C_\theta l \, e^{1/2} \tag{5}$$

$$K_e = C_e l \, e^{1/2} \tag{6}$$

$$\varepsilon = C_\varepsilon \frac{e^{3/2}}{l_e} \tag{7}$$

For the values of the constants C_e, C_θ and C_ε we follow Duynkerke and Driedonks (1987). We will assume for simplicity that the lengths for dissipation and mixing are the same. The main new assumption in our model is that the mixing length can be diagnosed as a function of TKE as:

$$l^* = \tau e^{1/2} \tag{8}$$

where τ is a time-scale that we will consider to be constant. The actual formulation used in the model is a match between equation (8) and the linear mixing length that is expected close to the surface:

$$l = l^* + (kz - l^*)e^{-\frac{z}{\alpha}} \tag{9}$$

where k is the Von Karman constant and $\alpha=100\ m$.

3. The Test Case

As a test case we consider that at the surface the heat flux is imposed as 0.06 Kms^{-1} and the TKE is imposed as zero (e.g. Wyngaard and Cote 1971). At the upper boundary (z=3 km) the fluxes of both variables are imposed as zero. The spatial discretization of the equations uses a finite difference method, and the time discretization of the equations is done implicitly, following Richtmeyer and Morton (1967). The vertical resolution for both the single column model (SCM) and the LES model is *20 m*, and the time step of the SCM runs is *60 s*. In this test case we have used $\tau=360\ s$. A sensitivity study to other values of the time-scale is also shown.

The time evolution of the simulated potential temperature profile is presented in fig. 1 together with the LES results (Siebesma and Teixeira 2000) after 8 hours of simulation. The analysis of the figure shows that the boundary layer's growth is quite well simulated by the 1D model. Comparing with the LES results it can be seen that the 1D model achieves a very realistic PBL height after 8 hours of simulation. However, and although this is a small problem, the 1D potential temperature is not so well mixed as in the LES model. The reason for this mismatch is associated with the buoyancy flux.

In fig. 2 the corresponding time evolution of the buoyancy flux profile is shown. It can be seen that the 1D model produces a very realistic linear buoyancy flux profile with about 20% of entrainment, as in the LES model. The lack of mixing of potential temperature in the 1D model is characteristic of an interesting aspect of the dynamics of the 1D model: the model adjusts to a linear buoyancy flux profile and the consequence of this is a potential temperature profile that is slightly unstable up to the level where the buoyancy flux changes sign. But the difference between the values of potential temperature from the 1D or the LES model are fairly small and can be considered negligible in terms of climate or NWP applications. It is relevant to mention that these results show that the counter-gradient terms may not be so important after all for a reasonably realistic simulation of the dry convective PBL and this confirms previous results from Stevens (2000) and Siebesma et al. (2001).

Since the formulation of the mixing length is the new aspect of this model, it is interesting to analyze its behavior during the simulation. Fig. 3 shows the time evolution for the mixing length profiles. It can be seen that the profiles look quite reasonable. From the values of mixing length shown, values for the TKE can be inferred that are greater than what the LES or mixed layer theory may indicate. The reason for this is that for the eddy-diffusivity closure to maintain a significantly positive value of buoyancy flux in the middle of the PBL, it needs a large value of TKE to balance the small gradient in potential temperature. This does not represent to us a major deficiency of the model, since we think that it is better to have a realistic simulation of the buoyancy flux, and consequently of the PBL height, than to have the perfect TKE values. In a way, we think of the TKE as a means to an end, which is to have a realistic PBL growth. In terms of large-scale models like climate or NWP this is definitely what we want to have.

In order to test the sensitivity to different values of τ, we performed several simulations and analyzed the results in terms of variables characteristic of dry convection situations like the boundary layer height (defined as the minimum buoyancy flux height), the entrainment ratio (defined as the absolute value of the minimum buoyancy flux divided by the surface buoyancy flux) and the maximum value of TKE. The results of these different simulations are summarized in table I. It can be seen that the PBL height and the entrainment ratio increase with τ, which is to be expected, since by increasing τ we are increasing the overall mixing in the PBL and consequently the entrainment. On the other hand it is interesting to note that the maximum value of TKE does not necessarily increase with τ, except for the first few values of τ. The reason for this difference in behavior between the PBL height and entrainment ratio, on the one side, and the maximum of TKE, on the other, is associated with the fact that the height at which the TKE is maximum (around 500 m as can be inferred from Fig.3) is quite far from the PBL top.

4. Discussion

In this short discussion we will focus on two aspects: the advection-diffusion nature of the eddy-diffusivity parameterization and the extension of the new mixing length formulation to LES models.

The success, as shown in this paper, of the k-diffusion approach in simulating the dry convective boundary layer is somehow contradictory with its assumed diffusive nature. It is well known that in this type of boundary layer, the transport due to strong thermals that are more "advective" in nature, is responsible for a substantial percentage of the total mixing.

We have seen how the k-diffusion closure tends to a linear buoyancy flux to the detriment of a well mixed potential temperature in the middle of the PBL and how that contributes positively to a realistic entrainment rate. In here, we will show that the "advective" component of the turbulent diffusion equation significantly contributes to the evolution of the thermal structure of the PBL. In fact, the turbulent diffusion equation due to the eddy-diffusivity closure can be written as:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K \frac{\partial \theta}{\partial z} \right) = K \frac{\partial^2 \theta}{\partial z^2} + \frac{\partial K}{\partial z}\frac{\partial \theta}{\partial z} \tag{10}$$

There are two terms on the rhs of eq.(10): the first one is more diffusive (although not pure Fickian diffusion since k is not constant) and the second one is an advective term. In this advection term the velocity is:

$$w_k = -\frac{\partial K}{\partial z} \tag{11}$$

It can be seen that this advection term will be probably larger in areas where the turbulent diffusion coefficient changes rapidly with height. In the dry convective PBL, these are the regions closer to the surface and the PBL top. The interesting question is: how large is the advection term when compared with the total and the more diffusive tendencies?

In order to answer this question the following diagnostic analysis was performed: for every time-step we calculated explicitly the discretized version of the advection term and estimated the diffusive term by subtracting the advection tendency from the total tendency. The mean values, between hours 7 and 8, for the advective, diffusive and total tendencies are shown in Fig.4. This figure shows the expected constant value of the total tendency from the surface to the PBL top, just below where it becomes negative above the inversion. It can be seen that in general the advective term has a fundamental role. Close to the surface and the top of the PBL, the advective and diffusive terms are of a comparable large magnitude, but while the advective term is strongly negative the diffusive term is strongly positive. Another striking feature is the fact that in the middle of the PBL the advective tendency is about more than half of the total tendency. But the most important feature is that above the top of the PBL, the advective term is responsible for most of the cooling associated with the entrainment.

This result can be understood by remembering that close to the top of the PBL the velocity from eq.(11) is largely positive since the diffusion coefficient is significantly decreasing with height. This advective term is then modeling the advection of properties from inside the PBL into the free atmosphere contributing to the entrainment. So in practice, the advective term is simulating the transport into the top of the PBL, due to strong thermals from the middle of the PBL.

This sort of analysis is quite simple and straightforward and this type of link between advection and diffusion equations has been recently used to develop numerical schemes for diffusion equations based on concepts initially used for advection equations (Teixeira 1999, Smolarkiewicz and Margolin 1998). This simple analysis gives some insight into how the eddy-diffusivity closure manages to realistically simulate the dry convective boundary layer. It also shows that interpreting the eddy-diffusivity closure as merely a diffusive process is simplistic and does not reflect what the parameterization is actually doing.

In LES models the formulation of the mixing length is usually based on more solid physical arguments. It is assumed that the eddy-diffusivity closure in LES models paramterizes the turbulence that occurs at the scale of the grid-size and that cannot be "resolved" by the dynamical part of the model. In this sense the mixing length should be of the order of the grid-size:

$$l \sim \Delta s = (\Delta x \Delta y \Delta z)^{1/3} \qquad (12)$$

It is interesting to investigate, even if only in a speculative and brief manner, if the new mixing length formulation proposed in this paper can reproduce a similar result. Let us first assume that the time constant τ changes with the horizontal resolution reaching a value of the order of Δt at typical LES horizontal resolutions (about 50 m). In principle, a time scale like τ should not be smaller than the time step, and should equal the time step when the parameterization is representing sub-grid motions that happen at a length scale that is smaller, or equal, than the grid-size.

On the other hand, in LES models, as mentioned above, the parameterization is only there to represent turbulence mixing at the scale of the grid-size and as a consequence it should then be:

$$\sqrt{e} \sim \frac{\Delta s}{\Delta t} \qquad (13)$$

which implies

$$l = \tau \sqrt{e} \sim \Delta s \qquad (14)$$

So it can be said, at least in a qualitative manner, that the new mixing length formulation is able to converge to the LES expected values when the horizontal resolution becomes fairly high. This means that a dependence of τ on the horizontal resolution may well be able to make the bridge between the scales where the turbulence is basically "unresolved" and the LES scales of tens of meters, where turbulent and convective motions are substantially "resolved". If this is the case then the new mixing length may allow an eddy-diffusivity parameterization that is universal enough to be used on large-scale, mesoscale and LES models

5. Summary

In this work, a new mixing length formulation for the eddy-diffusivity parameterization of turbulence was suggested. This new formulation directly relates the mixing length with the turbulent kinetic energy, through the use of a time scale.

This new relation was tested in the context of a 1D boundary layer model, for the case of dry atmospheric convection and turbulence. The results are quite satisfactory, with the model reproducing quite well the growth of the boundary layer. The profiles of potential temperature and buoyancy flux are compared with LES results and show a very realistic agreement. In particular the buoyancy flux compares extremely well with the LES model showing that an eddy-diffusivity parameterization is able to reproduce the linear buoyancy flux profile. As a consequence the potential temperature profile is slightly too unstable when compared with the LES results, but the differences between both models are quite small. It must be mentioned that the new mixing length formulation may be used even in models where the TKE is not a prognostic variable.

It was also shown that the eddy-diffusivity closure is not purely diffusive since the diffusion coefficient changes with height. The "advective" part of the equation was shown to have a significant impact in general, and, in particular, close to the boundary layer top, significantly contributing to the entrainment. It was speculated that the new mixing length formulation maybe flexible enough in order to be used on large-scale and LES models and to successfully make the bridge between the "unresolved" large scales and the typical LES horizontal resolution.

Overall, the results show that the new mixing length formulation, that directly links the mixing length with the TKE, is a promising alternative to fully close the turbulence problem in atmospheric models. The fact that the new formulation is so general has led us to follow this study with an investigation of its capabilities in simulating the moist boundary layer (Cheinet and Teixeira 2001). This formulation may also have a potential applicability in other areas of fluid dynamics where turbulence and convection have to parameterized.

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TAU (s)	TKE max (m^2s^{-2})	Entrainment ratio (%)	PBL height (m)
180	1.24	4.6	1844
240	1.39	9.5	1974
300	1.47	14.3	2068
360	1.50	18.6	2138
420	1.50	22.2	2191
480	1.49	25.3	2234
540	1.47	27.9	2267

TABLE I

TKE max, entrainment ratio and PBL height for different values of TAU.

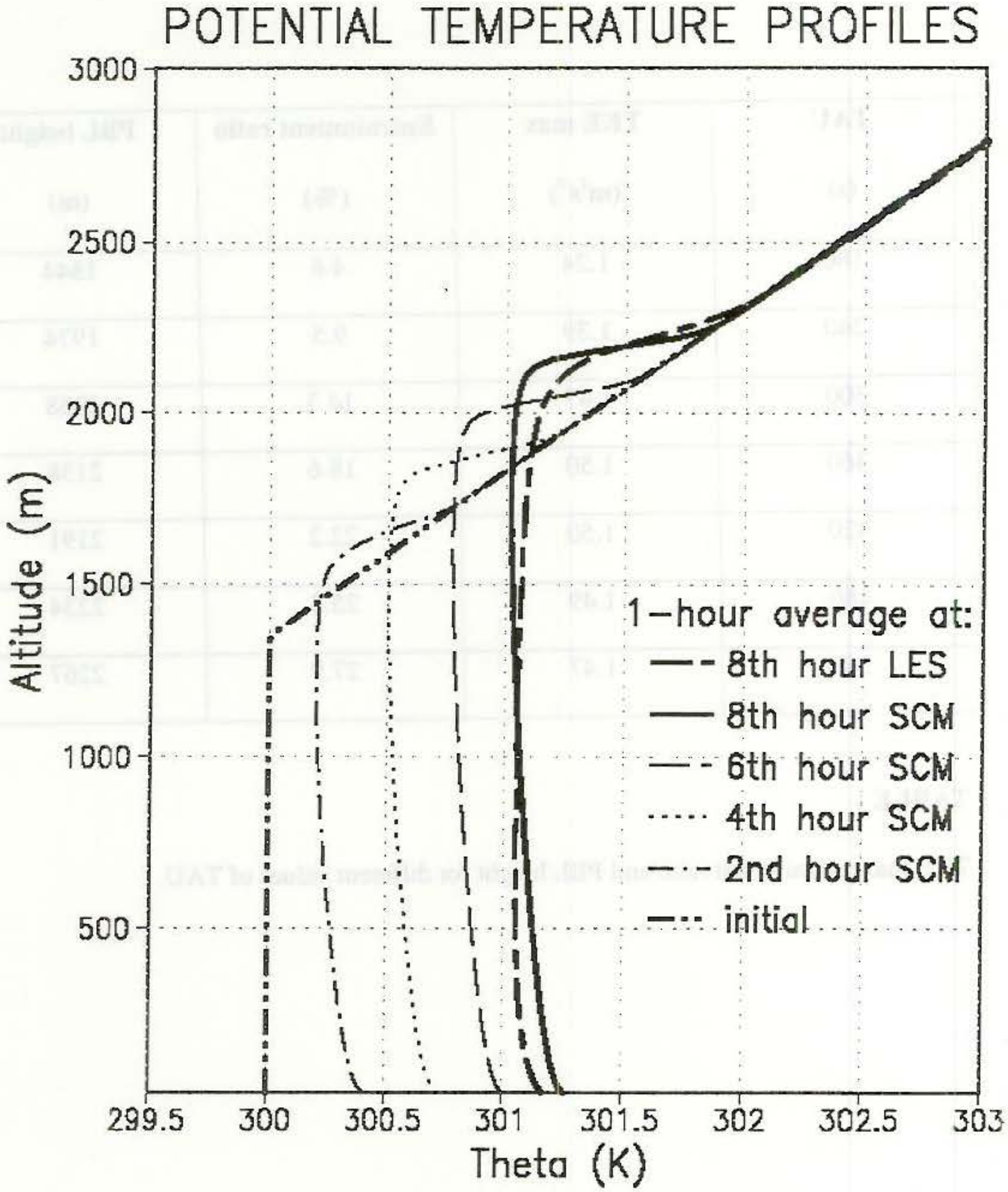

Figure 1 – The potential temperature (in *K*) profile simulated with the SCM model at initial time and at hours 2, 4, 6 and 8 (hourly means), together with LES results after 8 hours of simulation (hourly mean).

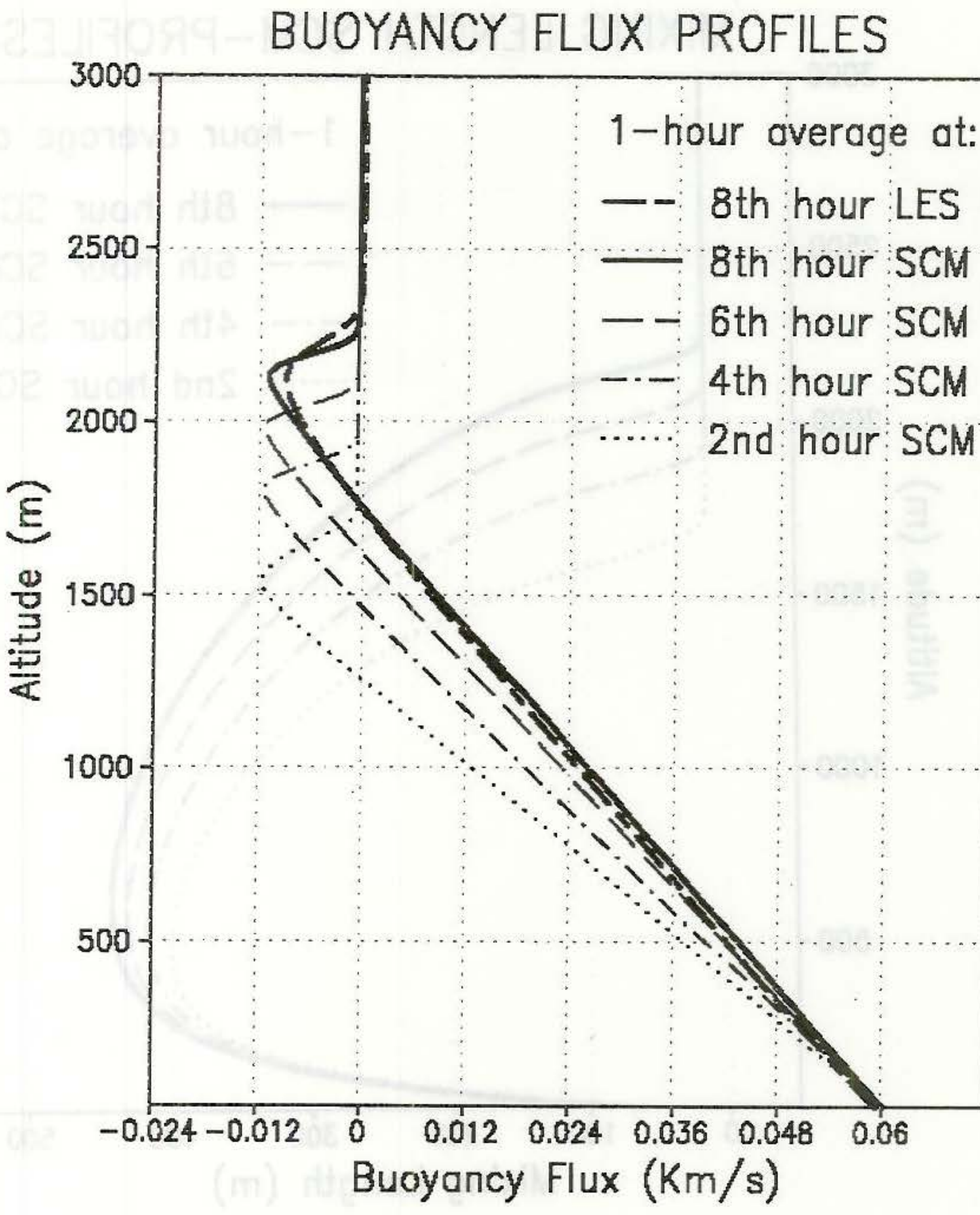

Figure 2 – As in figure 1 but for the buoyancy flux (in Kms^{-1}) profile.

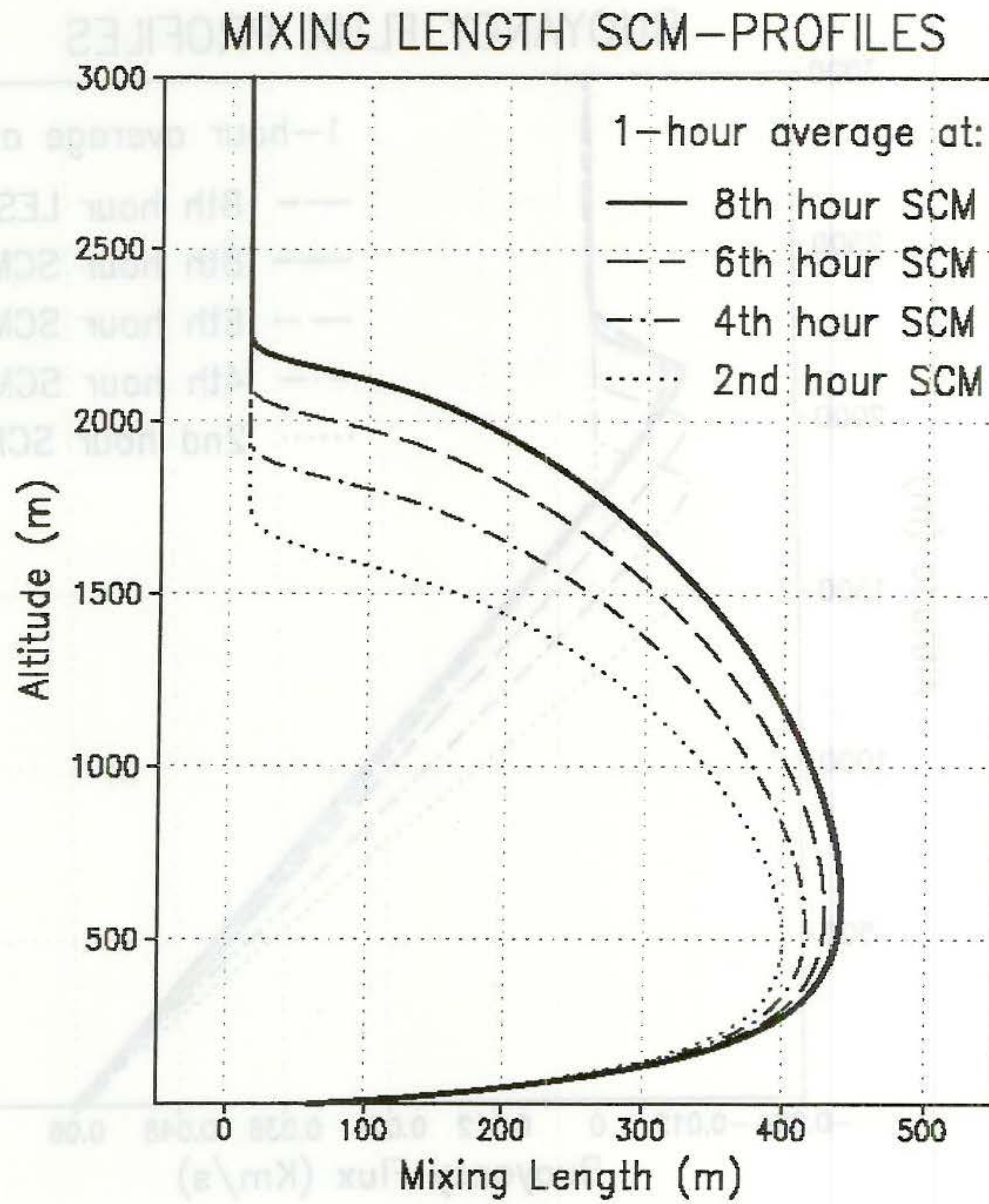

Figure 3 – As in figure 1 but for the mixing length (in *m*) and without LES results.

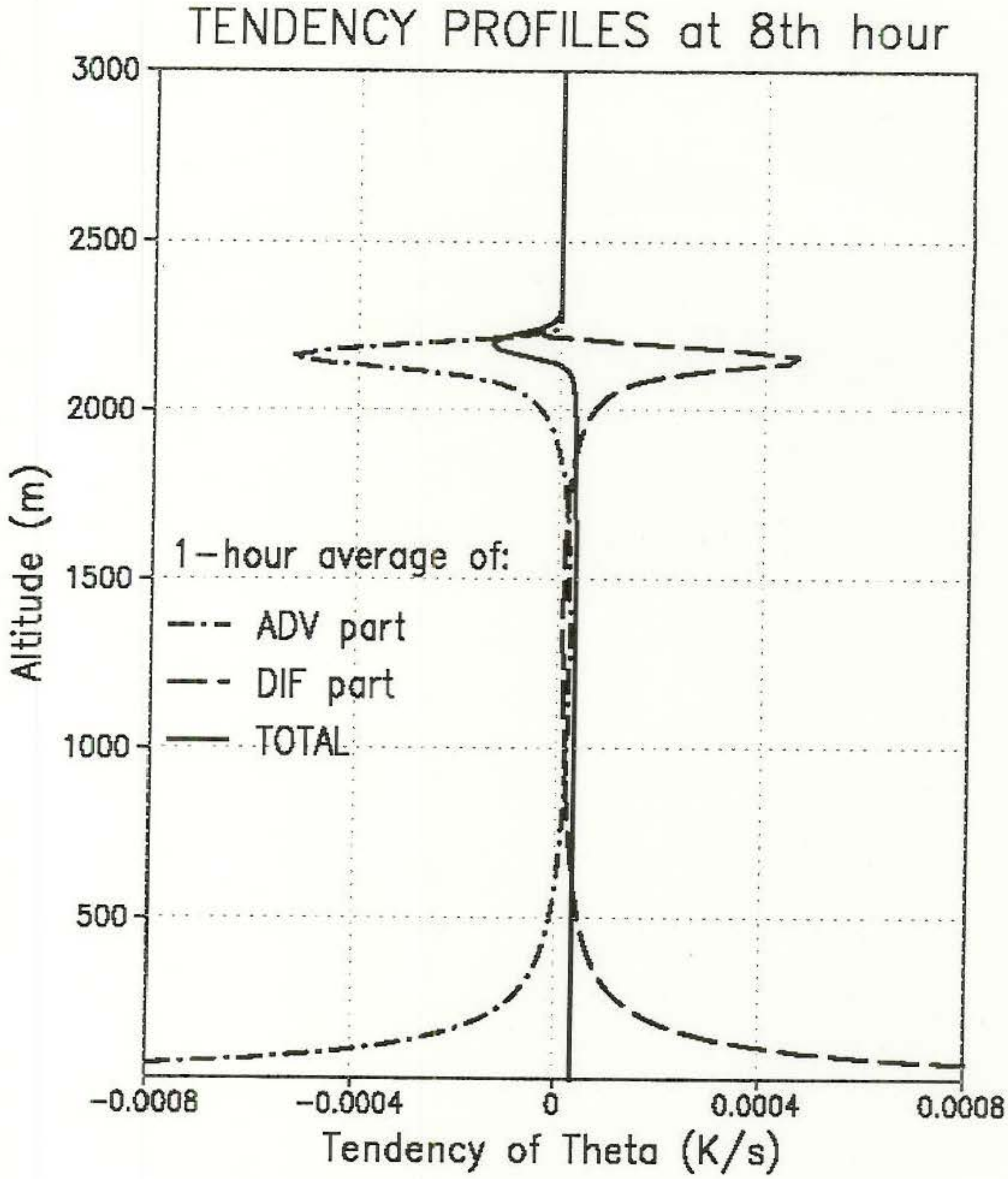

Figure 4 – The mean values, between hours 7 and 8, for the "advective", "diffusive" and total potential temperature tendencies (in Ks^{-1}) of the vertical diffusion equation. See text for details.