RC-LACE stay report

Improvement of TKE-based mixing length formulation in TOUCANS

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1 Introduction

During these two stays, previous work on TKE-based mixing length was continued. The first stay is directly connected to the previous one as it deals with the problem of the secondary maximum of TKE; its source, evolution and further attempts to remove it. In-between two stays, the question of the meaning of L_{TKE} length scale (average of L_{up} and L_{down}) was opened once again. After thorough discussion and additional inspection of the literature, it was found that the meaning of L and l_m length scales in TOUCANS is not as straightforward as it seamed previously, i.e. both of them are hybrid scales, rather than TKE-based and Prandtl type as it was thought so far. Based on these findings, during the second stay, the new formulation was coded and merged with the code for treatment of TTE induced oscillations. By the end of the stay it was validated and further updated. This report also points to major findings related to the work done after the second stay.

2 The problem of the secondary maximum of TKE

Since the problem of the secondary maximum of TKE will later prove to be practically irrelevant, the part of the research related to it will be only briefly described. With the purpose of thorough investigation of the problem, the time-step output analysis of TKE and l_m was performed. It was found that the secondary maximum problem exists already in the initial conditions (Fig. 1.; left panel), i.e. it also develops within the reference Geleyn-Cedilnik (GC) formulation. However, the design of the GC formulation, i.e. the existence of upper asymptotic (UA) limit and absence of direct dependence on TKE prevents further development of the problem. Contrary to the reference, in nearly neutral and shearless conditions, the secondary maximum of TKE within TKE-based formulation grows rapidly (Fig. 1.; right panel). After only five time-steps l_m values at model level 50 surpass 1500 m in the region along Eastern Adriatic coast (Fig. 2.; left panel), i.e. there is difference of almost two orders of magnitude compared to GC formulation. Simultaneously, the value of the TKE at the same level exceeds the value of 70 m^2s^{-2} (Fig. 2.; right panel). This value is larger for an order of magnitude than within the strong and gusty bora wind, which is common in this area.

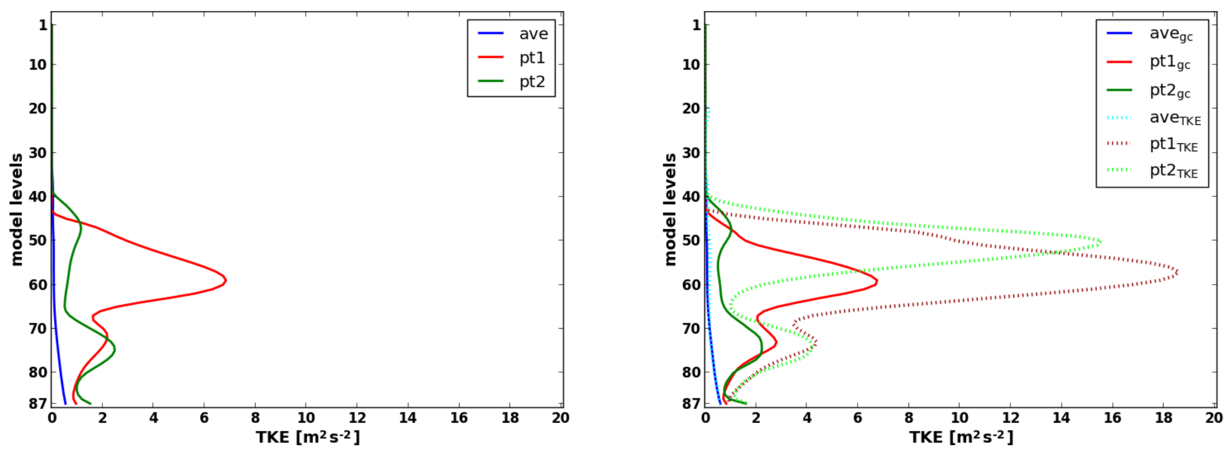

Figure 1: *The summer convection case 29.6.2017. Comparison of averaged TKE profile (blue) against two single point profiles (red and green) from columns with secondary TKE peak at the time of initialization (left) and after one time-step (right).*

Due to such a big disagreement with the GC formulation, after only five time-steps, it was thought that maybe there is some error within the algorithm for computation of L_{up} and L_{down}. In order to check this, the code was adapted to compute vertical displacements using the algorithm from the ARPEGE subroutine **acbl89.F90**. The computation was performed in fully diagnostic mode, i.e. using TKE obtained by GC formulation, on which the evolution of the forecast was based. Compared to TOUCANS, ARPEGE values are even bigger up to 10-15%. This is attributed to the impact of the shear term. Thus the doubt from the TOUCANS algorithm for computation of vertical displacements was removed and focus was shifted to finding the cure for removal of the secondary maximum of TKE.

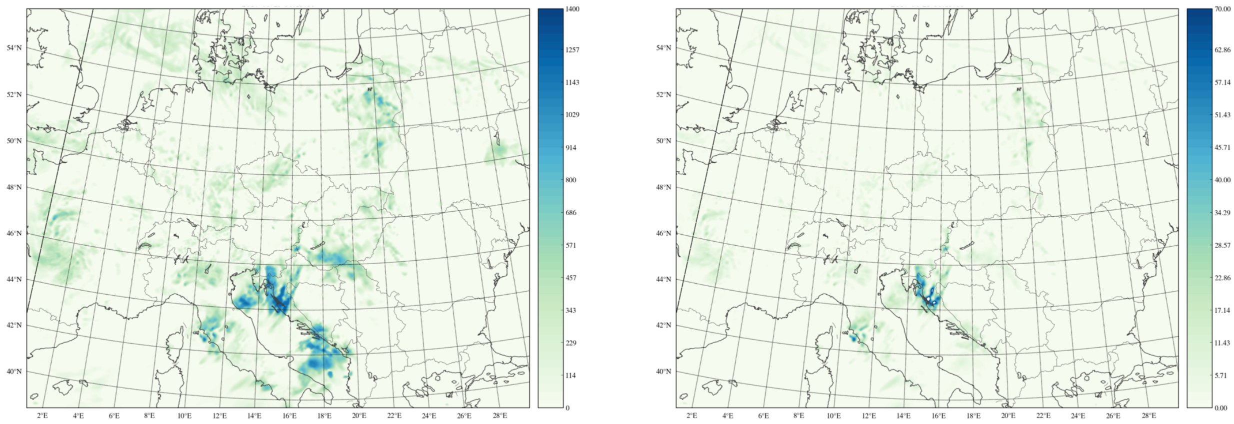

Figure 2: *The summer convection case 29.6.2017. Horizontal cross-section of mixing length (l_m; left) and TKE (right) through the model level 50 after 5 time-steps, i.e. 15 minutes of integration.*

Two options for solving the problem of the secondary maximum of TKE were proposed previously. The first one is based on addition of the third term into Bougeault-Lacarrère (BL89) integrals (cf. Chapter 4. or [1]):

$$C_1 \cdot \frac{1}{e}\left|\frac{\partial e}{\partial z}\right| \cdot g \cdot f_1(N_v) \cdot f_w(z) \tag{1}$$

where C_1 is a tuning constant, e is TKE, $f_1(N_v)$ is a stability-dependent function with maximum at neutrality and $f_w(z)$ is a height-dependent weight function aimed to tackle the region above the planetary boundary layer (PBL). The second option intends to utilize the formulation with upper asymptotic limit (λ_a) based on the following expression:

$$\lambda_a = C_2 \cdot \frac{\int_0^\infty \sqrt{e} z dz}{\int_0^\infty \sqrt{e} dz} \tag{2}$$

where C_2 is additional tuning constant. Finally, the l_m in this framework is:

$$l_m = min(\kappa z, L_{TKE}, \lambda_a) \tag{3}$$

The second option immediately proved as unsuccessful. Unfortunately, it was not able to cope with the profiles of TKE like those at Fig.1., i.e. the profiles which above PBL don't asymptotically close to a certain value. Not only that this option supports the existence of the secondary maximum of TKE, but it also enables its further growth (not shown). For this reason, it was abandoned. On the contrary, the first option was more successful. At first it was applied only above the certain model level (typically the level 65 or 70), which was safely above the surface layer where the primary TKE peak is found, but still below the levels where the secondary peak tends to occur. Of course, this is not ideal as in different conditions maximum can shift upwards or downwards and the index of cut-off level also depends on vertical resolution. The final solution in this context was to set the dependence, i.e. the inclusion of the third term, based on the PBL height. It proved as a very successful and almost matched the performance of the reference - GC formulation.

In the meantime another proposal appeared. This, so-called EL2 option, is based on the min(l_{gc}, L_{TKE}). Despite the success in removing the secondary maximum of TKE, it produced "jumpy" behaviour within the PBL. This is result of a sudden decrease of L_{TKE} when entering more stable layers. At this point it was decided to reconsider the concept and check basic equations of the TOUCANS scheme, including the comparison with equivalents from the ARPEGE model, where TKE-based formulation is also utilized.

3 Reconsidering the problem and change of the concept

Since the beginning of the work on TKE-based mixing length, the key question was related to the meaning of the L_{TKE} scale and its relationship to other length scales within the TOUCANS scheme, especially l_m and L. In order to give definitive response to this question, it was necessary to compare basic ARPEGE and TOUCANS equations, as well as to carefully read [2] and [3].

From the ARPEGE subroutine **acbl89.F90** it was found that L_{TKE} has the meaning of the Prandtl-type mixing length:

$$l_m = max[min(\kappa z, a), L_{TKE}] \tag{4}$$

where "a" is NAMPHY0 parameter ALMAVE. This can be further verified within the subroutine **acturb.F90** where the exchange coefficient is computed:

$$K_m \approx C_K \cdot l_m \cdot \sqrt{e_k} \tag{5}$$

The default value in ARPEGE is $C_K = 0.128$. Please note that there is no stability functions in (5) as we consider near neutral conditions, where they are approximately equal to 1. On the other hand, by default in TOUCANS it is assumed that L_{TKE} has the meaning of the main turbulence length scale L:

$$l_m = min\left(l_{gc}, \frac{C_K}{\nu} \cdot L_{TKE}\right) \tag{6}$$

where:

$$L = \frac{\nu}{C_K} \cdot l_m \tag{7}$$

while the exchange coefficient is computed according to:

$$K_m \approx \nu \cdot l_m \cdot \sqrt{e_k} \tag{8}$$

The default value in TOUCANS is ν = 0.5265 (C_K=0.0882). From [1] it can be confirmed that our current approach differs from default in treatment of L_{TKE} in (6), i.e. the conversion coefficient is assumed to be 1, or in other words l_m=L_{TKE}.

Now, let's consider the conditions within the surface layer and above it for ARPEGE and TOUCANS schemes. $l_{gc} \approx \kappa$z near the surface and it is likely to restrict L_{TKE} solution, i.e. expression (6) gives $l_m \approx \kappa$z there. Combining (6) and (8) in the surface layer for TOUCANS gives:

$$K_m = \nu\kappa z\sqrt{e_k} \approx 2.4 C_K z\sqrt{e_k} \tag{9}$$

where $\nu \approx 6C_K$ and κ is von Karman constant. On the other hand, combining (4) and (5) near the surface in ARPEGE gives:

$$K_m = C_K L_{TKE}\sqrt{e_k} \geq C_K z\sqrt{e_k} \tag{10}$$

If equations (5) and (8) are written outside the surface layer, supposing that L_{TKE} solution prevails there, i.e. limitations in (4) and (6) don't, one gets:

$$K_m = C_K L_{TKE}\sqrt{e_k} \tag{11}$$

Thus the only remaining difference between the two schemes is the value of C_K. Contrary to this, our current approach results in six times larger value of the exchange coefficient, which can explain the problem of appearance of the secondary maximum of TKE. On the other hand, within the surface layer we have more or less the same solution as in both κz limit is forced. The only remaining issue is to explain differences in the surface layer between TOUCANS and

ARPEGE. After reading [2] and its short summary in [4], it is found that length scale is used to achieve matching between the surface value of C_K and its free atmosphere value. Those two differ by almost an order of magnitude in reality; surface being larger of the two. For this reason, both in [2] and TOUCANS, the main length scale L was set as L=l_m above the surface layer and L=Az in the surface layer, with a smooth transition in-between (A=$\kappa \cdot \nu / C_K \approx 2.4\kappa$). Unlike in TOUCANS, within ARPEGE some variability around "const·z" is enabled. This depends on the value of L_{TKE}, which may prevail in near neutral and unstable conditions.

4 The new TKE-based formulation

Including the latest changes, we proceeded towards the definite form of TKE-based mixing length formulation in TOUCANS. We decided to stick to the former shape of the BL89 integrals, used to compute vertical displacements:

$$\int_{z}^{z+L_{up}} \left\{ \frac{g}{\theta_v(z')} \left[\theta_v(z') - \theta_v(z)\right] + C_0 \sqrt{e(z')} S(z') \right\} dz' = e(z) \tag{12}$$

$$\int_{z-L_{down}}^{z} \left\{ \frac{g}{\theta_v(z')} \left[\theta_v(z) - \theta_v(z')\right] + C_0 \sqrt{e(z')} S(z') \right\} dz' = e(z) \tag{13}$$

where θ_v is virtual potential temperature (at starting level - z or at actual parcel's point - z'), e(z) is TKE at the starting level, S(z') is local vertical wind shear, while C_0 is a constant controlling the magnitude of the shear term. Once when L_{up} and L_{down} are computed, the TKE-based scale is computed by averaging of the two:

$$L_{TKE} = \sqrt{L_{up} \cdot L_{down}} \tag{14}$$

Note that any other averaging operator vanishing with L_{up} or $L_{down} \to 0$ is equally justified.

As in (6), the TKE-based scale is now set as equal to the main length scale, i.e. L=L_{TKE}. However, the minimum of κz and L_{TKE} will not be declared as l_m anymore. Within the new formulation, depending on the height of PBL, there is a smooth transition from the surface "κz" layer towards the upper PBL and free atmosphere, where pure L_{TKE} solution prevails:

$$l_m = f_w \cdot \kappa z + (1 - f_w) \cdot \frac{C_K}{\nu} \cdot L_{TKE} \tag{15}$$

where f_w is a weight function given by:

$$f_w = 3 \cdot f_w'^{\,2} - 2 \cdot f_w'^{\,3} \tag{16}$$

while f'_w is given by:

$$f_w' = max\left[0, min\left(1, \frac{c_2 - \frac{Z_H}{H_{PBL}}}{c_2 - c_1}\right)\right] \tag{17}$$

where c_1 and c_2 are heights relative to the height of the PBL (H_{PBL}) and denote levels between which mixed solution is applied ($f_w \in \langle 0,1 \rangle$), and z_H is height of the model half-levels (l_m is computed there). Prior to any experiments, the new TKE-based mixing length code was merged with the code for treatment of TTE induced oscillations into local "CY43t2plus_op1" code. Furthermore, new cases (21-25.11.2019. and 17-21.6.2020.) were selected and everything is prepared for the switch to ALADIN-CZ non-hydrostatic 2.3 km configuration.

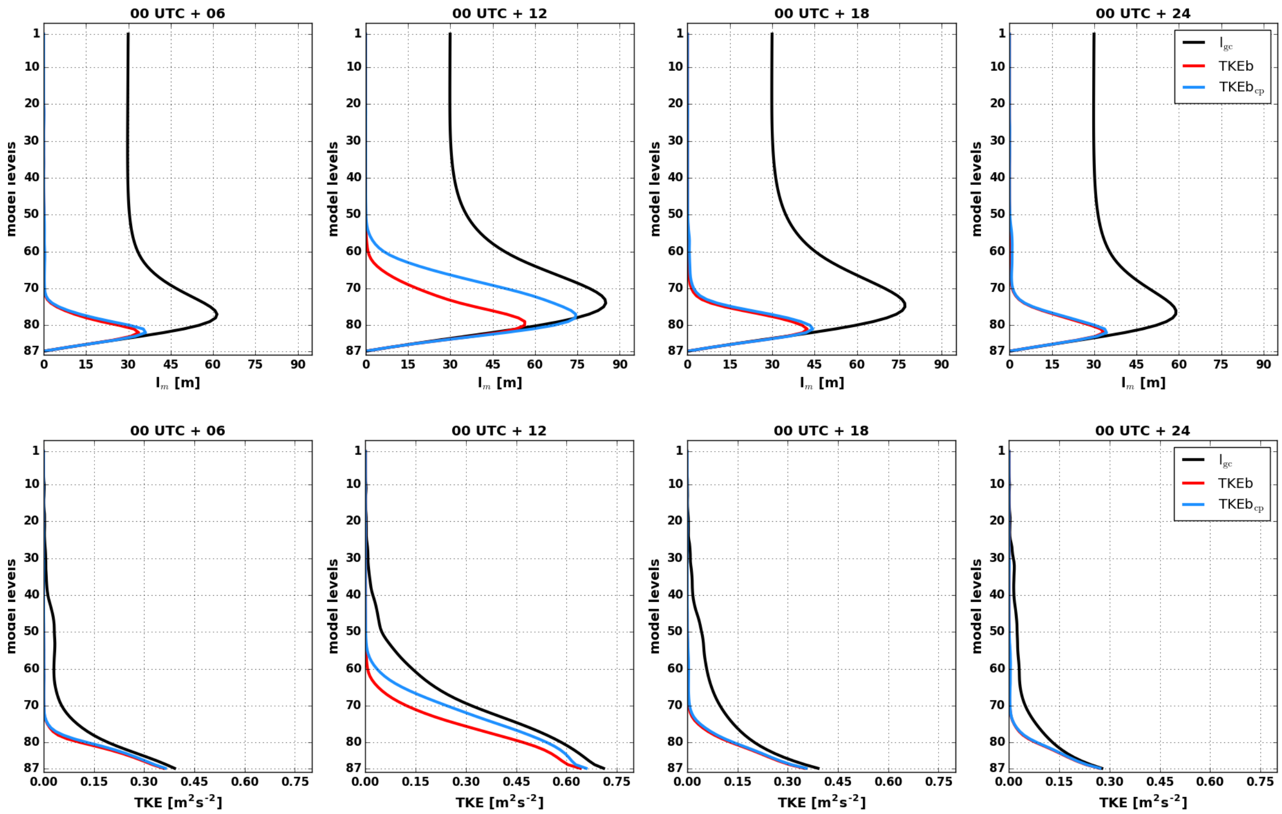

Figure 3: *The summer convection case 18.6.2020. Comparison of averaged l_m (upper panels) and TKE (lower panels) profiles for the reference (GC formulation; black), TKE-based formulation without crossing parcels method (red) and TKE-based formulation with included crossing parcels method (blue).*

Enabling the above mentioned smooth transition and extending the κz layer above the lowest model half-level prevents the collapse of TKE and ensures reasonable model performance in stable conditions. On the other hand, in unstable conditions there is not enough mixing, both near the surface and in upper PBL. This problem was tackled from several perspectives. Among other, the crossing parcels (CP) treatment (e.g. [5]) proved as the most successful one. It implies that after computation of L_{up} and L_{down}, entire profile is recomputed so that:

$$L_{up}(i) = max\{L_{up}(i), L_{up}(i+1) - [z(i) - z(i+1)]\} \tag{18}$$

starting from KLEV-1 and:

$$L_{down}(i) = max\{L_{down}(i), L_{down}(i-1) - [z(i-1) - z(i)]\} \tag{19}$$

starting from KTDIA+1.

As it can be seen on Fig.3., the impact of CP is huge during daily hours and summer convection (both for l_m and TKE). Contrary, during the night and especially winter (not shown) its contribution is practically negligible. This is in accordance with expectations and helps to increase turbulent transport across the PBL top (when needed). However, it is still not enough to overcame the reference.

In parallel with CP treatment, the moist potential temperature (θ_m; inverted from N_m^2) was also tested in (12) and (13). Despite the positive impact on few cases (further increase of mixing across the PBL top and in cloudy layer above it), it was decided to abandon this approach. First of all, it resulted with few unstable simulations. Secondly and conceptually more important, in convective environment N_m^2 is close to zero, which results in nearly constant θ_m. Thus the parcel displacement in (12) and (13) can be stopped only by the boundaries of this nearly neutral region, i.e. by the ground and tropopause. The above mentioned behaviour of θ_m is suggested in [6], where it is shown that in the case of stratocumulus moist entropy remains constant across the PBL, without a jump at its top. Moreover, the free atmosphere and in-cloud - clear sky variations also proved to be small. For our approach this is not acceptable as θ_m is obviously too conservative variable, possibly leading to double counting of the moist effects (I. Baštak Ďurán, personal communication).

Except the CP method, setting the free atmosphere value of l_m also proved as significant contributor in improving the performance of TKE-based mixing length. Furthermore, it is also very easily implementable. Several options between the UA value of l_{gc} and 0 were tested. The winter situation is less sensitive to this value, but it is evident that 0 is not a solution (not shown). During the summer, l_{gc} asymptotic value of 30 [m] proved as the most successful one so far. The impact of setting UA value can be seen on Fig.4. (upper panels; blue curve). Not only that it increases mixing in the free atmosphere, but also between the maximum of mixing region and cut-off point. To a smaller extent it works in the same direction within the surface layer. The latter one is a result of vertical communication between different layers (in this case it should come from above). The impact on TKE (Fig.4.; lower panels) is following the pattern of l_m, i.e. it decreases from the middle troposphere and PBL top towards the surface.

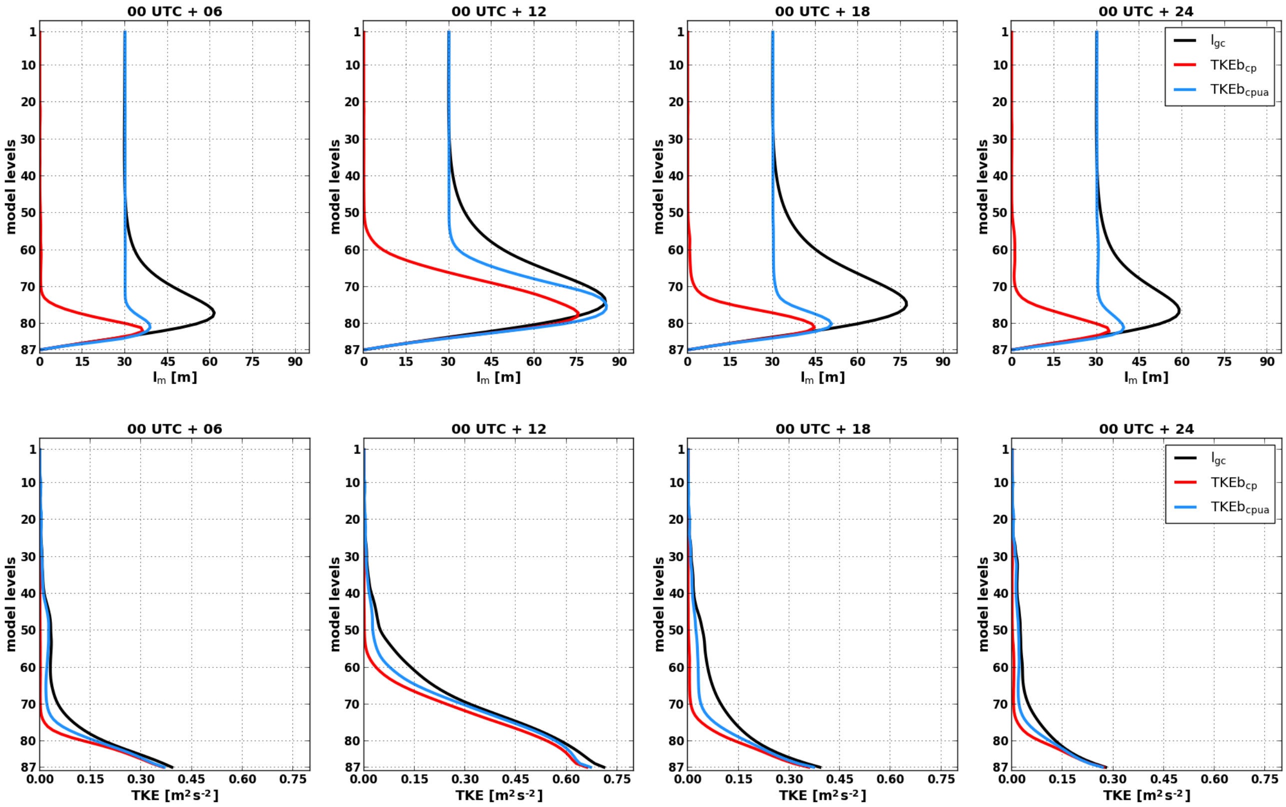

Figure 4: *The summer convection case 18.6.2020. Comparison of averaged l_m (upper panels) and TKE (lower panels) profiles for the reference (GC formulation; black), TKE-based formulation with included crossing parcels method and without upper asymptotic (UA) value (red) and TKE-based formulation with included crossing parcels method as well as with UA value set to 30 [m] (blue).*

The impact of the latest change on enthalphy and water vapour, i.e. increasing UA value, is shown on Fig.5. (enthalphy) and Fig.6. (water vapour). Apparently, it results in closing the gap between TKE-based mixing length and the reference (l_{gc}). For enthalpy, the impact is seen mostly near the surface, where reference is in generally colder than experiments. In the case of water vapour, it is evident that +/- pattern in tendency decreases in magnitude, i.e. the PBL moisture surplus decreases for experiment with UA limit, as well as deficit above the PBL. However, the scores for this case are still neutral (upper air) to slightly negative (surface) and also similar for the winter case (not shown).

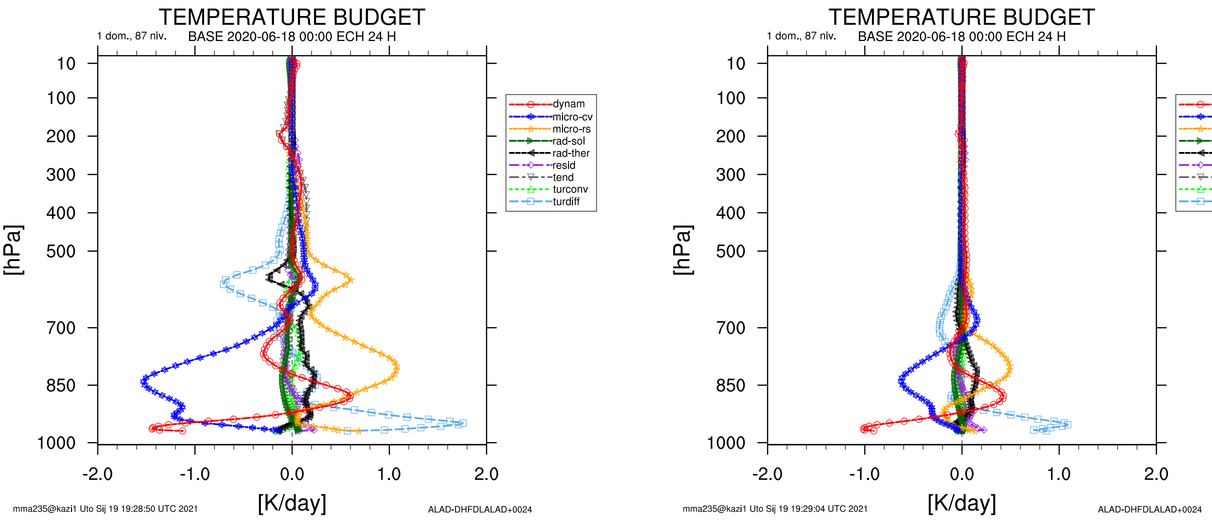

Figure 5: *The summer convection case 18.6.2020. DDH budget differences for enthalpy: reference-TKEb$_{cp}$ (left panel) and reference-TKEb$_{cp-ua}$ (right panel). Cf. Fig4. for more details on TKEb$_{cp}$ and TKE$_{cp-ua}$.*

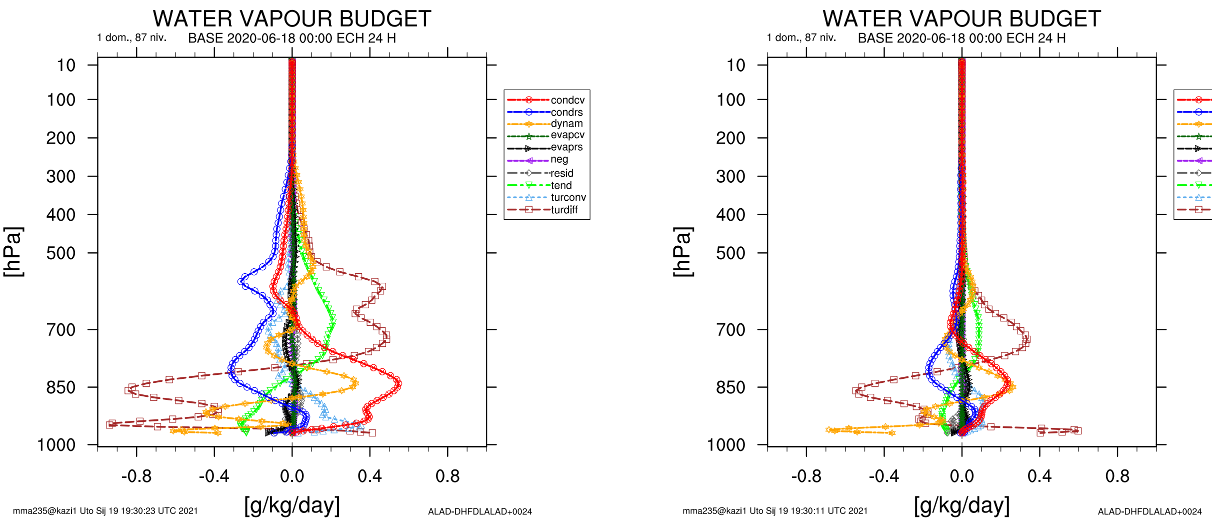

Figure 6: *The summer convection case 18.6.2020. DDH budget differences for vater vapour: reference-TKEb$_{cp}$ (left panel) and reference-TKEb$_{cp-ua}$ (right panel). Cf. Fig4. for more details on TKEb$_{cp}$ and TKE$_{cp-ua}$.*

Further experiments were focused on tuning the existing options, e.g. basic TOUCANS parameters (C_ϵ and C_K; without touching ν), value of C_0 in (12) and (13), c_1 and c_2 in (17) and ”invisible” TKEMULT which multiplies the right-hand side of (12) and (13). Neither of these proved as crucial. The first only pronounced the maximum of mixing, but didn't effect the target region near the PBL top. The impact of the shear term (C_0) is rather small and can be only used for fine tuning. c_1 and c_2, which determine the boundaries of the smooth transition region, mostly affect stable situations, but without the clear impact on scores. Similarly as C_0, they were left for later as there was no clear impact seen through scores. Finally, TKEMULT showed promising impact (increase of l_m above the maximum of mixing and towards the free atmosphere). Unfortunately, this was noted only when it was increased by 300%, which can't be justified. For this reason, TKEMULT approach is permanently abandoned.

5 Conclusion

This stay confirmed that definite formulation of TKE-mixing length in TOUCANS should be based on $L=L_{TKE}$, with a smooth transition towards $L=Az$ in the surface layer. The smooth transition from one to another is achieved through PBL height dependent weight function, with two tuning parameters.

After thorough inspection of the literature and further discussion, it was confirmed that the main length scale (L) is not TKE-based as it was thought, but a hybrid one. Precisely, L corresponds to the Prandtl- type mixing length above the surface layer and in free atmosphere, while near the surface it is a Prandtl-type solution scaled by $C_\epsilon/\nu^3 \approx 6$. The purpose of such scaling is to enable the usage of the same value of C_K, both in the surface layer and free atmosphere, i.e. to compensate for its different value in these layers (almost one order of magnitude). Contrary to L, l_m is a Prandtl-type scale in the surface layer, while outside it is scaled by reversed factor to that applied to L in the surface layer ($\nu^3/C_\epsilon \approx 1/6$).

The previous approach, where $l_m=L_{TKE}$, resulted in overestimated values of exchange coefficients ($K_{m/h}$) above the surface layer and appearance of the secondary (artificial) maximum of TKE. Obviously, such approach wasn't suitable. However, the related research pointed to the fact that TOUCANS (with reference mixing length formulation) can also produce TKE profiles with secondary maximum, but not nearly close in magnitude to the ones obtained by $l_m=L_{TKE}$ approach. The positive finding is also that having an upper asymptotic limit of l_m helps to prevent further (uncontrolled) growth of mixing and related TKE maximum above the PBL.

The new formulation was upgraded with the use of crossing parcels method and setting an upper asymptotic limit. The later one is prone to further modifications, depending on daily and/or seasonal cycling of TKE-based mixing length seen in analyzed profiles. Further work will continue from home.

6 Further work and perspectives

The behaviour of the new formulation is, unlike the previous, well balanced between different cases. Previously there were huge problems with convection, where the impact of the secondary maximum of TKE was more prominent. However, there is still some work to be done, including: i) testing the options to modify the buoyancy term of (12) and (13) in cloudy conditions, ii) inspecting the possibility of tuning both the convection and turbulence schemes, iii) modification of MD2 stability functions, iv) implementation and testing conditions-dependent upper asymptotic value of l_m and v) coding and evaluation of the complementary method for computation of PBL height (the current one is not suitable for stable conditions).

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