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Limited Area Modeling in Central Europe

RC-LACE stay report

Recent developments of the TKE-based mixing length formulation in TOUCANS

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1 Introduction

During this stay, the work on the improvement of the TKE-based mixing length formulation continued. Motivated by discussions during the TOUCANS brainstorming, we revised the issue of scaling the TKE-based mixing length as well as methods for computation of the Upper-air Asymptotic Mixing Length (UAML) and height of the Planetary Boundary Layer (PBL). In the first two weeks, most of the related development was done, followed by the evaluation on several cases, e.g., inversion, convection, and rapid change of cloudiness regimes. The report is organized as follows. The description of the changes in the TKE-based mixing length formulation is presented in Chapter 2, followed by an evaluation of selected cases in Chapter 3. Finally, a summary and plan to finalize the TKE-based formulation are presented in Chapter 4.

2 The settings of the TKE-based formulation

2.1 The basic setup and scaling

The starting point for determining the TKE-based mixing length is the computation of the air parcel's vertical displacements following the approach of [8]:

$$\int_{\mathrm{z}}^{\mathrm{z}+\mathrm{L}_{\mathrm{up}}} \left\{ \frac{\mathrm{g}}{\theta_{\mathrm{v}}(\mathrm{z}')} \left[\theta_{\mathrm{v}}(\mathrm{z}') - \theta_{\mathrm{v}}(\mathrm{z})\right] + \mathrm{C}_0 \sqrt{\mathrm{e}(\mathrm{z}')}\mathrm{S}(\mathrm{z}') \right\} \mathrm{dz}' = \mathrm{e}(\mathrm{z}) \tag{1}$$

$$\int_{\mathrm{z}-\mathrm{L}_{\mathrm{down}}}^{\mathrm{z}} \left\{ \frac{\mathrm{g}}{\theta_{\mathrm{v}}(\mathrm{z}')} \left[\theta_{\mathrm{v}}(\mathrm{z}) - \theta_{\mathrm{v}}(\mathrm{z}')\right] + \mathrm{C}_0 \sqrt{\mathrm{e}(\mathrm{z}')}\mathrm{S}(\mathrm{z}') \right\} \mathrm{dz}' = \mathrm{e}(\mathrm{z}) \tag{2}$$

where θ_v is a virtual potential temperature (at starting level - z or at actual parcel's point - z'), e is TKE, 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 known, the TKE-based scale (L_{TKE}) is computed by averaging the two. In our work, we utilize power averaging:

$$\mathrm{L_{TKE}} = \left(\frac{\mathrm{L_{up}^{p}} + \mathrm{L_{down}^{p}}}{2} \right)^{\frac{1}{\mathrm{p}}} \tag{3}$$

where p may be any real number, but preferably $-2 \leq p < 0$. Smaller values of p lead to insufficient mixing in the entire PBL, while larger values overemphasize the area near the maximum of mixing and thus deteriorate the forecast. Our starting choice is p=-1/2. However, it may be changed during the final tuning. Previously, we considered L_{TKE} as equal to one of the existing length scales in TOUCANS, i.e., L or l_m where:

$$\mathrm{l_m} = \frac{\nu^3}{\mathrm{C}_\epsilon} \cdot \mathrm{L} \tag{4}$$

In the above Eq. (4), C_ϵ=0.871 and ν=0.5265, i.e., $\nu^3/C_\epsilon \approx 1/6$. So, the choice of the length scale to which L_{TKE} is related (set equal to) strongly affects the turbulent mixing within the model column. If it is set that $l_m = L_{TKE}$, this results in too strong mixing, the appearance of the secondary maxima of TKE and l_m above the PBL and numerical instability in the most extreme cases [4]. Contrary, with $L = L_{TKE}$, there is insufficient mixing in the middle and upper PBL and too weak turbulent transport of heat and moisture across the PBL top [5]. The latter approach can be improved more easily by ([3, 5]): i) setting a smooth transition from $L = \kappa z \cdot C_\epsilon/\nu^3$ in the surface layer of the PBL to the aloft layer where $L = L_{TKE}$ solution prevails, ii) introducing the crossing parcels (CP) method, and iii) constructing a variable UAML in the free atmosphere.

A recent comparison of mixing length profiles with LES-based diagnostics revealed that L_{TKE} should be scaled with von Karman's constant (κ; personal communication with Ivan Bašták Ďurán):

$$\mathrm{l'_m} = \kappa \cdot \mathrm{L_{TKE}} \tag{5}$$

where l'_m is the same type of scale as l_m but applied above the surface layer (with smooth transition to κz in the surface layer; cf. sub-chapter 2.2). The newly proposed solution lies between our two previous attempts and presumably can improve the drawbacks of the recent one. Most notably, too weak turbulent transport of heat and moisture across the PBL top.

2.2 Inherited ingredients from the previous attempt

In previous work, i.e., when we assumed $\mathrm{L}=\mathrm{L}_{\mathrm{TKE}}$, the CP method proved essential to represent turbulence in statically unstable conditions. For this reason, we decided to keep it and validate it with the new scaling. As explained in [5], before using Eq. (3), vertical displacements L_{up} and $\mathrm{L}_{\mathrm{down}}$ should be updated for parcels crossing the computation level (i) in the following way:

$$\mathrm{L}_{\mathrm{up}} = \max[\mathrm{L}_{\mathrm{up}}(\mathrm{i}), \mathrm{L}_{\mathrm{up}}(\mathrm{i}+1) - \Delta\mathrm{z}] \tag{6}$$

$$\mathrm{L}_{\mathrm{down}} = \max[\mathrm{L}_{\mathrm{down}}(\mathrm{i}), \mathrm{L}_{\mathrm{down}}(\mathrm{i}-1) - \Delta\mathrm{z}] \tag{7}$$

where Δz is a distance between the height of the computation level and its preceding level in the direction of integration. Once $\mathrm{L}_{\mathrm{TKE}}$ is updated for CP and scaled by using Eq. (5), the mixing length is computed as:

$$\mathrm{l}_{\mathrm{m}} = \mathrm{f}_{\mathrm{w}} \cdot \kappa\mathrm{z} + (1 - \mathrm{f}_{\mathrm{w}}) \cdot \mathrm{l}'_{\mathrm{m}} \tag{8}$$

where f_{w} is a weight function given by:

$$\mathrm{f}_{\mathrm{w}} = 3 \cdot \mathrm{f}'^{2}_{\mathrm{w}} - 2 \cdot \mathrm{f}'^{3}_{\mathrm{w}} \tag{9}$$

while $\mathrm{f'}_{\mathrm{w}}$ is given by:

$$\mathrm{f}'_{\mathrm{w}} = \max\left[0, \min\left(1, \frac{\mathrm{c}_2 - \frac{\mathrm{z}_{\mathrm{H}}}{\mathrm{H}_{\mathrm{PBL}}}}{\mathrm{c}_2 - \mathrm{c}_1}\right)\right] \tag{10}$$

In the above Eq. (10), c_1 and c_2 are heights relative to the height of the PBL ($\mathrm{H}_{\mathrm{PBL}}$) and denote levels between which mixed solution is applied ($\mathrm{f}_{\mathrm{w}} \in \langle 0,1 \rangle$), and z_{H} is height of the model half-levels (l_{m} is computed there). The $\mathrm{H}_{\mathrm{PBL}}$ in ALARO-CMC is computed by utilizing the Weak-Capping-Inversion Method (WCIM; [1]):

$$\theta_v(z_i) = \frac{1}{z_i}\int_0^{z_i} \theta_v(z)\,dz + 0.25\,\mathrm{K} \tag{11}$$

where z_i is a height at which the local virtual potential temperature ($\theta_v(z_i)$) first time exceeds the vertical running average of the mixed layer virtual potential temperature by 0.25 K.

2.3 The upgrade of the TKE-based mixing length formulation

The previous work of [5] showed that setting the UAML is another way to increase the mixing near the PBL top. It also proved beneficial for the forecast of temperature and humidity. However, set to a fixed value is not representative for different stability conditions. Thus, the idea of having a variable UAML (VUAML) originated. The simplest option we figured out was to scale the maximum value of L_{TKE} within the H_{PBL} and impose it as a lower limit of L_{TKE}:

$$L_{TKE} = \max(L'_{TKE}, c_3 \cdot L_{TKE-max}) \tag{12}$$

where L'_{TKE} and $L_{TKE-max}$ are non-corrected value of L_{TKE} and its maximum value within the PBL while c_3 is a tunable parameter of order 0.2-0.3. Since it is based on vertical displacements, this method is a regime-dependent. However, it has its weaknesses due to the heuristic nature of L_{up} and L_{down}, and their averaging to L_{TKE}. During the TOUCANS brainstorming, another method was found. According to [2], the identification of different regimes within the PBL can be made from the vertical gradient of the moist entropy potential temperature ($\Delta\theta_s$):

$$\Delta\theta_s > C_{\beta_m} : L_{TKE} = L_{TKE1} \tag{13}$$

$$-C_{\beta_m} \leq \Delta\theta_s \leq C_{\beta_m} : L_{TKE} = \frac{1}{2}\cdot\left[L_{TKE2}\left(1-\frac{\Delta\theta_s}{C_{\beta_m}}\right) + L_{TKE1}\left(1+\frac{\Delta\theta_s}{C_{\beta_m}}\right)\right] \tag{14}$$

$$\Delta\theta_s < -C_{\beta_m} : L_{TKE} = L_{TKE2} \tag{15}$$

$$\Delta\theta_s = \theta_s(z = 1.5\cdot H_{PBL}) - \theta_s(z=0) \tag{16}$$

where C_{β_m}, L_{TKE1} and L_{TKE2} are calibration constants. The first constant sets the limits of $\Delta\theta_s$ above which the minimum and maximum upper-air lower limit values of L_{TKE} are applied. However, it also determines how L_{TKE} varies when $-C_{\beta_m} \le \Delta\theta_s \le C_{\beta_m}$. The other two constants denote the minimum and maximum values of L_{TKE}.

An important parameter whose calculation needs to be improved is the H_{PBL}. Within our approach it is utilized to: i) achieve a smooth transition of the TKE-based mixing length from the surface to the aloft layer, ii) determine the altitude above which VUAML is applied and iii) compute both VUAML solutions. In addition to the existing WCIM method, we implemented a more general method based on TKE and appropriate particularly for statically stable conditions:

$$H_{PBL} = \frac{z_{05}}{0.95} \tag{17}$$

where z_{05} is a height at which TKE decreases to 5% of its surface value. After the z_{05} is found, we linearly extrapolate to the level where TKE would vanish if its profile was linear. Due to weaknesses of the WCIM approach in statically stable conditions, the aim is to use it together with the TKE-based method, i.e., to take the minimum of the two. Finally, there is a method based on the integral of L_{up} which contains the impact of buoyancy, vertical wind shear and turbulence intensity [2]:

$$H_{PBL} = c_{pblh} \cdot \sqrt{\int_{z=0}^{z_{top}} L_{up} \cdot dz}, \qquad c_{pblh} = 1.75 \tag{18}$$

where c_{pblh} is a calibration constant and z_{top} is a height of the model top. Thus it has a potential to be used solely and more generally than the other two methods, i.e., in different stability regimes.

3 Validation of the updated TKE-based mixing length formulation

The preliminary validation is performed on the same set of cases as during the previous stay, i.e., inversion (23th November 2019) and convection (18th June 2020) case. Once satisfying performance is achieved, the number and types of cases will be increased. The results are presented in the following subchapters.

3.1 Preliminary validation and numerical instability issue

The impact of the new scaling, with and without the CP method, for the latter case is shown in Figure 1. As can be seen, the impact of scaling is most pronounced in convective conditions (Figure 1b). However, unlike the CP method, it is also notable in more stable conditions, i.e., during the night and morning (Figure 1a, c and d). Further, we notice an increase of the height at which the maximum of mixing occurs. This is in accordance with the finding of [7] for their cloudy case. Both scaling and CP also increase the magnitude of the maximum of l_m.

However, none of the options can sufficiently increase the turbulent transport of heat and moisture across the PBL top (not shown). For this reason, we opt to construct the formulation with the UAML as in [5]. Unlike there, we implemented the variable UAML (VUAML), as given by Eq. (7) and Eq. (8)-(11). Hereafter, the former is referred to as "VUAML option 1", and the latter as "VUAML option 2".

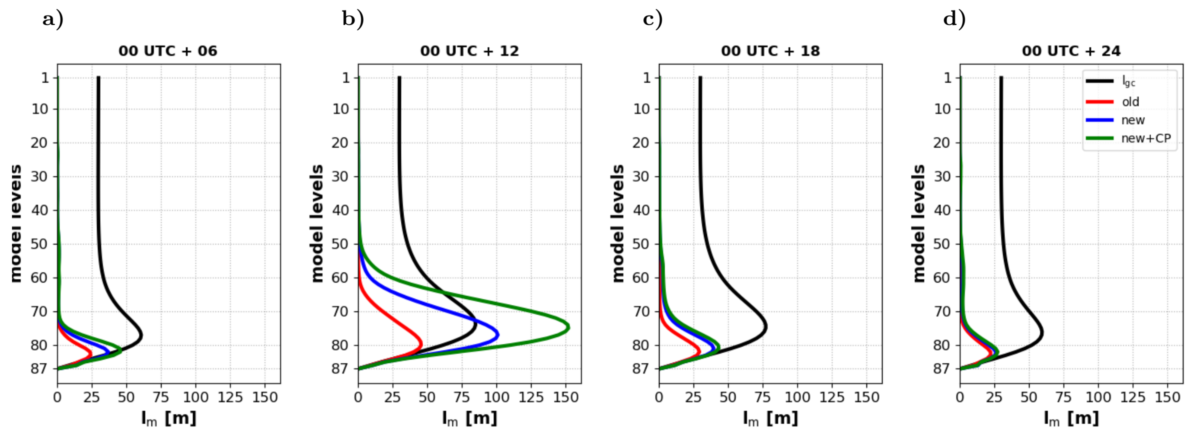

Figure 1: The impact of the new scaling and crossing parcels (CP) method on the domain averaged mixing length profile for the convection case of 18$^{\mathrm{th}}$ June 2020.

The "VUAML option 1" was also implemented for the configuration with old scaling and compared to the fixed UAML from [5] for the above mentioned cases. This led to improvement in the transport of heat and moisture across the PBL top in both stable and unstable conditions (not shown). By comparing two VUAML configurations with different scaling, we found that the new scaling somewhat improves the results in unstable conditions, while the impact in stable situations is relatively small.

Additionally, we launched the same experiments for the case with underestimated low cloudiness in CHMI's operational configuration (8^{th} November 2020). The experiment with new scaling crashed at 127^{th} time step, i.e., after $\sim$ 3 hours and 10 minutes of integration. The problematic point was found near the outer edge of the coupling zone, and it was identified as an inland water point, i.e., a lake in the northeastern Europe. The profile of L_{up}, L_{down}, l_m and TKE is shown in Figure 2. and points to unrealistically high values of all parameters near the PBL top and slightly above it.

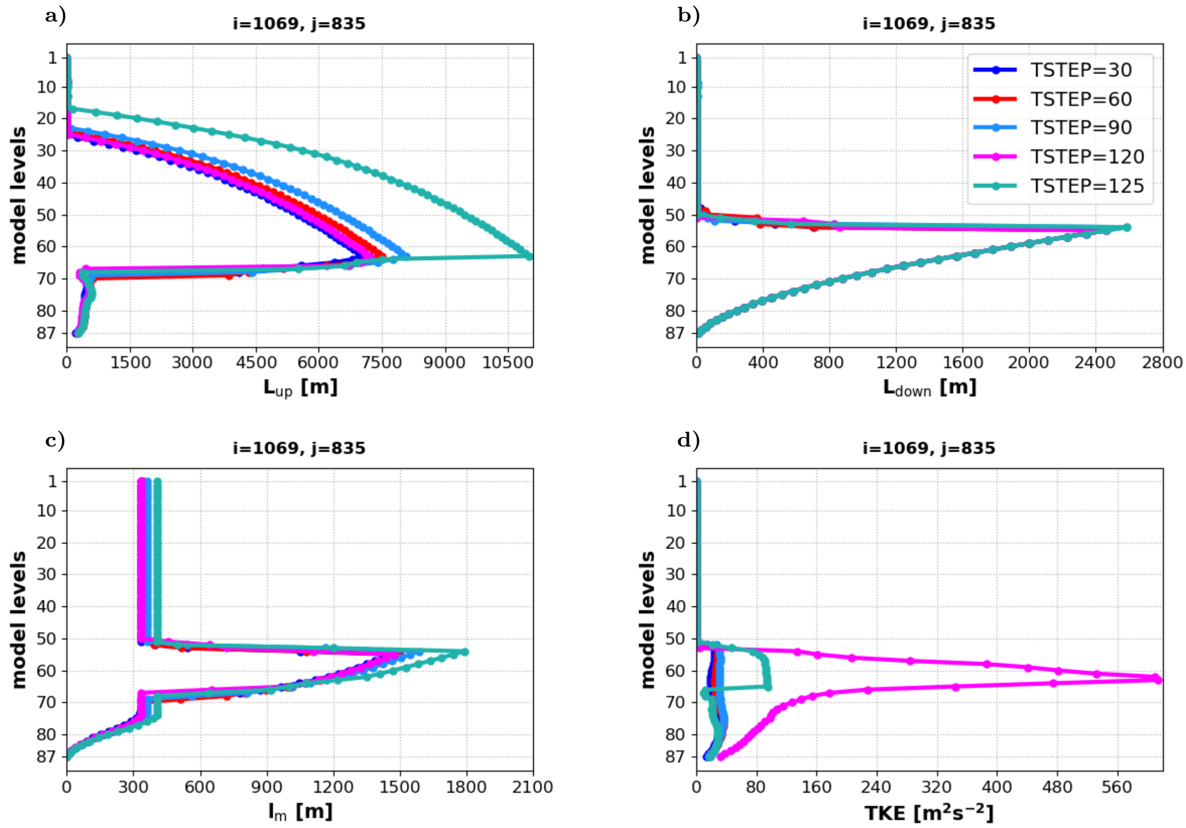

Figure 2: The profile of L_{up}, L_{down}, l_m and TKE for the unstable point within the coupling zone (i=1069, j=835) and chosen time steps of the 00 UTC 8^{th} November 2020. forecast.

We immediately suspected that there was a problem with the lateral boundary coupling. For this reason, we created profile plots of related fields at problematic point and found a sharp decrease in temperature and specific humidity fields near model level 60 (Figure 3a and b). Consequently, the buoyancy production of TKE was huge which created enormous amount of fuel for vertical displacement of air parcels (Figure 3c and d). The wind profile and TKE shear production term did not point to any irregularities (not shown). Before further experiments, we switched off the Apache treatment of the PBL for all parameters (LESCALE=.FALSE. in the e927 configuration). Previously it was switched off only for wind components. This resulted in the disappearance of jumpiness in vertical profiles of coupled fields and unrealistically high values in L_{up}, L_{down}, l_m and TKE profiles as well as the stabilization of the forecast. For this reason, we continue the development of the updated TKE-based mixing length formulation without Apache treatment. However, its impact on the forecast (in general) has to be evaluated as a separate task.

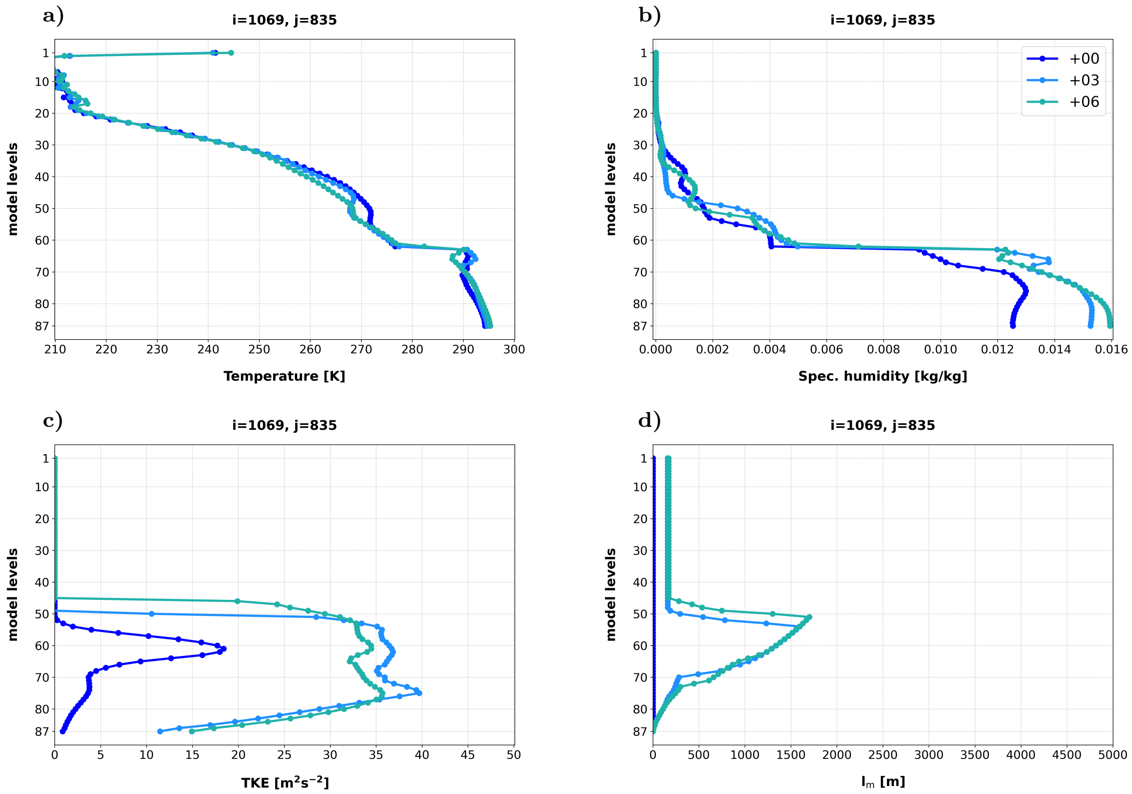

Figure 3: The profile of: **a)** temperature, **b)** specific humidity, **c)** TKE and **d)** l_m for the "unstable point" within the coupling zone (i=1069, j=835) at first few coupling times of the 00 UTC 8th November 2020. forecast. In this experiment c_3 was reduced to 0.1 to stabilize the simulation and extract the first few profiles.

3.2 Validation of the updated and stable TKE-based mixing length formulation

Here, the "VUAML option 2" is introduced, with its preliminary tuning (C_{β_m}=10 K, L_{TKE1}=6.25 m and L_{TKE2}=125 m). Additionally, the impact of different H_{PBL} computation methods is being assessed. First, we launched experiments that differ only in how the VUAML is being imposed. The "VUAML option 2" proved to be more successful in terms of general performance and cross PBL transport (not shown). Further, it should better recognize different regimes than the method solely based on L_{TKE}.

For this reason, testing the impact of H_{PBL} computation method was combined with the "VUAML option 2". In total, three methods were tested: i) WCIM, ii) min (WCIM, TKE-based), and iii) BD22. The first method is used as default in the ALARO-CMC. The second method aims to compensate for deficiencies of the first method in statically stable conditions. Finally, the third method has a potential to be applied generally, and its solution is also relatively smooth. So far, the best results are obtained with the second method and will be compared to the reference formulation in the following sub-chapters.

3.2.1 *Validation of the convection case on 24th June 2022.*

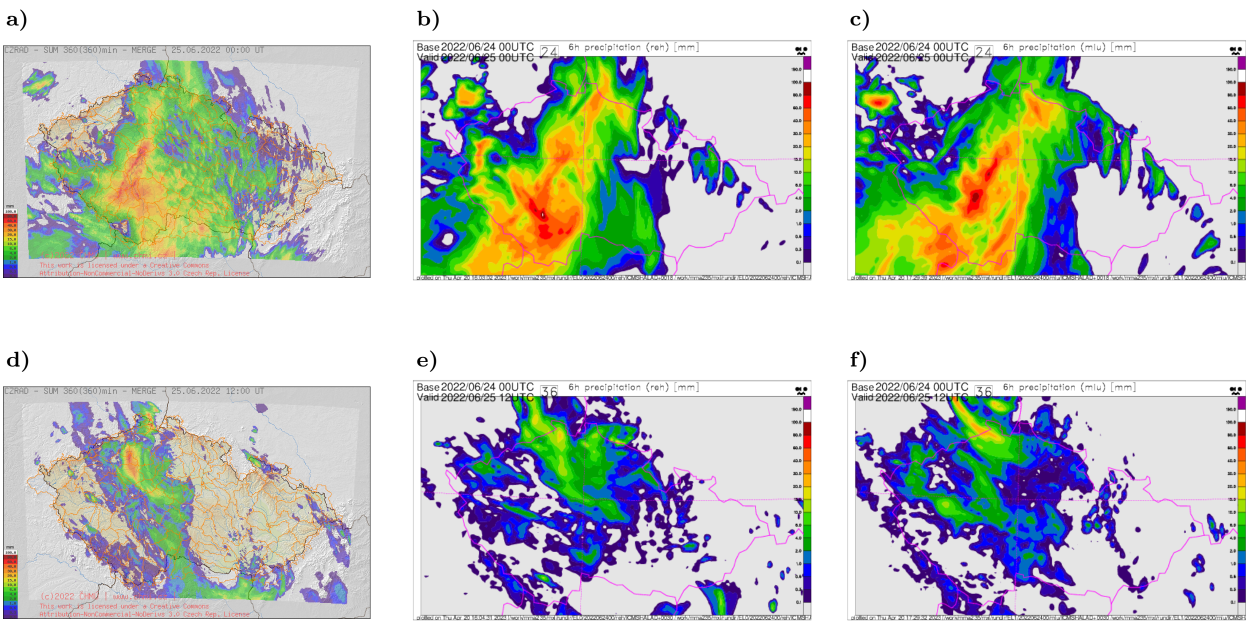

Figure 4: Comparison of CHMI's 6h precipitation estimates (radar values adjusted with rain gauges by krieging with external drift method; **a)** and **d)**) with the forecast obtained by the reference mixing length (ML) formulation (EL0; **b)** and **e)**) and TKE-based ML formulation (EL1; **c)** and **f)**) at +24 and +36 prognostic hours. The forecast was initialized at 00 UTC 24th June 2022.

The case of 24th June 2022. was characterized by the heavy precipitation in the western part of the Czech Republic during the evening hours, whose intensity gradually decreased during the night (Figure 1a and d). Some localized storms were still observed the following morning (Figure 1d). The TKE-based formulation better represented the shape and amplitude of the primary maximum and correctly reduced the excessive rain in the northwestern part of the country. Further, the precipitation amount in the northeastern region was also improved, i.e., increased. Among the drawbacks, we highlight the reduction of precipitation in the southeast (Figure 1a-c). The following morning, the most prominent feature was a localized storm in the northern part of the country. Unlike the reference, the TKE-based formulation reproduced its amplitude but slightly misplaced it in the space (Figure 1d-f). A more detailed analysis will follow after the stay.

3.2.2 *Validation of the inversion case on 23th November 2019.*

This case was isolated from the lengthier period with a similar weather pattern. Throughout the day, low clouds were standing over the entire Czech Republic (Fig 1a, b and d). The reference formulation did not maintain them in the western part of the country during the afternoon, while the TKE-based approach was more successful (Figure 1b, c, e and f). The differences were even bigger the following evening when the TKE-based formulation covered the entire country with low cloudiness while the reference was almost cloud free (not shown). To confirm this, we have to utilize the satellite-based product available 24 hours per day. However, it is striking that the following morning, the entire country was again covered by a low cloud system. Further analysis of this case will focus on comparison to atmospheric soundings and time series of the screen-level temperature in affected regions. The plan for further improvement is described in the following chapter.

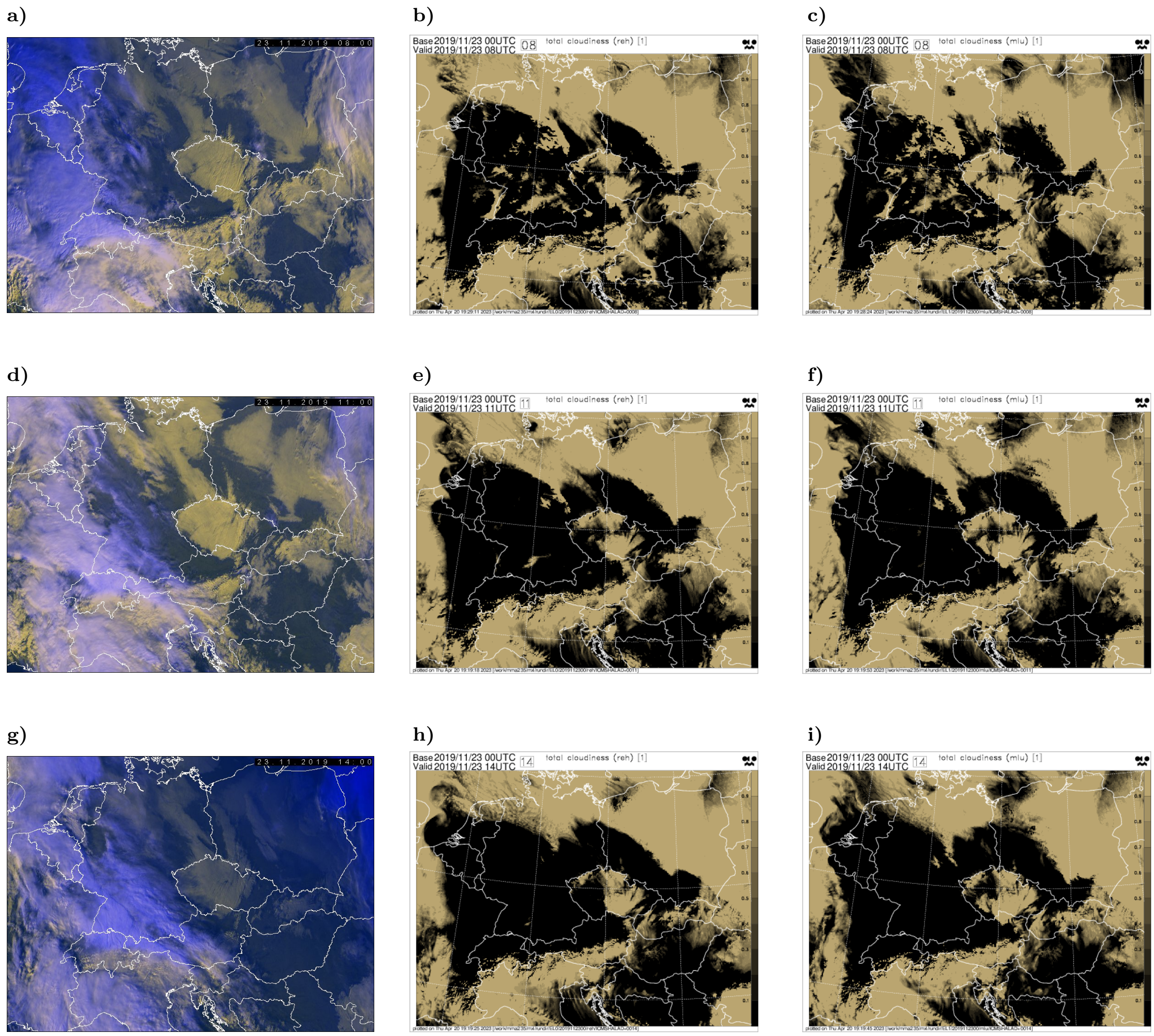

Figure 5: Comparison of the MSG VIS-IR low cloudiness (**a**), **d**) and **g**)) with the forecast obtained by the reference mixing length (ML) formulation (EL0; **b**), **e**) and **h**)) and TKE-based ML formulation (EL1; **c**), **f**) and **i**)) at +8, +11 and +14 prognostic hours. The forecast was initialized at 00 UTC 23$^{\text{th}}$ November 2019.

4 Summary and further work

During this stay, a new TKE-based mixing length scaling was implemented and validated. It is supported by the results of the mixing length diagnostics from the LES data. The fundamental ingredients of the formulation have been retained, such as the smooth transition of l_m from the surface κz layer to the upper-air layer where the TKE-based solution with CP method is applied. In addition to scaling, novelties include: i) the application of VUAML based on the scaling of the maximum of L_{TKE} within the PBL on the vertical gradient of $\Delta\theta_s$ and ii) the implementation of new methods to compute the H_{PBL}. The latter includes three approaches, wherein the one using a minimum value of WCIM and TKE-based methods seems to be the most successful if combined with the VUAL computed from $\Delta\theta_s$. This setup was validated for seven cases and provided either neutral or slightly positive results. We especially emphasize the inversion case, for which the new formulation, in contrast to the reference one, correctly predicted low cloudiness over a larger area.

Finally, it seems we have all ingredients to complete the TKE-based formulation but still need to find their optimal setup. To achieve this, we still need to: i) seek for the best setup of the BD22 method to compute H_{PBL} and compare it to other approaches, ii) adjust the tuning of VUAL based on $\Delta\theta_s$ and iii) optimize other choices, e.g., smooth transition parameters c_1 and c_2, averaging operator (the choice of p), the magnitude of the shear term (C_0), etc. After this stay, a more detailed analysis will follow to achieve the stated goals. The work will continue from home.

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