Implementation and Significance of TKE-Advection in COSMO 5.0 for itype_turb=3 and Other Turbulence-Related LES-like Sensitivity Studies Including 3D Turbulence

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1 Introduction

Up to now the advection of TKE was only implemented for the alternative turbulence schemes from the LLM-project (`itype_turb=5...8`). It can be activated by by choosing `lprog_tke=.TRUE.` and is only possible when using the Runge-Kutta-Core. This process has now also been implemented for the "standard" scheme (`itype_turb=3`), still only for Runge-Kutta-dynamics. This document describes the technical implementation and some simulations to investigate the significance of the process for simulations at 3 km horizontal grid spacing (today's "high resolution" weather forecasting) as well as for an LES-like setup for explicit shallow convection simulations at 200 m grid spacing.

Note that the switch `lprog_tke=.TRUE.` has a slightly different meaning in the different schemes, as will be explained below. Whereas it only denotes the advection process of TKE for `itype_turb=3`, it also switches on the vertical and horizontal TKE diffusion (depending on switch `l3dturb`) for the schemes `itype_turb=5...8`. The latter processes are active in `itype_turb=3` independent of `lprog_tke`.

For the LES-like setup, besides the effects of including TKE-advection, we will also investigate in more general the settings of other turbulence-related parameters, in particular in combination with considering full 3D turbulence effects (`l3d_turb=.true.`). This is relevant for future LES-like very high resolution simulations in idealized or real-case configurations, because it gives hints on how to properly choose and configure the turbulence scheme(s).

Although we mention the schemes `itype_turb=5/6` above and sometimes below, their use is not recommended!

Just to mention, the difference between `itype_turb=7` and `8` respectively `5` and `6` is that the latter employ moist conserved liquid water potential temperature instead of ordinary potential temperature to take into accound the effects of phase changes on local stability within clouds.

2 Implementation and technical testing

The implementation is along the lines of the COSMO tracer advection schemes. Semi-lagrange advection, flux-form density-based advection (Bott et al.) or the traditional formulation with divergence correction can be used.

For `itype_turb=3`, the transported quantity is the turbulent velocity scale $q = \sqrt{2\ \mathrm{TKE}}$, but for `itype_turb=5...8` it is directly the TKE. For the flux-form density-based advection schemes, the transported quantities are multiplied with the total density before the advection operator — to transform them to densities for the advection operator — and divided by the advected density afterwards, same as for the tracers. Because TKE is defined on half levels, the density values to multiply with have to be vertically interpolated to the half levels, which is done by linear interpolation. The same applies for the advected density to be divided by afterwards.

Technically, the advection is done slightly differently for the different turbulence schemes:

- `itype_turb=3`: The advective tendency $\mathrm{TEND}_{adv} = (q_{after} - q_{before})/\Delta t$ is stored on a new global field `tket_adv(1:ie,1:je,1:ke)` and added to q in the call to the subroutine `turbdiff()` in the next timestep, together with the other physical tendencies of q.
- `itype_turb=5...8`: "update in place" of the advected quantity on timelevel `nnew`

A slight complication arises for `itype_turb=3` because of the exponential filtering of q to damp numerical local oszillations during time integration. The relevant namelist parameter is `tkesmot`, which is the weight a in the recursive exponential time filter

$$q_{n+1} \ = \ (1-a)q^*_{n+1} \ + aq_n \tag{1}$$

where q_n is the "old" value, q_{n+1} the "new" and q^*_{n+1} is the result of an implicit time integration step,

$$q^*_{n+1} \;= \text{fct}\,(q_n, q^*_{n+1}, \text{TEND}(q_n), \Delta t) \tag{2}$$

It is obvious that, if we would include the advection in the total tendency TEND(q_n), the transport velocity of TKE structures would be reduced by the factor a, which is physically wrong. To mitigate this problem and at the same time to keep the possibility for time smoothing, the procedure is modified. In a first explicit Euler-Forward-step, only the advective tendency $\text{TEND}_{adv}(q_n)$ is applied to obain a provisional value q^{**}_{n+1},

$$q^{**}_{n+1} \;= q_n \;+\; \text{TEND}_{adv}(q_n)\Delta t \tag{3}$$

Then, the implicit scheme is applied to this provisional value, neglecting the advective tendency,

$$q^*_{n+1} \;= \text{fct}\,(q^{**}_{n+1}, q^*_{n+1}, \text{TEND}(q_n) - \text{TEND}_{adv}(q_n), \Delta t) \tag{4}$$

followed by the time filtering

$$q_{n+1} \;=\; (1-a)q^*_{n+1} \;+ a q^{**}_{n+1} \tag{5}$$

In this way, the time filtering is only applied to the non-advective part of the TKE-changes.

Note that, for the diffusion process of TKE, there is a similar problem with the spatial propagation speed of the diffusion signal, and in the future, the diffusion tendendy should also somehow be removed from the time filtering.

As a first testing step, a simple 2D idealized test case (flow over hill) has been set up. A cuboid package of high TKE values (50 m^2s^{-2}) is artificially introduced near the inflow boundary of the domain, and the output is analyzed every timestep. The spatial resolution was ΔX = 1.1 km, the time step ΔT = 10 s and 40 vertical levels up to 22 km height have been chosen. The initial wind speed is a constant U = 10 ms^{-1} everywhere (no lateral and vertical motion) and the temperature decreases linearily with height at the ICAO standard atmosphere gradient. With that, we have a stable stratification and very low windshear and expect pure horizontal transport.

This setup has been run for both `itype_turb=3` and `itype_turb=7` to test the two above-mentioned different implementations of TKE advection. Fig. 1 to 4 show the results for both runs for different simulation times, starting with the initial state (Fig. 1) and ending with 15 min (Fig. 4). Slight differences in the initial state are due to the fact that the output of TKE in the first timestep includes or excludes the time-changes during the first time step. For `itype_turb=7`, the output is on timelevel "nnow" as for the other prognostic model variables, so no changes occured. But in case of `itype_turb=3`, the local changes due to some TKE sources and sinks (not the advection and diffusion and possibly some others!) have already been added in the first time step.

One can see that in both cases the TKE-cuboid is transported with about the same speed, but there are differences in the vertical. Therefore, the advection is implemented properly and happens at the expected speed. We expect no advection errors in the other transport directions, because the same well-tested subroutines as for the tracers are applied in the same way.

However, the vertical differences require some more consideration. It turns out that these are due to differences in the turbulent diffusion of TKE. Note that the values of the Richardson Number $Ri = N^2/S^2$ (N = Brunt-Väisälä frequency, S = total shear) are quite high, so that in reality, we expect the TKE to die out very soon, associated with low turbulent mixing. This "stable" case is treated differently in both turbulence schemes. For `itype_turb=7`, the diffusion coefficients are simply set to a low value (0.1 m^2s^{-1}) regardless of the TKE, whereas they are still a function of stability and TKE in case of `itype_turb=3`. This explains why the blob of spuriously high TKE is strongly diffused in the latter case and nearly not diffused in the former.

The use of the already existing namelist parameter `lprog_tke` to switch on the advection of TKE for `itype_turb=3` requires some clarification, because its meaning is slightly different in case of the alternative schemes `itype_turb=7/8`. And in combination with the parameter `l3dturb` ("3D-turbulence"), different terms of the TKE-equation are actually considered. Tab. 1 summarizes these considered terms for `itype_turb=3` and Tab. 2 for `itype_turb=7` and 8. Note in particular that for `itype_turb=7/8` the metrical terms in horizontal differentials in case of `l3dturb=.true.` due to the terrain following coordinate system are not considered. This means that this scheme is strictly only valid for flat terrain, although the errors in case of "not too hilly" terrain should be tolerable.

Additionally Tab. 3 shows which processes are active for "3D-turbulence" in the other model equations for T, p, $\vec{v}$ and tracer(s), depending on `l3dturb` and the switch `l3dturb_metr`, which concerns the metrical terms due to terrain following coordinates in the horizontal diffusion part of the equations. In case of hilly terrain it is advisable to set `l3dturb_metr=.true.` if `l3dturb=.true.`.

Table 1: `itype_turb=3`: Considered processes in the TKE-equation for the different combinations of `lprog_tke` and `l3dturb`.

`lprog_tke`	**.false.**	**.false.**	**.true.**	**.true.**
`l3dturb`	**.false.**	**.true.**	**.false.**	**.true.**
∂_t	X	X	X	X
Therm. prod.	X	X	X	X
Horiz. Shear prod.		X		X
Vert. Shear prod.	X	X	X	X
Dissipation	X	X	X	X
Horiz. diffus.				X
Vert. diffus	X	X	X	X
Advection			X	X
Metrical terms in horiz. differentials in TKE-equation due to terrain following coordinates		X		X

Table 2: Same as Tab. 1, but for `itype_turb=7` and `8`.

`lprog_tke`	**.false.**	**.false.**	**.true.**	**.true.**
`l3dturb`	**.false.**	**.true.**	**.false.**	**.true.**
∂_t			X	X
Therm. prod.	X	X	X	X
Horiz. Shear prod.		X		X
Vert. Shear prod.	X	X	X	X
Dissipation	X	X	X	X
Horiz. diffus.				X
Vert. diffus			X	X
Advection			X	X
Metrical terms in horiz. differentials in TKE-equation due to terrain following coordinates				

Table 3: `itype_turb=3`: Considered processes in the equations for T, p, $\vec{v}$ and tracer(s) depending on `l3dturb` and `l3dturb_metr`.

`l3dturb`	**.false.**	**.true.**	**.true.**
`l3dturb_metr`	**(not relevant)**	**.false.**	**.true.**
Vertical diffus. of T, p, $\vec{v}$ and tracer(s)	X	X	X
Horizontal diffus. of T, p, $\vec{v}$ and tracer(s)		X	X
Metrical terms in horiz. differentials in diffusion tendencies of T, p, $\vec{v}$ and tracer(s) due to terrain following coordinates			X

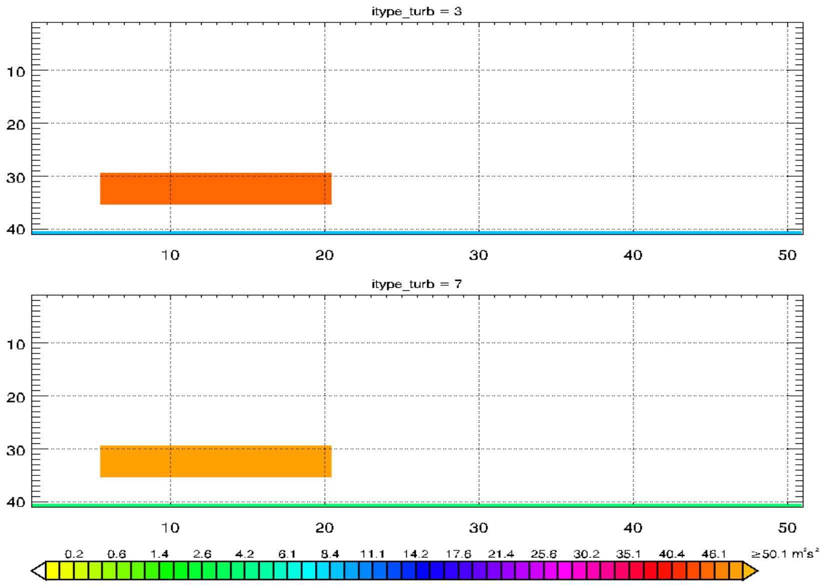

Figure 1: Simple test of the TKE advection for `itype_turb=3` and `7`. X-Z-cut along the 2D flow, $U = 10$ ms^{-1} everywhere from left to right, stable stratification (ICAO-standard atmosphere). Initial values for the TKE.

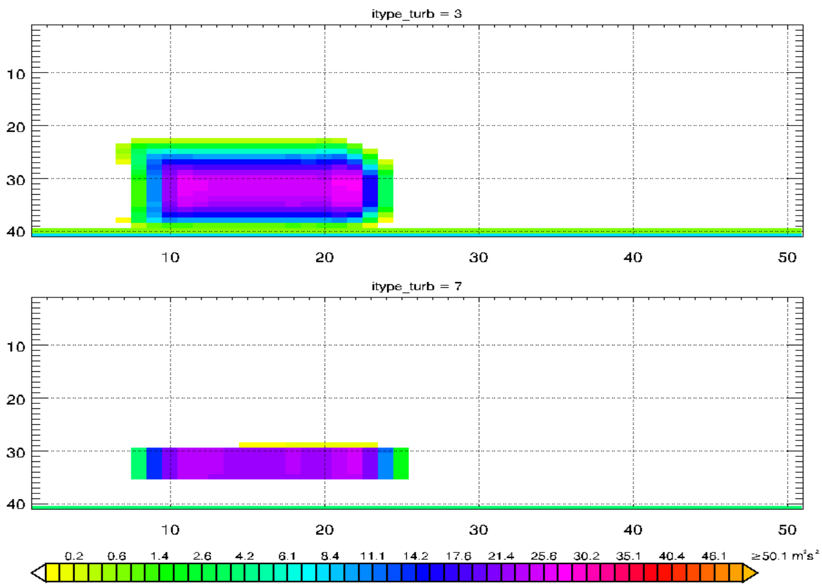

Figure 2: Same as Fig. 1 but after 2 minutes.

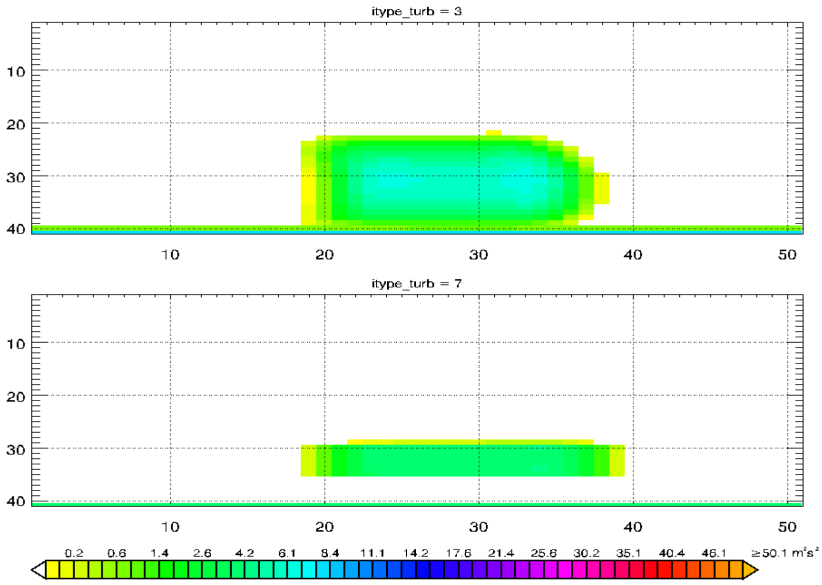

Figure 3: Same as Fig. 1 but after 10 minutes.

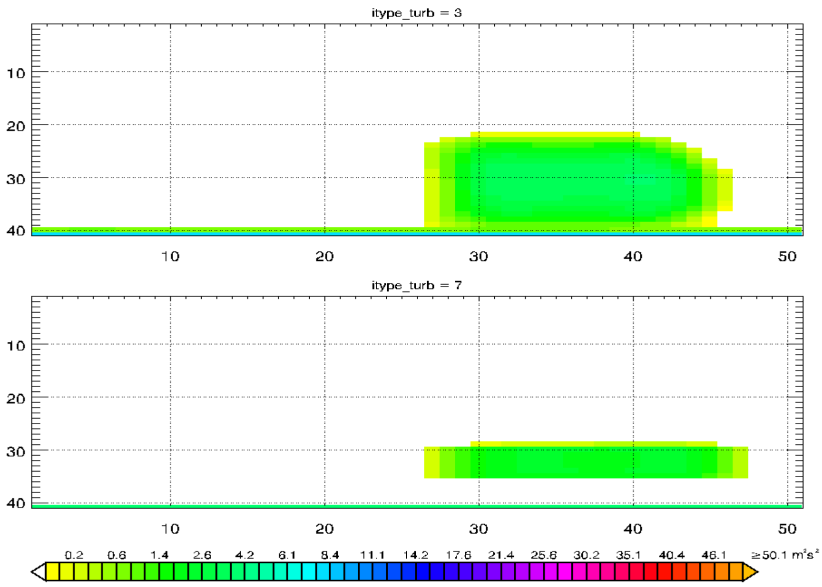

Figure 4: Same as Fig. 1 but after 15 minutes.

3 Meteorological significance for $\Delta X \sim 3\,\mathrm{km}$

For `itype_turb=3`, the activation of `lprog_tke` has been tested by a real case COSMO_DE hindcast of 31.5.2011, 12 UTC +21 h, driven by the operational COSMO_DE-analyses (`l3dturb` remained `.false.`). Two model runs were performed, one with `lprog_tke=.false.` and the other with `.true.`. The 3D-turbulence was deactivated, consistent with the operational setup of COSMO_DE. The only difference between the two runs is thus the consideration of TKE-Advection (cf. Tab. 1, first and third column).

Fig. 5 shows T_2M (upper row) and accumulated total precipitation (lower row) after 21 h at the end of the forecast. The left column is without TKE-Advection, the middle column with TKE-Advection and the right column is the difference with minus without. No significant differences for the T_2M can be observed, only a wave-like pattern, perhaps indicating spatial shifts, is visible in the difference plot.

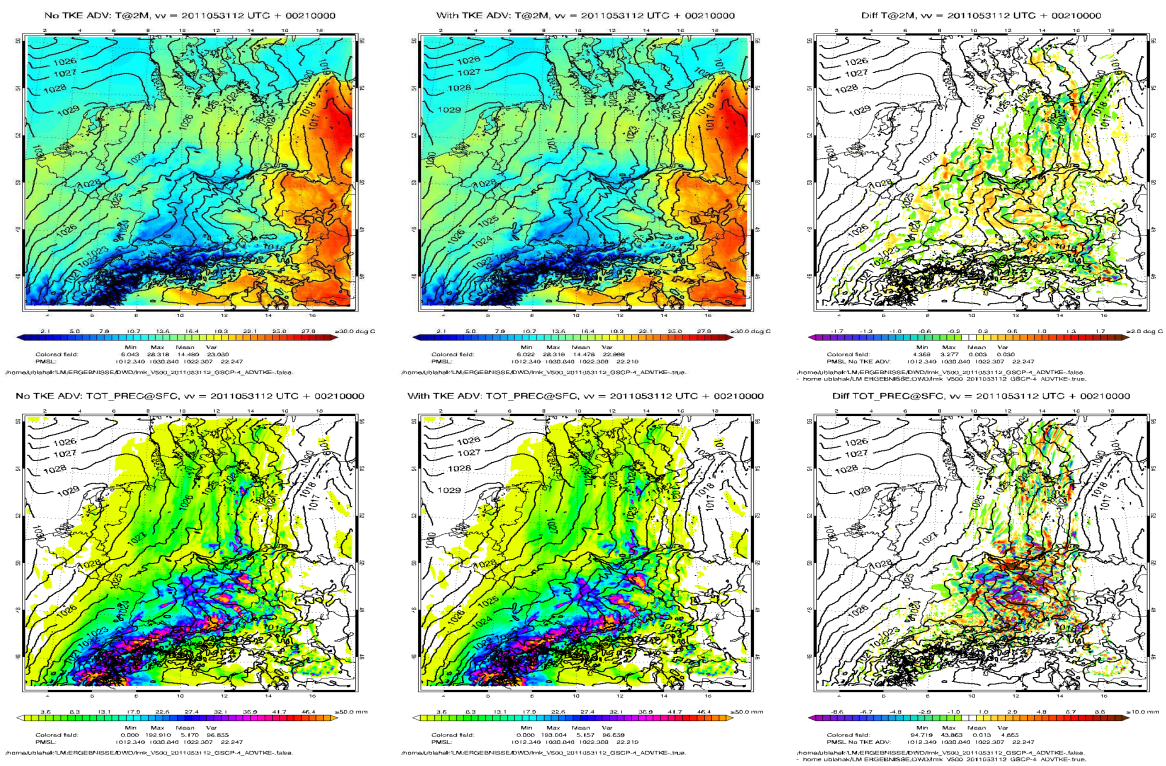

Figure 5: COSMO_DE hindcast, 31.5.2011 12 UTC + 21 h, `itype_turb=3`.
Upper left: T_{2m}, no TKE advection.
Upper middle: T_{2m}, TKE advection.
Upper right: Difference middle to left.
Lower left: Total precip, no TKE advection.
Lower middle: Total precip, TKE advection.
Lower right: Difference middle to left.

This is generally similar also for the total precipitation, except for a region south of the Erzgebirge, Eastern Bavaria and Western Czechia. Here, the consideration of the TKE-Advection shifted the precipitation pattern a little to the South.

However, for both quantities, the domain averaged systematic difference is very very small. The effect of considering the TKE-Advection has therefore no significant effect on the weather forecast in this case. However, this has to be checked by a longer term experiment.

4 Dependence on the different subswitches for 3D LES-like simulations

To further illustrate the effects of the different switches/processes in Tab. 1 and Tab. 2 on very high resolution runs, a series of idealized LES-like simulations with a horizontal grid spacing of $\Delta X = 200\,\mathrm{m}$ has been performed. The runs are characterized by 125 x 125 grid points in the horizontal, 64 levels in the vertical up to 15 km height, periodic boundary conditions, flat terrain, condensation and cloud microphysics switched off, soil model switched off, radiation switched off, deep and shallow convection parameterization switched off, usage of the new fast waves solver in the Runge-Kutta core, and a forced constant sensible heat flux of $H_0 = 300\,\mathrm{Wm}^{-2}$ at the surface.

The initial T-profile in the PBL is slightly stable with a T lapse rate of $\approx -0.007\,\mathrm{Km}^{-1}$, and the wind profile is $U(z) = U_\infty \tanh(z/z_{ref})$ with $U_\infty = 5\,\mathrm{ms}^{-1}$ and $z_{ref} = 3000\,\mathrm{m}$. Some small random noise on T and w is added at simulation start in the lowest 100 hPa of the atmosphere to initiate motions on different scales from which shallow convection will spin up later.

For each of the 4 possible combinations of the switches `lprog_tke` and `l3dturb` and each of `itype_turb=3` and 7, a model run has been performed out to +4 h. To make both turbulence schemes comparable, the full 3D isotrophic shear production of TKE has been switched on for `itype_turb=3` by choosing `itype_sher=2`. Fig. 6 shows horizontal cross sections of w at a height of about 700 m after 4 h for each of the 4 switch combinations in case of itype_turb=3. Fig. 7 is the same, but for itype_turb=7.

From convection theory and measurements, one would expect to see coherent and organized up- and downdraft structures with a more cellular pattern close to the ground and more isolated updrafts above ("Thermals") , growing from the cell corners with converging horizontal motions.

The updraft regions should be smaller than the downdraft regions, and the maximum updrafts "stronger" than the maximum downdrafts, but not more than, say, 5 – 6 ms^{-1}. The diameter of the cellular patterns respectively the average distance between the thermals should scale with the boundary layer height and be about 2 - 5 times this height.

With this in mind, an inspection of Fig. 6 for itype_turb=3 shows clearly that without 3D turbulence effects (upper row), the coherent structures are strongly overlayed by spurious noise, which turn out to be $2\Delta x$ waves caused by spurious energy accumulation at the smallest grid scales ("under-diffusive" turbulence scheme). Setting l3dturb=.true. completely changes the picture (lower row). The added horizontal diffusion effects (cf. Tables 1 and 3) cause a very strong smoothing of the structures, eliminating any $2\Delta x$ waves. The w structures seem qualitatively realistic, although in the opinion of the author somewhat overly smooth. A closer look at power spectra could shed more light on this in the future.

Clearly, considering TKE advection (by setting lprog_tke=.true.) is a second-order effect compared to the combined action of all other 3D effects (maybe because of the quite low windspeed).

The situation in Fig. 7 for itype_turb=7 is slightly different. The $2\Delta x$ waves vanish here when setting lprog_tke=.true. and l3dturb=.true. (lower right panel). Then, the w structures look very realistic (considering the relatively coarse grid resolution for this phenomenon) and are not overly smoothed. The author considers this as the best simulation of the series.

As mentioned previously, concerning the different behaviour of the two turbulence schemes, the meaning of the two switches l3dturb and lprog_tke is different among the two turbulence schemes (Tables 1 and 2). Whereas for itype_turb=3, lprog_tke concerns only the TKE-advection and the TKE horizontal diffusion in case of l3dturb=.true., it is connected to the prognostic treatment of TKE and to its advection and diffusion for itype_turb=7. Additionally, l3dturb=.true. switches on the horizontal diffusion of all other prognostic variables.

From the different behaviour visible in Figures 6 and 7, one possible conclusion is that mainly the consideration of the horizontal diffusion (l3dturb=.true.) of the model variables, including in the TKE-equation the TKE shear production and TKE diffusion, enhances the quality of the results in the presented case.

The different "degree of smoothing" of the w structures between the two turbulence schemes, perhaps associated with a different behaviour of the power spectra, deserves a closer look. As previously mentioned, the author considers the simulation with itype_turb=7 and lprog_tke=.true. and l3dturb=.true. (Fig. 7, lower right) as the best simulation of the series. For the standard scheme itype_turb=3, an unrealistically smooth w field was obtained here (Fig. 6, lower right). To improve the simulation here, M. Raschendorfer suggested, on physical grounds, to limit the horizontal length scale for 3D-turbulence by $0.5\Delta X$ instead of the current $1\Delta X$.

This can be motivated by the fact that each one of a pair of contrariwise rotating eddies, which are not resolved by the grid, can have a maximum horizontal diameter of $0.5\Delta X$. If the most energetic non-resolved eddies are assumed to be even smaller, the factor should also be smaller than 0.5.

To be separated from the vertical length scale, the factor 0.5 has been introduced in the code only at the 2 following places:

- turbulence_utilities.f90, subroutine turb_param():

```
l_scal=MIN( 0.5*l_hori, tur_len )
```

- turbulence_diff.f90, subroutine turbdiff():

```
IF (itype_sher.GE.2 .OR. PRESENT(tket_hshr)) THEN
!Separate horizontale Scherungsmode soll berechnet werden:
  DO j = jstart, jend
  DO i = istart, iend
    src(i,j)=(a_hshr*0.5*l_hori)**2 * hlp(i,j,k)**z1d2 !related horiz. ...
  END DO
  END DO
```

Fig. 8 compares a corresponding test simulation (right) with "standard" itype_turb=3 (upper left; same as Fig. 6 lower right) and with the abovementioned best simulation itype_turb=7 (lower left; same as Fig. 7

lower right). The w field of the test simulation appears much similar to the one from `itype_turb=7`, although still a little more smooth. However, the reduction of the limiting horizontal length scale by half is clearly an improvement. The question if the value should be even smaller than 0.5 should be addressed in the future, e.g., by inspection of the corresponding power spectra.

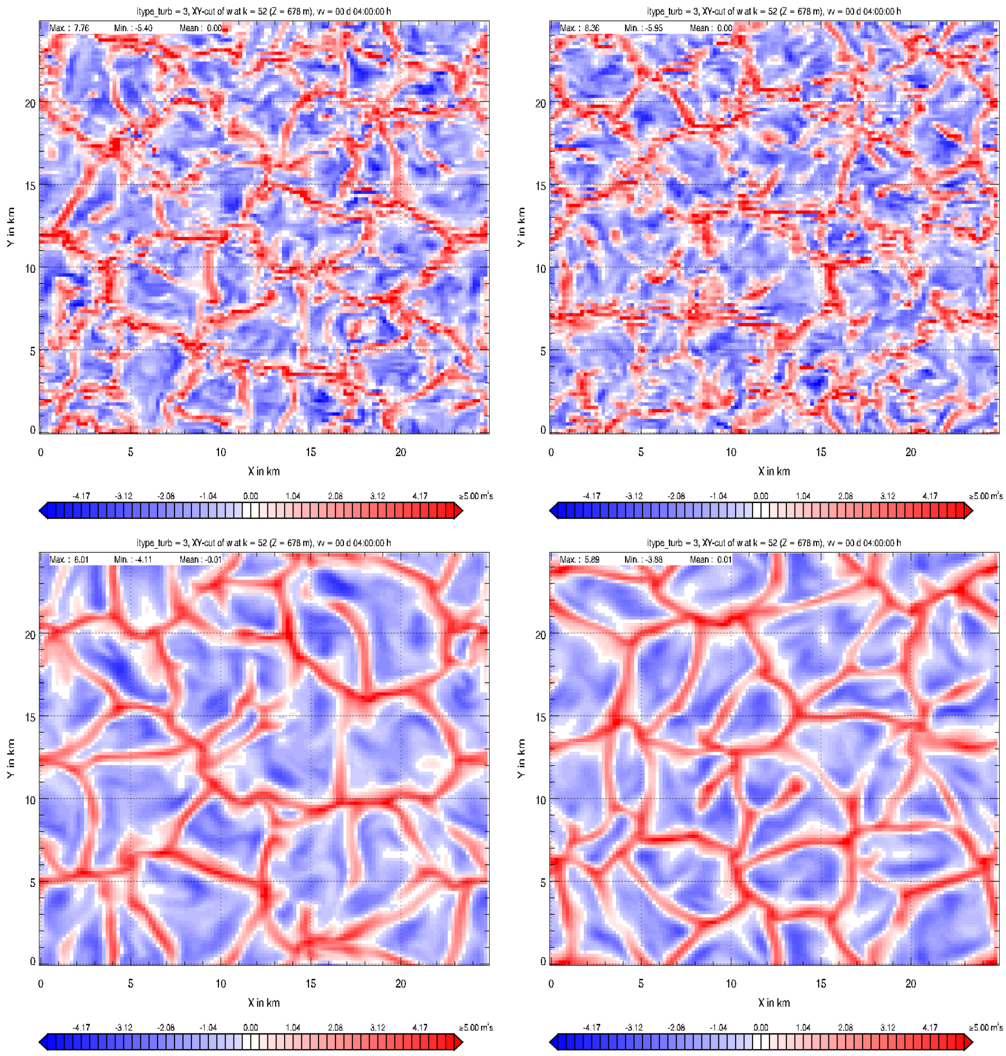

Figure 6: LES experiment: $H_0 = 300\,\mathrm{Wm}^{-2}$, $\Delta X = 200\,\mathrm{m}$, 4 h after simulation start, `itype_turb=3`, horizontal cross section of w at $Z = 678\,\mathrm{m}$.
Upper left: `lprog_tke=.false.`, `l3dturb=.false.`.
Upper right: `lprog_tke=.true.`, `l3dturb=.false.`.
Lower left: `lprog_tke=.false.`, `l3dturb=.true.`.
Lower right: `lprog_tke=.true.`, `l3dturb=.true.`.

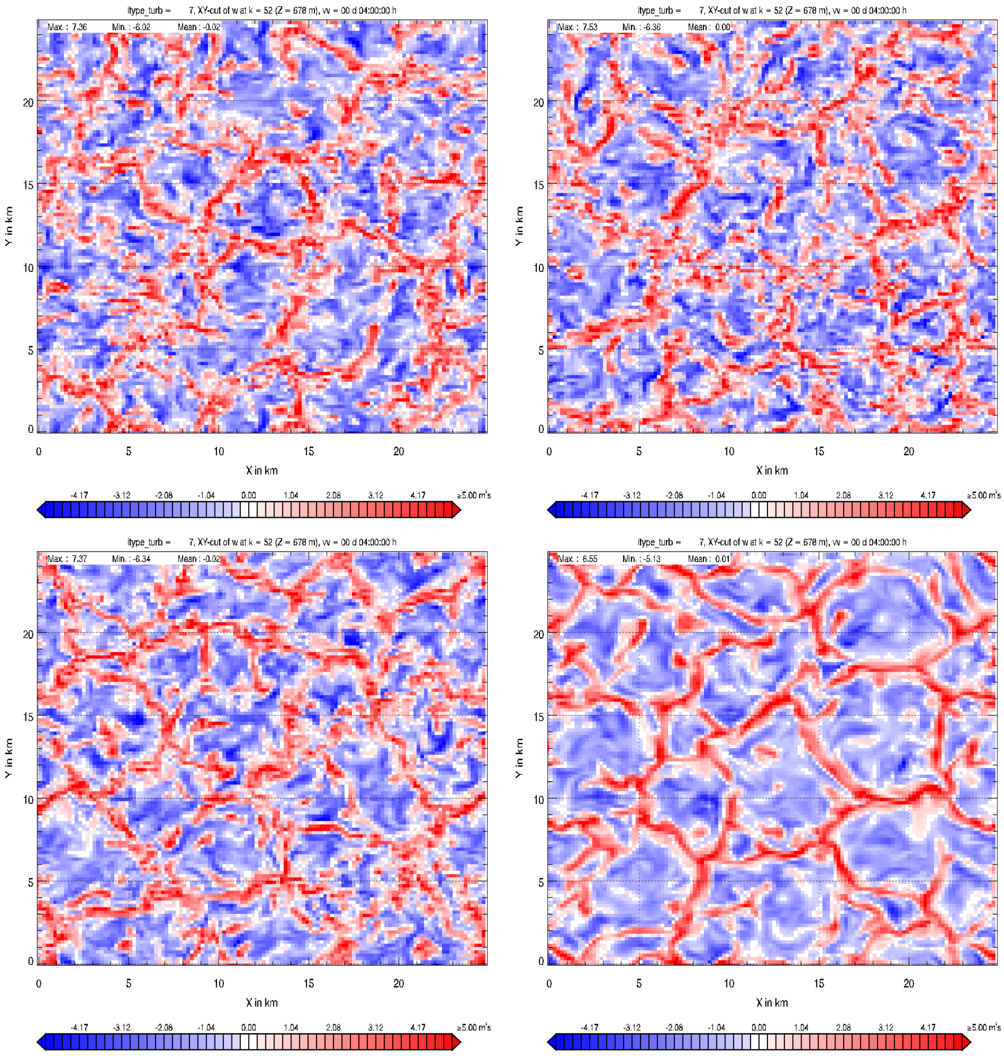

Figure 7: LES experiment: $H_0 = 300\,\mathrm{Wm}^{-2}$, $\Delta X = 200\,\mathrm{m}$, 4 h after simulation start, `itype_turb=7`, horitonal cross section of w at $Z = 678\,\mathrm{m}$.
Upper left: `lprog_tke=.false.`, `l3dturb=.false.`.
Upper right: `lprog_tke=.true.`, `l3dturb=.false.`.
Lower left: `lprog_tke=.false.`, `l3dturb=.true.`.
Lower right: `lprog_tke=.true.`, `l3dturb=.true.`.

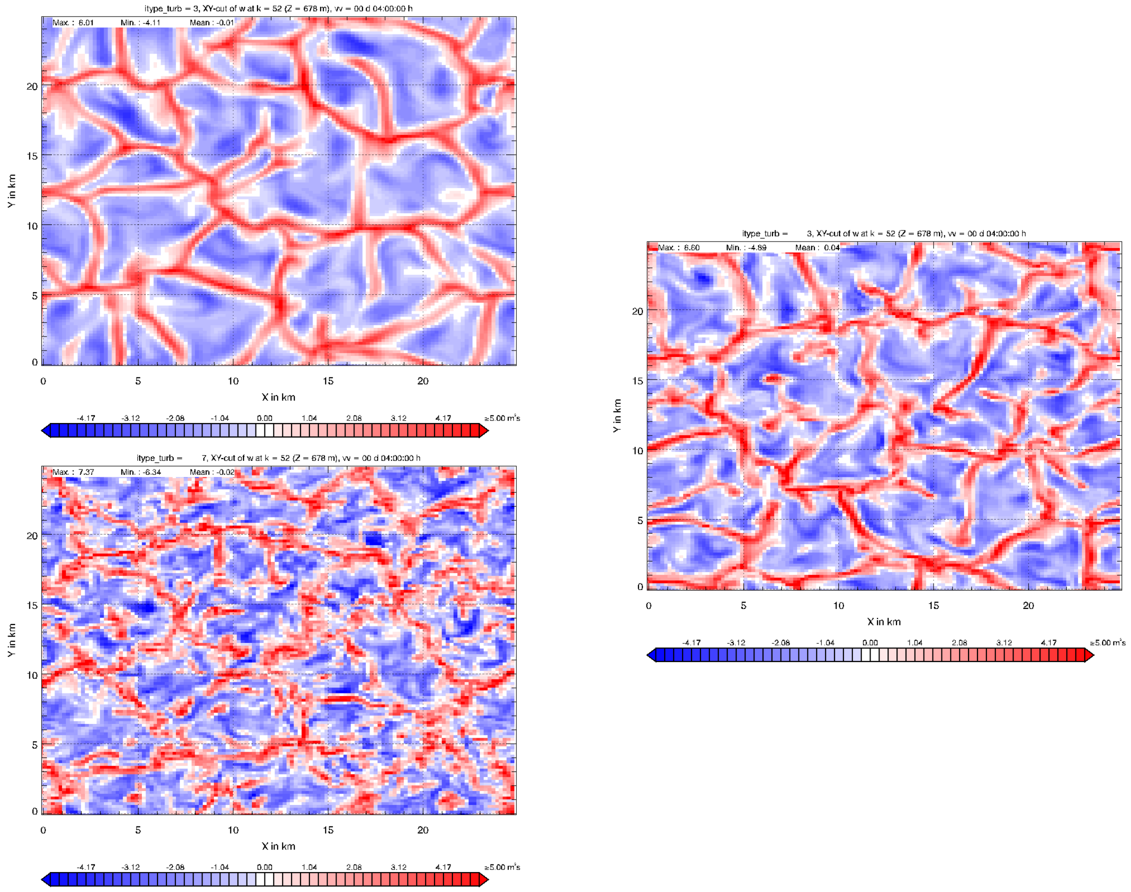

Figure 8: LES experiment: $H_0 = 300\,\mathrm{Wm}^{-2}$, $\Delta X = 200\,\mathrm{m}$, 4 h after simulation start, `lprog_tke=.true.`, `l3dturb=.true.`.
Upper left: `itype_turb=3` with original turbulent length scale formulation, same as Fig. 6 bottom right.
Lower left: `itype_turb=7` same as Fig. 7 bottom right, ("best" simulation).
Right: `itype_turb=3`, but with limitation of the horizontal length scale by $0.5\Delta X$ instead of $1\Delta X$. **Clear improvement compared to upper left!**

5 Summary and Outlook

The advection of TKE has been implemented into the COSMO-model for the standard turbulence scheme `itype_turb=3`, where it has not been present before. The implementation details have been described in Section 2. Section 3 shows that for todays "high resolution" NWP at a horizontal grid spacing of $\sim 3\,\mathrm{km}$ and the operational COSMO-DE configuration, its consideration does not lead to significant changes, although there might be some differences on small scales.

Further, for LES-like studies with the COSMO-model and full 3D turbulence closure, also the influence of other namelist configuration parameters for the turbulence scheme has been investigated. Here, in particular the consideration of horizontal diffusion (`l3dturb=.true.`) of all model variables (including in the TKE-equation the TKE shear production `itype_sher=2` and TKE diffusion) enhances the quality of the results in the presented case.

Here, the alternative hybrid Smagorinsky-/TKE turbulence scheme `itype_turb=7` lead to the most plausible and "realistic" results in terms of structure and smoothness of the w fields for shallow convection simulations. `itype_turb=3` produced overly smoothed structures. However, reducing the upper horizontal length scale limit from $1\Delta X$ to $0.5\Delta X$ leads to a considerable improvement towards the results of `itype_turb=7` and is promising for the future. It will have to be investigated in more detail, whether the reduction factor should be even smaller than 0.5 and how the corresponding power spectra behave.

If, for `itype_turb=3`, the spectra would follow reasonably well the -4/3 law without too much energy loss at small scales an without too much spurious buildup at $2\Delta X$, the COSMO-model would posess a universal turbulence scheme, usable from operational forecasting down to grid spacings in the LES range.