

## RC-LACE stay report

# Generalized TKE-based mixing length formulation in TOUCANS

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14.1-25.1.2019. and 18.2-1.3.2019.

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## 1 Introduction

During the previous stay<sup>[1]</sup> we implemented generalized version of the Bougeault-Lacarrère (BL89), TKE-based, mixing length formulation<sup>[2]</sup>, following the work of Rodier et al. (2017)<sup>[3]</sup>. The newly included shear term (on top of buoyancy term) represents the parcel slowdown effect due to vertical decoupling of turbulent eddies when local shear is strong. It is expected that combined buoyancy-shear (BS) scale will better represent local effects in stable stratification, as well as reduce excessive mixing near neutrality. The main goal of this stay is to thoroughly evaluate performance of the BS scale, including calibration of the constant controlling the magnitude of the shear term within the local  $\kappa$ -scaling framework. Depending on the outcome of evaluation procedure, there is a possibility of further upgrade of the BL89 formulation and/or re-tuning of the TOUCANS scheme, with emphasis on TKE budget equation.

## 2 Generalized Bougeault-Lacarrère (BL89) formulation

The generalized version of BL89 formulation is given by:

$$\int_z^{z+L_{up}} \left[ \frac{g}{\theta_v(z')} (\theta_v(z') - \theta_v(z)) + c_0 \sqrt{e(z')} S(z') \right] dz' = e(z) \quad (1)$$

$$\int_{z-L_{down}}^z \left[ \frac{g}{\theta_v(z')} (\theta_v(z) - \theta_v(z')) + c_0 \sqrt{e(z')} S(z') \right] dz' = e(z) \quad (2)$$

where  $\theta_v$  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 vertical displacements ( $L_{up}$  and  $L_{down}$ ) are known, the TKE-based length scale ( $L_{TKE}$ ) is obtained by their averaging, e.g.:

$$L_{TKE} = \frac{2L_{up} \cdot L_{down}}{L_{up} + L_{down}} \quad (3)$$

Finally,  $L_{TKE}$  is made equal to Prandtl type mixing length ( $l_m$ ) above the surface layer:

$$l_m = \min(\kappa z, L_{TKE}) \quad (4)$$

wherein the  $\kappa z$  limit is set to achieve matching with the Monin-Obukhov Similarity Theory (MOST) near the ground. However, the  $\kappa z$  limit also serves as a protection against too strong mixing in unstable stratification (cf. Fig.A2. in Appendix).

As already stated, the role of the shear term (red in eq. (1) and (2)) is to represent the parcel slowdown effect produced by vertical decoupling of turbulent structures in strong shear conditions. The decoupling depends on average size of turbulent eddies (larger eddies are decoupled more), which is here represented by TKE. In [3] it is not specified which value of TKE is taken as a measure of average eddy size along parcel's integration path. Initially we assumed that  $TKE=e(z)$ , i.e. the TKE at the starting level. However, as the value of TKE may significantly change over longer integration paths, we consider the local value -  $e(z')$  as more appropriate one in this context. The comparison of these two options was performed on three consecutive 72-hourly forecasts within the period 28-30.6.2017. The impact of  $e(z')$  on  $l_m$  is fairly small and verification scores are neutral (not shown). Taking this into account and having in mind the above mentioned, we decided to stick to the  $e(z')$  option.

Hereinafter we present the results of evaluation of the generalized BS scale for the case of a summer convection within the period 28-30.6.2017. Its performance was also tested for a winter case during the period 15-17.5.2017. There it outperformed the reference for most of the surface scores (cf. Fig.A1. in Appendix), while in upper layers the scores were mixed. However, during the summer we found that mixing above the Atmospheric Boundary Layer (ABL) is too strong, which leads to appearance of a secondary maximum of TKE and finally to degradation of the forecast through many feedback effects. Along with evaluation of the performance of the BS

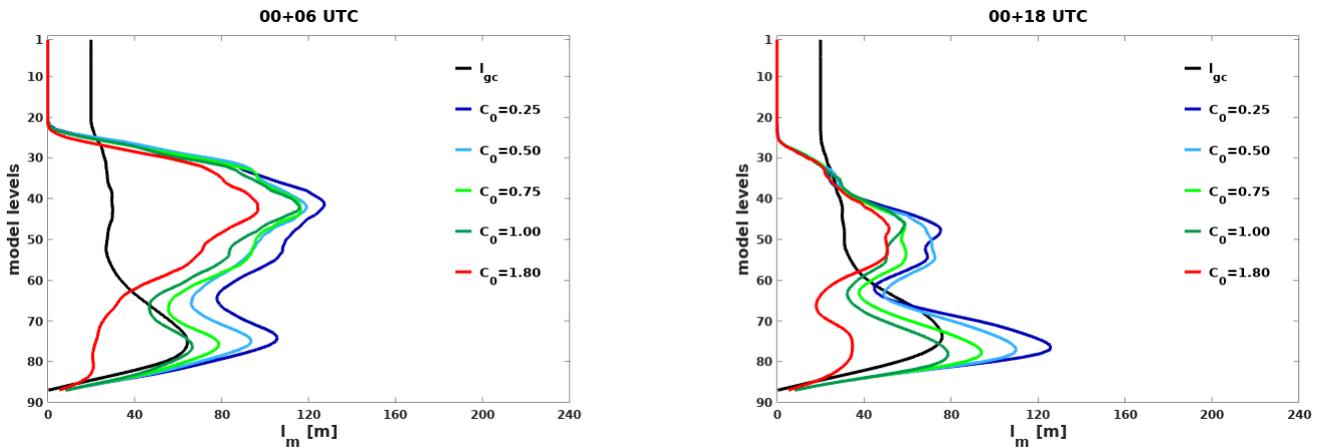
scale, we present few sensitivity studies and suggest how to fix the problems we observed.

### 3 Calibration of the constant $C_0$

As a starting option we have chosen the value of  $C_0$  constant from [3], which is further supported by several of their references. Furthermore, following [3] we tried to estimate an upper bound of the constant. In order to do it, we considered 1-D sheared flow and assumed that, after initialization, the (shear) production of TKE is greater than dissipation (otherwise the turbulence would be suppressed immediately):

$$-\overline{u'w'} \frac{\partial \bar{U}}{\partial z} > \epsilon \quad (5)$$

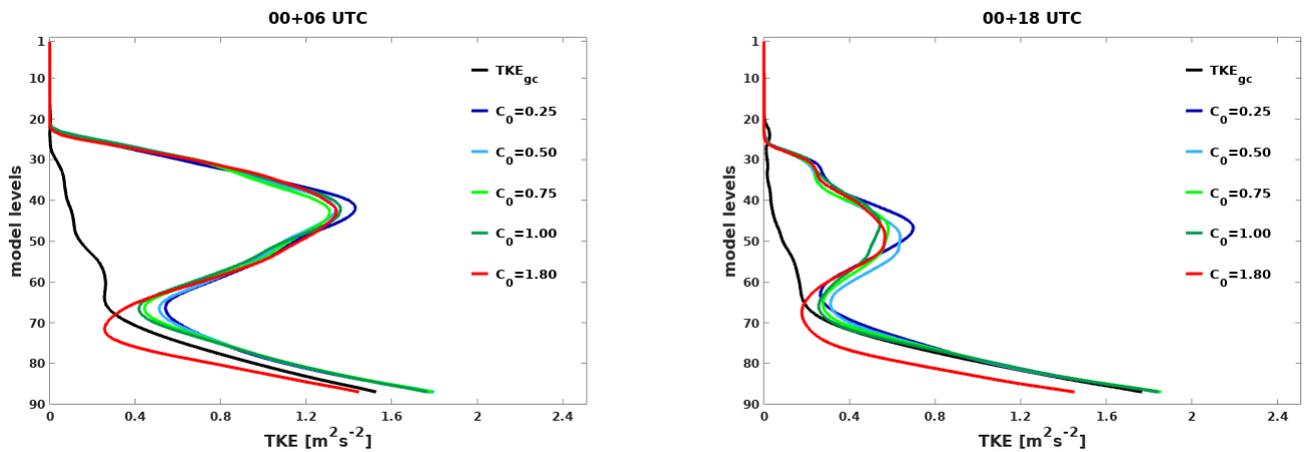
After the inclusion of corresponding TOUCANS expressions for momentum flux and dissipation of TKE, we obtained the condition for upper bound of  $C_0$ , i.e.  $C_0 < 1/\nu \approx 1.9$  (notice that this is valid only in near neutral conditions).



**Figure 1:** Comparison of averaged vertical profiles of the reference  $l_m$  (Geleyn-Cedilnik formulation) and generalized BL89 options which differ in the magnitude of the shear term ( $C_0$  constant).

Based on this, we constructed series of experiments trying to find an optimal value for our framework. In addition, we also tested the performance of BS scale in case when the value of  $C_0$  is on the edge of the criteria ( $C_0=1.8$ ). The domain averaged vertical profiles of  $l_m$  and TKE are presented on Fig.1. and Fig.2. As it can be seen, an increase of magnitude of the shear term significantly decreases  $l_m$  in the ABL, while the impact above the ABL is significantly smaller. The verification scores are clearly better than without the shear term, especially for

experiments with  $C_0=0.5$  and  $C_0=0.75$  (not shown). However, none of experiments is able to reduce too strong mixing (Fig.1.) and related maximum of TKE (Fig.2.) above the ABL. The problem itself appears very soon after the initialization, i.e. within the first 3 hours of the forecast and temporarily vanishes during the afternoon. By default, TKE is initialized using the corresponding value from the previous forecast. To confirm that there is no problem with the way how initialization is done, we initialized the forecast with  $TKE=0$ , but outcome was the same. Keeping this in mind, and knowing that even with the extreme value of  $C_0=1.8$  the observed problem above the ABL can't be solved, we decided to proceed in direction of further upgrade of our formulation.



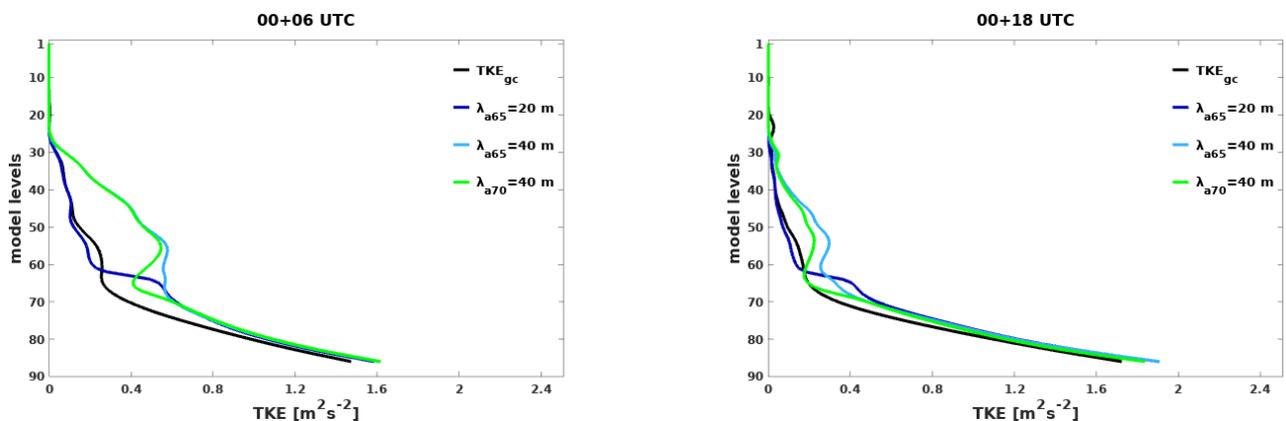
**Figure 2:** Comparison of averaged vertical profiles of the reference TKE (uses Geleyn-Cedilnik formulation) and those obtained by using generalized BL89 options which differ in the magnitude of the shear term ( $C_0$  constant).

## 4 Sensitivity studies

Before the upgrade of our formulation we decided to perform several sensitivity studies. Their goal was to see what is the impact of removal of a secondary, and to our opinion artificial, maximum of  $l_m$  on model performance, i.e. whether it will also remove the maximum of TKE and thus improve the model performance?

First we created an experiment in which the maximum of  $l_m$  above the model level 65 ( $\approx 1300$  m) was set to 20 m, wherein this value was chosen as it approximately corresponds to the asymptotic limit of Geleyn-Cedilnik formulation. The impact on domain averaged TKE is shown on Fig.3. As it can be seen, the maximum of TKE above the ABL is successfully removed (dark blue curve). The verification scores are significantly improved and now are comparable

to the reference (not shown). Two further experiments were created to see: i) how far can we push the limit of  $l_m$  and ii) what is the sensitivity to the height where we apply the limit? The results indicate (Fig.3.) that already with  $\max(l_m)=40$  m (light blue curve) we are heading towards the creation of a secondary maximum of TKE. When setting the cut-off point to model level 70 ( $\approx 850$  m) less sensitivity was found (green curve). In terms of scores the later two experiments are slightly worse than the first one. However, all the tests we made here clearly suggest that finding a physically supported way to remove the maximum of TKE above the ABL should push us towards completing the TKE-based mixing length formulation.



**Figure 3:** Comparison of averaged vertical profiles of the reference TKE (uses Geleyn-Cedilnik formulation) and those obtained by using generalized BL89 options which differ in the magnitude of the shear term ( $C_0$  constant).

## 5 Further upgrade of the generalized BL89 method

With clear signals that: i) inclusion of shear effects improves the performance of TKE-based mixing length formulation and ii) removal of a secondary maximum of TKE leads to further improvement of the model performance, we are confidently heading towards seeking physically-based principle to tackle the problem of excessive mixing above the ABL. Our attempts can be classified into those which: i) allow stability dependence of  $C_0$ , ii) introduce additional security constants and iii) introduce new term into generalized BL89 formulation.

### 5.1 Stability-dependent $C_0$ constant

Following [4], we adopted an idea of having a stability-dependent  $C_0$  within our framework:

$$C_0 = \frac{C'_0}{\sqrt{1 - \frac{Ri_g}{Pr_t}}} = \frac{C'_0}{\sqrt{1 - \frac{C_3 \cdot Ri_g \cdot \phi_3}{\chi_3}}} \quad (6)$$

where  $P_{rt}$  and  $C_3$  are Prandtl's turbulent number and closure constant, while  $\chi_3$  and  $\phi_3$  are TOUCANS stability functions. During the derivation of an upper limit for  $C_0$ , within the TOUCANS framework, we principally came to the following condition:

$$C_0 = C'_0 \cdot \frac{\chi_3}{\nu f(Ri_g)^{\frac{1}{4}}} \quad (7)$$

which at neutrality collapses to  $C'_0/\nu$ . For consistency with (6) we added  $C'_0$  as a further tuning constant. In (6) it is taken from [4], while in (7) it is set to  $C'_0=1$ . Both options are designed to be almost inactive in unstable stratification, while close to neutrality their strength significantly increases. Contrary to (6) which is also acting strongly in stable stratification, (7) is significantly suppressed there.

During the implementation phase, stability-related part of computations was done in **acm-rip.F90** subroutine and then passed to **acmixelen.F90**, where TKE-based mixing length is computed. Several experiments were done, including variations of the  $C'_0$  constant. Unfortunately, both of the methods were unsuccessful as they mostly affected the ABL. On the other hand, in the target region they almost did not have any impact.

## 5.2 *Additional security constant - $\epsilon$*

The idea which followed was to add a small security constant -  $\epsilon$  into (1)-(2) that would act similarly as asymptotic limit for the sensitivity test. However, this way we do not limit  $l_m$  directly. Also, with proper selection of that constant, we should avoid sharp transitions. As previously, we tried with two different approaches: i) to add  $\epsilon$  as a third term into (1)-(2) and ii) to add  $\epsilon$  as an addition to the shear term to ensure some effect (minimum shear) above the ABL, where shear is generally weak. Similarly as in previous chapter, the impact was stronger in the ABL than above it, i.e. when  $\epsilon$  was big enough to impact the above ABL layer then the structure of the ABL itself was practically destroyed.

## 5.3 *Addition of physically-based third term*

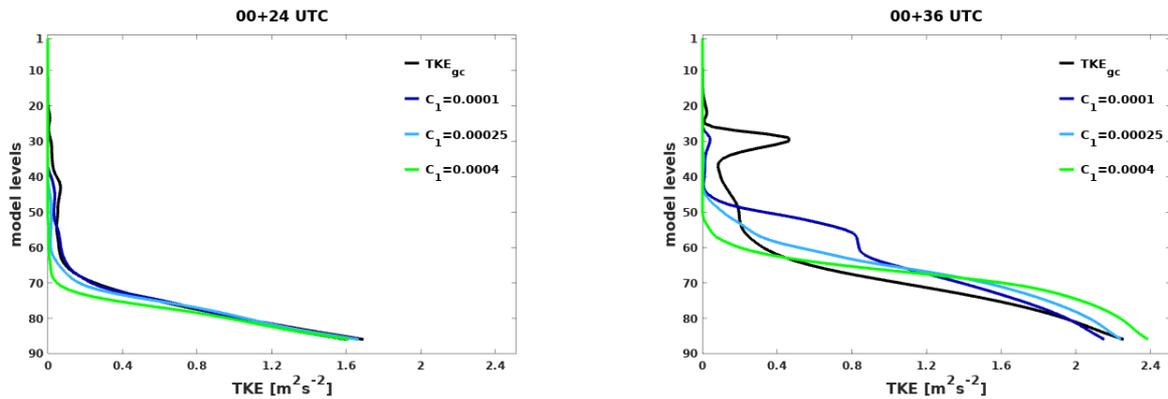
After two unsuccessful attempts we decided to add a new, physically-based, term into BL89 integrals, i.e. (1)-(2). The term is designed in a way to seek for sharp vertical changes of TKE and to act depending on the magnitude of that change. In order to work similarly both in and above the ABL, it seeks for relative, rather than absolute changes:

$$C_1 \cdot \frac{1}{e} \left| \frac{\partial e}{\partial z} \right| \cdot g \cdot f_1(Ri_g) \cdot f_w(z) \quad (8)$$

here  $C_1$  is a tuning constant controlling the magnitude of the term,  $f_1(Ri_g)$  is a stability-dependent function (different to the one used in TOUCANS) used to ensure maximum efficiency at desired stability range, while  $f_w(z)$  is a weight function which should diminish towards the surface. Due to dimensional reasons, as a first guess, we choose  $f_w(z)=z$ . Stability-dependent function  $f_1(Ri_g)$  is defined as:

$$f_1(Ri_g) = \frac{1}{(1 + |Ri_g|)^2} \quad (9)$$

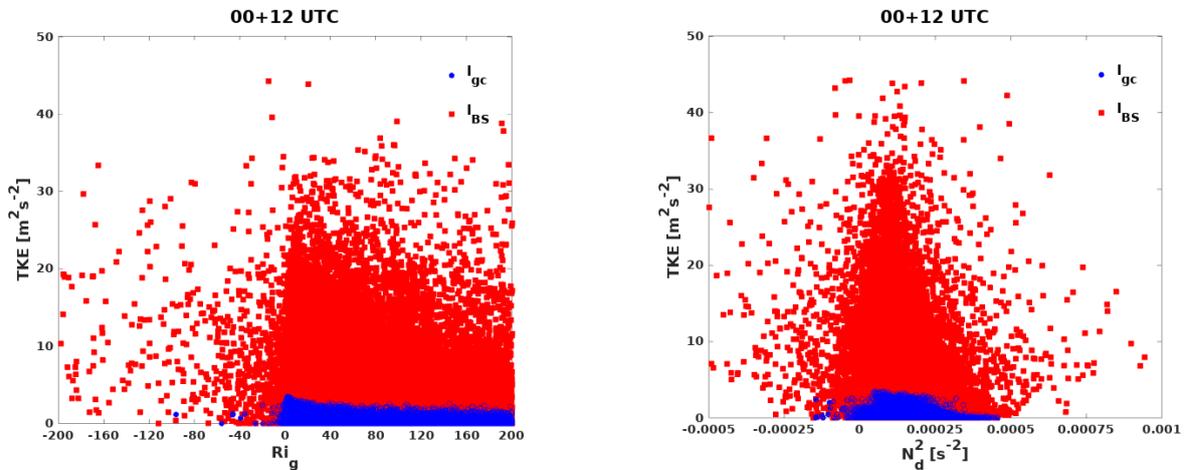
to ensure maximum efficiency as close as possible to neutrality.



**Figure 4:** Comparison of averaged vertical profiles of the reference TKE (uses Geleyn-Cedilnik formulation) and those obtained by using generalized BL9 options which differ in the magnitude of added third term ( $C_1$  constant).

The only affected subroutine by code changes is **acmixelen.F90**. In total, three experiments with different values of the  $C_1$  constant were performed. The most efficient one resulted in removal of a jet-stream signal (TKE profile; Fig.4.), which is obviously a result of poorly chosen weight function -  $f_w(z)$ . In the absence of a proper shape of  $f_w(z)$ , we decided to set it equal to one and apply the term only above some model level where the problem of excessive mixing is occurred, i.e. above the level 65. The goal here is only to test the term efficiency. After further testing we found that term efficiency changes depending on time of the day, as well as with height (within the layer where it is applied). We immediately suspected that the problem is related to stability, i.e. that we do not hit all the points with artificially strong TKE due to our choice of  $f_1(Ri_g)$ .

For this reason we decided to do the stability dependency analysis of  $l_m$  and TKE in different layers of the troposphere. We found that above level 60 huge number of high values (e.g. for TKE; Fig.5. - left panel) lie outside of  $Ri_g \in \langle -2, 2 \rangle$  which is mostly affected by the additional term. Contrary, if we use Brunt-Väisälä (BV) frequency as a stability measure (Fig.5. - right panel), then most of the high values are concentrated in the vicinity of zero. This is why in further work we will construct the stability-dependent part of third term as a function of BV frequency.



**Figure 5:** Scatter plot of TKE for the reference (blue) and generalized BL89 formulation with  $C_0=0.5$  (red) in dependence on stability parameters: i) Richardson gradient number (left panel) and ii) Brunt-Väisälä frequency (right panel) during the period 28-30.6.2017.

## 6 Conclusion and further work

We implemented and tested generalized BL89 formulation, i.e. the BS scale. The inclusion of shear effects, incorporated with local  $\kappa$ -scaling, reduces mixing within the ABL and outperforms the reference in terms of surface scores for tested winter case. On the other hand, upper level scores are mostly neutral. However, during the summer scores are mostly worse than for the reference. Despite favorable decrease of mixing within the ABL, the BS formulation is unsuccessful in removing artificial secondary maximum of TKE above the ABL.

Several sensitivity studies were performed and showed that reduction of mixing above the ABL leads to significant improvement of both surface and upper level scores, thus making them comparable to the reference. The inclusion of additional term, on top of buoyancy and shear, is direction in which we are currently heading. This term reduces mixing by identifying sharp

vertical changes of TKE and its intensity is controlled by stability function. During this stay we found that this function should be formulated using the BV frequency, rather than  $Ri_g$ . Formulation of this function is a main short-term goal. To make new term generally applicable we also need to define proper weight function, which should diminish the effect within the ABL.

Other aspects mentioned in the previous report, like work on smooth transition from  $\kappa z$  layer to the layer where full TKE-based solution prevails are currently put on hold. However, we open one additional direction in tackling the problem of excessive mixing above the ABL. This approach utilizes upper asymptotic mixing length ( $\lambda_a$ ) based on the following expression:

$$\lambda_a = C_2 \cdot \frac{\int_0^\infty \sqrt{e} z dz}{\int_0^\infty \sqrt{e} dz} \quad (10)$$

where  $C_2$  is additional tuning constant. Finally, the  $l_m$  in our framework should look like this:

$$l_m = \min(\kappa z, L_{TKE}, \lambda_a) \quad (11)$$

After the discussion with Ivan Bařtak Duran during "ALARO-1 working days 2019", we decided to keep the option of global  $\kappa$ -scaling opened for further revision. There we were pointed out to the fact that during the derivation of TOUCANS equations  $\kappa z$  was replaced with  $l_m$  outside of the surface layer, including free atmosphere. This may point out to global  $\kappa$ -scaling as preferable option, after all. However, until we clarify this aspect, we will stick to our choice - local  $\kappa$ -scaling, as the main problem we have (secondary artificial maximum of  $l_m$  and TKE) is observed with both options.

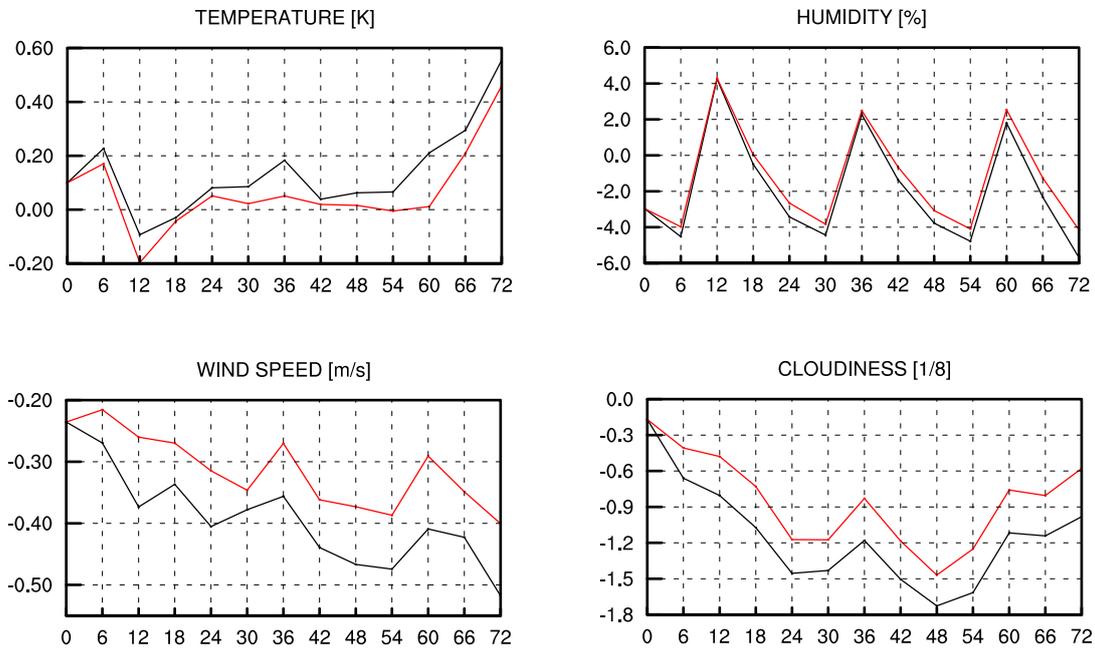
For the time being, the work on this topic will continue from home. Related to this, there is also an ongoing work on putting TKE and TTE prognostic equations into DDH. We consider this step as crucial for better understanding of the relationship between mixing length and TKE, as well as for tuning of the TOUCANS scheme in general. At this point, the implementation phase is completed and new DDH package is ready for testing. Hereby I would like to thank to Tomislav Kovacic for his work in the preliminary phase of this task, as well as for providing the support after retirement.

**Acknowledgment:** The author wishes to thank to Jan Masek and Radmila Brořkova for their support and cooperation, as well as to entire ONPP department for their warm welcome and hospitality. This stay is funded by the RC-LACE project.

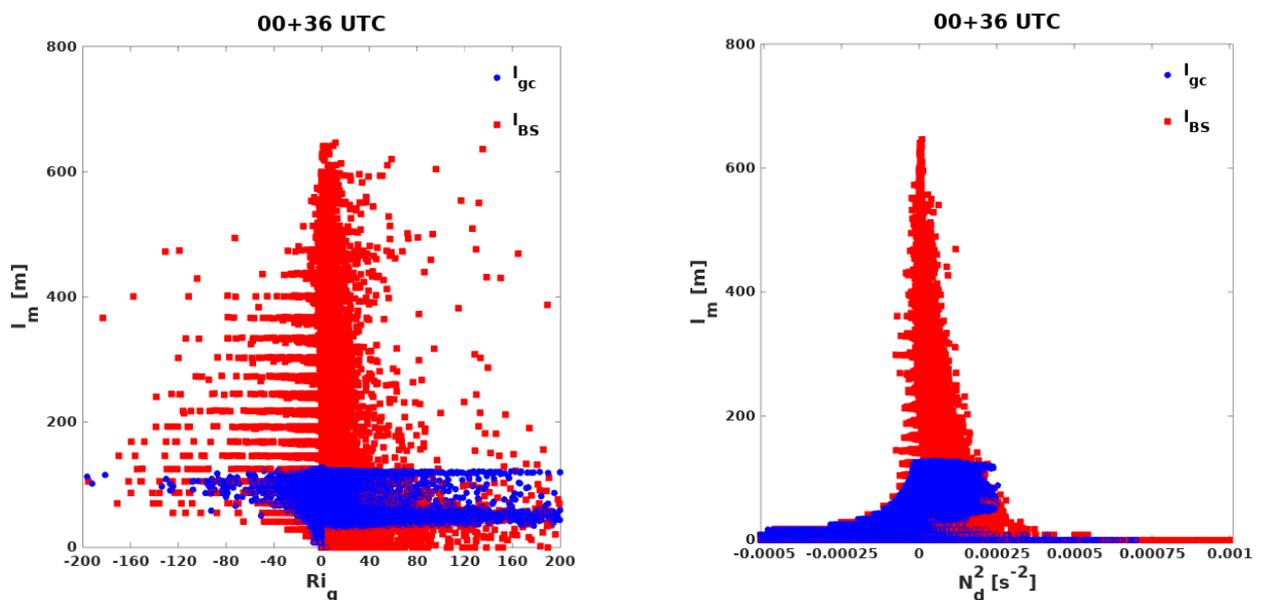
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- <sup>3</sup> Q. Rodier, V. Masson, F. Couvreux, and A. Paci. Evaluation of a Buoyancy and Shear Based Mixing Length for a Turbulence Scheme. *Front. Earth Sci.*, 5:65, 2017.
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## Appendix



**Figure A1:** BIAS of surface parameters for the reference (black) and generalized BL89 formulation with  $C_0=0.5$  (red) during the period 15-17.1.2017.



**Figure A2:** Scatter plot of  $l_m$  for the reference (blue) and generalized BL89 formulation with  $C_0=0.5$  (red) in dependence on stability parameters: i) Richardson gradient number (left panel) and ii) Brunt-Väisälä frequency (right panel) during the period 28-30.6.2017.