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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Parameterization of vertical diffusion and the atmospheric boundary layer height determination in the EMEP model" *by* A. Jeričević et al.

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Answer to the comments of the Reviewer2:

1. Grisogono parameterization

C1.1. By inserting Eqs. 11 and 12 into Eq. 10, one obtains K(z) = C(K).C(h).u*.eËĘ1 2.z.exp[-0.5(z/h)ËĘ2], which can be written as K(z) = C.u*.z.exp[-0.5(z/h)ËĘ2], where C is a constant. This does not depend on the boundary layer height H, even though the authors state that H is explicitly included (p. 9607), as H cancels out when introducing K_max and h. It should be clarified why Eqs. 11 and 12 are needed and why C and h are not fitted directly. A1.1: Constants C(K) and C(h), Eq. (11) and (12), were not directly included in Eq. (10) in order to stress that it is the same gradually varying form of the K(z) used to generalize the classical analytical solution for the Ekman layer flow using the WKB method (after Wentzel, Kramers and Brillouin who popularized this method in theoretical physics) in e.g., Grisogono, B.: A generalized Ekman profile with gradually varying eddy diffusivities, QJRMS, 121, 445-453, 1995. Furthermore, this profile has been applied to simulate katabatic flows, e.g., Grisogono, B., and Oerlemans, J.: Justifying the WKB approximation in pure katabatic flows, Tellus A, 54, 453-462, 2001. In this work the same K(z) formulation is applied, and the only difference is in chosen parameterization of the constants C(K) and C(h) which are here defined with H, u* and universally applicable parameters determined based on the LES data. Furthermore, note that H is still explicitly included in Eq. (10) through the exponent term and direct inclusion of C(K) and C(h) would still incorporate two empirical constants.

C1.2.: Based on the formula derived above, if the eddy diffusivity within the surface layer (z Âń h) can be approximated by K(z) = C.u*.z, i.e. by a linear profile (cf. Fig. 2 for z< 50 m). By using C(K) = 0.1 and C(h) = 3, one obtains C = 0.49, which is not very different from the van Karman constant. Thus the surface-layer K(z) profile effectively corresponds to the profile derived from Monin-Obukhov similarity in neutral conditions. It is thus surprising that this would provide a better fit than a model that includes stability effects. Please discuss. A1.2.: In neutral and stable conditions condition z«h is not fulfilled due to the relatively coarse model vertical resolution. The lowest model level is approximately at 45 m and by taking H=200 m in stable conditions as a referent experimental value we obtain h $\approx$ 66.7 m; therefore, z $\approx$ h, which means that the exponential part can not be disregarded from the Eq. (10). Furthermore the coefficient C is relatively close to von Karman constant but still different enough ($\sim$ 10 %) to produce differences in the modelled concentrations of the similar magnitude.

2. K(z) evaluation based on LES data C2.1.: Why did you compare the Grisogono scheme against the O'Brien profile, even though the latter is not used in the EMEP

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model in stable conditions? A2.1.: Grisogono profile is an approximation of the O'Brien third order polynomial and the comparison of those two approaches was provided to establish the differences of those two approaches and the effects of different parameterizations applied. Results are published in Jeričević and Večenaj, BLM 2009 where special emphasis was given to the parameterization of stable atmospheric conditions which are of great importance for application in air pollution. Although O'Brien approach is not used in the EMEP for the stable atmospheric conditions it is used in many other applications and it is even recommended for application in the stable conditions (e.g. Stull, 1988).

C2.2. The data presented in Section 3.1 are taken from a previous study (Jericevic & Vecenaj, 2009, ref. in MS). Instead of showing just two examples, it would be more useful to present a more complete summary of the results of that study. A2.2.: We are aware that only two examples could not describe the full work conducted in Jeričević and Večenaj (2009); hence, the reader is often pointed to the original paper. The main idea here was to show that comprehensive study on vertical diffusion evaluation has been started with intercomparison between the O'Brien and Grisogono K(z) schemes based on the LES data. Although it is possible to provide complete summary of the previous paper, there is a possibility to burden already quite an extensive material.

Q2.3. Why did you choose to show only stable cases, even though neutral cases were also included in the LES dataset? In fact, the K(z) values (and their vertical extent) shown in Fig. 2 seem quite large for stable conditions. If these examples are shown, it would be useful to report the basic flow variables associated with them. A.2.3.: A numerous of the LES runs were used from neutral to stable conditions and cases presented in the paper were randomly chosen. These selected LES cases of nocturnal and stable conditions were obviously characterized with stronger mechanical turbulence (see Figure 1, i.e. Fig. 3 in the revised paper) but the stability conditions were maintained in the LES.

C.2.4. Why did you compare K_m rather than K_h that is used for scalar diffusion in the

EMEP model? A.2.4.: In the EMEP model vertical diffusion coefficient is scalar K_h. Magnitudes of K_h and K_m differ only to a constant, therefore it is basically same which one is used for comparison.

3. K(z) evaluation based on EMEP model performance C3.1.: Why did you not include nitrate concentrations in the comparison? I know there are fewer stations measuring these compounds, but these would provide information on the balance between primary and secondary compounds (cf. sulphur with both SO_2 and sulphate included). A3.1. The reason why we did not include nitrate is that it is the most difficult inorganic aerosol to model; to get it right you need to get the HNO3-NO3 equilibrium right (which means you have to have NH3, SO4, HNO3, NH4+ right also) and in addition you need to get the split between fine and coarse nitrate right. Therefore, the resulting fine nitrate will be very sensitive to many processes which are difficult to model. SO4 (and even NH4+) is easier, as it depends on fewer processes one has to get right.

C3.2.: I am unable to follow the discussion in Section 3.3.1. Firstly, the authors explain that the model overestimates NO_2 concentrations at the SE02 station and that overestimation is larger in 2000 than 1990, and much larger in 2001. I do not understand how this trend is related to the exclusion of the measurement stations in the North Sea area. Secondly, the authors state that the "Grisigono method is less diffusive than O'Brien in stable conditions" (repeated on p.9613), but Section 3.1 demonstrates just the opposite. (See also the comment about the use of O'Brien scheme in the EMEP model.) A3.2.: The intention was to show that modeled NO2 values at some stations in the shipping area exhibit nonsystematic variations even in the long-term average NO2 concentrations due to influence of local emission sources. However, we agree that this is not significantly contributing to the results and it is considerably shortened. It is important to point that shipping emission paths are not sufficiently resolved due to the coarse horizontal resolution in the model, and therefore higher concentrations are horizontally diffused over larger areas (including analyzed stations, where obviously these high concentrations were not observed). The Grisogono method is generally less dif-

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fusive, e.g. annual averages of NO_2 at SE02 also confirm this finding. However, in this particular LES case (in section 3.1) it was not less diffusive. It will be fair to say that the Grisogono method represents surface concentrations in stable conditions better than the operational scheme. This is now rephrased also in the Conclusions and at other suitable parts in the text.

4. BL height comparison with observational data

C4.1. The same Ri_B-based criterium for the estimation of boundary layer height is used both within the analysis of observations (both radiosounding and tower data) and the proposed new modelling scheme. Thus the modelled and observation-based H values cannot be considered fully independent. I would like to see a comment on this. A.4.1.: The possibility to have biased results due to the same methodology applied is minimal because the RiB method depends considerably on the data resolution. Since the same RiBc was used in the model, radiosoundings and Cabauw data, there was no tuning or adjustment of the results in order to achieve better agreement of the calculated H values. Furthermore, the choice for determination of the H from the radiosoundings is basically limited by the data itself. For example, sensible heat flux is not available from the radiosoundings; therefore, it was impossible to apply the same method as in the operational EMEP model for the convective atmospheric conditions. On the other hand, in stable conditions H is determined based on K(z) calculated by the Blackadar equation, which also includes Ri number, and the same reasoning on the independency can be assumed.

C4.2. The Cabauw tower provides measurements up to a height of 200 m. Figure 15 indicates that the estimated H exceeds this for most of the daytime, which significantly limits the possibilities for model evaluation. Thus the conditions to which the presented results actually apply should be described and the limitations of these data quantified. It would be useful to discuss whether the seasonal variation in the agreement (Fig. 16) is related to the availability of data. A4.2.: In Fig. 2 number of hourly H values higher than 200 m, N (%), determined from the observations (white bars) and from the EMEP

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model (blue bars) per month during 2001 at the Cabauw tower is presented. It should be pointed that in this work RiB numbers are differently estimated from the observations and from the model. From the observations RiB numbers are estimated using values at 2 m as the lowest level, z1= 2 m, while RiB estimated from the EMEP model used the first model level (z1 $\approx$ 50 m) as the lowest level. As a consequence considerably more cases, $\sim$ 30 %, with H > 200m are found in the observations than in the model (Fig. 2) which is in the agreement with findings of Vogelezang and Holtslag (1996). Annual course has 2 maxima during spring and autumn N $\sim$ 80 % in the observations and N $\sim$ 70 % in the model (Fig. 2). During the winter N is expectedly smaller with N $\sim$ 60 - 70 % from the observations and N $\sim$ 30 - 40 % from the model. During the summer N $\sim$ 70 - 80 % of cases with H > 200 m is found in observations and N $\sim$ 50 - 60 % from the model. Since there was a considerable number of cases with H > 200 m, N, dependency of r and N is examined. In Fig. 3 relation between the r and N determined from the model is shown. Obviously N is related with r in the way that an increase in N is reflected in a decrease in r.

5. Presentation

C5.1. The authors should improve the presentation. The description of the EMEP model, in particular, is insufficient and partly confusing. The most recent and detailed documentation of the K(z) and H parameterisations used in the EMEP model (Simpson et al., 2003, EMEP Report 1/2003) should be used as the key reference. A5.1. We have now provided the model parameterizations description closer to those of Simpson et al., 2003.

C.2. The authors should describe the methods more accurately. On p. 9599, for example, it is stated that K(z) is based on Monin-Obukhov similarity theory in stable conditions, while Section 2.4 indicates that this is only true for the surface layer in unstable conditions. In Section 3.1, the Grisogono scheme is compared against the O'Brien profile. This appears puzzling, as the LES data used as a reference are for stable conditions, while according to Section 2.4 (and Simpson et al., 2003) the O'Brien profile is used in the EMEP model in unstable cases only. A5.2. Methods are now described more accurately according to Simpson et al., 2003. In the stable conditions K(z) is calculated based on MO theory (Eq (5)) on the first model level. Sentence between Eq. (3) and (4) is added: ‘To avoid non physically small exchange coefficients within the boundary layer K(z) value is evaluated at the top of the lowest model layer ($z \approx 90$ m) with Eq. (5) both in stable and unstable atmospheric conditions.’ For the second part please look the answer A2.1.

C5.3. The language should be revised. There are also many technical inaccuracies; see the detailed comments below. A5.3. The language is now improved in the revised manuscript; moreover, most of the former technical inconsistencies are now removed.

Detailed comments

C: p.9598, line 5, "especially in the stable conditions": Only stable conditions were tested. A p.9598, line 5: It was tested in the neutral conditions also.

C: p.9598, line 14 (and elsewhere), "ABL schemes": The ABL height is only considered. Please rephrase. A: It is rephrased into ‘ABL height schemes’.

C: p.9599, line 13, "vertical diffusion scheme K(z)": Please define the variable K (and z) properly. A: We do not fully understand the comment; however, we have rewritten this part of the Introduction and explained that z is height.

C: p.9599, line 17: "Deardorf" should read "Deardorff". A: Changed.

C. p.9600, line 7 (and elsewhere): Remove ’a’ from the reference. A: Done.

C: p.9604, Eq. 1: The use of K_min is not consistent with Simpson et al. (2003). A: Flore value of K(z), i.e. 0.001 value is here represented with a variable Kmin and the consistency is preserved.

C: p.9604, Eq. 1: Please explain how the mixing length is obtained. A: It is now explained after Eq. (1).

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C: p.9604-5, Eqs. 1 and 2: These equations should be written in terms of finite differences rather than derivatives. A: It is now rewritten.

C: p.9605, Eq. 3: This is not consistent with Simpson et al. (2003). A: It is now rewritten.

C: p.9605, lines 6 and 12: Please use different symbols for different model layers. A: It is now changed.

Q: p.9605, line 8: Why "recalculated"? A: Because K(z) values are firstly initialized on all model levels, regardless of the atmospheric stability, with the Blackadar profile and then replaced or recalculated for the boundary layer with different values for different atmospheric stabilities. Now it is changed into: ‘ In the unstable ABL, values are calculated with the O’Brien scheme:’

C: p.9605, line 12: As K_H is a constant, dK_H/dz = 0 by definition. Please reformulate to indicate that you mean dK(z)/dz = 0 at z = H. A: Done.

C: p.9605, Eq. 5: z/L should be replaced by H_S/L. A: We would like to use Eq (3.2.) from Simpson et al. (2003).

C: p.9606, line 20: These values are not taken directly from Jericevic and Vecenaj (2009). That study presents values for both K_m and K_h; C(K) = 0.13/0.06 and C(h) =1.52/3.73 for m/h. Please clarify. A: Constants determined in Jeričević and Večenaj (2009) for Km, C(K)=0.13 and C(h)=1.52, and for Kh, C(K)=0.06 and C(h)=3.73, are determined from a range of values which provide optimal K(z) values in neutral and stable conditions. Averages and standard deviations of the C(K) and C(h) coefficients determined based on the LES data are shown in Fig 4.

C: p.9607, line 8: "ABL" should read "ABL height". A: Done. C: p.9607, Eq. 13: Ri_B depends on the level j, so you could write Ri_B,j. A: Now the subscript j is avoided.

C: p.9608, line 5: But K_H is rather unimportant and K _H_S is obtained from Monin-Obukhov similarity theory. A: We presume your comment was for p.9607. It is true that

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KHs is determined based on the Monin-Obukhov theory. However, it is based on Hs which is not easy to resolve and depends on model resolution.

C: p.9608, lines 7-10: In the EMEP model, a Ri-based method is used in stable conditions. A: This is now commented: 'Furthermore, although the operational method in the stable conditions is based on Ri number and includes both sources of turbulence, it can be oversensitive to local turbulence and underestimate the ABL height.'

C: p.9608, lines 10-12: Repetition. A: Now it is changed into: 'Main advantages of this method over the operational approach are that RiB includes two major turbulence generators in the atmosphere, thermal and mechanical sources of turbulence, and it is applicable in stable and unstable atmospheric conditions. Equation (14) describes the H as an integral atmospheric property that relates surface processes to upper processes in the ABL and thus includes non-local effects.'

C: p.9608, line 13: Why "vertically integrated"? A: Changed into: 'The main weakness of the operational ABL method in stable conditions is dependence on K(z) profiles calculated with the Blackadar approach (Eq. 1).'

C: p.9609, line 5, "both schemes": Unclear which schemes are referred to. A: It is changed into: 'The unstable conditions are not simulated in the LES, however performance of the both schemes, the O'Brien and Grisogono, is evaluated in the EMEP model during July 2001 against surface NO_2 concentrations and lower underestimation, i.e. higher surface concentrations, is found with the Grisogono scheme.'

C: p.9609, line 11: Please define r. A: It is now defined.

C: p.9609, lines 21-24: This conclusion is not justified. It is of course possible that the differences could result from the processes mentioned but there is a number of other equally plausible explanations. A: It is changed now into: 'Overestimation of SO_2 and underestimation of sulphate indicates that other processes responsible for sulphate formation in the model should be investigated as well as meteorology, particularly pre-

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cipitation and moisture provided by the NWP model.'

C: p.9610, lines 10-11: The caption of Fig. 10 states that all stations are included. A: It is corrected in the caption of Fig. 10.

C: p.9610, line 12: The title is misleading, as most of this section is about trends and the problems around the North Sea. A: The title is changed into: 'Influence of local emission sources'

C: p.9611, line 10-11: Please explain why the coarse horizontal resolution in this case results in the overestimation of concentrations, while typically it overestimates horizontal dispersion and thus would underestimate concentrations. A: It is true that the coarser horizontal resolution leads to the greater numerical dispersion, however we think that in this particular case the numerical dispersion itself is the cause of the mentioned overestimations. This apparent contradiction can be easily explained on the example of Birkenes station. The station is located some 25km inland which is far enough inland not to be influenced by the shipping emissions directly. The real shipping lines are distributed through the pass between Norway and Denmark which is less than 100 km wide. However, looking from the framework of the model (50 km resolution), the station is at most a single grid cell away from the emission source (if not in the same cell). Therefore, numerical dispersion leads to the elevated concentrations in the grid cells adjacent to the cell with large emissions which in reality happens to cover the area of the measurement station.

C: p.9612, line 4, "used": For what? A: It is now clarified: 'Two stations with the highest altitude in the EMEP domain are used for evaluation of vertical mixing schemes in the EMEP model; CH01 and SK02.'

C: p.9612, lines 17-21: RD(BIAS) (where BIAS actually means the absolute value of BIAS) is a bit difficult to perceive. Please explain why the maximum value of this metric is 100% (cf. Fig. 7). A: Relative differences are now excluded and only differences D are shown in Figs. 7 and 8 in the revised MS. The maximum value was set to 100 %

in order to be able to put all stations at the same figure. Otherwise, stations with RD (BIAS) > 100 % would dominate and it would impossible to spot the variability among the stations with RD (BIAS) < 100 %. Now this is avoided.

C: p.9613, line 12: How did you define the "no change" case? Its frequency obviously depends on the number of significant figures recorded or a tolerance criterium applied. A: Criterion was that station with RD(r)=0 was declared as those without change.

C: p.9614, lines 7-8: All the stations that did not indicate improvement were not shown to have a "higher uncertainty in measurements". Please rephrase. A: Rephrased as: 'Obviously only few stations, some of them are those with higher uncertainty in measurements, did not follow the common trend of improvement with the new K(z) scheme.'

C: p.9614, lines 21-22: I would assume that the seasonal variation of emissions also plays a significant role here. A: We agree, added: 'This drop in is caused by increased photolysis of NO2 and more vigorous vertical mixing during the warmer period. Also seasonal variation of NO2 emissions also plays a significant role in the annual course.'

C: p.9614, lines 28-29: If this refers to Fig. 10, then it was previously explained that the stations with highest uncertainties were removed. Anyhow, this sentence can be removed. A: Removed.

C: p.9615, line 17: typo A: Corrected.

C: p.9616, lines 12-13: All the values shown in Fig. 11c are not within these ranges. A: Changed into: 'Average monthly H values for different stations are mostly in range: 200 m < < 400 m, while for the new method: 400 m < < 600 m.'

C: p.9616, line 18: According to Simpson et al. (2003), a minimum H of 100 m is enforced in the EMEP model. A: Indeed both schemes have minimum H=100 m and this is corrected now. First full sigma model level is on height of 100 m and that is a minimum H value set in the Shapiro filter. Height of the half sigma level is approximately at 50 m.

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C: p.9617, lines 19-20: Unclear which model is referred to. A: Now it is stated that it is a EMEP model: ‘Lisbon station is located near the boundary of the EMEP model domain where the modelled results are dominated by weakly varying boundary conditions.’

C: p.9617, lines 26-: Methods should be described in Section 2. A: Indeed RiB method is not described in this section therefore it is changed in: ‘In this section average hourly vertical profiles of RiB number, (), where j = 10, 20,. . ., 200 m are the measuring levels; and the corresponding H at the Cabauw tower are analyzed and described for every month in year 2001 (Figure 15).’

C: p.9619, line 2: Fig. 15m does not exist. A: Corrected.

Q: p.9619, lines 9-10: How do you compare the boundary layer height "in the surface layer"? A: Changed into: ‘Obviously the new ABL scheme gives significantly better results for all months except for Jun, July and August i.e. the summer period when both schemes performed similarly.’

C: p.9620, line 15: It is not clear why a less diffusive scheme would be an "important preference". Please rephrase. A: The whole paragraph is rephrased.

C: p.9620, lines 23-24: Unclear what is meant by this sentence. A: We wanted to point that NWP model preferences limit the performance of the air quality model and that improvements in the NWP would affect distribution of the pollutants. The effect of the changes will be investigated although improvements are expected to improve the results of air quality model. ‘Therefore improvements in the NWP model performance would yield to appreciable differences in terms of both, magnitude and spatial distribution of pollutants which would in the end improve the air quality model performance.’

C: p.9623, line 7: A wrong page number. A: Corrected.

C: Figs. 9, 12, 14 and 16: The data points should be indicated and connected by direct lines instead of a curve based on an unspecified function. A: Used smoothing function does not affect the data and contributes to the quality of the figures. However, we have

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made requested corrections.

C: Fig. 10: Units missing. The lines should be explained. I am not sure if this figure is needed (or could perhaps be enhanced by including some statistics). A: Fig. 10 is now excluded. Results are described in Sec 3.3.3.

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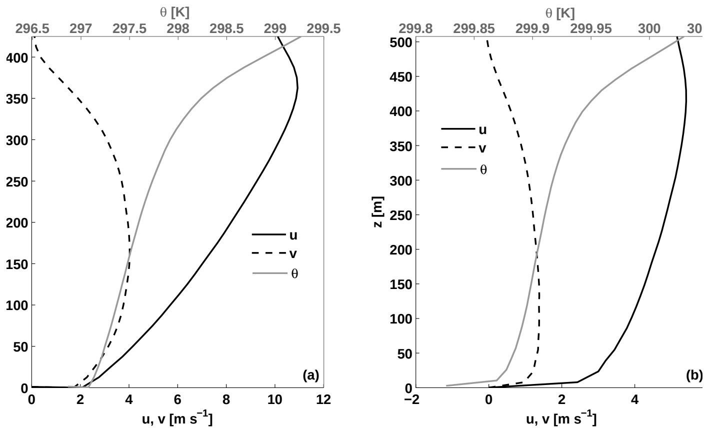

Fig. 1. Vertical profiles of wind components, u (thick black line) and v (dashed black line), and potential temperature (gray line) for the selected LES cases in a) nocturnal conditions and b) long-lived stab

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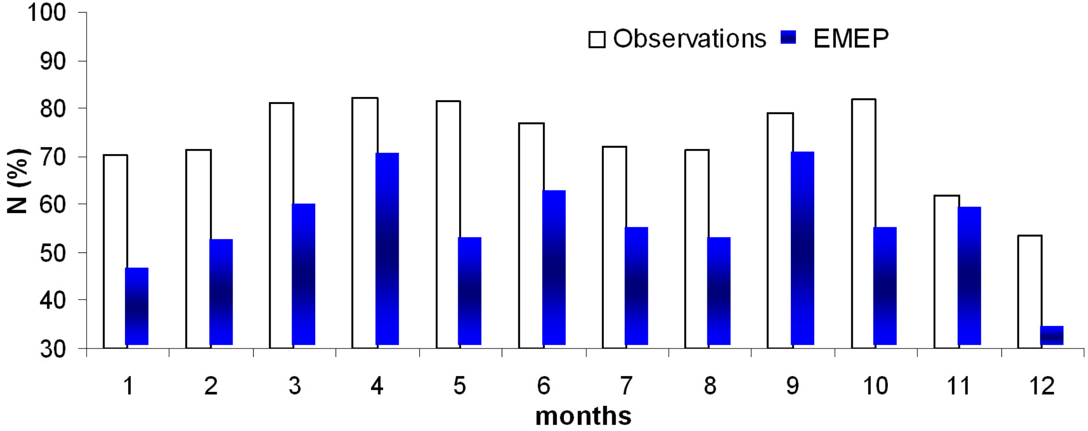

Fig. 2. Number of hourly H values higher than 200 m, N (%), determined from the observations (white bars) and from EMEP model (blue bars) per month during 2001 at the Cabauw tower.

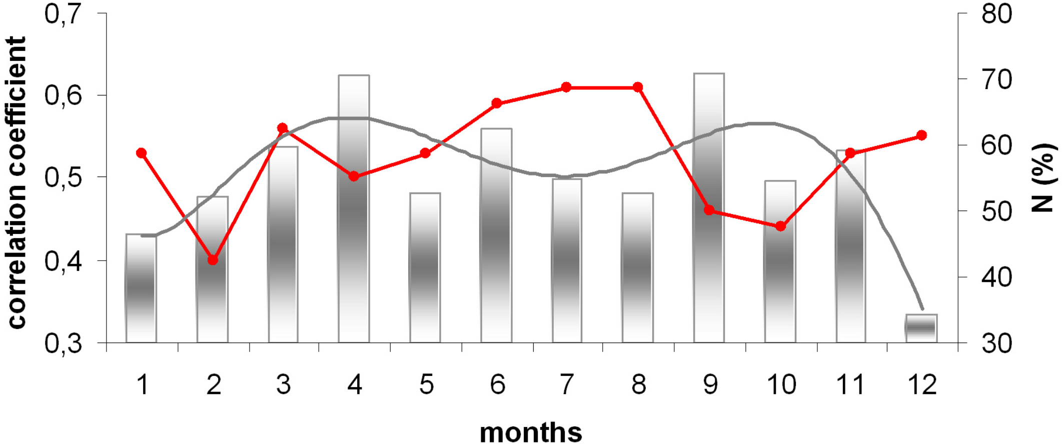

Fig. 3. Number of hourly H > 200 m values, N (%) determined from the observations (bars, right axes) and the corresponding monthly correlation coefficient (red line, left axes) at the Cabauw tower during the

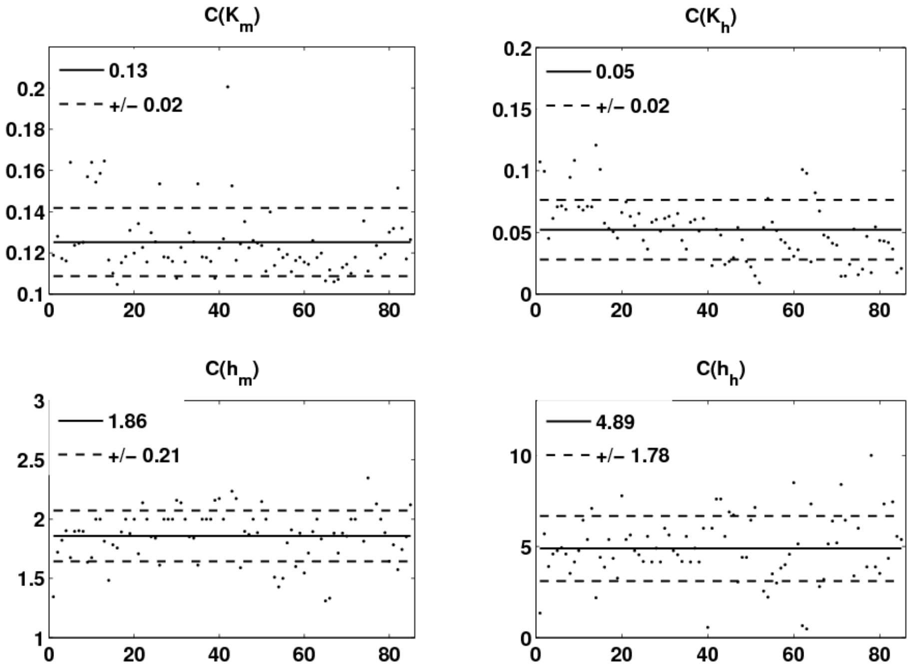

Fig. 4. Averages and standard deviations of the C(K) and C(h) coefficients determined based on the LES data.

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