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SCALING VARIANCES OF SCALARS IN A CONVECTIVE BOUNDARY LAYER UNDER DIFFERENT ENTRAINMENT REGIMES

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Abstract. For the presentation and analysis of atmospheric boundary-layer (ABL) data, scales are used to non-dimensionalise the observed quantities and independent variables. Usually, the ABL height, surface sensible heat flux and surface scalar flux are used. This works well, so long as the absolute values of the entrainment ratio for both the scalar and temperature are similar. The entrainment ratio for temperature naturally ranges from −0.4 to −0.1. However, the entrainment ratio for passive scalars can vary widely in magnitude and sign. Then the entrainment flux becomes relevant as well. The only customary scalar scale that takes into account both the surface flux and the entrainment flux is the bulk scalar scale, but this scale is not well-behaved for large negative entrainment ratios and for an entrainment ratio equal to −1. We derive a new scalar scale, using previously published large-eddy simulation results for the convective ABL. The scale is derived under the constraint that scaled scalar variance profiles are similar at those heights where the variance producing mechanisms are identical (i.e., either near the entrainment layer or near the surface). The new scale takes into account that scalar variance in the ABL is not only related to the surface flux of that scalar, but to the scalar entrainment flux as well. Furthermore, it takes into account that the production of variance by the entrainment flux is an order of magnitude larger than the production of variance by the surface flux (per unit flux). Other desirable features of the new scale are that it is always positive (which is relevant when scaling standard deviations) and that the scaled variances are always of order 1–10.

Keywords: Bottom-up, Entrainment, Scalar variance, Scaling, Top-down.

1. Introduction

Dimensional analysis and similarity theory are powerful tools in the analysis of surface-layer and atmospheric boundary-layer (ABL) data. One of the goals of similarity theory is the correct scaling of characteristic features of a flow through the choice of appropriate length, velocity and scalar

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scales (Garratt, 1992). In this way the absolute value of the scale of the flow, as well as the magnitude of the driving forces, are eliminated.

For the convective boundary layer (CBL, i.e. a boundary layer in a state of free convection with zero mean wind) the following set of scales is used (Deardorff, 1970; Holtslag and Nieuwstadt, 1986; Stull, 1988): the mixed-layer height z_i, a velocity scale w_* and a scalar scale s_*, where

$$w_* = \left(\frac{g}{\overline{\theta}_v}\overline{w'\theta'_v}_s z_i\right)^{1/3},$$

$$s_* = \frac{\overline{w's'}_s}{w_*},$$

and $g/\overline{\theta}_v$ is the buoyancy parameter, θ_v is virtual potential temperature, $\overline{w'\theta'_v}_s$ is the surface buoyancy flux and $\overline{w's'}_s$ is the surface scalar flux. If the scalar is θ_v, the scale is denoted as θ_{v*}. With these scales it is possible to form non-dimensional plots of observations or simulation results in order to explore the shape of the profiles of scalar statistics and the relative magnitude of those statistics between scalars. For a scaled scalar statistic to be useful:

- it should be of the order of 1;
- it should, for a given scalar, reveal similarities between flows, as far as the dominating forcings are similar (either forcing by the surface flux or the entrainment flux);
- it should, for a given flow, reveal similarities between different scalars, as far as the forcings are similar.

These requirements are met so long as the dominant driving force is included in the scale that is used to non-dimensionalise the scalar statistic. Thus, so long as the surface scalar flux dominates the scalar statistics throughout the CBL, the set of mixed-layer (ML) scales mentioned above is sufficient. However, if in the upper part of the CBL entrainment processes are the main determinant of scalar statistics, information on entrainment should be included as well.

For (virtual) potential temperature information on entrainment is automatically included in θ_*, because the magnitude of this entrainment flux ($\overline{w'\theta'_v}_e$) is mainly determined by the momentum of the rising air (relative to the strength of the capping inversion) and is thus coupled to the surface flux (taken into account in w_*). The strength of the capping inversion both *enhances* (entrainment of hotter air) and *suppresses* (less pentrative convection) the entrainment flux, leaving only a limited net influence of the capping inversion on the entrainment flux. Note that the process of entrainment is modified in the presence of shear (Pino et al., 2003; Sorbjan, 2004).

For other (passive) scalars, however, the entrainment flux $\overline{w's'}_e$ is determined by the mean gradient of the scalar in the interfacial layer around z_i (or the magnitude of the scalar concentration jump) and the strength of the penetrative convection. The scalar entrainment flux is *not* coupled to the scalar *surface* flux, and therefore can have any value or sign and can dominate over the influence of the surface flux on scalar statistics. Examples of the ABL in which the statistics of scalars (e.g., water vapour, CO_2 and reactive species) are mainly determined by the entrainment process can be found in e.g., Druilhet et al. (1983), Sorbjan (1991), Michels and Jochum (1995), De Arellano et al. (2004) and Jonker et al. (2004).

In this paper we will develop a *scalar scale* that can be used to normalise observed or modelled profiles of scalar statistics (particularly variances) for arbitrary entrainment regimes. Note that it is not our intention to derive new universal *profiles* for scalar variances as was done by Sorbjan (1988, 1990), for example. The analysis is restricted to the cloudless boundary layer.

In the next section we first discuss the entrainment regimes as they are observed for moisture and we will discuss the shortcomings of classic ML scaling when applied to scalar variances for which the entrainment flux dominates. Subsequently, we define the requirements for a new scalar scale, we discuss existing scales that might be useful and we develop a new scale: the generalised mixed-layer scale. All scales mentioned in Section 2 are tested in Section 4 according to a method described in Section 3. In Section 5 the features of the generalised mixed-layer scale will be discussed further. Finally, the most important conclusions are summarised.

2. Theory

2.1. Entrainment regimes

The relative importance of the entrainment flux can be expressed by the entrainment ratio, defined for a scalar s as:

$$R_s = \frac{\overline{w's'}_e}{\overline{w's'}_s}. \tag{1}$$

Mahrt (1991) distinguishes two types of prototype ABL, based on the entrainment flux ratio of humidity (which is generally positive). If the entrainment ratio of humidity is less than one, humidity is increasing and one has a moistening boundary layer (MBL); humidity transport is dominated by surface evaporation. On the other hand, if R_q is greater than 1, the ABL is drying: we term this an entrainment-drying boundary layer (EDBL), where the entrainment process drives the humidity transport.

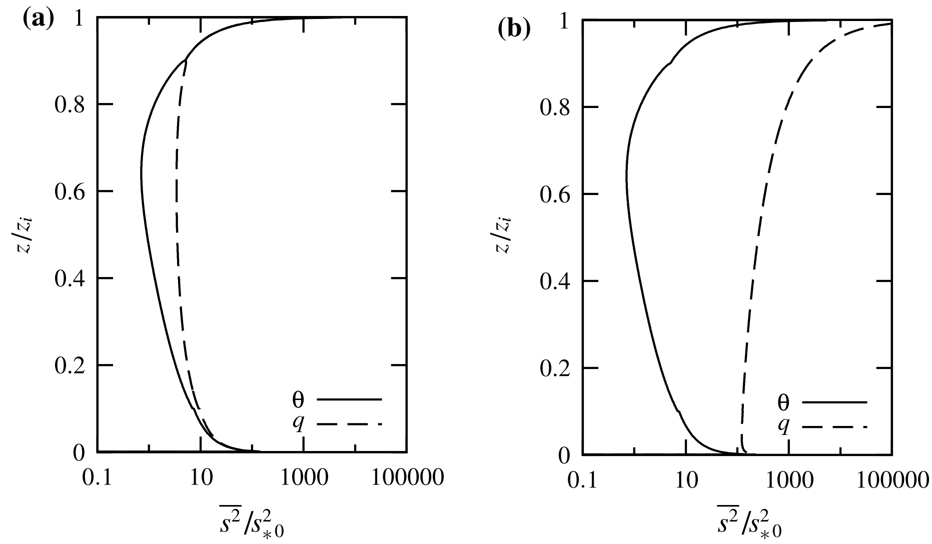

Figure 1. Scaled variance profiles for temperature and specific humidity as derived from the profiles of Moeng and Wyngaard (1989) (see also Appendix A) for a moistening ABL (left, $R_\theta = -0.2$, $R_q = 0.2$) and an entrainment drying ABL (right, $R_\theta = -0.2$, $R_q = 5$). The variances have been scaled with their respective mixed layer scales θ_* and q_*.

Mahrt's classification can be generalised for other scalars, making a distinction between a *surface-flux dominated* scalar regime (with small $|R_s|$) and an *entrainment-flux dominated* scalar regime (large $|R_s|$).

To illustrate the problem of scaling variance profiles in the ABL with contrasting entrainment regimes, we use the similarity profiles of Moeng and Wyngaard (1989) (further referred to as MW89), which they derived from large-eddy simulations (LES) of a convective ABL including a non-zero mean wind. Figure 1 shows the variance profiles of temperature and humidity for both a MBL and an EDBL, normalised with their ML scales. The shortcomings of the ML scaling for the EDBL are clear. First, the scaled humidity variance is orders of magnitude larger than one, which violates the requirement that a scaled variance should be of order 1 (see the Introduction). Second, the scaled humidity variance profiles are not of similar magnitude for the two types of prototype ABL at any height. In the EDBL, entrainment dominates; thus one would require that the scaled variance is similar to that in the MBL at the top of the ABL (where entrainment is relevant as well, but not dominating). Finally, the scaled variance profiles of temperature and humidity show no inter-scalar similarity at any height within the EDBL (whereas they do in the MBL). Figure 2, showing the profile of the correlation coefficient between both scalars, indicates however that there is a large (negative) correlation between temperature and humidity at the top of the ABL. Thus, as in the MBL, the EDBL

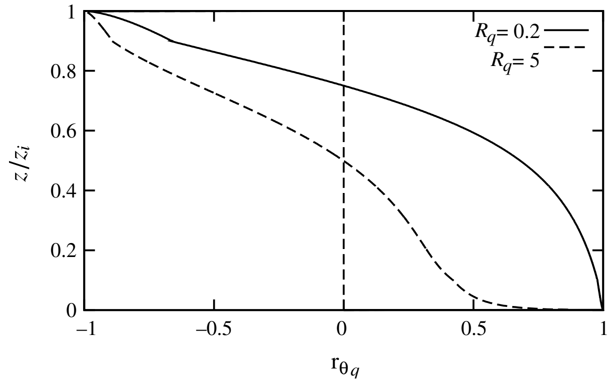

Figure 2. Comparison of correlation between θ and q for two entrainment regimes. as derived from the profiles of MW89. The entrainment ratio for heat is taken equal to -0.2.

profiles of the θ and q variances are expected to show similarity around $z/z_i = 1$.

2.2. Requirements for the generalised scalar scale

Above it was shown that for a CBL with varying entrainment regimes an alternative scalar scale is needed. Here the requirements for this new scale are developed.

First we look at the scalar scale that would be applicable for the limit of pure top-down transport. The *entrainment scalar scale* is defined as:

$$s_{*e} = \frac{\overline{w's'}_e}{w_*}. \tag{2}$$

This scale was used by MW89 to scale their top-down variances and by Druilhet et al. (1983) to scale aircraft data of humidity variances. In the same way as s_* is only suited for scaling scalar statistics in a surface-flux dominated ABL, s_{*e} is only suited for situations where the entrainment flux dominates. Therefore, neither s_*, nor s_{*e} is applicable to a wide range of entrainment regimes.

An alternative scale, valid for any entrainment ratio, should be consistent with ML scaling in the limit of pure bottom-up transport and with entrainment scaling for top-down fluxes. Another requirement for the scale is that it never becomes zero (since we use the scale to non-dimensionalise scalar quantities by *division*). Furthermore, when starting from pure bottom-up transport (zero entrainment flux) the addition of any entrainment flux (positive or negative) will enhance scalar fluctuations in (the top of) the ABL. Therefore both positive and negative entrainment fluxes have to increase the value of the scalar scale. Thus, the ML scale will be the minimum value of the scale.

Summarising, the new scalar scale should meet the following requirements:

1. The scalar scale exists and is non-zero, independent of the entrainment regime of the scalar.
2. For pure bottom-up transport the scale reduces (in order of magnitude) to the mixed-layer scale, and for pure top-down transport it reduces to the entrainment scale.
3. Any entrainment flux (positive or negative) increases the value of the scalar scale, as compared to pure bottom-up transport.
4. Scaled scalar fluctuations show (self-)similarity, when subject to the same processes.

Note, that if requirements 2 and 3 are fulfilled, requirement 1 is fulfilled as well.

A potentially useful scale that meets some of these requirements is the bulk scale of Cuijpers and Holltslag (1998), s_{*b}. Whereas Cuijpers and Holtslag used their scale for scaling flux budget terms, it might be considered as an alternative scalar scale for the entraining ABL. In order to retain the connection with s_* and s_{*e}, we use the ML definition of w_*, rather than Deardorff's bulk velocity scale used by Cuijpers and Holtslag. This gives:

$$s_{*b} = \frac{1}{z_i w_*} \int_0^{z_i} \overline{ws}(z) dz. \tag{3}$$

Since flux profiles in the quasi-steady ABL are linear profiles, ranging from surface flux to entrainment flux, the formulation for s_{*b} can be rewritten:

$$s_{*b} = \frac{1}{w_*} \frac{(\overline{w's'}_e + \overline{w's'}_s)}{2} = \frac{1}{2}(s_* + s_{*e}). \tag{4}$$

When checking this scale against requirements 1–3, a major disadvantage of this scale (for variance scaling purposes) becomes clear: requirement 3 is not fulfilled, since in the presence of an oppositely-signed entrainment flux the bulk scale is reduced rather than enhanced. In the case of $R_s = -1$ the scale becomes zero, creating a singularity in scaled fluctuations.

2.3. Generalised mixed-layer scale

Since the 'existing' scales (s_*, s_{*e} and s_{*b}) do not meet all requirements for an alternative scalar scale, we propose a new scale: the generalised mixed-layer scale, s_{*c}. Based on requirements 1–3 (see Section 2.2) we define s_{*c} as a (linear) combination of ${s_*}^2$ and ${s_{*e}}^2$:

$$s_{*c}{}^2 \equiv a s_*{}^2 + c s_{*e}{}^2, \tag{5}$$

where a and c are constants with a yet undefined value. In Appendix A the heuristic derivation of this generalised mixed-layer scale is elaborated, and the values of a and c are determined. The derivation is based on the requirement that s_{*c} should be of the order of the variance at that location in the mixed layer where the source of the variance is located: at the bottom for bottom-up transport and at the top for top-down transport. The values of the constants are based on the variance profiles given by MW89 for separate top-down and bottom-up transport (see Appendix A). It is found that the constant c has a value of order 10 and a has been set to 1 to meet requirement 2 (see Section 2.2). This results in:

$$s_{*c} = \sqrt{s_*{}^2 + 10 s_{*e}{}^2} = s_* \sqrt{1 + 10 R_s{}^2}. \tag{6}$$

In the new generalised mixed-layer scale the effect of the entrainment flux is amplified by a constant factor, c. A more detailed comment on the accuracy of this factor and its interpretation can be found in Appendix A.

The generalised mixed-layer scale obeys requirements 1 and 3. Requirement 2 is nearly fulfilled, except that for pure top-down transport the scale becomes $\sqrt{10} s_{*e}$ instead of s_{*e}. As for the other scales, requirement 4 will be tested in Section 4.

3. Method of Comparison

Here we describe briefly the means by which the skill of the scalar scales (s_*, s_{*e}, s_{*b} and s_{*c}) is assessed. The test will mainly examine the performance of the scales with respect to requirement 4: scaled scalar fluctuations should show (self-)similarity, for situations where the same processes dominate. Thus scalar variance profiles should be similar in the bottom part of the ABL (say $z/z_i = 0.1$) when the scalar regime is dominated by the surface flux of the scalar. When the entrainment flux dominates, the variance profiles should be similar near the top of the ABL (say $z/z_i = 0.9$).

In order to have a wide variety of test cases, scalar variance profiles were generated using the variance profiles given by MW89 (see Appendix A) with a variety of entrainment ratios. Two main groups of ABL can be distinguished. The surface-flux dominated ABL with $R_s = \pm 0.2$ and $R_s = \pm 0.01$ (nearly pure bottom-up transport). The scaled variances for these cases will be compared at $z/z_i = 0.1$. The second category is the entrainment-flux dominated ABL, with values for R_s of ± 1, ± 5 and ± 100 (nearly pure top-down transport). For these, such an ABL similarity is required at

$z/z_i = 0.9$. We add the case R_s of ± 0.2 to this category, to serve as a reference that is present in both categories. In that way we can check whether scaled variances are of similar magnitude in the upper and lower parts of the ABL when both surface processes *and* entrainment are relevant.

As stated before, scaled variables should be identical when and where the dominating processes are identical. The operational definition we will use here for 'identical' is 'identical (within an order of magnitude)': the scaled variance for a given entrainment ratio should be between 0.2 and 5 times the scaled variance for $R_s = -0.2$.

4. Results

Figure 3 shows the variance profiles for a variety of entrainment ratios, in each figure scaled with a different scale. From these figures, the shortcomings of each of the scales become clear.

The mixed-layer scale s_* (Figure 3a) leads to very large values of the scaled variance for $|R_s| > 1$, both at the bottom and at the top of the ABL. The similarity between the profiles for the entrainment dominated ABL is not apparent. For the profiles scaled with the entrainment scale s_{*e} (Figure 3b) the situation is reversed. In the entrainment zone the profiles are similar, but at the surface the profiles diverge. For $|R_s| = 0.01$, the variance profile is even dissimilar to the others at the the *top* of the ABL.

The variance profiles scaled with the bulk scale s_{*b} (Figure 3c) show a smaller range in values (about two orders of magnitude) than the profiles scaled with s_* and s_{*e}. This is due to the fact that the scale contains information both from the bottom and from the top of the ABL. The line for $R_s = -1$ is missing from the figure, since the scale equals zero for that value. Another shortcoming is that there seems to be no similarity between any of the profiles, neither for the ABL driven by the surface flux, nor for that driven by entrainment.

Figure 3d shows the profiles scaled with s_{*c}. The range in values is about two orders of magnitude smaller than those in Figure 3c, and it is evident that the ABL with $|R_s| \geq 1$ is similar at the top of the boundary layer, whereas that with $|R_s| \leq 0.2$ is similar near the bottom.

In Section 2 we required that 'Scaled scalar fluctuations show (self-) similarity, when subject to the same processes'. In order to judge the skill of each of the scales, the scaled variances are compared at the top of the ABL for the entrainment dominated ABL, and at the bottom for the surface-flux dominated the ABL (Table I). From this table we conclude that only one scale shows some or good similarity at the relevant heights for the entire range of entrainment ratios, viz. s_{*c}. The other scales only work well either in the surface flux dominated ABL, or in the entrainment dominated ABL.

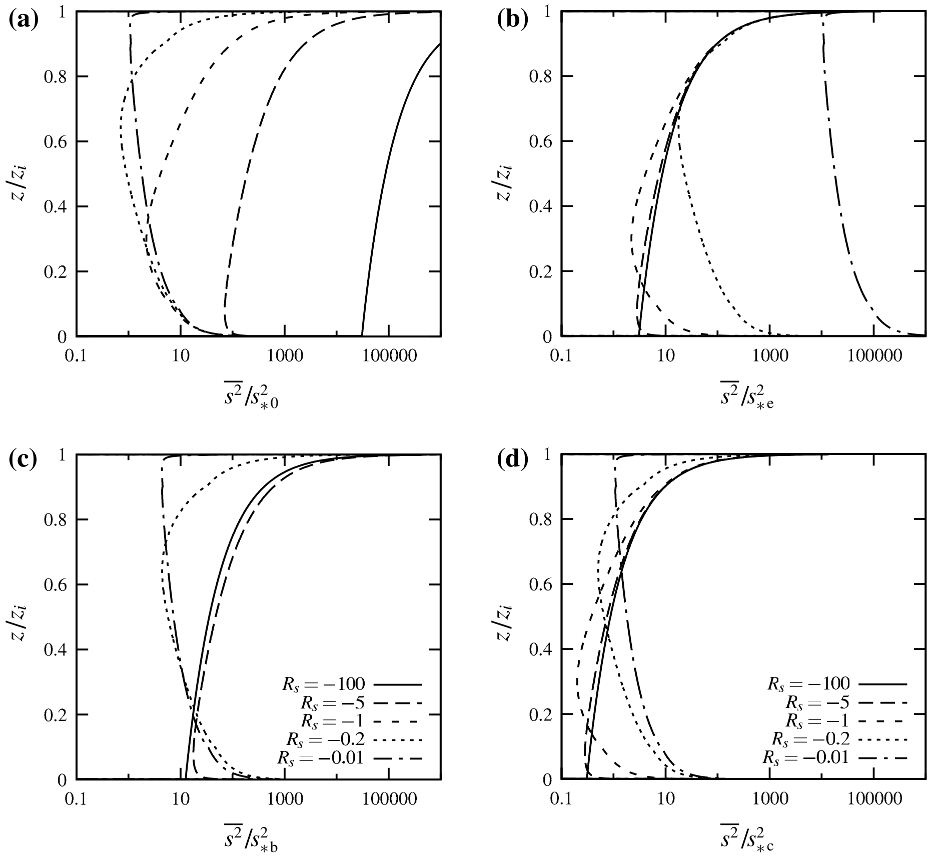

Figure 3. Variance profiles for a range of entrainment ratios R_s, scaled with various scaling parameters: s_* (top left), s_{*e} (top right), s_{*b} (bottom left) and s_{*c} (bottom right). Profiles are shown only for negative entrainment ratios. The profiles for the corresponding positive R_s are similar, though not identical.

Combination of the findings of Sections 2.2, 2.3 and 4 yields the total skill of the scales with respect to the four requirements put forward in Section 2.2. A summary of this skill is given in Table II. From this table we conclude that only s_{*c} gives a positive score on all four requirements. The bulk scale s_{*b} can be regarded as second best, with positive scores on some of the requirements.

We return to the anomalous scaling shown in Figure 1, and if we replot those variance profiles, non-dimensionlised with s_{*c}, we obtain Figure 4. From Figure 4 we can identify those regions where temperature and humidity behave similarly. In the MBL temperature and humidity are similar throughout the ABL, whereas for the EDBL both scalars are of similar magnitude only in the upper part of the ABL.

TABLE I

Scaled variances for the entrainment dominated ABL at $z/z_i = 0.9$ ('top') and for the surface flux dominated ABL at $z/z_i = 0.1$ ('bottom'). The judgement is based on the comparison of scaled variances for different entrainment ratios: values should be as constant and close to 1 as possible.

$\frac{z}{z_i}$	R_s	$\overline{s^2}/s_*{}^2$	$\overline{s^2}/s_{*e}{}^2$	$\overline{s^2}/s_{*b}{}^2$	$\overline{s^2}/s_{*c}{}^2$
0.9	−100	9.8×10^5	98	400	9.8
	−5	2.5×10^3	98	6.1×10^5	9.8
	−1	99	99	–	9.0
	−0.2	5.0	125	31	3.6
	0.2	5.0	125	14	3.6
	1	99	99	99	9.0
	5	2.5×10^3	98	272	9.8
	100	9.8×10^5	98	384	9.8
0.1	−0.2	7.0	175	44	5.0
	−0.01	7.9	7.9×10^4	32	7.9
	0.01	8.0	8.0×10^4	31	8.0
	0.2	9.2	230	26	6.6
judgement top		−−	+	−−	++
judgement bottom		++	−−	+	++

TABLE II

Judgement of scales, based on requirements 1–4 (see Section 2.2).

scale	requirement 1	requirement 2	requirement 3	requirement 4	conclusion
s_*	−	−	−	++/−−	−
s_{*e}	−	−	+	++/−−	+/−
s_{*b}	−	+	−	+/−−	+/−
s_{*c}	+	+	++	++	+

5. Discussion

5.1. Applicability

In our study, a new scale has been applied to scalar variances only. But given the close connection with the conventional ML scales, it should be applicable to other statistics as well (e.g. fluxes and skewnesses). Scaling of the scalar fluxes with $w_* s_{*c}$ has the disadvantage that the scaled flux will not be equal to unity either at the surface or at $z = z_i$ (except for $R_s = 0$).

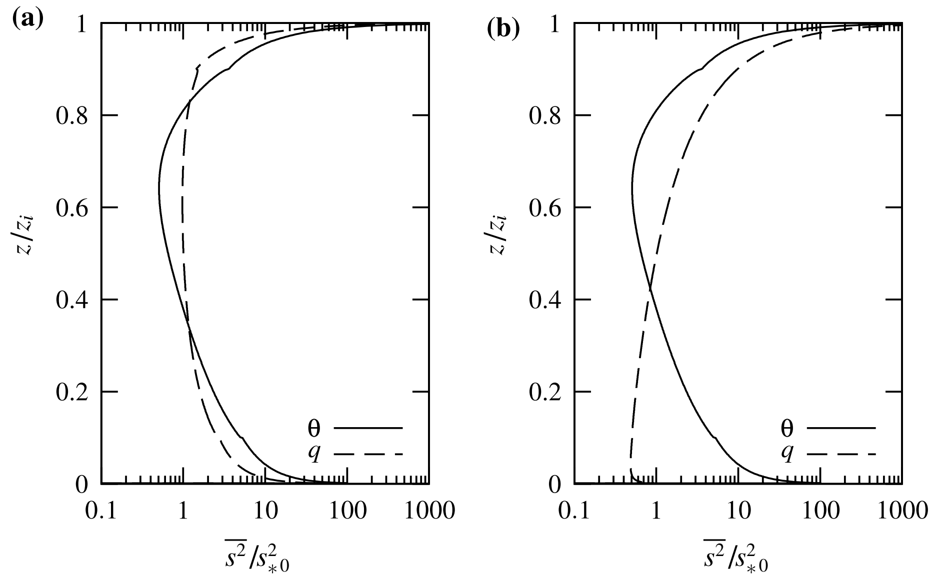

Figure 4. Scaled variance profiles for temperature and specific humidity as derived from LES for a moistening ABL ($R_q = 0.2$, left) and an entrainment drying ABL ($R_q = 5$, right). The variances have been scaled with the generalised mixed-layer scale s_{*c}.

For $|R_s| \to \infty$ the scaled flux will be $(\sqrt{10})^{-1} \approx 0.32$ at $z/z_i = 1$. However, scaling of fluxes with $w_* s_{*c}$ will reveal similarities if they are present (except for the sign).

The advantage of the classical ML scale s_* is that only surface observations and z_i are required to calculate it; the new scale also depends on the entrainment flux, which is not easily determined (even from aircraft data). Another objection may be that the entrainment flux is an internal parameter rather than an external forcing parameter. To circumvent one or both problems one could replace s_{*e} in Equation (5) by another interface scale, for example, the interface scale of Druilhet et al. (1983), based on a zero-order jump model (Garratt, 1992):

$$s_{**} = R_\theta \frac{\Delta s}{\Delta \theta} \theta_* \tag{7}$$

where Δs and $\Delta\theta$ are the jumps at the top of CBL of the scalar concentration and potential temperature, respectively. Both jumps could be considered to be exernal parameters and, although R_θ is an internal parameter, it is rather well-defined. Replacing s_{*e} by (7) in (5) is equivalent to the use of an empirical estimate for the entrainment flux from observed temperature and scalar profiles (e.g., Betts et al., 1990). Even if the observed profiles do not exhibit a clear jump, one could obtain Δs and $\Delta\theta$ by combining the observations with a mixed-layer template: extrapolate the constant mixed-layer concentration upwards, extrapolate the free-atmosphere concentration gradient downwards, and determine the jump from the distance between both lines at $z = z_i$.

Another option to eliminate the entrainment flux from s_{*c} is to use the interfacial scale S_s of Sorbjan (2005) instead of s_{*e}:

$$S_s = g_i w_* / N_i \tag{8}$$

where g_i is the scalar concentration gradient within the interfacial layer and $N_i = \sqrt{\frac{g}{\theta_v}\frac{\partial \theta_v}{\partial z}}$ (i.e., $2\pi \times$ the Brunt-Väisäla frequency). S_s implies a first-order jump model, and the use of S_s would result in $s_{*c}{}^2 = a s_*{}^2 + c' S_s^2$ (compare Equation (10b) in Sorbjan, 2005), where c' may differ from c.

The parameters occuring in (7) and (8) are external to the ABL in the sense that they describe the structure of scalar and temperature profiles above the ABL. However, as in the case of the entrainment flux, Δs, $\Delta\theta$, g_i and N_i are the result of the development of the ABL and cannot be known beforehand (e.g., to provide known forcings for large-eddy simulation).

5.2. Amplification factor for entrainment flux

The value of the amplifying factor c multiplying s_{*e} in s_{*c} is dependent on the choice of the height where we neglect the variance of the bottom-up scalar (now $0.9z_i$) and the variance of the top-down scalar (now $0.1z_i$). In Appendix A the sensitivity of c to those heights is explored. The choice for the levels $z/z_i = 0.1$ and $z/z_i = 0.9$ seems to be a reasonable compromise between, on the one hand, a sufficient distinction between bottom-up variance and top-down variance, and a sufficient invariance to the exact heights of both levels on the other hand.

The origin of the fact that in s_{*c} the entrainment flux part is an order of magnitude more important than the surface flux part is explored in Appendix B. The main conclusion is that for the top-down scalar the production of scalar variance at the top of the ABL is much larger than the production for the bottom-up scalar at the bottom. The scalar variance production is the product of scalar flux and mean scalar gradient so that the production per unit flux is directly proportional to the gradient of the mean scalar concentration. This gradient is generally much larger in the entrainment zone than near the surface. Furthermore, turbulent transport is a gain for the top-down scalar in the upper part of the ABL and a loss for the bottom-up scalar in the lower ABL.

6. Conclusion

Fluctuations of scalars in the atmospheric boundary layer are generated both by the surface flux and by entrainment. For temperature, the entrainment flux ratio is rather constrained, and as a result scaling of the temperature variance profiles with a scaling variable that is based solely on the surface flux (s_*) works well. For other scalars, however, the entrainment ratio can attain a wide range of values and the information contained in a surface-flux-based scaling variable is insufficient. This was shown for the case of humidity variance in an entrainment drying ABL.

In order to reveal possible similarity in scalar variance profiles a scale is needed that takes into account both the contribution of the surface flux and the entrainment flux. For scalars that are dominated by entrainment, scaling with a scale based on the entrainment flux works well. But for the more general case both fluxes should be taken into account. The bulk scale of Cuijpers and Holtslag (1998) does this, but this scale is not well-behaved for large negative entrainment ratios and for entrainment ratios equal to -1.

We propose an alternative scale, derived on the basis of the LES results of MW89. The scale is derived under the constraint that scalar variance profiles should show similarity at those heights where the variance producing mechanism are identical. If variance is mainly produced by entrainment, scaled variances should be similar at the top of ABL, whereas if the main production is due to the surface flux, the scaled scalar profile should be similar close to the ground. Furthermore, it takes into account that the production of variance by the entrainment flux is an order of magnitude larger than the production of variance by the surface flux (per unit flux). Other desirable features of the new scale are that it is always positive and that scaled variances are always of order 1–10.

With respect to practical applicability it might be problematic that the entrainment flux is more difficult to determine than the surface flux (used in s_*). This problem, however, can be circumvented by estimation of the entrainment flux from observed temperature and scalar profiles, or by replacement of the entrainment scale s_{*e} by the interfacial scale S_s.

Appendix A. Derivation of the Generalised Mixed-Layer Scale

Moeng and Wyngaard (1989) (further referred to as MW89) studied the behaviour of statistics of scalars in a CBL (including a mean horizontal wind). They distinguished between scalars with the source or sink at the bottom of the ABL (bottom-up) and at the top of the ABL (top-down), following Wyngaard and Brost (1984). Any scalar can be regarded as a linear combination of a scalar with pure top-down transport (t) and a scalar with pure bottom-up transport (b). MW89 developed the following general formulation for scalar variance profiles, using ML scaling and depending on the entrainment flux ratio of the scalar (R_s) and z/z_i:

$$\frac{\overline{s^2}}{{s_*}^2} = f_b\left(\frac{z}{z_i}\right) + 2R_s f_{tb}\left(\frac{z}{z_i}\right) + {R_s}^2 f_t\left(\frac{z}{z_i}\right), \tag{A1}$$

with f_t and f_b as given by MW89 and f_{tb} was derived from their Figure 12c ($f_{tb} = (f_t f_b)^{1/2} 1.8\left(\frac{z}{z_i}\left(0.9 - \frac{z}{z_i}\right)\right)^{1/2}$ for $z/z_i \leq 0.9$ and zero otherwise).

Since our new scale should be of the same order as the scalar variance, we use Equation (A1) to form the new scale (where the entrainment ratio has been eliminated):

$${s_{*c}}^2 = a{s_*}^2 + b s_* s_{*e} + c{s_{*e}}^2, \tag{A2}$$

where a, b and c are coefficients yet to be determined. We require that s_{*c} should be of the order of the variance at that location in the mixed layer where the source of the variance is located: at the bottom for bottom-up transport and at the top for top-down transport. Since the quality of LES results becomes questionable close to the surface and the functions in Equation (A1) degenerate close to the entrainment zone, the relevant heights were chosen to be $z/z_i = 0.1$ and $z/z_i = 0.9$, respectively.

The limit of pure bottom-up transport yields $a = f_b(0.1)$, the limit of pure top-down transport gives $c = f_t(0.9)$, and both limits leave b undetermined. We set $b = 0$. In Section 2.2 we pose the extra requirement that the new scale should reduce to s_* for pure bottom-up transport. Therefore, both a and b are divided by $f_b(0.1)$, giving $a = 1$, $b = 0$ and $c = f_t(0.9)/f_b(0.1)$.

Based on the functions of MW89, the value of c is 12 (between 11.7 and 12.3, depending on the expressions for used for f_b), whereas the profiles of Moeng and Wyngaard (1984) give 8.0 (see Figure A1a). Based on the uncertainty in c, its value is fixed to 10, which should be read as 'of the order of 10'. This results in the definition of the generalised mixed-layer scale given in Equation (6).

Sorbjan (1990) made a different distinction than MW89: he distinguished between non-penetrative convection and a residual (total minus non-penetrative). In his profiles, the variance of a passive scalar due to the penetrative part is dependent on the entrainment heat flux (and thus on R_θ). Then c can be defined as the ratio of the variance due to the penetrative part at $z/z_i = 0.9$ to the variance due to the non-penetrative part at $z/z_i = 0.1$. For $R_\theta = -0.2$ this results in a value of 10.0 when the thickness of the interfacial layer at the top of the ABL is ignored.

The MW89 profiles were derived for a given combination of scalar gradient, shear and stratification in the entrainment layer. In fixing the

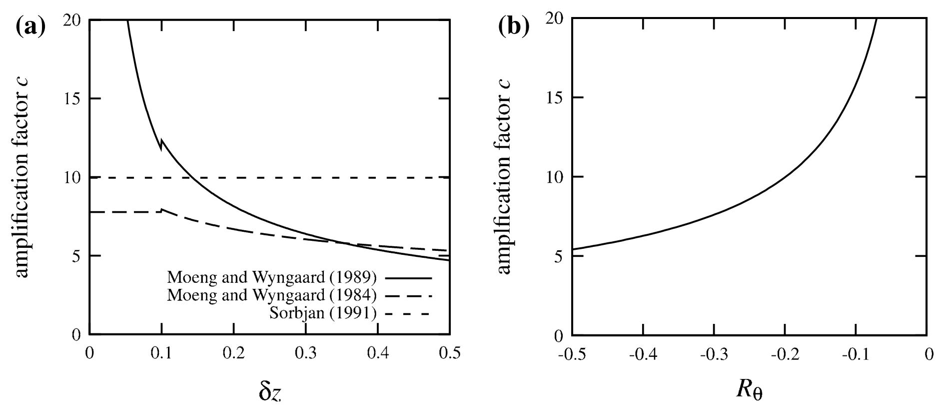

Figure A1. (a): Dependence of the amplification factor c for the entrainment scale on the height at which the factor is evaluated: δz is the distance (in units of z_i from either the surface (for f_b) or z_i (for f_t)). c was evaluated from the results of MW89 and Moeng and Wyngaard (1984), as well as the profiles of Sorbjan (1991) (with $R_\theta = -0.2$). (b): Dependence of c on R_θ as derived from the profiles of Sorbjan, ignoring the thickness of the interfacial layer.

value of c to a single value, we implicitly assume that those profiles are valid for other conditions in the interfacial layer as well. To assume that $\frac{\sigma_s}{s_{*e}}$ at the top of the ABL is independent of stratification, shear and convection, implies that $\frac{w_*}{r_{ws}\sigma_w}$ is independent of those parameters. The results of Sorbjan (2004) show that $\frac{\sigma_w}{w_*}$ in the interfacial layer does depend on the interfacial Richardson number, and thus c should depend on it as well. On the other hand, the effect of the interfacial scalar gradient does not influence the scalar variance (when scaled with s_{*e}, see Equations (19) and (20) in Sorbjan, 2004).

Another point of discussion may be the height at which the scalar profiles are evaluated to determine the value of c. Figure A1a shows that c is quite sensitive to that choice (at least for the MW89 results) and that c degenerates when the reference levels is taken too close to the top and bottom of the mixed layer. The value of c derived from the profiles of Sorbjan appears to be *independent* of the choice of the reference level. On the other hand, his profiles make the value of c dependent on the entrainment ratio of temperature (Figure A1b).

Appendix B. Origin of Large Variances Related to Entrainment Flux

In the previous section it was found that scalar variance related to the entrainment flux is an order of magnitude larger than the variance related to the surface flux. To investigate the origin of this difference, we start with

TABLE B1

Estimates of the scalar variance at $z/z_i = 0.9$ for a top-down scalar, and at $z/z_i = 0.1$ for a bottom-up scalar. Estimates based on a simplified budget Equation (B3) in combination with the LES results of MW89.

		parts of variance budget			resulting variance	
regime	height	τ_D	$-2\overline{w's'}\frac{\partial \overline{s}}{\partial z}$	$-\frac{\partial}{\partial z}\overline{w's'^2}$	$\overline{s'^2}$	$\frac{\overline{s'^2}}{s_*^2}$
top-down	$\frac{z}{z_i} = 0.9$	$0.4\frac{z_i}{w_*}$	$180\frac{\overline{w's'}_e^2}{w_* z_i}$	$25\frac{\overline{w's'}_e^2}{w_* z_i}$	$82\frac{\overline{w's'}_e^2}{w_*^2}$	$82{R_s}^2$
bottom-up	$\frac{z}{z_i} = 0.1$	$0.4\frac{z_i}{w_*}$	$36\frac{\overline{w's'}_s^2}{w_* z_i}$	$-14\frac{\overline{w's'}_s^2}{w_* z_i}$	$9\frac{\overline{w's'}_s^2}{w_*^2}$	9

the variance budget equation for a horizontally homogeneous flow:

$$\frac{D\overline{s'^2}}{Dt} = -2\overline{w's'}\frac{\partial \overline{s}}{\partial z} - \frac{\partial}{\partial z}\overline{w's'^2} - \chi \ , \tag{B1}$$

where the four terms signify the total rate of change, production, divergence of turbulent transport and dissipation.

First we assume a steady state and we replace the dissipation term by the following parametrisation:

$$\chi = \frac{\overline{s'^2}}{\tau_D} \ , \tag{B2}$$

where τ_D is a dissipation time scale.

The latter is a fair approximation near the surface and the top of the ABL. Combination of Equations (B1) and (B2) yields an explicit expression for the variance:

$$\overline{s'^2} = \tau_D \left\{ -2\overline{w's'}\frac{\partial \overline{s}}{\partial z} - \frac{\partial}{\partial z}\overline{w's'^2} \right\} . \tag{B3}$$

Next the production and transport terms are replaced by values derived from the results of MW89. For the production term, the results from their Figure 11 for $\frac{\partial \overline{s}}{\partial z}$ is used (the LES results, not the linear fits to the data) in combination with a linear flux profile. The turbulent transport term can be deduced from Figure 14 of MW89, for top-down and bottom-up transport separately. Finally, the dissipation time scale can be found in Figure 22 of MW89.

For the top-down scalar, the terms are evaluated at $\frac{z}{z_i} = 0.9$ whereas for the bottom-up scalar the level $\frac{z}{z_i} = 0.1$ is used. The resulting values can be found in Table B1. This crude approach indeed predicts that the entrainment flux generates an order of magnitude more scalar variance than the surface flux and thus corroborates the profiles in Equation (A1) and the resulting generalised mixed-layer scale (see Equation (6)). From Table B1 the mechanisms behind this asymmetry become clear,

- For the top-down scalar, the production is five times larger than for the bottom-up scalar. This is due to the fact that for the top-down scalar the entrainment flux is paired with a large gradient of the scalar in the upper part of the ABL. This combination gives rise to a high variance production per unit scalar flux. On the other hand, at the bottom of the BL (above the surface layer), the mean scalar gradient is smaller.
- For the top-down variance, the turbulent transport term is an extra gain term: variance produced elsewhere (in the entrainment zone) is transported downward. For the bottom-up scalar the turbulent diffusion is a loss term: variance existing locally is transported away.

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