Geosci. Model Dev. Discuss.

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Title: Large-eddy simulation and stochastic modelling of Lagrangian particles

for footprint determination in stable boundary layer

Summary Evaluation

Originality: Good
Technical quality: Good
Clarity of presentation: Fair
Practical significance: Good

Recommendation: Major Revisions – I would like to review the revised manuscript

General Comments

In this paper, Large-Eddy Simulation (LES) is used in order to determine flux footprint functions in a stable boundary layer for three different sensor heights. One individual case has been investigated and from this quite general conclusions are drawn. Results are compared to those from existing footprint models based on Lagrangian stochastic particle dispersion modelling, LPDM (in different sophistication) and a scaling-based footprint parameterisation applicable for a wide range of stability and receptor heights. It is concluded that the recovery of small-scale (sub-filter scale) turbulent motions and hence the spatial scale is relevant for the quality of the LES results and that Kolmogorov's constant for the Lagrangian structure function in the inertial subrange (C₀) has a strong impact on the footprints from LPDMs.

As the LES is treated as 'truth' (reference), a much more substantial discussion of the LES quality must be provided (major comment 1). Given sufficient information on this matter, the LES results for footprints in stable conditions could be used as a basis for fitting footprint parameterisations. Such data are very much welcomed. However, for a statistically relevant data set, not only one single simulation, but several simulations for a broader range of stable conditions would be necessary. It would be great to see such data being made available. Also, it seems that some ad hoc assumptions (e.g., 'absorption condition', normalisation) are employed, which need further explanation and consideration (major comments 2 and 3). The results concerning Kolmogorov's constant for the structure function in the Inertial Subrange are probably somewhat overstated (major comment 4). Finally, when comparing to other models, it appears that the authors have not correctly reproduced one of these 'other models' (major comment 5).

Before the paper can be recommended for publication in GMD, these major comments and some minor comments must be addressed. It is also suggested that the language should be assessed by a native speaker.

Main Comments

(1) Model validation and argumentation of approaches:

All conclusions are based on the inherent assumption that the LES provides the 'truth' – even if quite a number of ad hoc assumptions are being made in order to produce the LES-based footprints. For example:

- corrections of advection speed due to subgrid-scale turbulence (Eq. 36) are applied only in the lowest grid layer [why exactly one?], p. 13, l. 16 and somehow 'implemented' in the lowest three layers, p. 13, l. 20;
- furthermore, this correction is based on using a Langevin type of approach (Eq. 28), which employs a particular value for Kolmogorov's constant for the structure function in the Inertial Subrange [C₀] (which is not specified for this application);
- a further 'correction' is applied (Eqs. 33 and 34) with a somewhat arbitrary coefficient c=0.5, p. 14, l. 3
- particles are released at $z_0 = 0.1$ m, but reflected 'at the ground' (p. 12, l.17). Should this mean z = 0 m? And if so, how are the velocity statistics being evaluated below z_0 ?

All these settings are likely good (or reasonable) choices but should be substantiated. When serving as a reference for footprint calculations, the LES should be validated on a forward dispersion case from the literature. The reasoning for using LES as a reference comes from requiring 'scale invariance', i.e. independence of the results from grid resolution (p. 3, l. 17 – and Figs. 3c, d). This, first of all, is a good criterion in the absence of any true reference – but one would want to see to what degree the above choices influence this independence.

(2) Absorption condition:

Please provide more information on the absorption height and its impact (p. 12, l. 20 ff). I.e., provide a graph or a reference and list the tests undertaken confirming that "...the upper boundary condition does not have a large impact on the results of calculations of footprints...".

It seems that particles are absorbed at the absorption height and hence removed from the simulation domain. Figure 2 suggests that there is no vertical flux above the absorption height. However, turbulent fluxes should decline almost linearly from their surface value upwards to approach zero at the boundary layer height (i.e. in this case at z = 180 m and not at z = 100 m, cf. Stull, 1988 or Beare et al., 2006).

If the particles cannot reach the boundary layer height, they cannot be reflected at this height and cannot return to the surface. The consequence is that footprints consist of upwards flowing particles only. If so, this would result in an unrealistic increase in extent of flux footprints as downward flowing particles would weigh out upward flowing particles (when evaluating the vertical flux), with increasing tendency to do so with increasing distance from the measurement location. Please clarify how this is handled regarding the footprints from the LES.

(3) Normalisation of footprints:

On p. 13, l. 14, it is shown that the integral over the footprint function is normalised to one. Does this include negative footprint values, too? Or are these treated separately as mentioned on p. 15? Please clarify. The absolute values of the footprint function and hence the cumulated footprint will depend on how negative values are treated. Observed differences in the absolute footprint function values for different footprint approaches (cf. Fig. 11) may be partly due to differences in normalisation procedures.

Also, is there a threshold value for the distance from the measurement up to where footprint values are considered? The 'flat' trend of the cumulative footprint values suggests that the footprint function would only completely diminish at very large distances from the measurement location. If a threshold value is set, again the selected value will have an impact on the normalisation and the absolute value of the footprint function. Please provide more information on the applied procedure.

(4) Kolmogorov's constant for the structure function in the Inertial Subrange $[C_0]$:

First of all, this constant is referred to as 'Kolmogorov constant', a name that is usually associated with that in the energy spectra in the Inertial Subrange (and has a value of approximately 1.5). The authors discuss the range of proposed values in the literature, and it is felt that i) the paper by Rizza et al. (2010) might be a valuable addition to the discussion of possible values in the PBL and ii) the employed value in the LES subfilter correction (Eqs. 28 ff) should be provided. However, in the present paper it is demonstrated that the results of the LSMs (and in particular LSMT) are sensitive to the choice for C_0 – which is per se not particularly new (see, e.g., Rotach et al. (1996) who have sought the 'optimal' value based on comparison to water tank (dispersion) measurements of Willis and Deardorff – and many others, such as Du et al. (1995), Reynolds (1998), as cited in Rizza et al). If indeed the LES were fully validated and all the choices substantiated (see major comment 1), the present simulations would correspond to 'one more tessera' in the picture of a possible non-universality of C_0 , be it due to stability dependence or employed time scales (outside those corresponding to the Inertial Subrange). It is felt that the conclusions drawn in the present paper (one 'case' – even with three heights) do not warrant the quite general conclusions drawn (p. 21, l. 18), i.e. 'the optimal value is found to be close to 6'.

(5) Footprints plotted in Fig. 11:

The footprints plotted in Fig. 11 of the manuscript and listed as Kljun et al. (2015) do not coincide with FFP model results. Plotted below are footprints derived from FFP for the input values mentioned in the manuscript, and optimised parameters for neutral and stable conditions as listed in Kljun et al. (2015). (Note: using the universal FFP parameters, e.g. from the online footprint tool still results in different footprints than those plotted in Fig. 11). It can be seen in Fig. R1 that the peak location of FFP fits very well the peak of LSMT with C_0 =3 in Fig. 11. Footprint peak values, however, do differ, especially for larger measurement heights. Regarding the absolute values of these peak values please see major concerns (2 and 3) above. Also, the model of Kljun et al. (2004) is outdated; issues in stable conditions were known and were one of the reasons for the update to the model of Kljun et al. (2015).

As FFP compares well with the Lagrangian footprint model it is based on (see Fig. R2), and as different settings of C_0 produce similar shifts in footprints in LPDM-B (Kljun et al. 2002) and the LPDM used in this study (Fig. R2) – the main question boils down to: what is the 'ultimate truth' and what should a footprint parameterisation be based upon? (See comments above.) This is a very important question and I suggest that the authors highlight this fact even more in their manuscript.

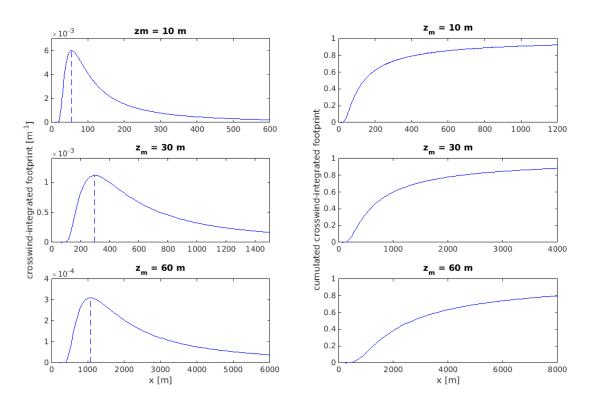


Fig. R1: Crosswind-integrated flux footprints for the three measurement heights as calculated with the parameterisation FFP of Kljun et al. (2015). The footprints are calculated using the FFP code available online at footprint.kljun.net and with the neutral/stable set of parameters.

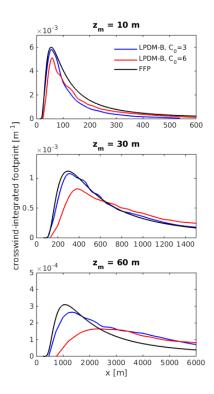


Fig. R2: Crosswind-integrated flux footprints for the three measurement heights as calculated with the parameterisation FFP (black line) of Kljun et al. (2015) and with LPDM-B of Kljun et al. (2002), setting $C_0 = 3$ (blue line) and $C_0 = 6$ (red line).

Minor Comments

- (a) The term "Analytical footprint model" is commonly used for footprint models based on analytical solutions of the diffusion equation by applying a K-theory approach. This is a distinctly different approach than used in the models of Kljun et al. (2004, 2015). The latter models are footprint parameterisations. Please correct throughout the manuscript.
- (b) p. 2, l. 5: '...commonly, the application of these models is limited by the constant flux approximation': this is not true at least for the Kljun et al. papers cited above.
- (c) p. 5, l. 26: If reference is made to 'the lake', this lake must be introduced beforehand. It is not appropriate to explain in brackets that the author apparently works on a 'lake problem'.
- (d) p. 8, l. 15: Euclidean: spelling?
- (e) According to Eq. 2, fys corresponds to the crosswind-integrated footprint. Please use this well-established term rather than 'crosswind averaged footprint' (e.g. p. 14, l. 3 or p. 20, l. 18). Further, in the captions of Figs. 9 and 11, the graphs are referred to as "One-dimensional footprints fys". This would suggest that the footprint at y=0 is plotted. Please clarify.
- (f) Wind profile: from Figure 1, it seems that simulated wind speeds in the surface layer part of the domain are smaller than the 'standard' wind profile for stable conditions (e.g., Stull, 1988; Högström, 1996). Please add a couple of sentences to explain why.

References

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