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Atmospheric Chemistry and Physics Discussions

Interactive comment on "In-canopy gas-phase chemistry during CABINEX 2009: sensitivity of a 1-D canopy model to vertical mixing and isoprene chemistry" *by* A. M. Bryan et al.

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In the following response, the line numbers refer to the lines in the revised manuscript.

1) The authors have added a discussion of non-Fickian diffusion and segregation, as suggested in my earlier review, but on p. 11, l. 7 they say that "Half-hour averaging filters out small-scale intermittent coherent structures (i.e., sweeps and ejections…" I think it is likely that such coherent structures are included in the half-hour averages. A better explanation might be that these coherent structures, that can extend throughout the PBL, are responsible for asymmetric transport that is not captured by the simple parameterizations used here.

We agree with the reviewer that coherent structures are included in half-hour averages, contrary to our statement in the original manuscript. We also agree that asymmetric transport is what model parameterizations cannot capture; however, due to restructuring and revisions in Sect. 2.2.1, we have moved this statement to the conclusions (lines 705–707).

2) p. 5, l. 14: Turbulence in the PBL occurs over a range of scales from mesoscale to sub-grid scales. In a 1-D model, as used here, all the turbulence is parameterized. This is not true of 3-D mesoscale or large eddy simulation models.

We have revised this sentence to address more accurately the range of turbulent treatment in models (lines 60–62).

3) p.5, l. 22: …due to the existence of intermittent coherent structures that encompass the entire depth of the canopy.

We have revised this sentence in accordance with the reviewer's suggestion (lines 68–69).

4) p. 6, l.4: The sentence, "Therefore, most models have…" seems to fit better preceding the sentence, "Large-eddy simulation models. . ." I also wonder whether it is really the case that LES lacks sufficiently detailed chemistry to capture the features... Is it possible that LES can do the job if the "right" set of reactions, even if abbreviated, could do an adequate job? I'm not enough of a chemist to answer that, but what is the evidence? I also know that LES practitioners are approaching the chemical complexity given on p. 7 for the RACM. It seems to me that the biggest advantage of the approach here over LES is the much lower resource requirements.

We have revised the sentence order as suggested by the reviewer (lines 73–75). Additionally, we have revised the LES discussion to account for recent enhancements to chemical mechanisms coupled with LES models (lines 78–81). While there are many advances on this front, coupled chemistry-LES models still require development to capture the BVOC oxidation discussed in this manuscript.

5) p. 6, l. 28: . . .suggest an unknown BVOC source,. . .

We have removed the word "potential," as suggested (line 97).

6) p. 8, l. 6: . . .which may reduce BVOC emissions and photochemical activity?

We have revised this text in accordance with the suggestion (lines 126–127).

7) p. 9, l. 7, eq. (1): You should use potential temperature instead of temperature and mixing ratio instead of "mass". It is the potential temperature gradient and mixing gradient that are relevant.

We have revised Eq. (1) and the term definitions according to the reviewer's suggestion (lines 152–154). We also added the subscript i to denote the different chemical species.

8) p. 10, l. 10: For completeness, perhaps you should include the stability dependence expressions for f.

We have substantially revised this section to include the full set of parameterized equations for the stability dependence (lines 191–192), the mixing length l (lines 184–188) and the wind profile used in the vertical wind shear calculation (lines 188–191).

9) p. 10, l. 15: In the micrometeorological literature, the asterisk in u_* is written as a subscript rather than a superscript.

We have corrected this throughout the manuscript.

10) p. 11, l. 4: The term on the right side of (7) should be raised to the 1/4 power.

We thank the reviewer for bringing this error to our attention, and we have revised it in the text (line 203).

11) p. 12, l. 2: How sensitive are the results to this assumed height scale? That is, if you change the maximum mixing height from, say 1 km to 2 km, or to 500 m, how much does this change the results? Presumably the height varies as a function of time

of day.

The maximum mixing height is not a prescribed input parameter that "caps" mixing at a specified height, as the original manuscript suggests. CACHE computes mixing strength and height as a function of daytime instability, which varies by the extent of surface heating. The typical mid-range mixing height reaches a daily maximum of approximately 1 km, but this height can vary under stronger surface heating (e.g. up to 1.5 km) or cloudy conditions (approximate mixing height of < 500 m). We have rephrased the sentence for clarity (lines 405–407).

12) p. 17, l. 9: Where does "measured" K_H" come from? is it from (5) or from (6)? Actually, in either case it is "K_H estimated from measurements. . ." Similarly in Figure 1, where do the "measured" and "modeled" K_H values come from? What is measured and what is modeled? Equation (6) is not K_H. It is an estimate of K_H obtained from measurements. You have no way of measuring K_H unless you have measurements of a flux and a gradient of a scalar.

We have revised the text in a several places to clarify this issue. First, we have rewritten the description of modeled turbulent transport (Sect. 2.2.1, lines 174–215) to provide the specific equations (Eqs. 5–11) and a detailed explanation of the differences between "measured" and "modeled" KH. Second, we distinguish between the modeled (KH,mod, Eq. 5) and "observed" (KH,obs, Eq. 8) eddy diffusivities throughout the manuscript. To clarify that KH,obs is an estimate of observed KH rather than a direct measurement, we replaced all instances of "observed KH" or "measured KH" with "KH,obs" throughout the revised manuscript. Third, we re-organized the paragraph structure in the evaluation of turbulent exchange (Sect. 3.1, lines 352–411) to distinguish the BASE and MIX turbulence schemes and clarified the equations used in each simulation. Finally, we revised Fig. 2 (Fig. 1 in the original manuscript) and its caption to include the new subscripts and equation numbers.

13) p. 18, l. 7: Why does "missing turbulence" have to be coherent structures or

counter-gradient terms? I don't see that there is a direct connection.

We attribute the discrepancies in model-measurement exchange to the known limitations of the model parameterization, including intermittent processes such as coherent structures that have been observed at the site during the campaign (e.g., Steiner et al., 2011). However, we acknowledge the reviewer's point that there could be many factors that contribute to the missing turbulence. Please see our revised sentence (lines 378–380).

14) p. 20, l. 28: Why should there be more subsidence at the end of the day? Subsidence is driven by large-scale processes. I have never heard of such a hypothesis. Couldn't the increase be due to the decreased mixing and shallower boundary-layer depth in the late afternoon and early evening?

We agree with the reviewer that use of the term "subsidence" does not accurately depict how recent studies (e.g., Barkley et al., 2011) explain the end-of-day buildup of isoprene. We have rephrased this sentence per the reviewer's suggestion (lines 476–477).

15) p. 21, l. 22: Figure 5 is referenced before Figure 4, I think.

Figure 4 (Fig. 6 in the revised manuscript) is referenced on p. 20, l. 15 in the original manuscript, prior to Fig. 5 (now Fig. 7).

16) p. 21, l. 29: . . .making it difficult to. . .

We have revised this sentence (line 503).

17) p. 28, l. 24: ". . .leading to an overly-strong diurnal cycle of ozone, and an overestimate of NOx, BVOC and their oxidation products. . ."

We have revised this sentence according to the reviewer's suggestions (line 694).

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 12801, 2012.