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## ***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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The paper presents a study on the application of a 1-D canopy-atmosphere exchange modeling system with a focus on the significance of a proper representation of turbulent transport in the exchanges of BVOCs and its oxidation products and the impact on the oxidizing capacity. The paper addresses a highly relevant topic also informing the atmospheric chemistry and atmosphere-biosphere exchanges community on an proper consideration of turbulent transport commonly being represented in a rather simplified way in chemistry studies which rely on these kind of the models. As such the paper fits in well with the scope of ACP. The paper is well written, sometimes does include a

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lot detail but which is then overcome by providing some short summary at the end of the sections. The main issue that really deserves more attention in this ms is the role of surface deposition in potentially explaining some of the discrepancies between the simulated and observed oxidation products that are now partly attributed to potential issues on the other processes (see also comments below).

Line 234: “Measured NO<sub>2</sub>, HCHO, and MACR concentrations are used to tune advection rates for the model scenario that incorporates both nudged turbulence and RACM-MIM chemistry”. Reading through your section on how you treated the role of advection I was wondering why you did not nudge (you state that you are nudging the models turbulence so you are familiar with such rather technical numerical simulation features) the model simulated boundary concentrations using the observed concentrations of some of the long-lived compounds such as NO<sub>x</sub>, CO and O<sub>3</sub>? This would secure your model to simulate the observed boundary layer concentrations and then let the canopy exchange model calculate how this “translates’ into the canopy exchange fluxes and concentrations. I have used this approach in the analysis of canopy exchange processes for different sites and this seems to secure a optimal way to ensure a fair evaluation of these models for those compounds with relative short exchanges timescales compared to that of advection.

Section 2.3; reading over the section on the model set-up this is only addressing the issue on how the BVOC (and NO) emissions have been included for this specific analysis but there is no information at all about how you have treated dry deposition and potentially relevant foliage NO<sub>x</sub> emissions associated with nitrate photolysis. I am aware that the focus is on BVOC cycling and the role of turbulence and chemistry but 1) because of the role of O<sub>3</sub>, NO<sub>x</sub>, oxidants (peroxides) but also oxygenated species in canopy photochemistry and exchanges and 2) recent findings that the dry deposition of some of those components might be quite different from what we always assumed (and how it is represented in CACHE?) (oxygenated species and VOC products; Karl et al., 2004 & 2011, peroxides; Ganzeveld et al., 2006), it is relevant to discuss how this process has

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been considered in your study. How is for example stomatal and non-stomatal uptake being considered in the model? A change in the representation of turbulent exchanges as you present in your study might have large (if VOC product and peroxide removal is  $\sim$ turbulent limited) or small (using the “traditional” Wesely approach removal rates) consequences on the efficiency of removal of some of these compounds and their simulated concentrations.

Lines 330-334: “Because the BASE model parameterization typically classifies stable conditions when PAR decreases at the end of the day, the modeled KH abruptly decreases at the onset of sunset resulting in an end-of-day decrease in mixing that is nearly two hours earlier than observed. We note that CACHE does not account for heat storage within the canopy biomass and this is also likely contributing to the early onset of stability in the model at the end of the day”. This issue of the model makes me wonder how well the model simulates the in-canopy energy balance and temperatures. You would expect that during the afternoon the soil (and understorey) warm up and that in the late afternoon, early evening, the lower part of the canopy and especially the soil is warmer compared to the crown-layer that would enhance the mixing. It would be interesting to see, also since CACHE calculates these feature explicitly, how the simulated lower-canopy and soil temperatures compare to observations for the BASE and MIX case. Because of the important role of in-canopy stability on mixing efficiency, the changes in temperatures due a change in mixing effect mixing conditions consequently introducing (“a numerical”) feedback mechanism.

Line 346; “This is an artifact of the use of two different equations to construct the in- and above-canopy wind profiles and turbulence schemes, which creates a discontinuity at the forest-atmosphere interface and prevents BVOC transport out of the canopy sub-layer in the model”. This apparently really addresses a potential model flaw that is now fixed having established the important role of turbulence in simulations of BVOC exchanges.

Line 355: “For the longer-lived species (formaldehyde, MACR+MVK, and acetalde-

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hyde), concentrations are decreased and gradients are weakened by the enhanced mixing". The analysis of the impact of a changed mixing of these component is especially dependent on the representation of their sinks including OH/O<sub>3</sub> oxidation but also potentially the removal by dry deposition or even some biogenic source (existence of compensation point for formaldehyde).

Line 374; This suggests that in-canopy O<sub>3</sub> concentrations are more influenced by local chemistry than regional transport at the canopy-scale, as observed, e.g., by Wolfe et al. (2011)". This stresses the weakness of this analysis. Misrepresentation of the in-canopy O<sub>3</sub> mixing ratios is attributed to chemistry whereas another quite important explanation might be the role of in-canopy sinks such as understorey vegetation- or soil deposition that would be anticipated to be rather efficient for expected organic soils at this site.

Line 383: "or a missing NO<sub>2</sub> source in the model". What would be a nocturnal NO<sub>2</sub> source besides the NO+O<sub>3</sub> reaction?

Having checked in detail figure 3 it is obvious that its layout should be changed. It took me a long time to understand the legend since these are plotted on top of the figures which suggests that these legend names are to be connected to the figures found under these names. Could you put the legends close to each other on the right hand side of the figure and include again the explanation of the colors fitting to the specific figures in the figure caption?

Line 401- ; and the modeled diurnal pattern is prevalent in many modeling studies (e.g., Sillman et al., 2002; Forkel et al., 2006; Barkley et al., 2011), which attribute the end-of-the-day increase to subsidence associated with the compression of the PBL". Are these your own wordings or those of the references you mention here?? I don't think that you really have a compression of the PBL in the evening. The forcing of the PBL growth will stop and you will actually get the onset of the formation of an inversion layer below the residual layer with a decrease in the sensible heat flux but the decrease in

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mixing might be not that large since you might have enhanced mixing conditions inside the canopy (warmer soil compared to crown-layer); in such situations I can imagine that the reference height of the observations that you use for the evaluation becomes very critical. But you also wonder to what extent your model (and the other models) properly represents the temperature that really controls the VOC emissions in the late afternoon. You might not expect that global model system, e.g., used by Barkley et al., would realistically simulate these day-night transitions but you could analyze with your model how well it simulates the decrease in crown-layer temperature associated with long-wave cooling.

Line 413; “Our evaluation of the BASE and MIX turbulence schemes presented in Sect. 3.1 discusses several observed model measurement discrepancies in BASE-case KH that are corrected in the MIX scenario, including the two-hour offset between the modeled and measured diurnal cycle of KH”. In a study on analysis of atmospheric chemistry observations over Guyana’s tropical forest (Ganzeveld et al., Atmos. Chem. Phys., 8, 6223–6243, 2008) we discussed the problem on a misrepresentation of the early morning transition in mixing for chemical exchanges and the evaluation by comparison with the models. In that case it turned out that part of the problem is also the representation of the energy partitioning with incoming energy in the morning being used to evaporate canopy water resulting in a further temperature drop in the morning after sunrise further delaying the onset of mixing. To what extent are such features also a potential explanation for some of the issues on turbulence in CACHE (recognizing the fact that Renate Forkel has also been working on the role of dew in chemical exchanges....)

Line 419-420 and paragraph; “While enhanced mixing improves the diurnal evolution of isoprene, modeled mixing ratios exceed observations on the second day by 1–3 ppbv, likely due to an underestimate of isoprene oxidation”. This is an interesting finding that stresses the difference between your analysis and that by Wolfe et al. (2011) who conducted an analysis focusing on one midday event. You discuss the noted discrep-

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ancy between the observed and simulated isoprene in terms of a misrepresentation of nighttime chemistry. However, this might only be part of the explanation. It would be interesting to see the results with your model system on the oxidation products for the second day where I would expect them to be also enhanced associated with the downward mixing of those products partly consuming the OH not being available for isoprene oxidation (this was also discussed in the 2008 ACP paper). Those products (e.g., CH<sub>2</sub>O) can accumulate overnight in the residual layer due to the ongoing nighttime chemistry and a decoupling from the surface avoiding any destruction by surface deposition. It would be nice to see if this feature is also present in your model (we also found this feature in the model analysis by Barkley et al. 2011) further confirming the importance of this boundary layer feature in chemical exchanges modeling.

Line 453: “measured-modeled comparisons improve above the canopy but not below the canopy, suggesting either that there is in-canopy production that the model does not capture”; is this not indicating the possible importance of the representation of dry deposition/the issue on the existence of a CH<sub>2</sub>O compensation point?

Line 472: “Consequently, modeled concentrations of the MACR RACM-MIM surrogate overestimate measured MACR+MVK by a factor of three throughout the profile”; also this finding really urges for some explanation how the deposition of the products are treated in CACHE.

Line 481: “(200 - 500 pptv)”.

Line 493: “At the PROPHET site, however, the correlation between MACR+MVK and isoprene is weak ( $r^2 = 0.03$ ) as a result of highly variable MACR+MVK advection with respect to wind direction;”. Here you attribute the low correlation between MACR+MVK and isoprene completely to advection. It would be interesting to see how much of the MACR+MVK during the second day can be attributed to the entrainment of residual air masses relative to the contribution by advection. Does your model include the specific process tendencies as a diagnostic tool to separate those two different contributions?

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Line 518: “Previously, other studies have attributed measured-modeled discrepancies to boundary layer dynamics, but our results suggest an important contribution from forest-canopy exchange”. I would say it is the combination of both, during the daytime large-scale BL turbulent motions might control the exchange between the forest and the atmosphere (sweeps) whereas at nighttime the strong long-wave cooling triggers the formation of the inversion layer decoupling the residual layer from the surface. I am making this point since according to me both components need a high priority in improving chemistry simulations in a suite of 1-D to 3-D models.

Line 557; “as does the explicit reaction of ISOP+ISOP”. I don’t get this one; could you explain in more detail what you mean with this?

Line 730; better refer to the paper that presented the analysis on the peroxide exchanges; Ganzeveld, L., Valverde-Canossa, J., Moortgat, G., Steinbrecher, R., Evaluation of Peroxide Exchanges over a Coniferous Forest in a Single-Column Chemistry-Climate Model, Atmos. Environ., 40, S68-S80, 2006.

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