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Atmospheric Chemistry and Physics Discussions

Interactive comment on "SOSA – a new model to simulate the concentrations of organic vapours and sulphuric acid inside the ABL – Part 1: Model description and initial evaluation" *by* M. Boy et al.

Anonymous Referee #1

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General:

In their manuscript Boy et al. adress the important point of climate feedback processes of the biosphere-atmosphere system. It is supposed to have a remarkable impact on the local climate. In order to do so they implemented the latest MEGAN emission code of Guenther et al. (2006) for the emission of volatile organic compounds. The boundary layer meteorology is accurate implemented according to similarity theory. The atmospheric chemistry scheme is adopted from the Leeds University Master Chemical Mechanism v3 (MCM) scheme treating inorganic and organic gas-phase chemistry reactions in detail. However due to a lack of scientific knowledge the scheme has to stop at two exemplary monoterpenes, i.e. α- and β-pinene depending on the location of the carbon-carbon doublebond, which determines the further chemistry. So far new particle formation and the very important aerosol dynamics are missing but will be implemented in a next step. Especially the process of new particle formation is one of the key questions in atmospheric sciences because of the growth of new particles up to a size at which they can affect cloud droplet formation and the cloud droplets size spectra. In order to verify the authors intercompare their model results with the field forest site in Hyytiälä, Southern Finland, which is globally the best equiped one with the magnitude of measurements performed routineously.

The authors have done well and I'd like to congratulate them so far. The implementation of the aerosol part however is a very essential future aspect that should be followed. The manuscript is written fairly well and merits publication after several comments and corrections listed in the following have been considered.

Specific comments:

* Application of a 1D-model requires a rather homogeneous surface to prevent disturbances by slanted wind pattern to affect the results. In this respect the field forest site SMEAR II in Hyytiälä is exemplary. Has the model been tested at other sites/conditions, too?

* How much detail and how many errors have been omitted by averaging for 30 min? I am aware that the usual data collection uses this time frame, but what about the model? What is the necessary time resolution essentially required?

* p. 18613/18614: Please check the variable(s) A_ϕ (p. 18613, eq. 12) and A_Φ (p. 18614, l.5). Are these two identical or not?

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* It seems that the nudging is essential. Interpolation has been made for datasets of every 6 hs. Would there be a benefit in increasing this for the results? How far the model deviates in the absence of nudging, thus for prognosis?

* The vegetation is known to have a slightly elevated temperature compared to the atmosphere. How is this treated in the model? I know that a model cannot capture everything but this would have strong effects on the emissions!

* What is the "negligible" deviation for a chemistry timestep of 60 s? It Would be nice to show a plot for deviations or agreement for the timesteps between 5-300 s with respect to chemistry. That would strengthen the arguments more and help others to use the approach later on.

* p. 18620, l.17f: Please write all the listed monoterpenes correctly: (α-pinene, β-pinene, **d**-limonene, Δ^3-carene, sab**in**ene and camphene).

* Please make a very important comment on using two exemplary monoterpene schemes for the complex mixture and its effects on inorganic chemistry. Since the entire mixture of monoterpene species represent reaction rate constants with the individual oxidants varying by about 4-5 orders of magnitude this is essential for closing OH budgets, ozone and NO$_x$-cycles etc. This interferes strongly with the supposed implementation of new particle formation and its link to OH.

* In general the model is a very interesting tool to study the important aspects such as missing OH-reactivity (OH-sink). However, the assumption of two selected monoterpenes I suppose only a single one of them can only represent the determination of the uncertainty range due to monoterpenes, not the exact pin down of the product k(X+OH)*X!!! This uncertainty taking into account the actual mixture and reactivity of the monoterpenes shoud be given for later investigations.

* Text comments on Fig.4: The Deviations between PTR-MS measurements (Rinne et al., 2005) and MEGAN approximations are nothing special. The empir-

ical approach ("simplification") by Guenther et al. (2006) is just an empirical relationship, not a strict plant physiological approach! Thus 8-14% are quite OK. One should keep in mind the different atmospheric lifetmes of the different monoterpenes e.g. from camphene to limonene. This will certainly affects the vertical and horizontal pattern simulated and its intercomparison with ambient measurements. Please take this into account when discussing Fig. 4.

- Fig.4: Plotting a logarithmic vertical axis would be beneficial. Moreover the indication of the measured values intercompared with would allow a direct visualization of the statements made. This can be either by averages as made for the modelling output or by individual days. If this is supposed to be shifted to a supporting online information, OK.
- The nighttime effects of the vertical monoterpene profile reduction includes not only physical, chemical and meteorological mechanisms but partially compensates each other. I.e. chemical reactions with NO_3 at nighttime do express at different and usually less intense speed than with OH at daytime resulting in a longer atmospheric lifetime. The mixture of indivual monoterpenes might also change throughout the day depending on the source terms and pools emptied for emission. At night the plants surface is expected to be wet (high humidity) and thus has different properties than during daytime. How is this being treated in the model?
- The remarks on nucleation mode particles and the shape of organic vapours as well as sulphuric acid and OH are worth a comment: Since OH (in combination with the atmospherically rather stable SO_2) is the basic source of H_2SO_4 the profile essentially depends on the sink terms. If short lived any compounds originating by an OH-related reaction will display the same behaviour and thus act as a good marker for OH. The monoterpenes emitted from the biosphere display certainly a notable vertical profile due to their source only at the surface

and their chemical degradation with increasing distance from the emission site. Monoterpenes however are not directly involved in particle formation and growth but their oxidation products. Thus, the rate of reaction with ozone and the one with OH will display different behaviour with the latter most likely similar to H_2SO_4. The similarity of nucleation mode particles with monoterpenes is an interesting phenomenon but is to be considered similar to a correlation with SO_2 if multiple oxidation pathways needed to be considered, that haven't to be.

- It would be beneficial to see a clear mechanism related vertical profile to distinguish. However, this is currently not available. But if so the complexity of the process might interfere because a multiple step related nucleation process is feasible complicating the intercomparison of simulation and reality.

- Conclusions: Reduce the starting paragraph. Challenges of 1D-models are apparent as well as the need but missing of meteorological as well as chemical values to run the code. Interesting would be the intercomparison of H_2SO_4 on the vertical scale to provide a base for mechnistic tests. Also the future implementation of the UHMA code (Korhonen et al., 2004) is highly encouraged and an exceelent idea.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 18607, 2010.

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