Atmos. Chem. Phys. Discuss., 10, C7650–C7655, 2010
www.atmos-chem-phys-discuss.net/10/C7650/2010/

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 #2

Received and published: 16 September 2010

1 Overall evaluation

I recommend the editor to accept the manuscript for publication in ACP after minor revision.

2 General comments

The paper addresses an important subject of atmospheric chemistry and physics, namely the elucidation of evolutionary formation pathways of aerosols and their precursors in the planetary boundary layer (PBL). Despite of enormous progress reached over decades in the survey of the phenomenology of precursor and aerosol formation, until now the community is still far away from formulating textbook knowledge. One reason for this is the large number of physicochemical possibilities to form ultrafine particles and subsequent aggregates under ambient conditions. Scale specific modelling approaches provide effective tools for the physical "inter- and extrapolation" of measured physicochemical properties and for the elucidation, e. g., of the genesis of new particle formation in the atmosphere. In the present paper, the authors proposed a state-of-the-art modelling approach in order "to reconstruct the emissions, transport and chemistry in the ABL in and above a vegetation canopy". The paper provokes a wide spectrum of very tricky scientific questions, which are not answered so far and which remain open also after the present paper. However, the modelling approach is very sophisticated, providing a high potential for future investigations of aerosol formation in the PBL.

The main features of the present approach are:

- application of a state-of-the-art PBL model, which is based on the coupled plant–atmosphere boundary layer model SCADIS of Sogachev et al.,
- application of a semiempirical emission model of volatile organic compounds, the model MEGAN of Guenther et al.,
- application of the Master Chemical Mechanism for the complete reaction paths for isoprene, 2-methyl-3-buten-2-ol, β-pinene, α-pinene, methanol, acetone, acetaldehyde, formaldehyde, methane and relevant inorganic reactions (including

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the Kinetic PreProcessor KPP for the translation of the chemical reaction annotation into a Fortran-code),

- employment of the Message Passing Interface (MPI) for numerical execution in parallelisation mode,
- application of a state-of-the-art aerosol dynamics model, the model UHMA of Korhonen et al. (option for the future).

With reference to previous works, the authors presented a brief model description, added by sound verification results, which demonstrate the predictive power of the model with respect to meteorological key parameters and some important aerosol precursor species. A more detailed evaluation of aerosol properties is intented to be performed in the future.

3 Specific comments

- p. 18609, line 4: I suspect that the ozonolysis of sesquiterpene leads to the formation of **low-volatile** oxidation products (but not to "very volatile" ones). The low volatility of these products favour their involvement in gas-to-particle conversion.
- p. 18612-18613, Eqs. (5)-(7), (9): To avoid confusion with standard deviation of velocity components (see Fig. 1e) I recommend the use of α for the Prandtl and Schmidt numbers (instead of σ^{-1}), respectively, as introduced in the original paper of Sogachev et al. (2002). Please check the paramerisation of the Prandtl number according to Eq. (5) for the case $\mathrm{Ri} \geq 0$. It does not agree with the formulation in the original paper.
- p. 18613, Eqs. (7), (14): Define or correct the parameter $C_{\omega 2}^{-}$.

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- p. 18613, Eq. (12): I found the canopy parameterisation very interesting. The ansatz to define S_T contains additional predictive parameters, such as the scalar properties of the sunlighted and shaded part of the canopy. Are the sunlit properties derived from an energy balance equation, the shaded ones from a diagnostic parameterisation? I recommend to add a few sentences to explain the closure of the canopy parameterisation, at least in a qualitative way.

- p. 18614, lines 5, 7: Use correct style A_φ and φ (instead of A_ϕ and ϕ). ... φ is the *placeholder* for the atmospheric value of the scalar.

- p. 18614, lines 9-11: Although described in the original paper of Sogachev et al. (2002), I recommend to add at least the physical unit of the integral exchange coefficients [m/s]. I have not rederived the parameterisation equations, but at least I have checked their consistency by the physical units.

- p. 18618, Fig. 1: (a) This figure shows the beta distribution (18), i. e., the abscissa depicts $f = A\,h/\mathrm{LAI}$. (c) The abscissa shows the normalised momentum flux, i. e., $\overline{u'w'}/u_\star$. Please add overline. (e) The measured values refer to the standard deviations of u, v, and w. To which velocity component the (predicted) solid lines refer? Owing to the dominant contribution of the vertical velocity variance to the TKE and the strong correlation between TKE and the plot in Fig. 1(e), I guess σ_w is depicted.

- p. 18619, line 28: The 1D model is per se not able to capture atmospheric fronts, which are defined by strong horizontal inhomogeneities.

- p. 18620, line 1: Replace “definition of R” by “determination of R”.

- p. 18620, lines 17-28, Fig. 4: From the presentation of time averaged vertical profiles (averaging over one month) I tentatively concluded, that the monoterpene precursors did not reveal any burst-like behavior. What can the authors say about

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the diurnal variation of monoterpenes over the plant canopy? (Please check the annotations of chemical compounds.)

- p. 18621, lines 9-13: I recommend the use of the notion "vertical gradient" in connection with the correct unit: "... vertical gradient of -2.15×10^9 cm^{-3} per ABL thickness", or "decrease of ... over the whole ABL" etc.
- p. 18621, line 25: Maybe "an inversion was located **at** about 1100-1200 m".
- p. 18621, line 26: Either "surface layer" (Prandtl layer) or "mixed layer". Here, maybe "lower part of the ABL below 600 m".
- p. 18622, lines 1-17, Fig. 5: The authors insinuate "strong evidence, that the amount of newly formed particles detected at sizes above 3 nm are more related to the concentrations of organic molecules than to the concentrations of sulphuric acid inside and above the ABL." I recommend the direct inclusion of the cited Figure 9 of O'Dowd et al. (2009) in the present paper. While the particle concentration around noon seems to be correlated with the mixed layer height (not shown but stated in the paper, see next item), there is obviously no jump of the sulphuric acid profile at the mixed layer height, i. e., sulphuric acid concentration scales with OH concentration. Is the sulphuric acid evolution influenced by any other reacting agents than OH? Seemingly, local ground sources of sulphur dioxide do not play any role. Here, I refer also to the specific comment nb. 13 on p. C7305 of the first reviewer.
- p. 18622, line 23: Please add the criterion for the determination of the mixed layer height. It is obviously not a predictive property. This is of importance because of the "excellent agreement with the measurements of vertical particle profile"! What is the vertical grid resolution at this height?
- p. 18623, line 22: "cannot"

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- Figures: The annotations in nearly all figures are to small in the ACPD format. Figures should be enlarged.

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