

Interactive comment on “MALTE – Model to predict new aerosol formation in the lower troposphere” by M. Boy et al.

Anonymous Referee #2

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Comments on

MALTE - Model to predict new aerosol formation in the lower troposphere

by Boy *et al.*

The paper is a very interesting attempt to extend the former box model approach with either simplified or neglected chemistry. Its advantages are clearly to get a more detailed picture of the atmosphere and the place of nucleation to happen. Impacts of

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pre-existing aerosols as well as pollutants mixed downward from the free troposphere can be studied in here as well. However, this requires the nucleation mechanisms to be understood in detail.

This leads to my conclusions about the results presented. Certainly the authors are not responsible for earlier proposed theories. When taking a look at the results presented, there are some things not captured by the boundary model, which should be if the vertical structure of temperature, wind etc is changing:

Figure 5 and 6 - although the nucleation is captured reasonable the Aitken mode maximum isn't accurate after the onset of nucleation, but significantly overestimated. The same applies to the time after 5 p.m. for the nucleation mode (Fig. 6). This seems to be caused by the underestimation of organics redistributing among the available aerosol particles (see Fig. 8). Very interesting in this context is the calculated ratio of the growth rate by sulphuric acid to the one by organics. This figure claims that nearly all particles are mainly growing by sulphuric acid except on the 25th of March 2003.

Figure 3 - The same observations with respect to the Aitken mode concentration overestimation can be made on the 20th of March too. What is notable, that nucleation doesn't stop at 3 p.m. but is simulated to continue even until midnight, with a lack of particle growth towards the Aitken mode particle size.

Figure 7 - On the 4th of April the nucleation event is not found by the model scheme. Although a slight nucleation appears at about 1 p.m., the 'real' event at about 5-6 p.m. is not captured.

Nevertheless, exactly this kind of study is needed to check for the current understanding of the processes as well as the vertical profile, which can be compared with e.g. tethered balloon measurements.

I have some questions with respect to approaches and comments made to the authors:

1) Are the monoterpene concentrations actually measured in accordance to the time resolution of the 1D-model or are the measured values interpolated? (p. 3481)

2) Why did the authors not use the monoterpene emissions in the canopy level of the model and allow it to mix and react afterwards within the boundary layer? This would

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reduce the uncertainty caused by any concentration approaches usually just obtained for the lowest level.

3) Why was an aerosol yield of 0.55 (0.05 non-volatile and water-soluble + 0.5 semi-volatile, insoluble) of monoterpene oxidation products used in this model? Earlier work by e.g. Hoffmann *et al.* (1997) have obtained maximum aerosol yields of 0.12 in their smog chamber even at elevated concentration levels compared to the atmosphere. Is there a further but unknown source related to monoterpenes?

The next to questions are not related to the paper work itself but to the usage and interpretation of results gained:

4) The correlation factor K for kinetic nucleation is varied and found best at $5 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$. Is there any explanation for this value? A collision limited nucleation would result in about $1.5 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$, which is about 300 times larger.

5) The factor γ given by Weber *et al.* (1996) used here is 0.001 - 0.003. Does this correspond to the condensation sink values?

One comment with respect to the production sulphuric acid at the bottom of page 3484: OH is not the precursor of sulphuric acid. In this case it would mean that any reaction of OH would lead to sulphuric acid, which is certainly not true for the atmosphere. Please switch this to SO_2 , the 'real' precursor.

Table 2: The density of sulphuric acid is 1850 kg m^{-3} not 1183 kg m^{-3} . About the value of organics we might argue, but a reasonable would be 1400 kg m^{-3} but certainly not 100 kg m^{-3} as given for compound 2. The molar masses of the organics used here are rather large. Monoterpene aerosol products measured are all below 185 g mol^{-1} with a mean probably at $160\text{--}170 \text{ g mol}^{-1}$. But a larger mass like 200 g mol^{-1} used would correspond to sesquiterpene oxidation products. There might be doubts if sulphuric acid really possesses a saturation vapour pressure of 0 Pa, but there is clearly a lack of knowledge in here. So the value used is at least a good first guess.

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Appendix A: Switch 'alfa' to 'alpha' or ' α ' in the reaction list.

To conclude the presented new boundary layer nucleation model MALTE seems to be a very good tool to test our current understanding of different processes occurring during new particle formation and will extend the present knowledge hopefully in the near future. One question might be needed to be asked before using it: Which are the limits with respect to boundary layer inhomogeneity? If this point is not too critical it might be even used for urban studies in a sufficient distance to large buildings. Good work done.

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