

Interactive comment on “An aerosol dynamics model for simulating particle formation and growth in a mixed flow chamber” by M. Vesterinen et al.

Anonymous Referee #2

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General comments

Vesterinen et al. describe a new numerical model for the simulation of (secondary organic) aerosol formation and growth from a condensable gas in a flow reactor. The condensable gas itself is formed by oxidation of organic species released from spruce seedlings. The model is kept simple and necessary parameters are fitted to the results of experiments with the flow reactor.

Unfortunately, my feeling is that the paper does not achieve its goals.

1) In the introduction the authors state that different processes can lead to secondary organic aerosol and understanding of these processes requires information on forma-

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tion mechanisms of low and semi-volatile organics. I cannot see that the paper helps to gain this understanding. While this might be due to lack of my expertise in this field, I must nevertheless say that the paper is poorly written and therefore not easily comprehensible. I give some examples:

- Page 388, l. 17: "...made a qualitative conclusion that the oscillation of the aerosol number concentration was a net result of nucleation and flow processes in the volume..."; this sentence explains nothing.
- Page 392, after Eq. 2: It is unfortunate that the model needs two different formulations for zero and non-zero γ . It is not at all necessary to make a formulation in a way that the unit of A depends on the value of γ .
- Page 393, around Eq. 4: The physics of the effect is not clear. Assume that all processes but the flow effect were switched off in eq. 1. Then from eq. 4 we see that the concentration of N_j decreases. What makes it decrease is not clear. I think it simply flows through the reactor tube when there is no other process at work.
- Eqs. 6, 7: These two equations should have the same form, i.e. in eq. 7 it should read $[O_3]_{outlet}$ as in eq. 6 it is $[HC]_{outlet}$.
- Eq. 8: What is CG_1 compared to CG ?

This list could easily be extended.

2) There are three occasions where I think that there have been mistakes in planning of the experiments: a) Only the inlet concentration for ozone was measured, b) the flow reactor was not free of HC at the beginning of the experiments, and c) HC and O₃ concentrations were measured 3 times during the first hours of the experiment (these hours have later been discarded from comparison with modelling results) and then

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another three times in the end of the experiment. In between there has not been a measurement for about 15 hours (including light on/off/on variations in the experiment conditions). See Figure 3a. The linear interpolation in this figure between the first and second set of measurements is just a guess. Furthermore, there is some strange variation in the first three measurement points at the inlet, so that I conjecture that there is some noise in the data. Unfortunately, nothing is said about error bars in this respect. I believe that these mistakes could have been avoided.

3) The comparison of model and experiment does not convince me. From Figures 4, 5, and 7 I cannot see that there is a big difference in the results for various choices of γ . The significance of figure 6 is not clear as well, in particular if the first couple of hours are not considered, as stated in the paper. What remains then is constant functions and it is not clear at all, which values is the correct one, therefore, which γ is the most appropriate one. Figure 8 shows some structure in the experimental results (after 6 or so hours) that is absent in the simulations. The size distribution in the experiment seems to peak at about 100 nm (it has a mode, i.e. lower numbers for smaller and larger particles), while that of the model peaks at the smallest considered size. This difference is indication of a fundamental problem in the model, and it is not discussed. On page 402 in the discussion section the authors indicate that another model with molar yield 0.001 and higher gas concentration could give results similar to their results with their special choices. I wonder if this is possible what one might be able to learn from their model.

In view of these major problems I cannot recommend to publish this paper.

Interactive comment on Geosci. Model Dev. Discuss., 4, 385, 2011.

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