

Interactive comment on “Development and evaluation of the aerosol dynamic and gas phase chemistry model ADCHEM” by P. Roldin et al.

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We would especially like to thank the referee for giving us the motivation on how to improve the 2D-VBS model for SOA formation.

We would like to clarify which changes in the model that we have performed after considering the comments from referee #1 as well as the comments on the companion paper (Roldin et al., 2010). The changes concern the organic gas to particle partitioning which is described in Sect. 2.2.2 and 2.4 and new model results from 2D-VBS and two-product model simulations are presented in Sect. 4.2.1.

1) The 2D-VBS model has been changed and it now tracks all the 2D-VBS surrogate species in every size bin. Running this model with 200 size bins is however computa-

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Interactive Discussion

Discussion Paper

tionally expensive and we therefore changed to 100 size bins between 1.5 and 2500 nm in diameter. We have also decreased the number of 2D-VBS bins from 11x16 to 11x10. This is possible since we no longer consider the non-oxidized SOA-precursors in the VBS (e.g. benzene, toluene and xylene) but only their generally less volatile oxidation products. The volatility distribution in the VBS is now between $C^*=10^{-2}$ and $C^*=10^7 \mu\text{g}/\text{m}^3$ instead of $C^*=10^{-4}$ and $C^*=10^{11} \mu\text{g}/\text{m}^3$ which was the range we used for the model runs presented so far.

2) The 2-product model has been changed. It no longer uses the 2-product yield parameterizations from experimental work in smog chambers. Instead, it keeps track of each 2-product model surrogate species (2 products for each oxidation reaction). In total this gives 40 surrogate species (35 for SOA, 2 for POA non-oxidized POA, 2 for non-oxidized IVOCs and 1 for oxidized POA and IVOC products). In the same way as for 2D-VBS model, the 2-product model keeps track of all 40 species in each particle size bin. However, since the number of organic compounds is fewer (40 instead of $11 \times 10 = 110$) this model is faster. Another advantage is that each of these 40 products can be traced back to the original non-oxidized molecules and therefore it is possible to distinguish between ASOA, BSOA and POA. This is not possible with the 2D-VBS which keeps track of the O/C-ratio (an indirect measure of the origin of the organic compounds).

1. Page 18668 line 20: “. . .for 13 different compounds. . .” I assume these are aerosol compounds. Please specify.

Yes, it is aerosol compounds and we will clarify this in the updated manuscript. Now with the updated 2D-VBS model the number of different aerosol particle compounds is 8 for the inorganic compounds and 110 for all the organic compounds, in total 118 aerosol particle compounds.

2. Section 2.2.4 2nd paragraph: Does it rain simultaneously with the same rainfall intensity to all of the 20x20 grids? Please explain.

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Not necessarily but for the modeled case study presented in the article it did. We always assume that the rainfall intensity is uniform in the horizontal direction perpendicular to the air mass trajectory, however the rainfall only occur below the estimated cloud base. The estimated cloud base is derived from the vertical RH profiles along the trajectory. For the simulated case study the RH was however never near 100 % within the model domain (up to 2000 ma.g.l.). Hence, for the modeled case study the cloud base was above the model domain and the rainfall affected all 20x20 grids with the same intensity. We will clarify this better in the text.

3. Section 2.2.6 line 27: Please provide a reference for the cloud droplet size distribution parameters (diameter and σ).

Yes, thank you for clarifying this to us. We will include a reference in the text. For the final simulations we changed the cloud droplet mode diameter to 10 μm because this value is in better agreement of what we have found in the literature about realistic droplet sizes distributions (see e.g. Rogers and Yau, 1989).

4. Page 18678 line 10: “. . .Eqs. (5) and (4)” should be “. . .Eqs. (5) and (6)”

Yes, thank you we will change this in the text.

5. Section 2.4 2nd paragraph: The authors suggest that an advantage of the two product theory against the VBS scheme is that using the latter you have to lump all the organics based on their volatility and therefore loosing the individual characteristics of the VOCs (i.e. specific yields, molecular weights etc.). I assume that when the model use the VBS theory, the VOCs are lumped on the high volatility bins (10^7 - 10^{11}) and then they participate in the same chemical reactions using the same parameters in each of the volatility bins. If that is the case then I suggest using some speciation for the VOCs and then only lumping the oxidation products of each VOC (and not the VOCs themselves) depending on their volatility and O/C ratio. In that way you can still have different VOCs participating in different chemical reactions with different characteristics. Moreover, using this treatment, the volatility bins will be reduced from

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10^{11} to 10^6 as all the products of the oxidation of the VOCs will be distributed in lower volatility bins.

Yes, thank you for these good suggestions. We have adapted them and changed the 2D-VBS model accordingly. The 2D-VBS now considers the species specific first oxidation step before the oxidation products are included into the 2D-VBS. We have thereby been able to decrease the upper volatility bin to $10^7 \mu\text{g}/\text{m}^3$.

6. Page 18685 line 22: I found the low limit of the volatility distribution ($C^* = 10^{-4}$) extremely low. Based on figure 7 the total OA concentration never goes below $2 \mu\text{g}/\text{m}^3$. Therefore, the organics that are distributed at the 4 first volatility bins (10^{-4} - 10^{-1}) are always in the aerosol phase. Probably a higher low limit at 10^{-1} or 10^{-2} would be enough to describe the phase state of these species.

Yes, thank you we have now changed so that the first volatility bin starts at $10^{-2} \mu\text{g}/\text{m}^3$.

7. Page 18686 lines 16-26: What is the change on the O/C ratio and the saturation concentration after each aging reaction?

Yes, thank you for this good question. This was definitely not clear in the submitted manuscript. We will clarify this in the new manuscript where we will include a table that describes the probability functions of adding 1, 2 or 3 oxygen atoms after each oxidation reaction and the probability functions for how much these added oxygen atoms change the saturation concentration.

8. Page 18687 lines 18-22: The discussion here is not in accordance with what was stated on the Eqs. 14 and 15.

Yes, thank you for clarifying this error to use. Equation 14 was used for high NO_x conditions and eq. 15 for low NO_x conditions and not the other way around as was written in Eq. 14 and 15. With the updated version of the 2D-VBS model Eq. 14 is now used both for low and high NO_x conditions and the difference between the low

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and high NO_x conditions is instead considered with the first oxidation step before the compounds are included in the 2D-VBS. This will be described in more detail in the updated manuscript.

9. Table S3: The SVPOA emission fractions at 10⁵ and 10⁶ volatility bins should be equal to zero. Yes, thank you we will change this in the table.

References

Rogers, R. R., and Yau, M. K.: A Short Course in Cloud Physics 3rd Edition, Pergamon Press, Oxford, Great Britain ISBN: 0-08-034864-5, 1989.

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