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Atmospheric Chemistry and Physics Discussions

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

Anonymous Referee #1

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In this paper, a model for aerosol dynamics, gas phase chemistry and radiative transfer calculations (ADCHEM) was developed in order to estimate the ageing processes within urban plumes. The authors explore the model sensitivity to the number of size bins, size structure method, coupled or uncoupled condensation, the volatility basis set (VBS) or traditional two product model for secondary organic aerosol formation, different aerosol dynamic processes and vertical and horizontal mixing. This is a very comprehensive sensitivity analysis. This paper is certainly worthy of publication in ACP. Prior to publication I recommend a few changes, listed below.

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

2.Section 2.2.4 2nd paragraph: Does it rain simultaneously with the same rainfall in-

tensity to all of the 20x20 grids? Please explain.

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

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

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

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 μg 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.

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

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

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9.Table S3: The SVPOA emission fractions at 10ˆ5 and 10ˆ6 volatility bins should be equal to zero.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 18661, 2010.