

Interactive  
Comment

## ***Interactive comment on “A computationally-efficient secondary organic aerosol module for three-dimensional air quality models” by P. Liu and Y. Zhang***

**Anonymous Referee #2**

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### **General comments**

The representation of SOA is an important part of modeling  $\text{PM}_{2.5}$  in atmospheric chemical transport models and it is also computationally expensive. The Liu and Zhang paper presents general areas (calculation of activity coefficients, solving SOA partitioning equations) where CPU calculation time in aerosol models can be reduced. Simulations are performed in a box model in which species concentrations are set at initial values to represent urban and rural conditions with either high or low biogenic VOC concentrations. Runs are performed for 24 hours with only gas and aerosol-phase chemistry (no emissions, transport, or deposition). The optimization of particular pa-

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rameters is relevant to MADRID 2. The optimized version of MADRID 2 represents significant speed-up over base case simulation while sacrificing some accuracy.

### Specific comments

1. Page 7089, lines 1 through 5: Are the hydrophobic and hydrophilic categories mutually exclusive? Are there any OCs that would be included in both hydrophobic and hydrophilic categories?
2. Page 7090, line 5: Do hydrophilic compounds form SOA if water is not present? More detail on the hydrophilic SOA model would be helpful.
3. Page 7091, line 3-5: How much error does holding  $M_{om}$  constant over the time-step introduce?
4. Page 7091, line 26: Should urban and rural air have the same NMHC speciation? Probably not. Comment on using the same distribution for rural and urban air. In Table 1, indicate which NMHCs use the Griffin distribution.
5. Page 7093, line 1: Why do rural HBG calculations take more time than urban HBG calculations?
6. Page 7094, lines 4-17: Were other combinations of speed-up parameters examined or just the three solvers mentioned here?
7. Page 7095, Section 3.4: The parameterization of activity coefficients is for the hydrophilic SOA only. Did you investigate parameterizing the activity coefficients for the hydrophobic SOA?
8. Page 7096, equation (3): Consider removing the  $c$  parameter from the equation and discussion since it is set to zero. Identify which species the subscripts stand for in Table 4. Why did you choose this parameterization over tabulated activity coefficients?
9. Page 7097, line 2: What is the difference between MADRID 2 Fast and comb\_all mentioned on the previous page?

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10. Page 7097, Section 3.5: Species concentrations (like NO) decrease to very low levels during simulations presumably due to the fact that emissions are turned off. What PM concentrations do you have at the end of 24-hour simulation? Since the VOCs are essentially oxidized during the 24 hours and aerosol is not removed by deposition, do SOA concentrations become unrealistically high? Have you run MADRID 2 Fast for 24 hours in CMAQ in one box with emissions, deposition, transport etc. turned on? How do the gas phase and PM concentrations compare to a base case simulation (with SMVGEAR and no optimization in the SOA module)? I know you mention in the conclusions that this will be put into CMAQ, but an initial examination of MADRID 2 Fast with CMAQ would be helpful since species concentrations would remain more realistic throughout the simulation.

11. Figure 3d: PM deviates by almost 20% under some conditions. Is any of this deviation due to the inorganics? What PM concentration (in  $\mu\text{g}/\text{m}^3$ ) does the largest deviation correspond to?

### Technical corrections

Paper should have been edited more thoroughly for errors and clarity before submission.

1. Page 7096, line 24 through page 7087, line 1: Rewrite sentence The formation of SOA . . . condensable products. for clarity
2. Page 7087, line 4: Replace posts with poses
3. Page 7087, line 22: Are hydrophilic compounds treated in MADRID 1 or are they treated using something other than Henry's law? Please clarify sentence.
4. Page 7087, line 16 through 20: Rewrite sentence First, both . . . derived by Pankow et al. 1994. for clarity
5. Page 7088, line 1: Replace SOA module with the SOA module

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6. Page 7088, line 4: Rename section
7. Page 7088, line 19: Replace SOA module with the SOA module
8. Page 7089, line 13, 20: Equation 1 & 2 citation should be Pankow not Pun/Zhang.
9. Page 7090, line 3: Replace stop with continue
10. Page 7091, line 6: Replace condition with conditions
11. Page 7091, line 11: Replace , with :
12. Page 7092, line 26: Replace second with seconds
13. Page 7093, lines 6-9: Rewrite sentence
14. General comment: MAXIT and MAXITS are both used. Pick one name. Also  $M_{om}$  sometimes has a bar over it and sometimes does not.
15. Page 7095, line 26: Rewrite sentence Multiple linear . . . process. for clarity
16. Page 7097, line 16: Figure 4 is missing.
17. Table 2: What do column headings Sect. 1 and Sect. 2 mean? Are they size sections? What sizes?
18. Table 3: Is  $x$  the same as  $A_i$  (the aerosol phase concentration of species  $i$ )?
19. Table 3: Clarify the purpose of ALF.
20. Figure 3: Specify in the caption that MADRID 2 Fast is used.

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Interactive comment on Atmos. Chem. Phys. Discuss., 8, 7085, 2008.

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