Atmos. Chem. Phys. Discuss., 6, S2707–S2713, 2006
www.atmos-chem-phys-discuss.net/6/S2707/2006/


Atmospheric Chemistry and Physics Discussions



# *Interactive comment on* "Implementation of a Markov Chain Monte Carlo Method to inorganic aerosol modeling of observations from the MCMA-2003 Campaign. Part II: Model application to the CENICA, Pedregal and Santa Ana sites" *by* F. M. San Martini et al.

**O. Hellmuth (Referee)**

olaf@tropos.de

Received and published: 25 August 2006

## 1 General comments

As for Part I, here I also want to apologise to the authors for the delay of my referee comment.
The present Part II of the paper is an evaluation study to apply the new Markov Chain

Monte Carlo (MCMC) method, presented in Part I, to several test sites from the Mexico City Metropolitan Area (MCMA) 2003 Field Campaign. With respect to its overall scientific relevance and importance I can refer to my referee comment to Part I. The authors presented an useful paper. It is well-understandable after one has been worked through Part I. Most of my questions refer to the method applied in both manuscripts. They were already ask in my comment to Part I.

**I recommend the editor to accept the paper after minor revisions. But as both Part I and Part II belong together, the present manuscript deserves the editorial acceptance of the first one.**

## 2 Evaluation according to the guidelines for ACP referee comments

1. Does the paper address relevant scientific questions within the scope of ACP?
   Yes, the subject of the paper fits into the ACP profile.
2. Does the paper present novel concepts, ideas, tools, or data?
   Yes. A new MCMC tool, developed in Part I, is applied to several test sites of the recently performed MCMA-2003 Field Campaign.
3. Are substantial conclusions reached?
   Yes.
4. Are the scientific methods and assumptions valid and clearly outlined?
   Yes.
5. Are the results sufficient to support the interpretations and conclusions?
   Yes.



ACPD
6, S2707–S2713, 2006





EGU

6. Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)?
In connection with Part I and the referee comments given to it, yes.

7. Do the authors give proper credit to related work and clearly indicate their own new/ original contribution?
Yes.

8. Does the title clearly reflect the contents of the paper?
Yes.

9. Does the abstract provide a concise and complete summary?
Yes.

10. Is the overall presentation well structured and clear?
Yes.

11. Is the language fluent and precise?
See my response given to Part I.

12. Are the mathematical formulae, symbols, abbreviations, and units correctly defined and used?
Yes.

13. Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated?
Not necessary.

14. Are the number and quality of references appropriate?
Yes. A reference regarding organic aerosols is recommended to add.

15. Is the amount and quality of supplementary material appropriate?
Yes.



ACPD
6, S2707–S2713, 2006





EGU

## 3 Specific comments

1. Section 3: A brief synoptical characterisation of all measurement periods might be instructive (synoptic situation, air mass influence, fronts, advection/ turbulence etc.). For April 9–11, this has been partially done.

2. Section 6: With respect to organic aerosols I recommend to consider also the comprehensive assessment study of Fuzzi et al. (2006, ACP, 6, 2017–2038).

3. Nitrate underprediction: With reference to Ansari and Pandis (2000) the $NO_3^-$ underprediction of ISORROPIA is supposed to be related to the impact of SOA's on the aerosol water content. This effect decreases with increasing relative humidity. Hence, the nitrate prediction capability of ISORROPIA should depend on the relative humidity. Is it possible, to classify your nitrate prediction error according to the observed relative humidity? This would give at least an empirical hint to verify/ falsify your hypothesis on the SOA influence. Apart from the call for experimental data on water uptake on SOA and corresponding models, as stated in lines 5–8 on p. 6017 and which is absolutely right, one might also consider to perform dedicated model evaluation studies using pre-classified field measurements including SOA characteristics. Perhaps, the model prediction capability in dependence on pre-classified scenarios contains further information on the contribution of SOA.

4. p. 6021, lines 2–6: As already stated in Part I, ISORROPIA predicts pH values comparable to observed ones during an "acidic" period (9–11 April). The authors added, that the predicted pH, especially of the aqueous aerosol in the MCMA was 3–4, despite the high concentrations of gas phase ammonia observed. Can you physicochemically explain this finding?



ACPD
6, S2707–S2713, 2006

# 4 Technical corrections

The corrections are adressed as follows: “6001/6“ ≡ “see p. 6001, line 6”

## 4.1 Text

1. 6001/6: “**to** predict”
2. 6001/6: “In general, ...”
3. 6001/14: I recommend to generally use “particle phase”, when the liquid/ solid component of an aerosol is meant.
4. 6001/15: Central Daylight Time (CDT)
5. 6001/17–18: “... is able to both accurately predict the aerosol chloride **mass concentrations** ...”
6. 6002/4: “**emission** control strategies” (several times)
7. 6002/16: ”hydrochlorid acid **concentrations.**”
8. 6002/22:”modelling **the** aerosol behavior”
9. 6002/24–27: comma placement to disburden readability
10. 6002/27: “Therefore, ...” (several times), also: “Note, that ...”
11. 6002/29: “is required/ is needed”
12. 6003/1–4: comma placement: “...model, introduced in Part I, to three ...”



ACPD
6, S2707–S2713, 2006





EGU

13. 6003/3: Check the brackets of all of your citations (several times).

14. 6003/12: Add full stop.

15. Please add in Section 2 or 3 the measurement periods (!) for the diffent sites. Your figures refer sometimes to different measurement periods.

16. 6003/14–18: Split this sentence: "... Cerro de la Estrella. It is in ..."

17. 6003/24: "It is considered **as** a 'boundary' site ..."

18. 6005/6: Remove comma: "The speciation and mass concentration ..."

19. Subsection 5.1: Please explicitly add the measurement period.

20. Eqs. (5),(6): Remove brackets for prefactor "0.3"

21. 6007/5: "and due to observed negative **values.**" I think the value of the variable is negative, but not its observation.

22. 6008/6: "excellent agreement" (several times). See my comment to Part I.

23. 6011/29: "HCl(g)"

24. Subsection 5.2: Please explicitly add the measurement period.

25. Subsection 5.3: Please explicitly add the measurement period.

26. Comments on Eqs. (11)–(20)

    - Eq. (16): Please explain explicitly the symbols RH and R. Make the difference between RH and radical ($R\cdot$) clear.
    - Introduce the rate constant $k_{17}$ immediately after Eq. (17).



ACPD

6, S2707–S2713, 2006

- Perhaps, it might be more consistent, to denote radicals also in the equations by a dot (such as in Eqs. (18), (19)).
- 6019/6–7: What the values $3 \times 10^{12}\mathrm{cm}^3/\mathrm{molecules} \cdot \mathrm{s}$ and $2 \times 10^{10}\mathrm{cm}^3/\mathrm{molecules} \cdot \mathrm{s}$ are standing for?
- 6019/17: In the sentence just before you were talking about the ratio $k_{20}/k_{16} \approx 1/90 - 1/14$. In the just following sentence, you derive a ratio of $\approx 400$. Which ratio you are talking about here?

27. 6021/14–15: "... to a better understanding **of the** aerosol behavior"

## 4.2 References

1. The name of the author is: **Hämeri**.

## 4.3 Figures

1. Figs. 4, 5, 6: Hopefully, these figures will be sufficiently enlarged in the final version. Excuse me, but they are a challenge for eyes, having been getting a bit long in the tooth ...
2. Fig. 15: "15–16 April"



ACPD
6, S2707–S2713, 2006