

Interactive comment on “Importance of mineral cations and organics in gas-aerosol partitioning of reactive nitrogen compounds: case study based on MINOS results” by S. Metzger et al.

Anonymous Referee #1

Received and published: 27 January 2006

In this work the authors analyse the importance of accounting for both mineral components and organic acids in gas-aerosol partitioning of reactive nitrogen species. They do so by comparing results from three thermodynamic equilibrium models of different complexity and measurements (18 day episode from MINOS campaign) describing three different pollution situations with sea salt or mineral dust dominating. The authors show that the EQSAM model, which is the only one accounting for both mineral salts and lumped organic acids, manages well to reproduce measurements of fine ammonium and coarse nitrate. I think this is an interesting and promising result as accurate calculation of gas-aerosol partitioning is important for sound regional and global gas

and aerosol pollution modelling. The issues addressed in the paper definitely fall within the scope of ACP. The results/conclusions made here support those made in Trebs et al. (2005). The new was to extend comparative analyses of size-segregated gas-aerosol partitioning for different types of pollution episodes (sea salt/anthropogenic K+ and Saharan dust). Probably the authors could give a brief consideration to the main findings in Trebs et al. (2005). In general, the paper is written fairly well, but I found that sometimes it was difficult to follow discussions because of some repetitions, text fragmentation and long sentences including additional comments in parenthesis. It would be advisable to structure up the paper and make it more transparent and focused. I think the paper is well worth being published in ACP with some revisions.

Comments/questions to the paper:

1. Abstract, last paragraph: needs to identify more clearly the main purpose (to study the effect of accounting for mineral components an organic acids on gas-aerosol partitioning), which is masked by the model descriptions.
2. It is not clear from the paper what the setup for model runs was: whether measurements were only used for initiation or also assimilated during the runs (e.g. the initial calculated and measured concentrations do not coincide in time-series (fig. 6, 7, 8).
3. Please, explain what you mean by "gas concentrations for fine and coarse mode" (in 4.1, 20 and Fig. 4)
4. Table 1 states that runs F/C5 were performed only with EQSAM and runs F/C4 were performed with EQSAM and SCAPE2. In this case, what the results for F/C5 from ISORROPIA and SCAPE2 and CF/4 for ISORROPIA represent (e.g. in fig. 5 and 6)?
5. (related to 4) Please explain large formation of ammonium aerosols in the coarse fraction in runs C1, if no coarse fraction minerals are present in this run: NH_4NO_3 and $(\text{NH}_4)_x\text{SO}_4$ are largely fine mode particles (Fig.5 and 4.2.1-150 In 4.2.1-15: you conclude that there is not enough anions in F/C1 system to produce the observed

[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)[Discussion Paper](#)

amount of fine NH₄. However, at the same time coarse NH₄ is greatly overestimated. Doesn't that rather indicate that coarse particles steal anions (NO₃⁻) from fine particles?

6. In 4.2.3 the authors introduce "threshold input values" for organic acids and minerals in order to achieve the best match between calculations and measurements for fine NH₄ and coarse NO₃, respectively. Could the authors support the statements (like "Obviously, there is a threshold for the input value.." p.12872-20) with more sound arguments and if possible substantiate the selected input values with e.g. observations (content of insoluble minerals p.12875-5).

7. The main finding and conclusions should be more highlighted in sect 5. Sect. 5 is rather long and its discussion part contains some repetitions from the earlier sections. I recommend that the authors consider splitting Section 5 to two or moving part of the discussion to section 4.

Minor comments to the text:

Repetitions: on p. 12860: from line 28, on p. 12865:10-13 and on p. 12868: 1-8. Recommended to give one model description/differences and refer to it whenever relevant.

p.12868: 20-24 - re-write the sentence (too heavy).

p.12869: 4 remove "However"; check the sentence, I suggest "The EQMs underestimate the fraction of fine ammonium"

p.12869: 5 and 6 - shouldn't it be F4 and C4 instead of F5 and C5

p.12869: 17 - "add into FINE aerosol phase".

p.12869: 22 Change "Nevertheless' with e.g. "It can/should be noted" or "The results show.."

p.12870: 11- Simplify "observed aerosol fine and coarse mode ammonium concentrations"; 15: suggested e.g. "partitioning of fine mode ammonium for period I " 20:

change "i.e. with pyrogenic potassium.." with e.g. "as indicated by enhanced concentrations of pyrogenic potassium .." 23: suggested "..considered in EQSAM2, the model manages to reproduce measured ammonium concentrations in the fine mode" 25: suggested: "Since both minerals and organic acids are not accounted for in the other EQMs, the results do not improve....." again, what is the run F5 in case of ISORROPIA and SCAPE2

p.12871: 3 and 5 contradicting "similar' and "in strong contrast" 8-11: rephrase the reasoning (at least the high dust concentrations cannot be the reason for ISORROPIAs failure to calculate coarse ammonium). 15-16: Needs a better connection to the previous, e.g. instead of "However, both seem to be important.." write "As EQSAM2 calculations show.."

pp. 12872-12873: For easier reading I suggest to move EQSAM2* input description (12873:10-14) after the 1-st paragraph

p.12873: 24-25 unnecessary, as it was already explained in Sect. 2.

p.12874: 17-19 re-phrase to make clearer; line 23 remove i.e. according to 25-28 check/re-phrase;

p.12875: 1 "Thus, the result show" instead of "Obviously"

p.12876; 1-4 - Re-phrase 7-8 - "not all sodium neutralized nitric acid" change with "not all measured sodium was needed (or went for) neutralization of observed nitric acid". But how can we tell that about measurements from Fig. 8? That is calculations which suggest that. This is in fact repeated on lines 12-15. line 26: "distinct chemical composition" of what?

p.12877: 6-10 re-phrase

p. 12878: 6-12 consider moving to section 4.2

p. 12879: 1-4 - I think it was enough to point it out in 4.2.2

[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)[Discussion Paper](#)

p. 12880: 9 The statement that "including .. is most important in aerosol composition studies" seems to be a bit too strong.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 12857, 2005.

Interactive
Comment

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper