

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.

S. Metzger et al.

Received and published: 24 April 2006

We thank the two anonymous referees for their valuable and constructive comments.

Anonymous Referee #1

The paper has been structured up to be more transparent and focused. Also, a brief consideration to the main findings in Trebs et al. (2005) is added.

1. The abstract has been extended and now includes a new paragraph.
2. Also a paragraph has been added at the end of 4.2 to clarify the setup for the model runs.
3. The gas concentrations for fine and coarse mode (in 4.1 and Fig. 4) are observed

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper

and the same - note the different scaling. They have been included in both panels for consistency. A note has been added and a table showing the numbers are now included in Fig 4 (similar to Fig 5). 4. To clarify, a paragraph has been added at the end of 4.2.1. 5. To clarify, the sentence (in 4.2.1) starting with “On the other hand, ...” has been extended. 6. Unfortunately it is not possible within the scope of this work to substantiate the introduced “threshold input values” for organic acids and minerals (4.2.3), due to the limitations by the available measurements - as noted the “threshold input values” were derived from applying EQSAM2 twice, i.e. once in the so-called reverse approach. However, this will be subject for further investigations. 7. Sect. 5 has been split as suggested into two (5. Discussion, 6. Conclusions) with the main finding and conclusions more highlighted.

Minor comments - Repetitions on p. 12865 (10-13) and on p. 12868 removed. - Sentence re-written (p.12868, 20-24). - p.12869 (4): “However” removed and the sentence changed to begin with: “The EQMs underestimate the fraction of fine ammonium ...” - p.12869 (5 and 6): F5 and C5 are correct. - p.12869 (17): “fine” added. - p.12869 (22): Changed accordingly. - p.12870 (all): Simplified/modified accordingly. - p.12871 (all): Sentences revised to: “In contrast to SCAPE2 the predictions of ISORROPIA fails particularly for the relatively dry period II, which is mainly a consequence of the overall lower total anion and in particular chloride concentrations (see table below Figure 4b).” and “As EQSAM2 calculations show...” - p.12873 (10-14): Moved accordingly. - p.12873 (24-25): Removed accordingly. - p.12874 (17-19): Rephrased accordingly. - p.12875 (1): Rephrased accordingly. - p.12876 (all): Rephrased accordingly. - p.12877 (6-10): Rephrased accordingly. - p. 12878 (6-12): Moved from the conclusions to the new discussion section. - p. 12879 (1-4): Removed accordingly. - p. 12880 (9): Changed to “probably most important”.

Anonymous Referee #2

A brief summary of the major EQSAM2 update is appended to this paper. Further a qualitatively discussion has been added to address whether a less constrained ap-

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

proach of the three equilibrium models would still yield such comparable results, especially under different chemical conditions.

Detailed comments

1. In the abstract (and throughout the whole paper) it is now clearer that model experiments were constrained by measured gas(g) and aerosol(a) concentrations, i.e. by total ammonia ($\text{NH}_3(\text{g})$ and $\text{NH}_4^+(\text{a})$), total nitrate ($\text{HNO}_3(\text{g})$ and $\text{NO}_3^-(\text{a})$), total sulfate ($\text{H}_2\text{SO}_4(\text{g})$ and $\text{SO}_4^{2-}(\text{a})$), total chloride ($\text{HCl}(\text{g})$ and $\text{Cl}^-(\text{a})$), sodium ($\text{Na}^+(\text{a})$), calcium ($\text{Ca}^{++}(\text{a})$), magnesium ($\text{Mg}^{++}(\text{a})$), potassium ($\text{K}^+(\text{a})$) and organic acids(a), from which the equilibrium composition and the phase partitioning between the gas/liquid, gas/solid and liquid/solid aerosol phase is calculated. 2. p. 12858 (15): Changed accordingly. 3. p. 12859 (5): Changed accordingly. 4. p. 12860 (10): Included reference to Schaap et al.. 2002. 5. p. 12860 (20): Reference given to Wexler and Seinfeld, 1990. 6. p. 12862 (4): Changed accordingly. 7. p. 12862 (18): Equation included. 8. p. 12862 (19): Changed accordingly. 9. p. 12863 (9): Equilibrium is assumed and sufficient for fine mode particles as the equilibrium timescales are much shorter than the measurement intervals of about 2-3 hours. This and the limitations are explained at the third paragraph of section 3. 10. p. 12863 (9): Changed accordingly. 11. p. 12863 (9): Changed accordingly. 12. p. 12870 (2): Changed accordingly. 13. p. 12870: Changed accordingly. 14. p. 12871 (25): We discuss here potential disequilibrium, e.g. due to insoluble matter that did not react within the measurement interval of 2-3 hours. In case all cations measured in the coarse mode would have been associated with the anions, the system would have been in chemical equilibrium. But this was obviously not the case as the measurements and our results indicate (Figure 8). 15. p. 12872 (15): Changed to "in agreement". 16. p. 12872 (20) vs. p. 12873 (11): Clarified in various parts of the text.

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

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper