

Interactive comment on “The simulations of sulfuric acid concentration and new particle formation in an urban atmosphere in China” by Z. B. Wang et al.

Anonymous Referee #1

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General: This study aims to recapture ambient urban new particle formation events measured in Peking (China) during the CAREBeijing campaign in 2008. Therefore the established box-model version of the Model to predict new Aerosol formation in the Lower Troposphere (MALTE, Boy et al., 2006; Lauros et al., 2011) was initialized with the present observations with a particular focus on the particle formation via linear or squared functionality to sulfuric acid. This is nevertheless an ambitious task since an urban area doesn't represent a homogeneous surface with constant emission of pollutants and in Beijing there is one measurement available only. Consequently a number of a priori assumptions are required and performed.

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All previous work is cited correctly and the aim of this study clearly defined. The study is in line with former studies and extends the investigated area to China. Quite interesting is the trial with the so-called kinetic (Riipinen et al., 2006) and the linear relationship of formation rate and sulfuric acid concentration, with the latter connected to some organics. Unfortunately the outcome does not make much progress although some tendencies are apparent: OH source, short-lived and condensation sink dependent. This would have been a major progress, but is not available using a model only. Therefore the study needs to concentrate primarily on H₂SO₄ measurements and on MCM reactions. Using this, the investigation is acceptable after minor corrections listed in the following and merits publication thereafter.

Detailed comments:

- * Provide the instruments used for basic gas concentrations (ozone, NO, NO₂, SO₂, CO) and detection limits (p. 14982) to allow readers to check for methods and detection sensitivities compared to other measurements.
- * Uncertainties are 1%? I am sure the authors mean on average. However the NO detection limit is dependent on ambient concentrations.
- * Organic chemistry is rather complex and a multitude of species not measured may show up. It is being stated that (calibrated) PTR-MS measurements are used instead of emission modules in MALTE. That's reasonable. However what about compounds with different structures but of the same mass, e.g. monoterpenes, xylene and ethylbenzene as well as ketone, alcohols or alkenes with the same number of basic atoms? This is not distinguishable by PTR-MS and would have implications to atmospheric chemistry. What about transport effects and vertical or horizontal gradients? How may those have affected the results?
- * p. 14984, l. 18: What is meant by ' K_{net} is chosen as $3.0 \pm 3.4 \times 10^{-12} \text{ m}^3 \text{ s}^{-1}$ '

C5257

'? Did the authors use a negative K_{het} ? Please correct with different upper and lower uncertainty ranges.

- * The aspect of 0.5% partitioning of all organic compounds is highly critical. Certainly the exact identity is so far unknown. But having the first order compounds saturation vapour pressures can be estimated by a number of simple methods (e.g. Stein and Brown, 1994) and applying a certain organic fraction, again unknown this may be a more realistic description since the primary compounds will further affect the local chemistry, i.e. the aromatic ones will. Everything seems to work like a big tuning of processes specific to the site. It may be appropriate it may be not. But at least those have been considered.
- * p. 14986: The fit of MATLE data with sulfuric acid data essentially depends on getting OH correct. How accurate the NO measurements and as the authors suggested the HONO simulation (in comparison with other sites) are, because that's commonly the weak point?

References:

Boy, M., et al. (2006), Atmos. Chem. Phys., 6, 4499–4517.

Lauros, J., et al. (2011), Atmos. Chem. Phys., 11, 5591–5601.

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Stein, S. E. and Brown, R. L. (1994), J. Chem. Inf. Comp. Sci., 34, 581-587.

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