Atmos. Chem. Phys. Discuss., 12, C3317–C3318, 2012
www.atmos-chem-phys-discuss.net/12/C3317/2012/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Sensitivities of sulfate aerosol formation and oxidation pathways on the chemical mechanism employed in simulations" *by* A. F. Stein and R. D. Saylor

WRS Stockwell (Referee)

william.r.stockwell@gmail.com

Received and published: 6 June 2012

The authors have produced an excellent study on the differences between the predictions of sulfate formation by CMAQ with three different chemical mechanisms. Although the three versions of CMAQ predict reasonably similar concentrations of sulfate, the relative importance of gas-phase HO and the various aqueous-phase oxidants are very different between the three mechanisms.

Overall this research leads to two important conclusions. The first is that while agreement between data and model results is necessary for model verification it is not sufficient. The response of the model to changing conditions needs to be tested against

the responses of measurements to change as well.

The second point is that the paper shows the importance of process research. More attention needs to be paid to understanding chemical processes in order to reduce the uncertainty in chemical mechanisms. Many important reactions remain poorly measured. Also more process analysis needs to be performed on measurement data and on modeling results to be certain that the models are producing the right results for the right reasons.

Therefore for making these points I commend the authors for their excellent study.

The concept of potential sulfate was first published in: Stockwell, W.R, Milford, J.B., McRae, G.J., Middleton, P., and Chang, J.S.: Nonlinear coupling in the NOx-SOx-reactive organic system, Atmos. Environ., 22, 2481-2490, 1988.

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 8169, 2012.