General comments

In this study, the authors attempted to implement a SO2 heterogeneous reaction parameterization into chemical transportation models to improve simulation of the sulfate rapid growth during haze pollution periods. The proposed parameterization focused on the treatment of the Fe^{3+}-catalyzed oxidation of SO2 by O2 in aerosol water. Simulations using WRF-CHEM model were conducted on haze episodes at two cities in China to evaluate the performance of the new parameterization. The authors found that the new parameterization could improve the representation of sulfate heterogeneous formation in WRF-CHEM model since the simulations with the parameterization could reproduce the observed rapid growth of sulfate aerosol and diurnal variations. Given that current models still underestimate the conversion of SO2 to sulfate, the SO2 heterogeneous reaction parameterization proposed here to improve sulfate simulation would be interesting to the readerships of the ACP journal. However, some issues related to the clarity of discussions and latest refs need to be addressed before its publication.

Specific comments

1) In the abstract and a statement on p. 3 lines 80-82, it appeared that the observed filter measurements in Xi'an, China since 2003 was used to develop SO2 heterogeneous reaction parameterization, but how to apply these filter measurements to parameterize SO2 heterogeneous reaction was not clearly explained. According to the parameterization section (section 3.1), it was more like that the filter measurements was only used to illustrate the relationships between sulfate, iron, humidity and PM2.5. None of values for the parameters in parameterization equation (line 208) was derived based on the filter measurements.

2) At several places (e.g., p. 7, lines 166-175; p. 9, lines 210-213) the authors stated that oxidation of sulfite by NO2 in aerosol water was proposed to contribute considerably to the sulfate production when NH3 concentrations were high. A very recent paper (Wang et al., PNAS, 2016, 113, 13630–13635) has provided the elucidation of this specific mechanism for sulfite-sulfate conversion. In addition, this work also pointed out the critical role of sulfate formation in haze development in China, including promoting the formation of SOA (Zhao et al., Environ. Sci. Technol. 40, 7682, 2006) and nitrate (Zhang et al., Geophys. Res. Lett. 22, 1493, 1995). Those references should be discussed when discussing the aerosol chemistry.

3) Some statements regarding to the discrepancies between simulation and observation were confused and speculative. For example, in both lines 293 and 314, it was stated that the model had difficulties in reproducing the long-range transport of pollutants like sulfate and nitrate. My concern was that the long-range transport contribution to pollutants could be negligible in this case since Guanzhong Basin was under the control of stagnation condition based on wind fields shown in Fig. 7. Therefore, the long-range transport may be not the reason why the simulated concentrations differ from the observations. Also in lines 302-307, the discrepancies between

simulated and observed sulfate mass was attributed to inaccurate simulations of wind fields, but there was no direct comparison between simulated and observed wind fields to demonstrate this point.

4) To be consistent with Figs. 11 and 12, how about adding one panel for time series of NH3 (in gas phase) to Figs. 9 and 10 to evaluate the model performance on NH3?

Technical corrections

1) On p. 5 in the equation for defining IOA, $|P_i - \bar{O}|$ in the denominator should be $|P_i - \bar{P}|$

2) Line 321: “sulfate aerosols play a more important role” than what? Nitrate aerosol?