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The effects of heterogeneous reactions on atmospheric chemistry and aerosol properties

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A new aerosol module is developed for the STEM model (the Sulfur Transport and dEposition Model) to better understand the chemical aging of dust during long range transport and assess the impact of heterogeneous reactions on tropospheric chemistry. The new aerosol module is verified and first applied in a box model, and then coupled into the 3-Dimentional STEM model. In the new aerosol model, a nonequilibrium (dynamic or kinetic) approach to treat gas-to-particle conversion is employed to replace the equilibrium method in STEM model. Meanwhile, a new numerical method solving the aerosol dynamics equation is introduced into the dynamic aerosol model for its improved computational efficiency and high accuracy. Compared with the equilibrium method, the new dynamic approach is found to provide better results on predicating the different hygroscopicity and chemical aging patterns as a function of size. The current modeling study also takes advantage of new findings from laboratory experiments about heterogeneous reactions on mineral oxides and dust particles, in order to consider the complexity of surface chemistry (such as surface saturation, coating and relative humidity). Modeling results show that the impacts of mineralogy and relative humidity on heterogeneous reactions are significant and should be considered in atmospheric chemistry modeling with first priority. The new dynamic approach for gas-to-particle conversion and RH-dependent heterogeneous uptake of HNO_3 improve the model performance in term of aerosol predictions under different conditions. It is shown that these improvements change the modeled nitrate and sulfate concentrations, but also modify their size distributions significantly.