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The efficiency and sensitivity analysis of observations for atmospheric transport model with emissions

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Air quality and climate change are influenced by the fluxes of green house gases, reactive emissions and aerosols in the atmosphere. But observations of the chemical states in the atmosphere typically have low temporal and spatial density. Therefore, many works are introduced to spatio-temporal data assimilation methods in atmospheric chemistry in recent years.

There is no doubt that the optimization of the initial state is always of great importance for the improvement of predictive skill. However, specified to the chemistry transport model with high dependence on the emissions in the troposphere, the optimization of the initial state is no longer the only issue. The lack of the ability to observe and estimate surface emission fluxes and important inner atmospheric fluxes with necessary accuracy is a major roadblock of hampering the progress in predictive skills of the atmospheric transport model. However, in many cases, the better estimations for both the initial state and emission rates are not always obtained with certain observational network configurations via various popular data assimilation methods, such as the ensemble Kalman filter and smoother and 4D-variation. It leads to the waste of resource by optimizing the improper parameters or brings the inaccuracy of the optimization by unsuitable weight between the initial state and emission rates.

Hence, in order to make a scientific and quantitative decision about which parameters to be optimized and how to balance them before any data assimilation procedure, we establish the dynamic model for emission rates with the constraint of diurnal profile shape and extend the state vector of atmospheric transport model so that the emission rates are included. Then, a theoretical approach, based on Kalman filter and smoother and their ensemble cases, to evaluate the potential improvement is introduced. By singular value decomposition, the efficiency of observations to optimize initial state and emission rates of the extended atmospheric transport model can be easily determined. Further, with the same singular vector analysis of the efficiency of observations, the sensitivity of observations can be identified by determining the directions of maximum perturbation. Finally, a 3D advection-diffusion toy model is presented to test the approach.