4.085 On inferring the unobserved chemical state of the atmosphere: box model experiments.

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Abstract:

Chemical data assimilation in numerical models of the atmosphere has to deal with strongly non-linear interactions. Commonly assimilated observations (i.e. retrieved satellite products) exist for only a selected few of those key gas phase compounds (CO, O_3, NO_2, CH_2O), and assimilating those in models assuming linearity begs the question of: To what extent we can infer the remainder to create a new state of the atmosphere that is chemically sound and optimal? In our work we present systematic investigation of sensitivities that exist between chemical compounds under varying ambient conditions in order to inform scientists on the potential pitfalls when assimilating single/few chemical compounds into complex 3D chemistry transport models.
In order to do this, we developed a box-modeling assimilation tool (BOXMOX/BEATBOX) based on the Kinetic PreProcessor (KPP) in which we can conduct simulations with a suite of 'mechanisms', sets of differential equations describing atmospheric photochemistry. The box modeling approach allows us to sample a large variety of atmospheric conditions (urban, rural, biogenically dominated, biomass burning plumes) to capture the range of chemical conditions that typically exist in the atmosphere. Included in our suite are 'lumped' mechanisms typically used in regional and global chemistry transport models as well as the Master Chemical Mechanism (MCM). We will undertake an Observing System Simulation Experiment approach using the MCM prediction as 'nature' or 'true' state and assimilate idealized synthetic observations (from MCM) into different mechanism under various environments. Different chemical sensitivity approaches will be compared: 1) adjoint, 2) ensemble and 3) hybrid: using an ensemble of adjoint sensitivities, in order to derive gain matrices to optimally infer the unobserved part of the atmospheric chemical modeled states.