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Ozone Data Assimilation with GEOS-Chem: a Comparison Between 3D-Var, 4D-Var, and Suboptimal Kalman Filter Approaches

K. Singh[1], A. Sandu[1], K. W. Bowman[2], M. Parrington[3,4], D. B. A. Jones[4], and M. Lee[2]

[1]Department of Computer Science, Virginia Polytechnic Institute and State University, 2202 Kraft Drive, Blacksburg, VA 24060, USA
[2]Jet Propulsion Laboratory, 4800 Oak Grove Drive, Pasadena, CA 91109, USA
[3]School of GeoSciences, University of Edinburgh, Edinburgh, UK
[4]Department of Physics, University of Toronto, ON M5S 1A7, Canada

Correspondence to: Adrian Sandu (sandu@cs.vt.edu)

Abstract. Chemistry transport models determine the evolving chemical state of the atmosphere by solving the fundamental equations that govern physical and chemical transformations subject to initial conditions of the atmospheric state and surface boundary conditions, e.g., surface emissions. The development of data assimilation techniques synthesize model predictions with measurements in a rigorous mathematical framework that provides observational constraints on these conditions.

Two families of data assimilation methods are currently widely used: variational and Kalman filter (KF). The variational approach is based on control theory and formulates data assimilation as a minimization problem of a cost functional that measures the model-observations mismatch. The Kalman filter approach is rooted in statistical estimation theory and provides the analysis covariance together with the best state estimate. Suboptimal Kalman filters employ different approximations of the covariances in order to make the computations feasible with large models. Each family of methods has both merits and drawbacks.

This paper compares several data assimilation methods used for global chemical data assimilation. Specifically, we evaluate data assimilation approaches for improving estimates of the summertime global tropospheric ozone distribution in August 2006 based on ozone observations from the NASA Tropospheric Emission Spectrometer and the GEOS-Chem chemistry transport model. The resulting analyses are compared against independent ozonesonde measurements to assess the effectiveness of each assimilation method. All assimilation methods provide notable improvements over the free model simulations, which differ from the ozonesonde measurements by about 20% (below 200 hPa). Four dimensional variational data assimilation with window lengths between five days and two weeks is the most accurate method,

with mean differences between analysis profiles and ozonesonde measurements of 1-5%. Two sequential assimilation approaches (three dimensional variational and suboptimal KF), although derived from different theoretical considerations, provide similar ozone estimates, with relative differences of 5-10% between the analyses and ozonesonde measurements.

Adjoint sensitivity analysis techniques are used to explore the role of of uncertainties in ozone precursors and their emissions on the distribution of tropospheric ozone. A novel technique is introduced that projects 3D-Variational increments back to an equivalent initial condition, which facilitates comparison with 4D variational techniques