Atmospheric Chemistry and Physics
An Interactive Open Access Journal of the European Geosciences Union

Atmos. Chem. Phys., 8, 5603-5614, 2008
www.atmos-chem-phys.net/8/5603/2008/

A method for evaluating spatially-resolved NO_x emissions using Kalman filter inversion, direct sensitivities, and space-based NO_2 observations

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Abstract. An inverse modeling method was developed and tested for identifying possible biases in emission inventories using satellite observations. The relationships between emission inputs and modeled ambient concentrations were estimated using sensitivities calculated with the decoupled direct method in three dimensions (DDM-3D) implemented within the framework of the Community Multiscale Air Quality (CMAQ) regional model. As a case study to test the approach, the method was applied to regional ground-level NO_x emissions in the southeastern United States as constrained by observations of NO_2 column densities derived from the Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY) satellite instrument. A controlled "pseudodata" scenario with a known solution was used to establish that the methodology can achieve the correct solution, and the approach was then applied to a summer 2004 period where the satellite data are available. The results indicate that emissions biases differ in urban and rural areas of the southeast. The method suggested slight downward (less than 10%) adjustment to urban emissions, while rural region results were found to be highly sensitive to NO_x processes in the upper troposphere. As such, the bias in the rural areas is likely not solely due to biases in the ground-level emissions. It was found that CMAQ was unable to predict the significant level of NO_2 in the upper troposphere that was observed during the NASA Intercontinental Chemical Transport Experiment (INTEX) measurement campaign. The best correlation between satellite observations and modeled NO_2 column densities, as well as comparison to ground-level observations of NO_2, was obtained by performing the inverse while accounting for the significant presence of NO_2 in the upper troposphere not captured by the regional model.

Final Revised Paper (PDF, 6326 KB) Discussion Paper (ACPD)

Citation: Napelenok, S. L., Pinder, R. W., Gilliland, A. B., and Martin, R. V.: A method for evaluating spatially-resolved NO_x emissions using Kalman filter inversion, direct sensitivities, and space-based NO_2 observations, Atmos. Chem. Phys., 8, 5603-5614, 2008. Bibtex EndNote Reference

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