Diagnostic Evaluation of Emissions via Top-down Inverse Modeling (2.4)

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In model evaluation studies, deficiencies in emissions are often a likely culprit for model biases or errors. Unlike meteorological and air quality model predictions, regional-scale emissions estimates cannot be validated against direct measurements (with the one exception being measurements available from Continuous Emissions Monitoring Systems (CEMS) on electricity generating units). For mobile emissions, flux measurements can be made directly at the tailpipe to develop emission factors, but the aggregate estimate across national roads and highways is an extrapolation that includes numerous assumptions. Diffuse area sources, such as fertilizer applications, are much more difficult to characterize at individual sites, especially for gridded, regional-scale modeling.

To complement the immense effort required to develop “bottom-up” emission inventories, inverse modeling approaches have been introduced as a tool for evaluating and refining emission estimates. While some have referred to inverse modeling as running the model “backwards,” that is a misnomer. Instead, based on the estimated sensitivity of the pollutant concentration to emission changes (the Jacobian or K_t) and on estimated uncertainties, inverse methods can be used to infer how much the emissions would need to change to get optimal agreement with the observations. While originally used in global-scale modeling for long-lived species such as chloroflourocarbons, the Division’s work in this area has demonstrated that similar approaches can be effectively applied to regional-scale air quality modeling problems. In general, inverse modeling approaches estimate the emission levels that would minimize the differences between modeled and observed concentrations. The methods rely on the response of air quality model predictions to emission changes and uncertainty estimates of concentrations and emissions. There are two studies summarized here:

- The NH_3 study demonstrates that inverse methods can be used to characterize seasonal changes in NH_3 emissions, and it also shows that overestimating these emissions during cooler seasons causes large biases in total nitrate concentrations in the model.

- The NO_x study, which is focused on urban areas of high mobile NO_x emissions and surrounding rural areas, demonstrates that NO_2 satellite retrievals can serve as observational data for NO_x inverse modeling. The study also expands on the inverse modeling approach by characterizing individual source regions, which is possible only because of the denser satellite data and incorporating the CMAQ-DDM capabilities into the approach. The importance of considering modeling uncertainties is also highlighted in the NO_x study, where model uncertainties in the free tropospheric NO_x chemistry severely affected NO_2 comparisons in rural areas.