**The influence of boundary conditions on inverse analyses**

**1. Introduction**

Option 1 : Methane focus

All modelled pathways that limit global warming to 1.5°C require deep reductions in methane emissions (IPCC). The sources of methane emissions, including livestock, oil and natural gas, waste management, and wetlands, are well known, but significant uncertainty exists in their spatial and temporal distribution. Regional inverse studies use chemical transport models (CTMs) and observations of methane concentrations to improve methane emission estimates at the high resolution needed to identify emission sources. However, the optimized emissions are sensitive to the methane concentrations used by the CTM at the boundary of the domain. Here, we present a theoretical and numerical framework to quantify, predict, and correct the influence of these biases on the improved emissions estimates.

Option 2 : General inverse study

Satellite observations of atmospheric composition can improve estimates of …

Satellites increasingly provide high-resolution observations that can be used to quantify emissions on a regional and facility scale (e.g., Zhang et al. 2020, Varon et al. …., Miller et al. …). These regional inverse studies use chemical transport models ….

[Past attempts to address errors in boundary conditions:

* Wecht?
* Maasakkers
* Shen
* Miller?]

**2. Analytical solution to the inverse problem**

Given a vector of gridded emissions and the vector of observations , both with normally distributed errors, the optimal emissions estimate is obtained by minimizing a Bayesian cost function

where and are the prior emissions estimate and error covariance, respectively, is the observational error covariance, and is the chemical transport model (CTM) that simulates observations as a function of emissions (Brasseur and Jacob, 2017). If the CTM is linear, then where is the Jacobian matrix and is constant defined so that . An analytical solution then exists for the cost function minimum that yields the optimal (posterior) state vector estimate

where

is the gain matrix that represents the sensitivity of the posterior emissions to the observations.

**3. Boundary condition sensitivity in a simple model**

We quantify the influence of boundary conditions on inverse analyses by conducting a series of inversions using a one-dimensional model for the transport of a passive tracer. Figure 1 shows a schematic of this model for grid boxes of length (m), though the model can be extended to any . The tracer sources are the boundary condition (ppb) and the emissions (ppb). The sink is transport defined by wind speed (km/hr). The model simulates the atmospheric concentrations (ppb) in each grid box at a given time . We conduct a series of sensitivity inversions in which we change the boundary condition and compare the posterior emissions. Section 3.1 solves for the influence of boundary condition perturbations on the posterior analytically. Section 3.2 confirms the analytical solution numerically. Section 3.3 demonstrates the same principle in an inversion that uses a complex three-dimensional chemical transport model.



**Figure 1: [insert caption]**

**3.1 Analytical solution**

Assuming the model has achieved steady state so that , we solve the system of differential equations for the one-dimensional model (Figure 1) yielding the dependence of the simulated observations on the emissions . The solution takes the form , shown here for an example with 3 grid boxes:

The Jacobian matrix is a function of the grid box length and wind speed , and the constant term is a function of the boundary condition alone.

[Define the state vector here and define “standard inversion”] We consider the effect of a constant perturbation to the boundary condition on the posterior emissions obtained by an inversion. We use this forward model in an analytical inversion (equation 2) with prior , observations , and prior and observational error covariance matrices and , respectively. We first solve the inversion using the “true” boundary condition that corresponds to the observations, yielding the “true” posterior . We then solve the inversion with a, yielding . The difference between the two posteriors gives the sensitivity of the posterior emissions to the boundary condition:

If the boundary condition is optimized as part of the inversion (BC inversion), the expression What happens if we optimize the boundary condition as part of the inversion?

where . We’re going to call this Jacobian

In this case, the gain matrix can be written in terms of the terms used in the

The term is orders of magnitude larger than the other terms in the inverted expression. As a result, the terms of the gain matrix for the BC inversion are much smaller than the terms in the standard inversion

**3.2 Numerical solution**

We solve for advection using the Lax-Wendroff scheme in grid boxes 1 through and an upstream scheme for grid box (Brasseur and Jacob, 2017).

Pseudo-observations are generated by adding random noise to the steady-state concentrations, and we define the prior and the prior and observational error covariance matrices and , respectively. We solve for the “true” posterior emissions with the “true” boundary condition used to generate the pseudo-observations, perturb the boundary condition, and and compare the posterior emissions

We define generate pseudo-observations by using the “true” emissions to generate a set of steady-state observations to which we add random noise with