**Predicting and correcting the influence of boundary conditions on inverse analyses**

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**Abstract**

[Insert]

**1. Introduction**

Satellites now measure atmospheric trace gas concentrations at sufficiently high-resolution to quantify emissions on a regional and facility scale (e.g., citations). These regional inverse studies compare observed concentrations to a chemical transport model (CTMs) to find the emissions that best explain the observations. However, the optimized emissions are sensitive to the boundary conditions used by the CTM. We present a theoretical and numerical framework to quantify, predict, and correct the influence of these biases on the improved emissions estimates.

[Regional inverse analyses description]

[Past attempts to address errors in boundary conditions:

* Wecht?
* Maasakkers
* Shen
* Miller?]

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

Given an *n*-dimensional vector of gridded emissions and the *m*-dimensional 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 matrix, respectively, is the observational error covariance matrix, 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 by the boundary condition so that . If the boundary condition is optimized by the inversion and therefore included in , the boundary condition is instead defined by and . In both cases, an analytical solution then exists for the cost function minimum that yields the optimal (posterior) emissions estimate and its error covariance matrix :

where

is the gain matrix that represents the sensitivity of the posterior emissions to the observations. The relative decrease in error is quantified by the averaging kernel , a measure of the information content of the observing system. The diagonal elements of are often referred to as the averaging kernel sensitivities and give the sensitivity of the posterior emissions to the true emissions in each grid box.

We solve the inversion assuming the “true” boundary condition is known and compare the resulting posterior emissions to the posterior emissions given by an inversion with a perturbed boundary condition. The sensitivity of the posterior emissions to the boundary condition is then given by:

where and are the constants associated with the perturbed and true boundary conditions, respectively, calculated for an inversion that does not optimize the boundary condition. This solution holds in inversions that both do and do not optimize the boundary condition.

**3. Sensitivity of the posterior to the boundary condition**

We show how equation (5) and the gain matrix can be used to predict and correct the influence of boundary conditions on posterior emissions in a series of inverse analyses. Section 3.1 solves for the influence of boundary condition perturbations on the posterior in steady state systems analytically. Section 3.2 confirms the solution numerically. Section 3.3 considers oscillating boundary condition perturbations. Section 3.4 demonstrates our approach for predicting and improving boundary condition errors in a one-week inversion of TROPOMI observations over the Permian basin.

**3.1 Analytical steady state solution**

We first 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). The tracer sources are the boundary condition (ppb) and the emissions (ppb). The sink is transport with wind speed (km/hr). The model simulates the atmospheric concentrations (ppb) in each grid box at a given time .

We solve the system of differential equations for this one-dimensional model to find the dependence of the observations on the emissions assuming the model is in steady state. The solution takes the form , where is the Jacobian matrix and is constant. In an inversion that optimizes only emissions, is lower diagonal with entries equal to the inverse lifetime of the tracer in each grid cell and . In an inversion that optimizes the boundary condition, the Jacobian is lower diagonal other than the column corresponding to the boundary condition, which is given by , and .

We solve the inversion (equation 2) assuming the “true” boundary condition is known to find the “true” posterior state vector . We then perturb the boundary condition by a constant and solve the inversion again, yielding . In both the standard and boundary condition inversions, the sensitivity of the posterior emissions in the th grid box to a constant error in the boundary condition is given by:

The sensitivity of the posterior emissions to a constant error in the boundary condition is therefore given by the row-wise sum of the gain matrix , which is in turn dictated by the structure of the matrix. Because optimized emissions are most sensitive to nearby observations, is banded. is positive for observations downstream of grid cell and negative for upstream observations, which preserves mass in the inversion. The magnitude of the sensitivities decreases as the distance between the observations and emission grid cell increases. The influence of the boundary condition is therefore largest for upstream grid cells, where has fewer negative entries, and decreases with the distance from the boundary.

The width of the gain matrix bands depends on the Jacobian matrix , theprior error covariance matrix , and the observational error covariance matrix . As demonstration, we consider a case with observations in each of grid cells. We assume hr (corresponding to grid cells of length km with wind speed km hr-1), constant observational errors of 15 ppb, and constant prior errors of 50 ppb d-1. We evaluate the structure of the gain matrix with two parameters: the gain matrix band width and the influence length scale. The band width is the maximum number of entries in a row of that are larger than 1/1000 of that row’s maximum value. The influence length scale is the number of grid cells before decreases below 10 ppb d-1, or 20% of the prior errors.

Figure 2 shows the change in the band width (top) and influence length scale (bottom) as the lifetime, prior errors, and observational errors are scaled across the inversion domain (left column). As the lifetime increases, the posterior emissions become less sensitive to distant observations, decreasing the gain matrix band width and, accordingly, the influence length scale. As the prior error decreases or the observational error increases, more observations are needed to alter the prior emissions, increasing the gain matrix band width and influence length scale.

Figure 2 also shows the sensitivity of the band width and influence length scale to changes in the inversion parameters in the first grid cell alone (right column), which could theoretically absorb errors in the boundary condition. However, the band width and influence length scale are relatively insensitive to changes to the inversion parameters in the first grid cell. Neither change in response to changes in the observational error, and the influence length scale decreases only slightly after the prior error doubles.

**3.2 Numerical solution**

We simulate concentrations of an inert tracer advected through grid cells of length km with wind speed km hr-1. Initial conditions are given by the steady state concentrations. We assume constant emissions of 100 ppb d-1 in each grid cell and a true boundary condition ppb. Advection is solved using the Lax-Wendroff scheme in the first grid cells and an upstream scheme for the last grid cell (Brasseur and Jacob, 2017). We solve for concentrations every 2.5 hours, corresponding to a Courant number of 0.5.

We solve a series of inversions with this model. Figure 3 shows a sample of a prior (top) and associated observational (bottom) inversion parameters for the base inversion. The prior emissions vector is given by random values with mean 70 ppb d-1 and standard deviation 40 ppb d-1. We test the sensitivity of our results to the prior by conducting inversions with 50,000 unique prior emission vectors. For each of these, we assume uniform relative errors of 50% unless the prior emissions are less than the mean prior emissions, in which case we use relative errors corresponding of 50% of the mean. We construct the prior error covariance matrix assuming no error covariance. The observation vector is composed of pseudo-observations, generated by adding random noise with mean 0 ppb and standard deviation 10 ppb to the steady-state concentrations. The 300 data points correspond to one observation per grid cell at 15 evenly spaced intervals between 150 and 300 hours from the start of the simulation. We assume constant observational errors of 15 ppb and construct the observational error covariance matrix assuming no error covariance. We construct the Jacobian matrix using a finite difference approach.

Figure 4 shows the true posterior emissions for a demonstration inversion assuming the true boundary condition is known. We show results that do and do not optimize the boundary condition. Both inversions produce similar posterior emissions and are most accurate in the middle of the domain, where emissions have a larger relative influence than the boundary condition on simulated concentrations and where there are many downstream observations. The inversion that optimizes the boundary condition has lower information content at the upstream edge and therefore an increased deviation from the truth because the observations are used to inform the boundary condition rather than the emissions.

**3.2.1 Numerical steady-state solution**

We perturb the boundary condition by a constant value, solve the inversion, and compare the posterior emissions. Figure 5 shows the difference in posterior emissions for a range of boundary condition perturbations for the inversions that do not optimize the boundary condition. As predicted by equation (5), the error scales with and agrees with the row-wise sum of the gain matrix. In all cases, the error decreases exponentially as the distance from the upstream boundary increases and is lower than 10 ppb d-1 within 6 grid cells. This result is invariant to the choice of prior. Across this influence length scale, the inversion absorbs errors in the boundary condition by correcting emissions in upstream grid cells. The inversion that optimizes the boundary condition has , or an influence length scale of 0 grid cells, demonstrating that the inversion can correct constant errors in boundary condition specification. However, as noted above, the correction of the boundary condition may result in a decreased ability to accurately constrain emissions in the upstream grid cells.

Figure 6 shows the sensitivity of the gain matrix band width and influence length scale to inversion parameters. For each inversion, we scale the prior and observational errors across the entire inversion domain (left column) and in the first grid cell alone (right column). The numerical result largely agrees with the theoretical result shown in figure 2: on average, as prior errors decrease and observational errors increase, the band width and the influence length scale increase, and both quantities are less sensitive to changes in the first grid cell. However, while the theoretical band width and influence length scale increase monotonically as the errors change, the numerical values initially decrease. This discrepancy results from differences between the numerical and theoretical Jacobian matrices. The theoretical Jacobian matrix is lower diagonal with constant entries equal to the inverse lifetime of the tracer in each grid cell . The numerical Jacobian matrix is approximately lower diagonal, with deviations resulting from the Lax-Wendroff advection scheme. It also has larger than predicted values for the sensitivity of the observations to the first grid cell that result from an attempt to capture the sensitivity to the boundary condition. These numerical artifacts occur in both the standard and boundary condition inversions and explain the discrepancies between figures 2 and 6.

Figure 6 shows that scaling the variances for observations in the first grid cell by a factor of about 10 will more than halve the influence length scale. This functionally discards the observations over the first grid cell, decreasing the observational constraint so that the inversion can alter emissions in the first grid cell to compensate for the error in the boundary condition. The optimal scaling factor for a given inversion can be determined by recreating this analysis, which is trivial for an analytical inversion with a pre-defined Jacobian matrix.

**3.2.1 Numerical non-steady state solution**

In the case that the error in the boundary condition changes in time, the steady state assumption made in our previous analyses fails. In this case, the sensitivity of the posterior to the boundary condition is given by:

We also test a series of oscillating boundary condition perturbations, shown in Figure 8. These perturbations all have a vertical shift of 75 ppb relative to the true boundary condition, but vary in the amplitude, period, and phase shift. Figure 9 shows the difference in posterior emissions for these perturbations for the standard inversion and boundary condition inversion. In all inversions, the errors in the posterior resulting from the perturbation to the boundary condition persist after the initial enhancement

The influence length scale is shorter for the standard inversion than for the boundary condition inversion because a single correction term is insufficient to correct the oscillating error in the boundary condition. Moreover,

**3.3 Demonstration inversion of TROPOMI observations over the Permian**

[Insert]

🡪 next step.

**4 Discussion**

[To write]

**5 Conclusions**

[Insert]