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

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**Abstract**

[Insert]

**1. Introduction**

Regional simulations of atmospheric trace gases provide insights into emissions and chemistry at relatively high spatiotemporal resolution. Errors in the boundary conditions used to drive background concentrations may have a spatially and temporally variable influence on model output, resulting in systematic biases in the inferred emissions, chemical loss, or chemical production. Understanding the sensitivity of the simulated observations to boundary conditions is critical to avoiding these biases. We characterize the sensitivity of simulated concentrations to boundary conditions to predict and correct the influence of boundary condition errors. We consider the case of inverse analyses of satellite observations used to infer emissions, but our analysis is generalizable to any regional simulation of atmospheric trace gases.

Boundary conditions for regional simulations define the background concentrations of atmospheric trace gases and their precursors. These conditions are often provided by coarse-resolution global simulations adjusted to be unbiased with respect to observations (e.g., Lauvaux et al., 2012, Gockede et al., 2010, Qu et al., 20xx). However, the observations may be insufficient to correct the boundary condition at the spatial and temporal resolution necessary to capture background variability (citation—maybe Lu’s paper?). Other studies use smoothed atmospheric observations as boundary conditions (e.g., Estrada et al., 2023). These approaches are limited to spatiotemporally dense data and may also remove systematic variability..

Residual biases in the boundary condition are particularly significant for analyses of long-lived gases for which the inflow dominates the observed concentrations, or for which the variability of inflow dominates observed variability.

Biases in simulated concentrations resulting from boundary conditions can propagate to inferred emissions, chemical loss, or chemical production. Inverse analyses compare observed concentrations to a chemical transport model (CTMs) to find the emissions, chemical loss, or chemical production that best explain the observations. However, any systematic biases in the CTM or CTM parameters, including boundary conditions, can propagate to the optimal solution. For example, in the case of emissions optimization, an inversion could attribute a positive bias in the boundary condition to emissions, resulting in an overestimate. To address this problem, boundary condition elements are often optimized as part of the inverse analysis (e.g., …). However, it is often unclear the temporal and spatial resolution necessary to capture boundary condition variability (e.g., Lauvaux et al. 2012).

… Satellites now measure atmospheric trace gas concentrations at sufficiently high-resolution to quantify emissions on a regional scale (e.g., citations).

* Challenge is that state vector is limiting factor

Lauvaux, etc

*4th: what motivates you and your setup, and tease at broader impacts*

We present a theoretical and numerical framework to quantify, predict, and correct the influence of these biases on the improved emissions estimates. We use a simple one-dimensional model for the transport of an inert tracer to demonstrate

Thoughts

Is there a way to use a very simple inverse analysis to get at the errors in BCs for non-inverse problems? For example, could you look at the sensitivity of the observations to the first grid cell, second grid cell, etc, without characterizing the jacobian/gain matrix for the entire domain?

[Regional inverse analyses description

* Include differences/similarities with regional AQ BC problems]

[Past attempts to address errors in boundary conditions:

* Wecht?
* Maasakkers
* Shen
* Miller?
* U of M paper]

[To do:

* Add analysis of “buffer” grid cell approach—this is missing]

**2.**

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 h-1). The domain is ventilated with wind speed (km/hr). The model simulates the atmospheric concentrations (ppb) in each grid box at a given time .

**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 and the vector of boundary conditions (Brasseur and Jacob, 2017). If the CTM is linear, then where is the Jacobian matrix and is a vector function 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 posterior emission estimate can therefore be understood as a prior emission update, with contributions from the observations (**)**, the prior emissions (**)**, and the boundary condition (**)**. We then define a fractional boundary condition contribution vector with individual elements that represent the relative contribution of the boundary condition to the total adjustment from the prior to the posterior emissions in grid cell so that

where indicates the absolute value. We can use this fractional contribution to define an boundary condition influence length scale such that all grid cells beyond the length scale have less than some threshold.

We define the influence length scale threshold by solving 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. We can then

**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 h-1). The domain is ventilated 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 with the “true” boundary condition, perturb the boundary condition by a constant, and solve the inversion again. Following equation (5), the sensitivity of the posterior emissions to a constant error in the boundary condition is given by the row-wise sum of the gain matrix weighted by the error in the boundary condition. The row-wise sum of is 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 . To demonstrate the sensitivity of the gain matrix to these parameters, 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 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. 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 baseline relative errors of 50%. If the prior emissions are less than the mean prior emissions, 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 no error covariance. We construct the Jacobian matrix using a finite difference approach.

Figure 4 shows the posterior emissions for the base inversion assuming the true boundary condition is known. The inversion 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.

**3.2.1 Numerical steady-state solution**

We use our simple numerical model to perturb the true 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. We also show the influence length scale threshold of 10 ppb d-1 or 20% of the baseline prior errors. As expected, the error scales with and agrees with the row-wise sum of the gain matrix. For all priors and perturbation magnitudes, the error decreases exponentially as the distance from the upstream boundary increases and is lower than the influence length scale threshold within 6 grid cells. 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.

Figure 6 shows the sensitivity of the gain matrix band width and influence length scale to inversion parameters in the numerical model. 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 , which reflect the inversion’s attempt to capture the sensitivity of the observations 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 also 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 boundary condition constant is no longer uniform. However, the gain matrix can still be used to predict the influence of boundary condition errors on the posterior emissions. As demonstration, we 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 the oscillating perturbations for inversions that do and do not optimize the boundary condition. In all cases, the errors in the posterior persist beyond the initial, upstream enhancement that defines the influence length scale. The inversions that correct the boundary condition result in marginally smaller errors in the downstream grid boxes. However, these inversions also exhibit a longer influence length scales because a single correction term is insufficient to correct the oscillating error in the boundary condition. The longer influence length scale also cannot be predicted using equation (5) with a constant perturbation, which would suggest that correcting the boundary condition would result in an influence length scale of zero. By contrast, the inversions that do not correct the boundary condition all exhibit influence length scales consistent with those predicted by the constant perturbation results. This allows for estimation of the influence length scale even with no knowledge of the boundary condition error.

The consistency of the influence length scale between the oscillating and constant boundary condition perturbations for the inversion that does not optimize the boundary condition results from the significance of the gain matrix in equation (5). This expression shows that the sensitivity of the posterior to the boundary condition is given by the product of the row-wise sum of the gain matrix with the change in the constant term between inversions with true and perturbed boundary conditions. While the constant term associated with the oscillating boundary condition perturbation varies in space and time, it remains on the same order of magnitude as a constant boundary condition perturbation. Moreover, the scaling provided by the row-wise sum of the gain matrix remains the same between the two inverse models.

The consistency of the gain matrix across boundary condition errors and its significance for predicting the influence of these errors on the posterior means that the corrections suggested by figure 6 can be used to decrease the influence length scale even for oscillating boundary condition errors. Figure 9 shows that scaling the observational variances over the first grid box by a factor of 10 significantly reduces the influence scale of the oscillating perturbations (from about 5 to about 2). This correction is consistent with what is predicted by the constant boundary condition perturbation result. In both cases, increasing the observational errors loosens the observational constraint to allow larger corrections to the prior in the first grid box than would otherwise occur. However, while increasing the observational errors in this way decreases the influence length scale, the posterior errors later in the domain persist.

The significance of posterior errors beyond the influence length scale can be predicted using equation (5) if the difference between the true and perturbed constant is known. In practice, it isn’t. However, in the case of oscillating (time-varying) boundary condition perturbations, is a

* Can we model the “true” BC as some unknown sine wave and the known BC as a known sine wave and then maybe come up with a simplified expression for their difference

is in theory a function of the period of the oscillating error in the boundary condition and the ventilation time scale. However, characterizing these errors and their dependence on these quantities remains challenging.

* does the phase matter? Could we check that as long as you get the period right, the rest is easy to predict?
* We find that the BC is corrected to a relatively constant level regardless of the number of temporal elements optimized
* We find that that optimized BC level is slightly above the true BC. This is probably because the accumulation of methane across the domain, which means that the emissions are a large fraction of the observed methane

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

[To write]

* This section needs to discuss how these results interact with the buffer grid cell approach

**4 Discussion and Conclusions**

[To write]