Characterizing and mitigating the impact of model transport errors on CO_2 flux estimates in the assimilation of XCO_2 data from OCO-2

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1. Introduction

Inverse modeling of atmospheric CO_2 holds the promise of providing better estimates of regional sources and sinks of CO_2. However, discrepancies in the atmospheric transport models employed in these analyses have posed a challenge to obtaining robust estimates of the sources and sinks. Here we use a weak constraint four-dimensional variational (4D-Var) data assimilation scheme to assimilate atmospheric CO_2 data from the Orbiting Carbon Observatory (OCO-2) to optimize the distribution of atmospheric CO_2 in the GEOS-Chem chemical transport model. We investigate the adjustments to the CO_2 distribution produced by the weak constraint 4D-Var scheme to characterize transport errors in GEOS-Chem.

2. Model and Data

- We use version v35j of the GEOS-Chem adjoint model, driven by GEOS-FP meteorological fields, at a horizontal resolution of 4° x 5°.
- The configuration of the CO_2 simulation is as described in Byrne et al. (2018)
- We use OCO-2 XCO_2 data (version 9), preprocessed to 10s means by D. Baker.
- All modes of the OCO-2 observations (nadir land, glint land, and ocean glint) are assimilated.

3. Data Assimilation Approach

Strong Constraint (SC) 4D-Var

In SC 4D-Var we assume that the model (M) is perfect in evolving the model state (**x**) from time i to i+1

$$\mathbf{x}_{i+1} = M_i(\mathbf{x}_i, \mathbf{p}).$$

Here **p** represents the model parameters (i.e., the CO_2 fluxes). The SC 4D-Var cost function is then given by

$$J(\mathbf{x}_0,\mathbf{p}) = \tfrac{1}{2}\sum_{i=0}^{N}[\mathbf{y}_i - H_i(M_i(\mathbf{x}_0,\mathbf{p}))]^T \mathbf{R}_i^{-1}[\mathbf{y}_i - H_i(M_i(\mathbf{x}_0,\mathbf{p}))]$$
$$+\tfrac{1}{2}(\mathbf{x}_0-\mathbf{x}^b)^T \mathbf{B}_x^{-1}(\mathbf{x}_0-\mathbf{x}^b) + \tfrac{1}{2}(\mathbf{p}-\mathbf{p}^b)^T \mathbf{B}_p^{-1}(\mathbf{p}-\mathbf{p}^b),$$

where **y** are the observations, H is the observation operator, **R** is the observation error covariance matrix, and $\mathbf{B}_x$ and $\mathbf{B}_p$ are the a priori error covariance matrices.

Weak Constraint (WC) 4D-Var

In WC 4D-Var we account for errors ($\boldsymbol{\eta}$) in the model as follows:

$$\mathbf{x}_{i+1} = M_i(\mathbf{x}_i, \mathbf{p}) + \eta_{i+1},$$

where $\boldsymbol{\eta}$ are the forcing terms that capture the errors. We augment the cost function with an additional term to solve for these errors:

$$J(\mathbf{x}_0,\eta) = \tfrac{1}{2}\sum_{i=0}^{n}[\mathbf{y}_i - H_i(\mathbf{x}_i,\mathbf{p})]^T \mathbf{R}_i^{-1}[\mathbf{y}_i - H_i(\mathbf{x}_i,\mathbf{p})]$$
$$+\tfrac{1}{2}\sum_{i=1}^{n}\eta_i^T \mathbf{Q}_i^{-1}\eta_i + \tfrac{1}{2}(\mathbf{x}_0-\mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x}_0-\mathbf{x}^b).$$

Experiments

- We assimilate OCO-2 data from 1 July – 30 September 2016 to:
  1. solve for monthly mean fluxes using the SC approach;
  2. solve for the CO_2 state and the forcing terms (only between 66°S – 66°N) using the WC approach.
- The model is spun up by assimilating OCO-2 data using the SC 4D-Var from September 2014 to September 2015, and then by running it without assimilation from 1 June 2015 to 1 July 2016 to generate initial conditions for 1 July 2016 (the beginning of the analysis period).
- Here we focus only on the results for August 2016, the middle of the assimilation period.

4. Results

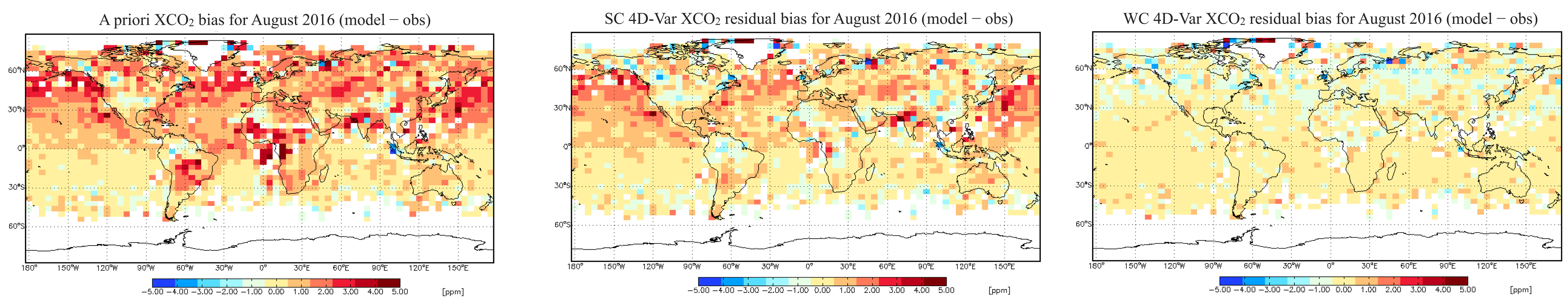

Figure 1. A priori XCO_2 bias (left), SC 4D-Var residual bias (middle), and WC 4D-Var residual bias (right). The bias is calculated as model − observations and is given in ppm.

- The SC assimilation reduced the XCO_2 biases over the continental regions, but large residual biases remain over the oceans in the extratropical NH.
- The WC assimilation successfully removed the a priori XCO_2 bias and reduced the standard deviation by a factor of 2 (Table 1).

Table 1. Mean and standard deviation of the model − observation differences.

	Mean (ppm)	StDev (ppm)
A priori	0.73	1.99
SC 4D-Var	0.27	1.58
WC 4D-Var	-0.02	1.01

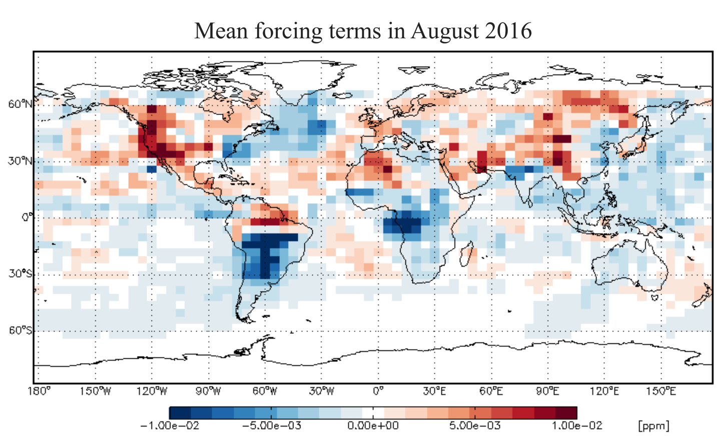

Figure 2. Monthly mean WC forcing (η) in August 2016, vertically averaged from the surface to 11 km.

- The large-scale forcing pattern is consistent with the a priori bias, with negative forcing where there are large positive biases, such as over South America, central Africa, and the northwestern Atlantic and Pacific oceans.

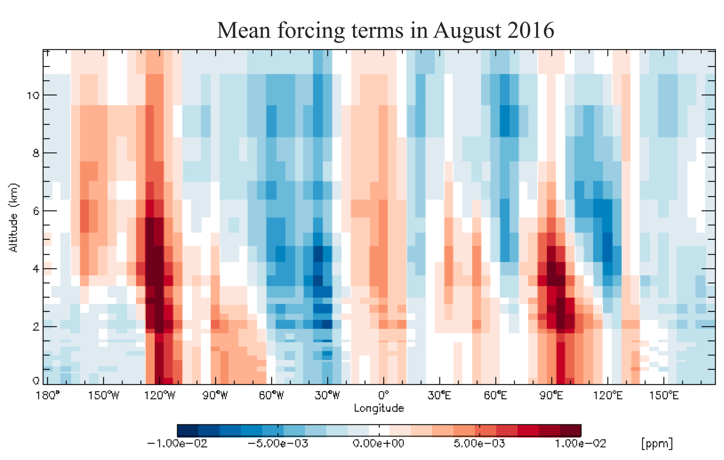

Figure 3. Altitude-longitude cross section of the monthly mean WC forcing, averaged between 40°N – 55°N.

- The forcing increased CO_2 in the lower troposphere over North America and East Asia, while decreasing it in the upper troposphere and downwind of the continental regions.

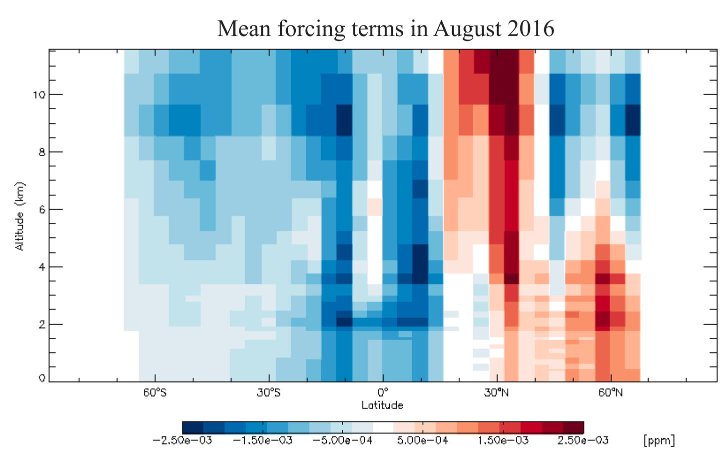

Figure 4. Zonal mean WC forcing for August 2016.

- The zonal mean forcing has a dipole structure poleward of 45°N, consistent with the vertical transport bias identified by Schuh et al. (2019).

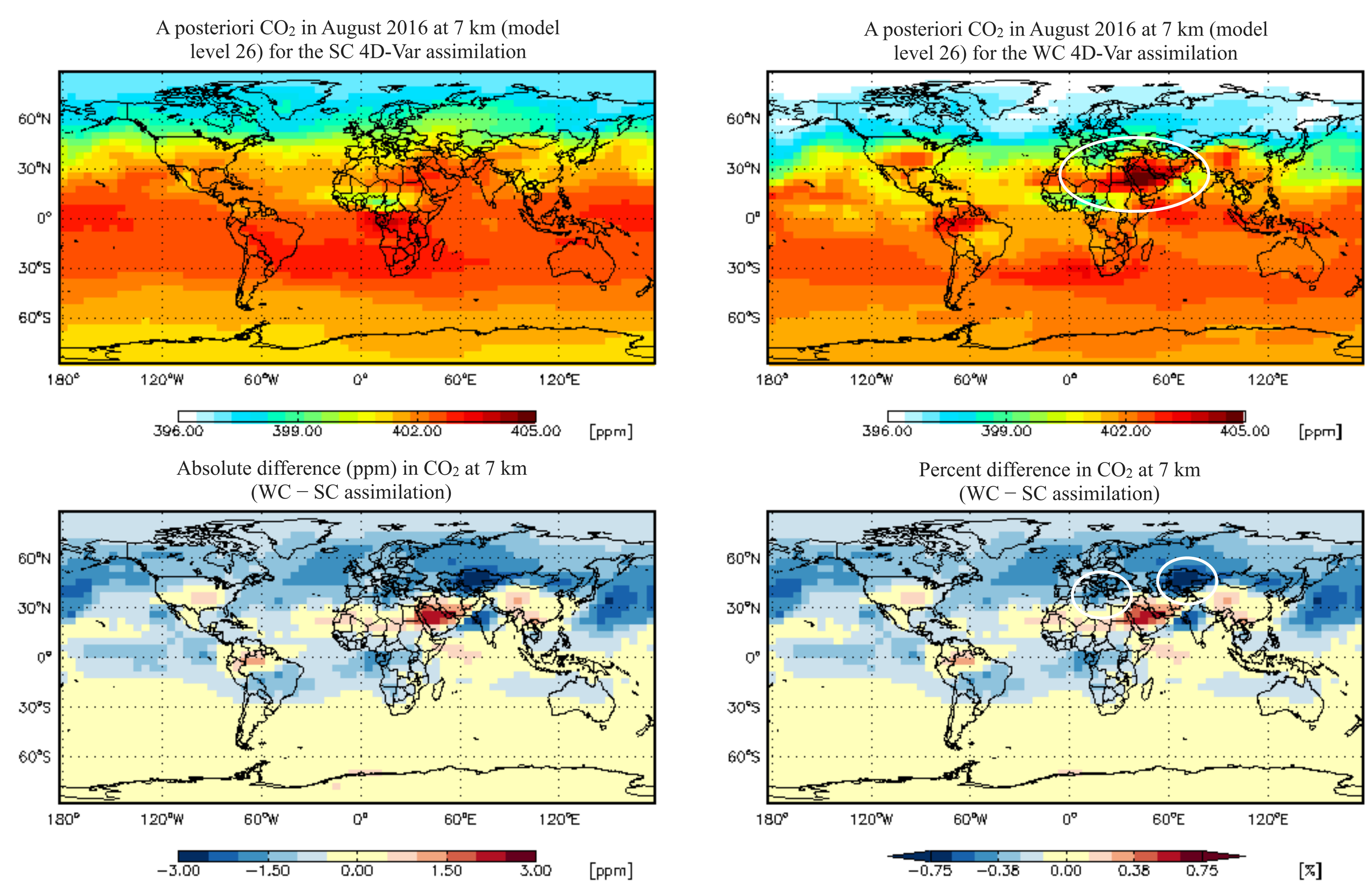

Figure 5. Monthly mean a posteriori CO_2 at 7 km for the SC (top left) and WC (top right) assimilation, and the absolute (bottom left) and percent (bottom right) differences between the a posteriori fields.

- A prominent feature in the upper troposphere in the WC assimilation is the CO_2 maximum over the Middle East, which is similar to the observed Middle East ozone maximum (Li et al., 2001; Liu et al. 2009).
- The Middle East ozone maximum is linked to the Arabian anticyclone and descent over the Mediterranean and central Asia, where the WC assimilation produces a reduction in CO_2.
- Discrepancies in capturing this transport feature could have implications for inferred European and North African fluxes.

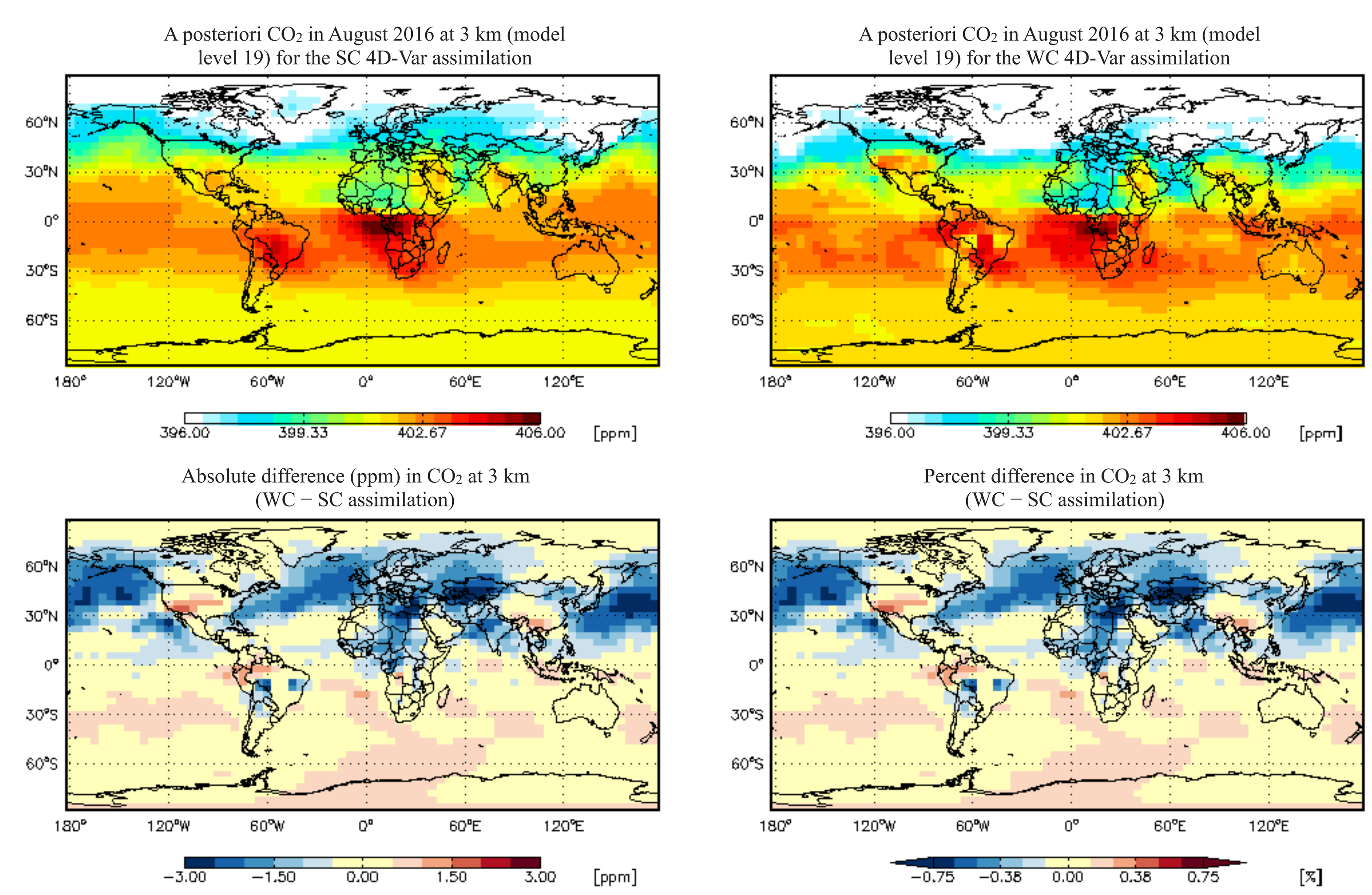

Figure 6. Monthly mean a posteriori CO_2 at 3 km for the SC (top left) and WC (top right) assimilation, and the absolute (bottom left) and percent (bottom right) differences between the a posteriori fields.

- In the lower troposphere the WC assimilation produces lower CO_2 abundances along the storm tracks over the northern Atlantic and Pacific oceans, which could be associated with discrepancies in synoptic transport in the model.

5. Summary

- The WC 4D-Var scheme provides a means of mitigating systematic errors in the assimilation of XCO_2 data.
- The estimated WC forcing terms suggest the presence of errors associate with summertime synoptic transport in the extratropical northern hemisphere.

6. References

Byrne, B., et al. (2018). Evaluating GPP and respiration estimates over northern midlatitude ecosystems using solar-induced fluorescence and atmospheric CO_2 measurements. Journal of Geophysical Research: Biogeosciences, 123. https://doi.org/10.1029/2018JG004472.

Li, Q., et al. (2001). A tropospheric ozone maximum over the Middle East, Geophys. Res. Lett., 28(17), 3235– 3238, doi: 10.1029/2001GL013134.

Liu, J. J., et al. (2009). Analysis of the summertime buildup of tropospheric ozone abundances over the Middle East and North Africa as observed by the Tropospheric Emission Spectrometer instrument, J. Geophys. Res., 114, D05304, doi:10.1029/2008JD010993.

Schuh, A. E., et al. (2019). Quantifying the impact of atmospheric transport uncertainty on CO_2 surface flux estimates. Global Biogeochemical Cycles, 33, 484–500. https://doi.org/10.1029/2018GB006086.