Supplemental Material

Joint inverse estimation of fossil fuel and biogenic CO_2 fluxes in an urban environment: An observing system simulation experiment to assess the impact of multiple uncertainties

Kai Wu[1*], Thomas Lauvaux[1], Kenneth J. Davis[1], Aijun Deng[1], Israel Lopez Coto[2], Kevin R. Gurney[3], Risa Patarasuk[3]

[1]Department of Meteorology and Atmospheric Science, Pennsylvania State University, University Park, Pennsylvania, USA

[2]National Institute of Standards and Technology, Gaithersburg, Maryland, USA

[3]School of Life Sciences, Arizona State University, Tempe, Arizona, USA

*Corresponding author: kzw151@psu.edu

December 20, 2017

List of Contents:

Text S1: In this section, we present the impact of varying both the Root Mean Square Error (RMSE) and the Spatial Correlation Length (SCL) in the prior flux error structures on the Degree of Freedom in the Signal (DFS). We express the DFS = Trace(KH) with K the Kalman Gain and H the influence function (Rodgers, 2000). Figure S1 illustrates the relationship between the DFS and the SCL from 1 km to 100 km. Three modes are observed depending on the values of SCL. For low values of SCL (less than 2 km), the DFS becomes very small instead of converging to the maximum DFS (assuming no spatial coherence in the inverse emissions). This problem has been illustrated by Bocquet (2005) as a singularity of the Continuum Limit. The Gram matrix $G = HBH^T$ (i.e. the Hessian of the dual problem) is not well defined and requires regularization at high resolutions. This regularization is performed here by the introduction of correlations in B matrix. For intermediate values (2 km < SCL < 8 km), the tower footprints overlap over the city which limits the impact of the SCL as the state space is already coherent, at least around the tower locations. The values of the DFS are nearly constant over the 2 - 8 km range of SCL

values. For the last segment of the plot, when SCL is larger than 10 km, the DFS decreases steadily as the impact of the prior error correlation artificially extends the optimization to the entire state space, beyond the city limit.

Text S2: We present the averaging kernel sensitivity for four cases in scenario 1 corresponding to Figure 5 in the main text (Figure S2). Compared to the error reduction maps, the averaging kernel sensitivity maps show marginal differences across the different cases for low error variance (Figure S2A) and intermediate error variance while the SCL is varying from 2 to 8 km (Figure S2C and S2D). Despite the changes in SCL values, the DFS remains similar. Considering higher values of error variance, DFS shows more sensitivity when the RMSE is 4 μmol m^{-2} s^{-1} (Figure S2B), but no dependence for smaller values (i.e. 1 or 2 μmol m^{-2} s^{-1}). The overall spatial extent of the different maps remains similar, with small variations compared to the error reduction maps presented in Figure 5. We conclude here that DFS values, as a product of prior error assumptions and observational constraints, is inadequate to estimate the impact of prior emissions errors in our inversion system.

Figure S1: The change of Degree of Freedom in the Signal (DFS) corresponding to different Spatial Correlation Lengths (SCLs) in prior flux error structures.

Figure S2: The diagonal elements of the averaging kernel matrix (*i.e.* S = KH) for four cases in scenario 1 corresponding to Figure 5 in the main text.

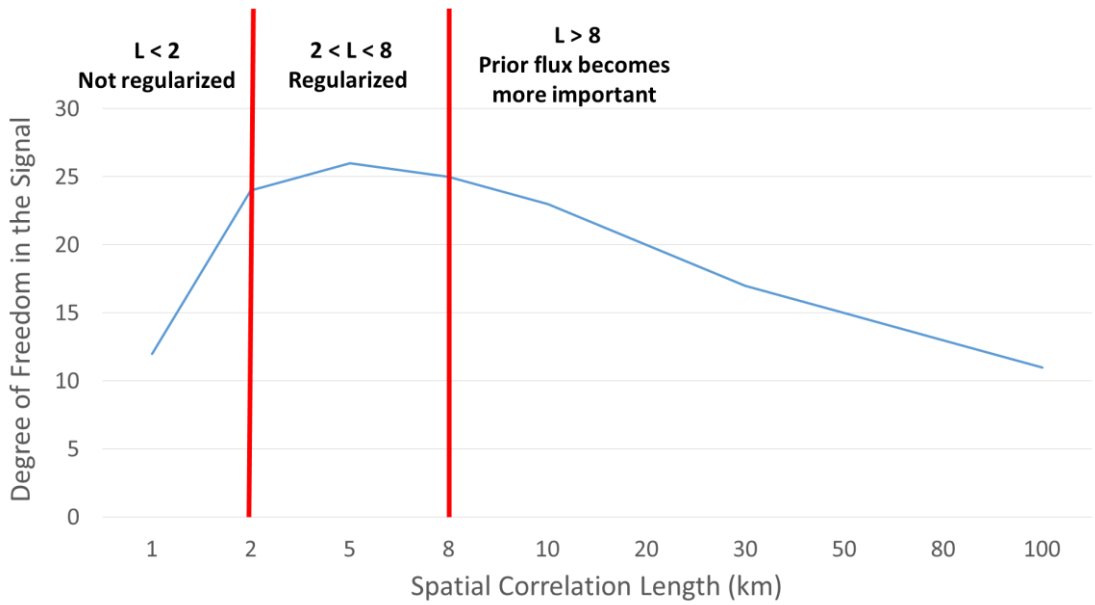

Figure S1: The change of Degree of Freedom in the Signal (DFS) corresponding to different Spatial Correlation Lengths (SCLs) in prior flux error structures.

Using 12 towers with 1 ppm observation error at each tower to analyze the relationship between the DFS and the SCL in prior emissions errors. The Root Mean Square Error (RMSE-B) is 2 μmol m^{-2} s^{-1}.

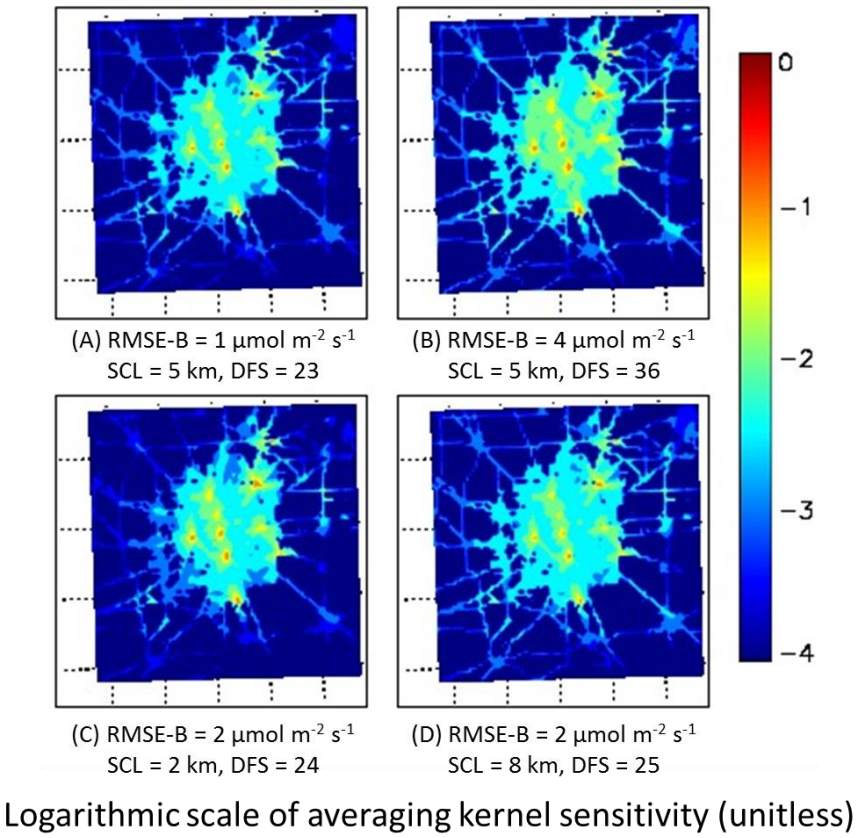

Figure S2. The diagonal elements of the averaging kernel matrix (*i.e.* S = KH) for four cases in scenario 1 corresponding to Figure 5 in the main text.

Test of the averaging kernel sensitivity and the Degree of Freedom in the Signal (DFS) for different Root Mean Square Errors (RMSE-Bs) and Spatial Correlation Lengths (SCLs) in prior flux error structures. Values are displayed on a logarithmic scale.

References:

Rodgers, C. D. (2000). *Inverse methods for atmospheric sounding: theory and practice* (Vol. 2). World scientific.

Bocquet, M. (2005). Grid resolution dependence in the reconstruction of an atmospheric tracer source. *Nonlinear Processes in Geophysics*, *12*(2), 219-233.