Supplementary Materials for “Observed impacts of COVID-19 on urban CO₂ emissions”

Alexander J. Turner, Jinsol Kim, Helen Fitzmaurice, Catherine Newman, Kevin Worthington, Katherine Chan, Paul J. Wooldridge, Philipp Köhler, Christian Frankenberg, & Ronald C. Cohen

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Introduction

This supporting information contains seven additional sections of text and 13 figures. Associated code for this project can be found here: https://github.com/alexjturner/UrbanInversion/. Figure S1 shows a map of the region. Figure S2 shows a timeseries of all observations used and the number of sites at a given hour. Figure S3 shows the cumulative influence on the BEACO₂N network for different background criteria. Figure S4 shows a timeseries of CO₂ concentrations from the AmeriFlux network that is to the east of San Francisco. Figure S5 shows a distribution of travel times for airmasses to travel from the AmeriFlux sites to the Bay Area. Figure S6 shows information on the airmasses as they pass by the AmeriFlux sites. Figure S7 shows the prior fluxes for one week in March 2020. Figure S8 shows the time-dependent model error. Figure S9 shows a subset of the prior error covariance matrix. Figure S10 shows the cumulative influence on the BEACO₂N network. Figure S11 shows a k-fold cross evaluation of observed and simulated CO₂ concentrations using prior and posterior fluxes. Figure S12 shows a timeseries of CO₂ concentrations at one site using prior and posterior fluxes, Figure S13 shows the residuals and comparison to the network for the same site.

Text S1. BEACO₂N measurements

We use hourly-averaged level two observations from the BEACO₂N network. Data can be found on the project page here: http://beacon.berkeley.edu/. Level two indicates they were automatically calibrated and inspected by a person. Figure S2 shows a timeseries of the observations and the number of active sites over our study period.

Text S2. Atmospheric transport

The methodology used here is adapted from previous work by Turner et al.[1]. We use meteorological fields from the NOAA High Resolution Rapid Refresh (HRRR [2]), to drive the Stochastic Time-Inverted Lagrangian Transport (STILT [3]) model, a Lagrangian particle dispersion model. Meteorological fields from HRRR are generated at 3 km horizontal
Figure S1: Map of the San Francisco Bay Area. Same as main text Fig. 1A but overlaid on a map of the region. Highways are in yellow.
resolution. The STILT model advects an ensemble of 1000 particles 30 hours backward in time, each with a small random perturbation, from the spatio-temporal receptor points using the meteorological fields from HRRR. These trajectories can be used to construct measurement footprints, representing the sensitivity of the measurement to a perturbation in emissions from a given location. See [1] for example trajectories and footprints in the San Francisco Bay Area.

Text S3. Specifying the upwind concentrations

We are inverting for emissions over a domain centered on San Francisco (dashed box in Fig. S7). As such, we need to know the concentration upwind of our domain. More specifically, we need the background concentration ($b_i$) to relate the measurements to the emissions:

$$y_i = h_i x + b_i.$$  \hspace{1cm} (1)

We estimate the background concentration using the ensemble of STILT trajectories. The majority of the airmasses that reach our sensors come from the west (see Fig. S10). However, a small fraction of trajectories come from the east through the Sacramento Delta (see right panel of Fig. S3). We have two sets of observational data to infer background concentrations for our domain: 1) NOAA measurements in the Pacific and 2) AmeriFlux measurements in the Sacramento Delta. The AmeriFlux sites are primarily located within the green circle shown in Figure S3.

Fig. S4 shows the timeseries of AmeriFlux CO$_2$ measurements. The AmeriFlux measurements are located approximately 55 km away. It would take 6 hours for the airmasses to travel from the AmeriFlux sites to our nodes at a windspeed of 2.5 m/s. As such, we have used a 6-hour moving window to smooth the AmeriFlux measurements.
Figure S3: **Region of influence for different background conditions.** Cumulative surface influence on the BEACO\textsubscript{2}N network using data from February 1, 2020 through April 31, 2020. Left panel shows results for trajectories that reach the NOAA “pacific curtain.” Right panel shows results for trajectories that pass within 25-km of the AmeriFlux sites. Green dot indicates mean location of AmeriFlux sites and the green circle indicates a 25-km radius.

Figure S4: **Timeseries of CO\textsubscript{2} concentrations at AmeriFlux sites.** Black dots are all of the AmeriFlux CO\textsubscript{2} measurements. Blue line is a 6-hour moving mean. Gray lines are the uncertainties.
We classify each observation based on whether or not it passed near the AmeriFlux sites. That is to say, we check each trajectory to see if it passed through the green circle shown in Fig. S3. Here, “near” is defined as within 25 km of the AmeriFlux sites. The right panel of Fig. S3 shows the cumulative influence for observations with trajectories that passed within 25 km of the AmeriFlux sites and the right panel shows the cumulative influence for all other observations. We can see that this classification does a good job separating the two dominant flow patterns at this time of year.

Fig. S5 shows the time required for airmasses to travel from the AmeriFlux sites to a BEACO₂N node. The mode of the distribution is just under 5 hours, consistent with our back of the envelope calculation above. Some trajectories take longer due to lower windspeeds and because they do not take a straight path between the two locations. Fig. S6 provides additional information about the trajectories that come from the east. We find that most of the trajectories are below 1 km when they pass the AmeriFlux sites and likely within the boundary layer, as such the AmeriFlux sites should be a good measure of the upwind CO₂ concentration.

Figure S5: Travel time from AmeriFlux sites. Histogram showing the number of hours required to travel from the AmeriFlux sites to the corresponding BEACO₂N node. Travel time is computed using the STILT back trajectory. Figure only shows data for trajectories that pass within 25-km of the AmeriFlux sites.

Text S4. CO₂ fluxes from the biosphere

We estimate net ecosystem exchange (NEE) from the biosphere using Solar Induced chlorophyll Fluorescence (SIF) data from the space-borne TROPOMI instrument. Here, we use SIF data that has been downscaled fo 500-m spatial resolution following Turner et al.[4]. Turner et al. (in prep) extended this to develop ecosystem-specific scalings from SIF to gross primary productivity (GPP) that we partition over the course of the day based on the cosine of the solar zenith angle. Baldocchi & Penuelas, [5] find that annual mean respiration scales linearly with annual mean GPP over a range of ecosystems. Specifically, they find that respiration = GPP×0.822. Following this, we assume that respiration can be related to the annual mean GPP (inferred from TROPOMI SIF) over the previous 365 days. We then partition that respiration based on a seasonal temperature scaling and apply a diurnal scaling based on Yang et al.[6].
Figure S6: **Trajectory information for AmeriFlux backgrounds.** Left panel shows a histogram of particle heights when they are within 25-km of the AmeriFlux sites. Right panel shows a histogram of the minimum distance between the AmeriFlux sites and the STILT trajectory. Orange shading indicates those trajectories are within the 25-km AmeriFlux radius. Vallejo nodes are 50 km from the AmeriFlux sites, thus increase in the histogram at that distance (the minimum distance occurs at the starting location for trajectories that come from the Pacific).

Our seasonal temperature data is taken from the Oakland National Weather Service office.

**Text S5. Inferring the posterior fluxes**

We infer the most likely CO$_2$ fluxes from BEACO$_2$N observations using Bayesian inference. Here we estimate hourly fluxes at 900-m spatial resolution over the San Francisco Bay Area. The inversion domain can be seen as the black/white dashed box in the top left panel of Figure S7. Our horizontal domain is $m_x \times m_y$ where $m_x = 157$ and $m_y = 127$. We estimate emissions for overlapping 96 hour windows ($m_t = 96$) to allow observations to constrain emissions prior to that day. The windows are centered on an individual day with a 36 hour buffer on both ends (36+24+36). As such, our state vector ($\mathbf{x}$) is a vector of length $m = 1, 91, 144$. We assume Gaussian errors and include off-diagonal terms in both error covariance matrices. Following [7], we solve for the posterior fluxes as:

$$\hat{\mathbf{x}} = \mathbf{x}_a + (\mathbf{HB})^T (\mathbf{HB}^T + \mathbf{R})^{-1} (\mathbf{y} - \mathbf{Hx}_a). \quad (2)$$

$\hat{\mathbf{x}}$ ($m \times 1$) is the posterior emissions, $\mathbf{x}_a$ ($m \times 1$) is the prior emissions, $\mathbf{y}$ ($n \times 1$) is the BEACO$_2$N observations, $\mathbf{H}$ ($n \times m$) is the matrix of footprints from HRRR-STILT, $\mathbf{R}$ ($n \times n$) is the model-data mismatch error covariance matrix, and $\mathbf{B}$ ($m \times m$) is the prior error covariance matrix.

The prior emissions are adapted from previous work (Turner *et al.*[1]) but now use a biosphere derived from TROPOMI SIF observations (Turner *et al.*[4]). Additionally, we manually inspected the 20 largest point sources to ensure their emissions were allocated to plausible locations. Figure S7 shows the mean emissions for a week in March 2020.

The model-data mismatch error covariance matrix ($\mathbf{R}$) has three contributions: instrument error, background error, and model error that we assume can be added in quadrature:

$$\mathbf{R} = \mathbf{R}_I + \mathbf{R}_B + \mathbf{R}_M. \quad (3)$$
Figure S7: **Prior fluxes used in the inversion.** Top left panel shows the mean fluxes over Northern California from March 15, 2020 through March 21, 2020. Dashed box indicates region used for the flux inversion. Right panel shows same fluxes over the inset region. Blue line indicates the region of influence for the BEACO$_2$N network (see discussion in Section S4). Bottom panel shows the total CO$_2$ flux over the region of influence. Panel shows total flux (black), point sources and residential heating (purple), traffic (orange), and net ecosystem exchange from the biosphere (green). The yellow-to-blue shading is the cos(SZA) to indicate daytime and nighttime.
The instrument error is derived from the standard deviation of the BEACO$_2$N measurements over an hour with a lower bound on the error of 1 ppm. We assume the model error is time dependent and can be seen in Figure S8, this assumes that our model has less error during the well-mixed afternoon, the most error in the morning (evening) when the PBL height is rising (falling), and the evening is in between because the boundary layer will be lower. We use the ensemble of STILT trajectories to estimate the background error by looking at the standard deviation of the background value over the 1000 trajectories for each BEACO$_2$N observation (Section S2). We impose a correlation length scale of 2 km based on a variogram analysis from a mobile measurement campaign (Turner et al., in prep) and a temporal correlation length scale of 1 hour.

Finally, this leaves the prior error covariance matrix: $B$. The dimension of this matrix is $m \times m$ and contains more than $10^{12}$ elements, making it computationally intractable to write out explicitly. Following Meirink et al.[8], Singh et al.[9], and Yadav & Michalak[10], we express our prior error covariance matrix as a Kronecker product of a temporal covariance matrix ($D; m_t \times m_t$) and a spatial covariance matrix ($E; m_x \times m_y \times m_x m_y$). This allows us to write $B$ as:

$$B = D \otimes E = \begin{pmatrix}
    d_{(1,1)}E & \cdots & d_{(1,m_t)}E \\
    \vdots & \ddots & \vdots \\
    d_{(m_t,1)}E & \cdots & d_{(m_t,m_t)}E
\end{pmatrix}$$

(4)

where $\otimes$ is the Kronecker product. Our implementation is adapted from Yadav & Michalak[10].

The temporal and spatial covariance matrices can be expressed in terms of correlation matrices and diagonal variance matrices:

$$\Sigma = \sqrt{f_\sigma} V^{1/2} M V^{1/2}$$

(5)

where $\Sigma$ is an $p \times p$ covariance matrix, $M$ is an $p \times p$ correlation matrix, $V$ is an $p \times p$ diagonal matrix of variances, and $f_\sigma$ is an uncertainty scaling factor (here we have chosen $f_\sigma$
Figure S9: **Prior error covariance matrix.** Top left panel shows the upper left block of the temporal error covariance matrix (D). Top right panel depicts a single row of D and the temporal decay parameters ($\tau_A$ and $\tau_B$). Bottom left panel shows a 256x256 block of the spatial error covariance matrix (E). Bottom right panel depicts a single row of E and the spatial decay parameter ($\tau$).
= 0.5, corresponding to a 50% uncertainty). Thus, the temporal covariance matrix is \( D = \sqrt{\tau_D} V_D^{1/2} M_t V_D^{1/2} \) and the spatial covariance matrix is \( E = \sqrt{\tau_S} V_S^{1/2} M_s V_S^{1/2} \).

We construct \( M_t \) and \( M_s \) from the prior emission inventory on the assumption that road grid cells should be correlated with other roads, the biosphere grid cells should be correlated with other biosphere grid cells, etc. We then impose an exponential decay in the correlation for grid cells should be correlated with other roads, the biosphere grid cells should be correlated with other biosphere grid cells, etc. This can be clearly seen by looking at the gain matrix. Posterior emissions will reflect the prior emissions in regions with low sensitivity from the measurements. This occurs when the sensitivity to a region is low and means that our posterior emissions will be unchanged from the prior emissions. As such, we focus our study on regions with high sensitivity because those are the regions that our observations can constrain.

Ideally this region of influence would be defined based on the posterior error covariance matrix or averaging kernel, but those matrices are dimension \( m \times m \) and computationally intractable for our state vector size. Instead, we define our region of influence based on the magnitude of the footprint. A similar approach was taken by Rigby et al. [11].

The footprint from STILT for the \( i \)th receptor is a third order tensor with dimensions \( m_x \times m_y \times m_t \): \( F_i(x, y, t) \), where \( m_x = 157 \), \( m_y = 127 \), and \( m_t = 30 \). The total network sensitivity is computed by summing the over the time dimension and summing over all receptors: \( S(x, y) = \sum_i \sum_t F_i(x, y, t) \). We then define the “cumulative influence” in a manner similar to a cumulative

\[
G = (HB)^T (HBH^T + R)^{-1}.
\]
distribution function. That is to say, we sort all values in $S(x, y)$ from smallest to largest, perform a cumulative sum, and normalize by $\sum_x \sum_y S(x, y)$. The resulting cumulative influence (right panel of main text Fig. 1) shows the percentile of influence for each grid cell. Figure S10 shows the cumulative influence over the full STILT domain (left) and the smaller inversion domain (right). The white contour indicates the most compact region containing at least 40% of the total network influence. The dashed lines show the same contour if we just consider data before or during shelter in place. The main differences between the two dotted contours is over water where fluxes should be negligible.

Figure S10: Region of influence. Cumulative surface influence on the BEACO$_2$N network. Figure uses data from February 1, 2020 through April 31, 2020. Darker colors indicate those grid cells contain XX% of the total influence on the network. Left panel shows influence over Northern California. Right panel is an inset for the San Francisco Bay Area. Solid white line is the 60$^{th}$ percentile. Dotted lines indicate the 60$^{th}$ for before and during shelter-in-place.

Text S5. Partitioning the posterior fluxes to specific sectors

Sources can be distinguished at high resolution due to spatial separation. McDonald et al.\cite{12} showed this for traffic emissions where freeway emissions were indistinguishable (or blended together) with arterial roads at resolutions coarser than 1-km. In this study, we are solving for fluxes at sub-kilometer spatial resolution.

We remove the biospheric signal before partitioning the posterior fluxes because that is a more diffuse signal and we have observational constraints from TROPOMI SIF. We then define a mask where we classify each grid cell based on the sector. A grid cell is only classified if a single sector (e.g., traffic) accounts for more than 50% of the total emissions.
Text S7. Evaluation of inversion results

Figure S11 shows a $k$-fold cross-validation of the posterior CO$_2$ fluxes. We find the posterior fluxes to explain 23% more variability than the prior CO$_2$ fluxes. Figures S12 and S13 show example timeseries results for a site in the network using both prior and posterior fluxes.

References


Figure S11: **Comparison of observed and simulated CO\textsubscript{2} concentrations.** Points are from a \(k\)-fold cross validation (i.e., data shown was withheld from the inversion). Top row shows all of the data points and their uncertainties. Bottom row is a 2-D histogram (note the log-scale for the colorbar). Left column uses the prior emissions. Right column uses the posterior emissions. Colored lines are from a York Fit allowing for errors in both \(x\) and \(y\).
Figure S12: **Timeseries of observed and simulated CO$_2$.** Timeseries of observed CO$_2$ concentrations (black), simulated CO$_2$ concentrations using prior fluxes (blue), and simulated CO$_2$ concentrations using posterior fluxes (red). Data shown for Cooper Elementary School in Vallejo, CA (38.126°N, 122.240°W).
Figure S13: Timeseries of residuals. Expanded comparison of simulated and observed CO$_2$ at Cooper Elementary School in Vallejo, CA (38.126°N, 122.240°W). Top row shows observed CO$_2$ (black), simulated CO$_2$ using prior fluxes (blue), simulated CO$_2$ using posterior fluxes (red), and the median CO$_2$ concentration across the BEACO$_2$N network (orange). Middle row is the residual between the observed CO$_2$ and the network median. Bottom row is the residual between the observed CO$_2$ and the simulated CO$_2$ (with prior fluxes in blue and posterior fluxes in red).