Supporting Information for "Emissions and topographic effects on column CO$_2$ (X$_{\mathrm{CO}_2}$) variations, with a focus on the Southern California Megacity"

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S1. Detailed description of simple model (Sect. 2.5).

This simple model was constructed with one purpose, namely to answer: How much of a difference in X$_{\mathrm{CO}_2}$ is there between Caltech and JPL if the ML is perfectly well-mixed with a top at the same pressure height at both locations? It does not represent the full true state of the atmosphere. It was constructed using 5 inputs including:

1. A function for the ML height.
2. Average in situ ML enhancements of CO$_2$.
3. Profiles of CO$_2$ for the remainder of the column above the ML.
4. 'Background' values of ML enhancements if there were no enhancements from local emissions.
5. Surface pressures at the different sites.

This is only meant to be a climatology model, showing what the average behavior could look like. It is not meant for direct single day comparisons with measurements.

We also include the AFRC site in the model, but for the purpose of evaluating the model performance rather than extracting results. AFRC is treated differently from Caltech and JPL in that the simulated X$_{\mathrm{CO}_2}$ is simply the integrated a priori column. The Caltech-AFRC difference is discussed in Sect. S1.6.

S1.1. Mixed layer height

For the ML height we make a simple assumption of a Gaussian shape with a peak at 1300 (UTC-8). Again, we note the true atmosphere is more complex (see Ware et al., 2016); our assumption is made simply to get a picture of how the atmosphere may behave on average with high and low values averaging out to get the mean estimate. The peak and base of the daily ML estimates were set to have annual sinusoidal variations. Sinusoidal variation values were set by fitting ECMWF model data from 2010–2014. The maximum daily peaks seemed too large and were scaled down by a factor of 2 to better match the values reported by Ware et al., [2016] and Newman et al., [2013]. These variations were (in km):

$$\text{max ML height} = 0.5\,(0.333\sin\left((yr + 0.848) \times 2\pi\right) + 1.443) \tag{S1}$$

$$\text{min ML height} = 0.0239\sin\left((yr + 0.887) \times 2\pi\right) + 0.106 \tag{S2}$$

where yr is the fraction of the year passed since Jan 1. Further, the width of the daily peaks depend on the length of the day, and have 1σ values that are $\frac{1}{3.4}$ the length of the solar day (between morning and evening SZA=88°).

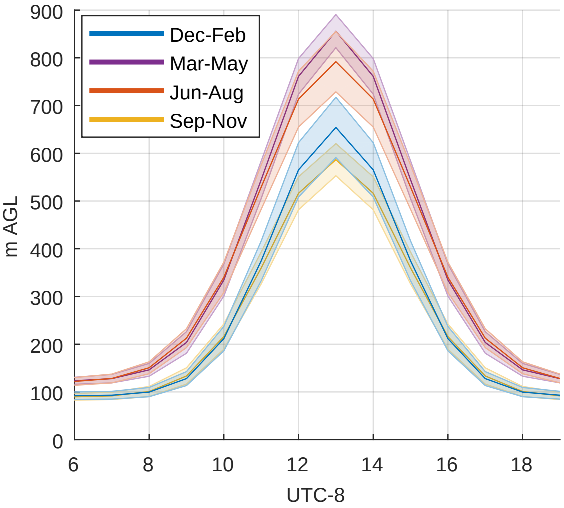

Figure S1. Mixed layer heights for different seasons in the model. Center lines are means and shaded areas are 1σ across the full season.

Seasonal averages are shown in Fig. S1. There is general agreement here with the results of Ware et al., (2016). We find the final results of this model are not particularly sensitive to errors in ML height. This is illustrated in Fig. S2 where once the ML height reaches the altitude at JPL, a change from 200 to 1100 m a.g.l. only causes about a 0.05 ppm change in ΔX$_{\mathrm{CO}_2}$.

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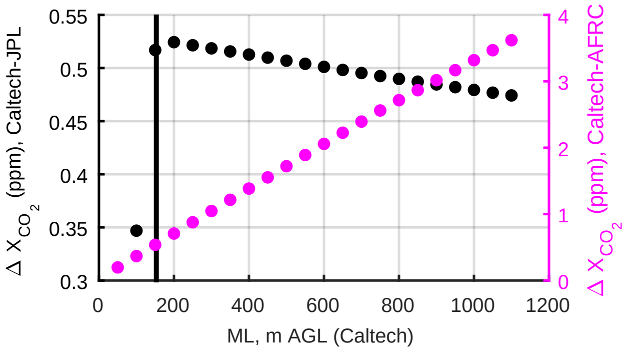

Figure S2. X_{CO_2} differences for different mixed layer heights (above Caltech). The black line indicates the difference in altitude between the 2 sites. Data are from 1 June 2013 with a fixed 30 ppm CO_2 surface enhancement. Note the difference in scale compared to Caltech−AFRC.

S1.2. ML CO_2 enhancement

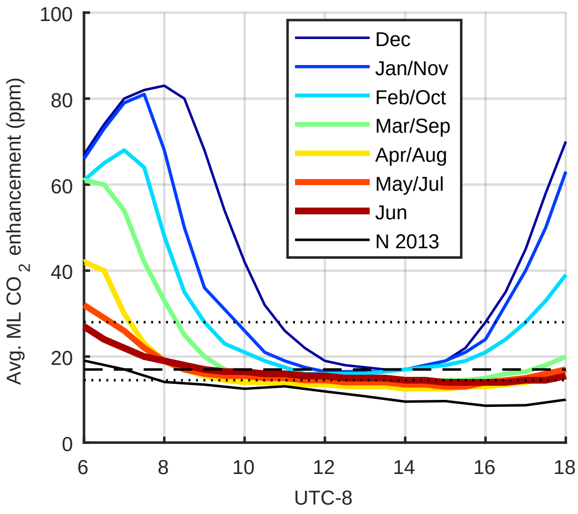

Figure S3. Parameterized average mixed layer CO_2 enhancements at Caltech. The black line is from Newman et al., (2013) using data from May–June 2010. Dashed lines indicate the 25th, 50th, and 75th percentiles.

The true average ML CO_2 enhancement is a complex function of biosphere activity, fossil fuel emissions, dilution from an increased ML volume, and vertical extent of mixing. We do not attempt to account for all of these individually. Instead, we make approximations in our model here based on the average diurnal behavior noted by Newman et al., [2013] and McKain et al., [2012]. We create a lookup table, with estimates of diurnal profiles for each month with some added noise. These profiles have draw-down during the daytime, as shown in Fig. S3. We added additional fossil fuel emissions to the ML enhancement as compared to Newman et al., [2013] because during May–June 2010 when they made their measurements meteorology conditions were atypical which resulted in lower pollution levels than normal [Hersey et al., 2013]. Other months have larger enhancements from less biospheric uptake and a shallower ML.

Despite the generalization of the surface CO_2 behavior at Caltech, the median of 17 ppm is within the 50% confidence interval of the full and mid-day medians noted by Verhulst et al., [2016] at both the USC and FUL sites. Any median value in the 10–20 ppm range would match this criteria.

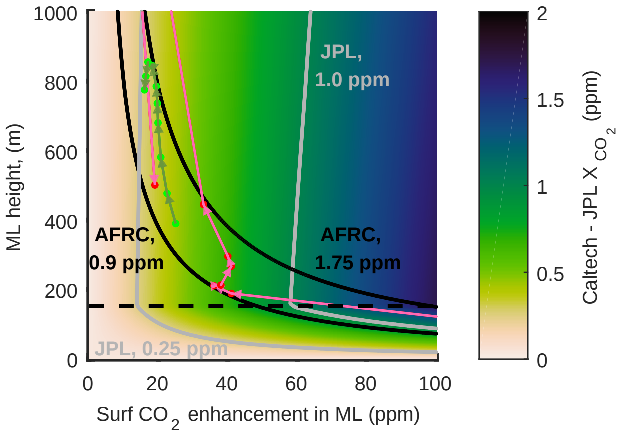

Figure S4. Depiction of what the Caltech-JPL X_{CO_2} differences would be for various ML heights and CO_2 enhancements using 20 May as a test day. Gray and black isopleths are for fixed differences that would be seen for Caltech-JPL and Caltech-AFRC respectively. The green dots are for values observed by Newman et al., (2013). Pink arrows are from constraining values based on the average behavior of the Caltech-JPL and Caltech-AFRC differences (where the isopleths cross for each pair of hourly averaged points).

Figure S4 can be thought of as a lookup table for what the difference in X_{CO_2} between Caltech and JPL would be for different ML heights and surface CO_2 enhancements. Note that for ML heights that are 200 m or higher, there is much greater sensitivity for the range of surface CO_2 values (left and right) than there is for ML height (up and down).

S1.3. CO_2 profiles

Profiles for the remainder of the column are from TCCON a priori mixing ratio profiles. These are the base estimate profiles used in the GGG algorithm when fitting spectra. They are generated based on the secular CO_2 increase with annual variation that depends on latitude. Upper parts of the profiles are adjusted for shifts in the tropopause height. In conjunction with the mixing ratios, profiles are generated that include the pressure at different atmospheric levels based on NCEP/NCAR reanalysis data.

For the AFRC site, the column abundances are calculated by integrating the a priori columns.

S1.4. 'Background' CO_2 values

'Background' CO_2 levels are estimated from a pressure weighted average between 5–9 km in the a priori mixing ratios of CO_2. They are an estimate of how much CO_2 would be seen at the surface without local emissions.

S1.5. Site surface pressure

Site surface pressures are derived by interpolating to the site altitude (240 m for Caltech, 390 m for JPL) using the a priori pressure profiles.

S1.6. AFRC and model evaluation

The modeled-measured mismatch for ΔX_{CO_2} between Caltech and AFRC was about 1.77. Because the 'toy' model underestimates the observed difference between Caltech and AFRC (Fig. 5), it suggests our model needs more CO_2 over Caltech. If this was due to an underestimated enhancement of CO_2 in the ML it would cause an underestimation of the Caltech-JPL difference by about 45%. If it was due to an underestimated ML, or a residual layer with enhanced CO_2 above the ML, it would cause a slight overestimation of ∼0.1%.

We do not take further action here to correct for the model-measured mismatch. The scale factor of 1.77× seems unreasonably large to scale either the surface enhancement or the ML height in the model. Our model only has two layers, and does not include a residual layer disconnected from the surface and observed by Ware et al., [2016]. It seems likely that at least part of the reason for the under-predicted ΔX_{CO_2} is from a residual layer, so we do not attempt to further correct for the measured-model mismatch.

S2. WRF wind vector field

In Fig. S5 is a depiction of the average latitudinal and vertical wind directions. The prevailing surface wind is inland, but winds aloft return to the ocean. Returning winds are enhanced in CO_2 in the uniform emissions scenario. This leads to enhanced X_{CO_2} over the ocean.

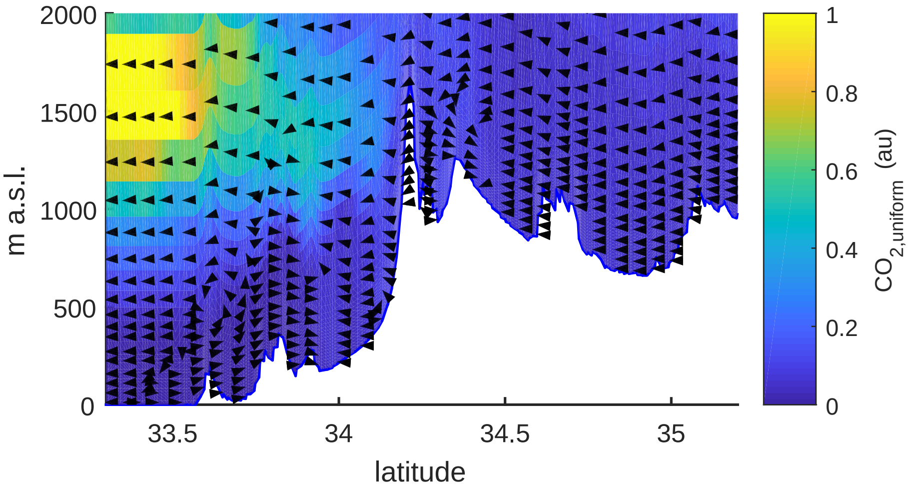

Figure S5. Average wind vector field for the cut shown in Fig. 8 in the main text.