Simulation of Carbonyl Sulfide (COS) to better understand the urban biosphere signal

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Background

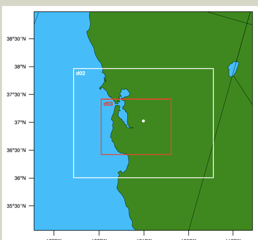
Currently, anthropogenic CO_2 emissions over urban regions can be calculated in several ways: 1) bottom-up approaches (or inventories) based on energy consumption within city limits and emission factors that depend on type of fuel and processes, 2) using $^{14}CO_2$ as tracer for fossil CO_2, and 3) subtracting the biosphere signal from observation (measured) CO_2 data. All of these approaches have their limitations. Given the immense amount of time and resources needed to develop inventories (1), generic emission factors and data assumptions are often used which result in a high degree of uncertainty. Additionally, temporal extrapolation and spatial redistribution lead to further uncertainties. Albeit $^{14}CO_2$ is an ideal tracer for fossil CO_2 because ^{14}C is entirely lost to radioactive decay in fossil fuels, the high costs and technological requirements of radio isotope measurements make method (2) hardly reproducible in the long term and high frequency required to monitor urban emissions. There are many biosphere models that can be used to determine the biosphere signal to apply method (3), but it is not always clear which one has the best approximation of net ecosystem exchange (NEE) and the differences are significant.

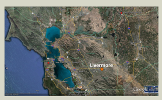
Abstract

We suggest that COS can be used to determine which ecosystem model best represents the biosphere signal. Just like CO_2, COS is taken up by photosynthesis but is not given off in respiration and can thus be used as a trace gas to estimate GPP. We begin with COS surface fluxes provided by SiB and CASA, regridded to lower resolution using NDVI values, for a 9, 3, and 1 km-resolution domain over the Bay Area of San Francisco and part of the San Joaquin Valley. Simulations using the atmospheric model WRF provide the meteorological data, which along with the COS fluxes, are used to run the transport model STEM over a 20-day period in March 2015. Simulations of COS mixing ratio based on the various surface flux models are compared to observed data available from several locations. The model that best represents COS uptake consequently also provides the most accurate simulation of CO_2 biosphere signal, and can be used to estimate fossil fuel CO_2 emissions.

Methods

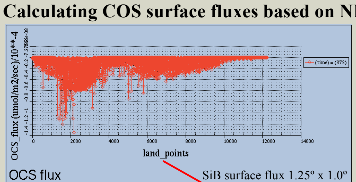
Domain





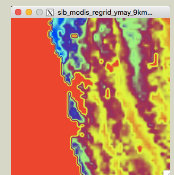
3 nested domains are centered over the city of Livermore, CA.
Resolutions: d01 9km, d02 3km, and d03 1km.

Calculating COS surface fluxes based on NDVI



SiB surface flux 1.25° x 1.0°

MODIS NDVI 1km or 250 m



$$\text{SiB COS flux value (entire STEM domain)} \times \frac{\text{NDVI value for 1 NDVI pixel}}{\text{NDVI value for entire STEM domain}} = \text{COS flux value for 1 pixel}$$

Model

WRF
Model version: 3.7.1 (August 13, 2015)
Simulation period: March 5-25 2015
PBL scheme: Mellor-Yamada-Janjic (Eta) TKE
Land surface model: NOAH
Cumulus: Grell-Devenyi ensemble scheme

STEM Sulfur Transport. dEposition Model

Calculations:

Where:

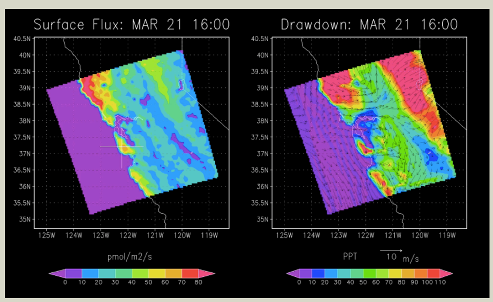
$$\text{COS flux} = GPP \frac{[COS]}{[CO_2]} V_{cos/co_2}$$

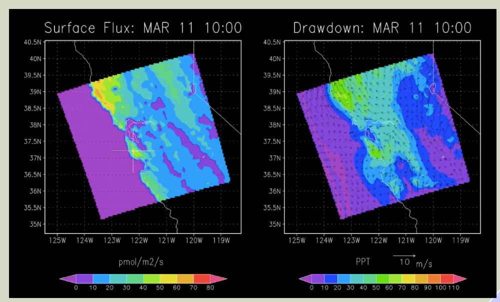
Gross Primary Productivity (photosynthesis)
Ambient concentrations of COS and CO_2
Relative plant preference for COS vs CO_2 during photosynthesis

1.84: LRU (Stimler et al 2012)
1.1: average ambient [COS]/[CO2] ratio from INTEX/NA experiment (Blake et al 2004)

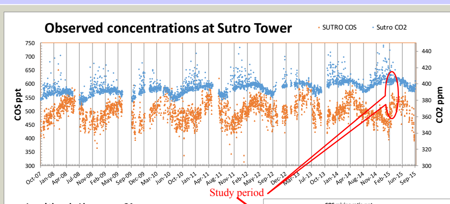
Using STEM to determine COS mixing ratios

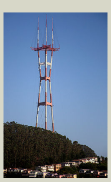
Surface flux and drawdown (difference between 450 ppt and simulated COS surface concentrations) is shown below on left for a typical day reflecting mean flow conditions, north-westerly winds, significant drawdown over the continent and less drawdown over the ocean. The model also showed some synoptic events in which continental air is brought to the ocean, and is brought back to the land again, showing atypical drawdowns such as is shown below on the right.

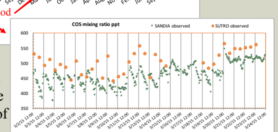




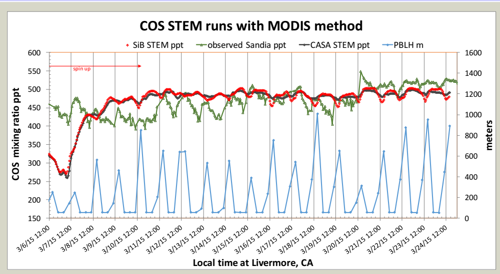
Results





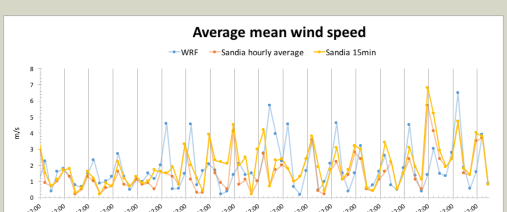


✓NOAA Sutro tower measurements in San Francisco (Montzka JGR, 2007) are on average upwind from study area of Livermore and provides background COS and CO_2 mixing ratios (average of 505 ppt and 405 ppm, respectively, for study period).
✓Seasonal variations are about 10-15%, and are similar to previous studies).
✓Synoptic variation during study period shown in zoomed-in box, is about 10%.
✓COS measurements are taken twice daily, not every day (15 measurements during study period).

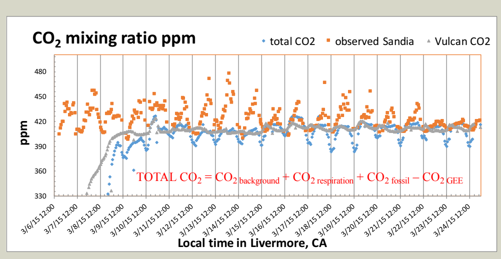


✓ Sandia location.
✓ 505 ppt background included.
✓ Amplitude: approx 20 ppt
✓ Wave: 24-hour variation, min 450, 461 ppt and max 503, 500 ppt, for SiB and CASA respectively.
✓ Synoptic event happening on 3/21 after which COS concentrations rise by 20 ppt. Potential continental influence until 21, after which marine air (less plant influence) seems more prominent.
✓ Observed is highest in the middle of the day coinciding with deepest boundary layer, which has a greater effect on the mixing ratio (due to increased mixing) than the capture of COS by photosynthesis. These findings are coherent with previous studies of forested areas.

✓Modeled COS mixing ratios are high at night (up to 503 ppt), then start to drop late morning/noon, reaching lowest values between 12:00 and 16:00 (down to 460 ppt for CASA and 450 for SiB).
✓Model results are not in phase with observations, by about 10 hours during continental influence (before March 20th), and by about 5 hours during marine influence (after March 21st). We found this discrepancy between observed and modeled results in another COS study of the Redwoods in California, and are presently working on tweaking STEM to improve mixing ratio calculations.



✓Mean wind speed at z=1 (Sandia tower at 13 meters).
✓Similar patterns and phases.



✓CO_2 background value of 405 ppm.
✓modeled total CO_2 underestimates observed CO_2, suggesting higher fossil CO_2 than determined by Vulcan inventories.
✓better model results during marine influence.
✓ highest concentrations of total CO_2 occur in early am, confirming other studies (Feng et al.,ACF, 2016).

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