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Special Section:

Carbon Weather: Toward the next generation of regional greenhouse gas inversion systems

Key Points:

- Characterizing non-stomatal fluxes of carbonyl sulfide (OCS) is necessary to use OCS as a tracer of stomatal conductance
- We construct an empirical model of soil-OCS fluxes based on long term field flux observations and lab incubation data
- The cause of deviations between model output and observations are explored using field observations from in-tact surfaces

Supporting Information:

Supporting Information may be found in the online version of this article.

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Soil Carbonyl Sulfide (OCS) Fluxes in Terrestrial Ecosystems: An Empirical Model

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Abstract Measurements of carbonyl sulfide (OCS) enable independent estimates of regional stomatal conductance provided that non-stomatal OCS fluxes are well constrained. OCS is taken up through plant leaves, following the same pathway as CO₂; in contrast to CO₂, OCS is irreversibly destroyed in plant leaves and plants do not typically exhibit OCS emissions. Ecosystem uptake of OCS can indicate changes in stomatal opening. Here we present an empirical model to assess the potential impact of soil OCS exchange, the non-Stomatal OCS exchange Empirical Model (SOCSEM, version 0). We created biome-specific response curves characterizing soil OCS exchange and restricted the model design to require only knowledge of soil moisture and surface temperature because remote sensing observations are available for these two features. Comparing the model to field-based chamber observations reveal deviations that can be attributed to missing complexity of the ground surface (having excluded litter and plants without regulated stomata), shortwave radiation, or the soil environment. For agricultural regions with known net emissions, we use remotely-sensed surface temperature data and demonstrate that data resolution can affect anticipated fluxes. We further investigate the influence of regions with unknown soil OCS responses, for example, Arctic tundra. We compare our model to a process-based and respiration-based soil OCS exchange model that has been implemented in a land surface model. Further field study of tropical and arctic ecosystems in conjunction with studies of non-stomatal surfaces in addition to soil (e.g., bryophytes) will increase confidence in applying OCS as a regional tracer for stomatal conductance.

Plain Language Summary Carbonyl sulfide (OCS) uptake over ecosystems is a good proxy for land carbon uptake via photosynthesis when non-plant OCS exchange is small or at least knowable. From what we have observed, soil OCS fluxes are typically overwhelmed by plant-based OCS uptake except in the case of wetland soils or when agricultural fields have become hot and dry. In this paper we constructed a model that estimates where soil OCS “hot spots” occur and how important they are for the global balance of OCS. Although this process is known to be fairly complicated, our model uses only soil moisture and surface temperature because these are the two most impactful parameters that can also be observed from space. We identify several potential causes of model-observation mismatches. For some regions of the world, like the Arctic tundra, there are no published observations and we hypothesize what the OCS exchange might be based on other ecosystems with similar traits. Overall, we note that soil OCS exchange is still much smaller than other surface sinks despite uncertainties.

1. Introduction

Most land uptake of carbonyl sulfide (OCS) is physically linked to gross primary production (GPP), the largest flux in the global carbon cycle (Berry et al., 2013; Protoschill-Krebs et al., 1995). However, outstanding questions remain that prevent the straightforward use of OCS as a tracer for GPP. In particular, there is a significant budget gap because the anticipated OCS sinks from plants, soils, and oxidation in the atmosphere are larger than all of the sources we have currently accounted for. Estimates of the missing source vary from 230 to 800 Gg S y⁻¹ (Lennartz et al., 2017). One possibility is that we have overestimated the plant sink although it would require an order of magnitude overestimation to account for the entire budget gap, unlikely based on laboratory and field data (Whelan et al., 2018). Two other possibilities have generated more debate: a large source in the tropical

Pacific or a large anthropogenic source in Southeast Asia, both supported by evidence from inversion studies but not yet observed directly (Berry et al., 2013; Kuai et al., 2015; Remaud et al., 2022). The relative contributions of the two possible sources have recently been constrained by isotopic data (Davidson et al., 2021). A final possibility is underestimated soil OCS production from specifically agricultural land, explored here.

Soils experience simultaneous OCS uptake and production. Soil OCS uptake is attributed to carbonic anhydrase in microbial communities, with fungi playing an important role (Sauze et al., 2017). OCS production is controlled by oxic, abiotic degradation of soil organic matter (Whelan & Rhew, 2015; Whelan et al., 2016) and redox reactions in oxygen-limited soils (Whelan et al., 2013). Previously, two models of soil OCS exchange were developed in parallel by different groups. There was not enough information at the time to describe the soil OCS production that accompanies soil OCS consumption in nearly every system observed: Ogée et al. (2015) did not include a term for oxic OCS production and Sun et al. (2015) relied on data from two sites with likely low OCS production for comparing model outputs. The process-based models require parameterizing variables that are not typically measured (e.g., soil carbonic anhydrase activity) and for which gridded global estimates with sufficient resolution do not exist. New information was discovered by Kaisermann et al. (2018) linking soil OCS fluxes to microbial carbon biomass and nitrogen content, which also do not have fine resolution data products on regional scales. Here we developed an empirical model to anticipate soil OCS exchange using biome classification as a proxy for more complex soil processes.

To link terrestrial OCS uptake with CO₂ uptake, we need to constrain OCS sources and sinks aside from plant leaves. We believe soils are the largest non-stomatal influence on OCS fluxes in natural systems (Whelan et al., 2018). This study provides global, gridded estimates of soil OCS exchange based on observed empirical relationships and compares the results to a process-based and a second empirical model. Using remote sensing data, we identify soil OCS “hot spots” and demonstrate the importance of spatial resolution for temperature data in calculating the net OCS flux over agricultural areas. There are two regions that are still data-poor: the Tropics and Arctic tundra. Hypotheses of how ground surfaces in these two regions exchange OCS are explored. Combining available data streams and exploring their implications provides direction for impactful studies on surface OCS exchange for the future. The resulting model can be used to make first estimates of non-stomatal OCS fluxes wherever surface temperature, soil moisture, and biome are estimated.

2. Methods: Model Approach and Description

The model developed here uses the available information to characterize what we know about non-stomatal fluxes of OCS in natural ecosystems. Many datasets come from soil samples with the top layer of organic matter removed (Table 1). This (version 0) of the non-Stomatal OCS exchange Empirical Model (SOCSEM) is based on soils without a litter layer or organisms without regulated stomata (e.g., mosses) due to lack of data. Soil OCS production and consumption are occurring simultaneously (Kaisermann et al., 2018) and we assumed the relationships are independent for the time scale of observations. We take the approach developed in Whelan et al. (2016): the overall OCS exchange of soil is calculated as

$$F_{\text{total}} = F_{\text{production}} + F_{\text{uptake}} \quad (1)$$

where F_{total} is the net soil OCS flux, $F_{\text{production}}$ is soil OCS production to the atmosphere, positive by convention, and F_{uptake} is the soil OCS uptake from the atmosphere, negative by convention.

We assume that OCS exchange from soils for each biome class (e.g., temperate forest) are similar enough within themselves and different enough from other biomes that the biome class will indicate the fundamental relationship between OCS total flux with soil temperature and soil moisture. Data was not available to define all features for each biome. In lieu of waiting for the extensive field work required for a robust empirical data set, lab incubations were scaled up and assumptions were declared to relate biomes with little data to better studied areas. Below we report the main assumptions that were made to bridge these data gaps.

2.1. Oxic Soil OCS Production

Through heating soils in controlled experiments, Whelan et al. (2016) found that the relationship of OCS production with temperature does not increase exponentially beyond conditions typically found in vegetated ecosystems.

Table 1
Empirical Data Used to Inform Models in This Study

Biome	Soil incubations	Field measurements
Grassland	Oak savannah Stunt Ranch, CA (Whelan et al., 2016)	Mediterranean grassland Santa Cruz, CA (Whelan & Rhew, 2016) Oak savannah Stunt Ranch, CA (Sun et al., 2016)
Desert	Colorado desert Boyd Deep Canyon Reserve, CA (Whelan et al., 2016) Moab, UT (Meredith et al., 2018)	None reported
Forest—broadleaf	Deciduous forest Willow Creek, WI (Whelan et al., 2016)	Deciduous forest, Petersham, MA (Wehr et al., 2017)
Forest—boreal or needleleaf	Boreal forest in Central Siberia Maiskoe, Russia (Van Diest & Kesselmeier, 2008) Douglas fir old growth forest Wind River Forest, WA (see Figure S8 in Supporting Information S1)	Douglas fir old growth forest Wind River Forest, WA (Rastogi, Berkelhammer, Wharton, Whelan, Meinzer, et al., 2018) Boreal Scots pine managed forest (Sun et al., 2018)
Forest—tropical	Rainforest Los Amigos Biological Station, Peru (Whelan et al., 2016)	None reported
Agricultural	Wheatfield Southern Great Plains ARM site, OK (Whelan & Rhew, 2015) Soy/Corn field Bondville, IL (Whelan et al., 2016) Wheatfield Mainz, Germany (Kesselmeier et al., 1999)	Wheatfield Southern Great Plains ARM site, OK (Maseyk et al., 2014) Fertilized hay meadow Neustift, Austria (Kitz et al., 2017)
Wetlands	Coastal salt marsh Louisiana Gulf Coast (Devai & DeLaune, 1995)	Coastal salt marsh Port Aransas, TX (Whelan et al., 2013)
Tundra	None reported	None reported

Note. Except where “none reported” is indicated, additional soil studies exist, but many did not investigate a range of conditions that could inform this environmental model driven by soil moisture and temperature.

To make this empirical model as widely applicable as possible, we use a logistic function to describe soil OCS production, $F_{\text{production}}$, in $\text{pmol OCS m}^{-2} \text{s}^{-1}$, where the maximum flux a is scaled to the highest observed OCS flux for that ecosystem, regardless of soil moisture:

$$F_{\text{production}} = \frac{a}{1 + be^{-kT}} \quad (2)$$

where $F_{\text{production}}$ is soil OCS production in $\text{pmol OCS m}^{-2} \text{s}^{-1}$, T is temperature in $^{\circ}\text{C}$, and b (unitless) and k ($^{\circ}\text{C}^{-1}$) are parameters fit to OCS flux observations from air-dried soils from field experiments (Maseyk et al., 2014) or laboratory incubations (Whelan et al., 2016) (Figure 1). This is a departure from the exponential equations reported in Whelan et al. (2016). To leverage as many possible observational datasets, we did not restrict our definition of a to only soils that are air-dried in a laboratory (see Table 2). Desert soils yielded little OCS exchange when dry and no convincing empirical relationship was found. The results of the fits are presented in Table 2 with data plotted in Figure 1.

2.2. Non-Wetland Soil OCS Uptake

Following Van Diest and Kesselmeier (2008), OCS uptake has an optimum temperature and soil moisture, with the exception of wetland ecosystems. In all cases, we first subtracted the modeled abiotic OCS production term from observations (Figure 1, Table 2) before attempting to fit OCS uptake relationships (Table 3). We then repurposed a model for soil NO production presented by Behrendt et al. (2014) for describing soil OCS exchange, an approach used in Whelan et al. (2016). To model OCS uptake, three factors needed to be characterized: (a) the optimum soil moisture for maximum OCS uptake at a given temperature, (b) the uptake at some secondary soil moisture, and (c) how the optimum and secondary OCS uptake change with temperature. Soil moisture here is reported in volumetric water content % between 0 and percentage of total soil porosity, typically ~ 50 . To describe the shape of the uptake curve with soil moisture, we formulate a variable to capture the overall curve shape α :

$$\alpha = \frac{\ln(F_{\text{opt}}/F_{\theta_g})}{\ln(\theta_{\text{opt}}/\theta_g) + (\theta_g/\theta_{\text{opt}} - 1)} \quad (3)$$

Where F_{opt} is the optimum soil moisture for maximum OCS uptake for a given temperature, θ_{opt} is the soil moisture at the optimum flux, θ_g is a secondary soil moisture where the OCS uptake is estimated as F_{θ_g} , and $\theta_g > \theta_{\text{opt}}$.

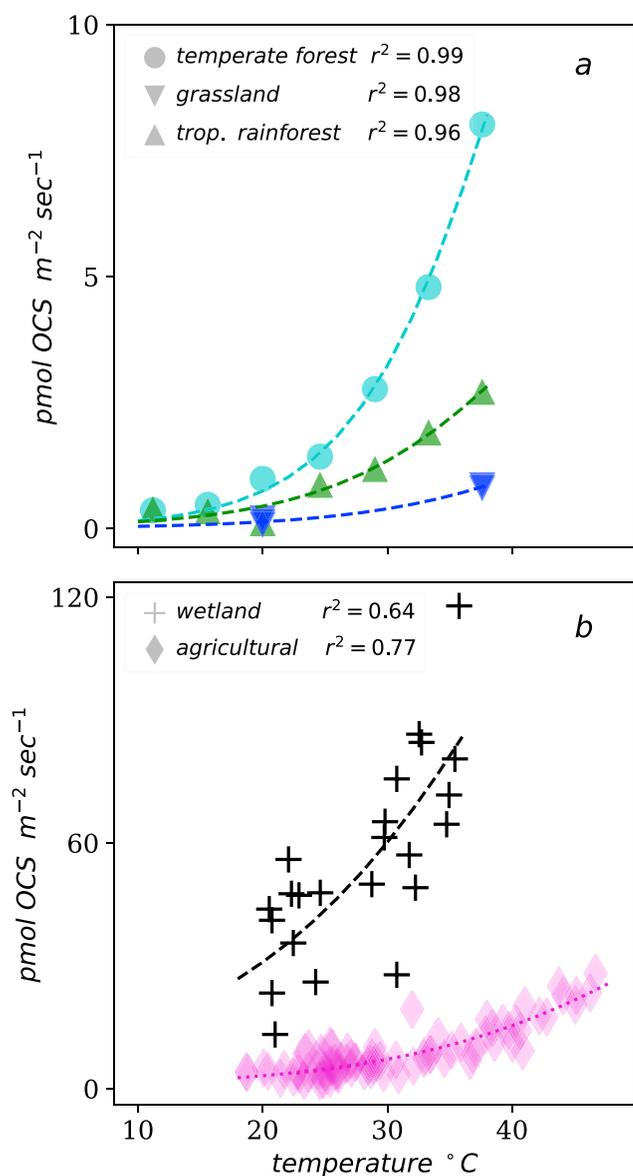


Figure 1. Estimated response of abiotic carbonyl sulfide (OCS) production to temperature for various field sites. (a) Non-tropical (temperate/boreal) forest and grassland sites exhibited low OCS production in lab experiments when soil was hot and dry (Whelan et al., 2016). (b) In situ measurements from wetlands (Whelan et al., 2013) and agricultural soils (Maseyk et al., 2014) were often an order of magnitude higher than OCS production for biomes in panel (a).

The uptake for any soil moisture θ is determined by the product of a power function and an exponential function:

$$F_{\text{uptake}} = F_{\text{opt}} \left(\theta / \theta_{\text{opt}} \right)^{\alpha} \exp \left(-\alpha \left(\theta / \theta_{\text{opt}} - 1 \right) \right) \quad (4)$$

In the absence of appropriate data, the optimum uptake F_{opt} is assumed to be constant with temperature; however, F_{opt} has been observed to vary with temperature with the same relationship described by Equation 4 (Van Diest & Kesselmeier, 2008). Where data is available, observations are binned by temperature and the F_{opt} is determined for each bin. The resulting set of F_{opt} over temperature was then fit to Equation 3 using least squares regression, replacing θ_g and θ_{opt} with temperature T_g and T_{opt} in $^{\circ}\text{C}$. An identical fitting approach is used to find the relationship of F_{θ_g} and F_{T_g} with temperature and soil moisture at a second soil moisture θ_g and a second temperature T_g , respectively. For any pairing of θ and T , first F_{opt} is calculated for a given T if information relating T and F_{opt} is available, then F_{uptake} is calculated for a given θ . The results are presented in Table 3. More detail on overcoming data gaps is provided in Text S1 of Supporting Information S1.

2.3. Anoxic Soil OCS Fluxes

Wetlands are known, large sources of atmospheric OCS due to anoxic production (Whelan et al., 2013, 2018). Diurnal OCS flux observations from a salt marsh with high sulfur mobility indicated a compelling relationship with temperature (Figure 1b). Fluxes from freshwater wetlands are likely different in magnitude given the lower concentrations of sulfur-containing compounds (DeLaune et al., 2002); however, all wetland soils investigated to date have demonstrated net OCS production (see summary in Whelan et al., 2018). In this study, we compare the anoxic OCS production from wetlands calculated using a redox relationship and the land surface model ORCHIDEE in Abadie et al. (2022) to the simple relationship shown in Figure 1b and Table 2. We use the weighted average of the upper 9 cm of the soil column temperature generated by ORCHIDEE to drive our model.

2.4. Model Validation With Field Investigations

We compare several OCS surface flux datasets (Figure 2) to our empirical model using the reported soil temperature and soil moisture. Many of these soil OCS flux observations did not capture a wide enough range of soil moisture and temperature to derive robust relationships to OCS fluxes and were not included in the formulation of this empirical model. The exception is agricultural soils, where we used the dry (<20% volumetric water content) observations from Maseyk et al. (2014) to create a new logistic model for agricultural soil OCS production. We examine the difference between field observations and calculated model fluxes in a violin plot (Figure 3), then generate root mean squared errors (RMSE) and model efficiency of fit (MEF) estimates (Table 5).

2.5. Investigating Issues of Fine Spatial Scale

To investigate the issue of small scale changes creating “hot spots” with large scale effects, we used remote sensing data for soil moisture from the soil moisture active passive (SMAP) satellite and surface temperature from the ECOsystem Spaceborne Thermal Radiometer Experiment on Space Station (ECOSTRESS) over a small region near the original Maseyk et al. (2014) study (Figure 5). Surface temperature measurements reflect soil surface temperatures where no vegetation is present, so we calculated NDVI using the most timely clear sky LANDSAT image to link high temperatures with likely bare soil remote sensing observations.

Table 2

Results of the Logistical Fit (Equation 2) of Observed Carbonyl Sulfide (OCS) Fluxes and Temperature

Site (r^2)	a (error) pmol OCS $m^{-2} s^{-1}$	a reference	b (error) unitless	k (error) $^{\circ}C^{-1}$	Number of observations
Agricultural (0.79)	83 (2.1)	Whelan et al. (2016)	147 (31)	0.0877 (0.006)	77
Tropical rainforest (0.96)	8.1 (2.7)*	Whelan et al. (2016)	205 (101)	0.124 (0.015)	8
Temperate/boreal forest (0.99)	20 (8)	Commane et al. (2015)	645 (132)	0.161 (0.006)	8
Grassland (0.98)	3.9 (1)	Whelan and Rhew (2016)	286 (158)	0.115 (0.015)	6
Wetland (0.64)	295 (48)	DeLaune et al. (2002)	41.1 (19)	0.0786 (0.016)	24
Tundra	Insufficient data				

Note. Errors for a are standard deviations uncertainty of the observations and for b and k are covariance from the statistical fit. At high temperatures, the OCS flux approaches a , set to the max flux observed. At low temperatures, the OCS production flux approaches 0, with the y -intercept at $a/(1 + b)$. *The maximum production for tropical forest soils was estimated by tripling the highest production rate found from soil incubations because it yielded the best goodness of fit to the incubation data. The uncertainty reported is the magnitude of the original incubation observation.

2.6. Comparing to Estimates From Global Approaches

Applying this model to the global scale, we compared the oxic soil exchange described by our empirical model to process-based (Ogée et al., 2015) and soil respiration-based (Berry et al., 2013) estimates calculated in Abadie et al. (2022) (Figure 4). To examine the uncertainty introduced by ecosystems for which we have no observations, we performed a simple sensitivity test where we calculated global fluxes based on whether it is assumed that a boreal grassland responds more like another grassland or the groundcover of a temperate forest. To drive our empirical model, we use the plant functional types (Table 4) and soil moisture and soil temperature averaged over the top 9 cm of soil used in the ORCHIDEE land surface model in Abadie et al. (2022).

3. Results: Non-stomatal OCS Empirical Model (SOCSEM) Evaluation

The major obstacle for estimating global non-stomatal terrestrial ecosystem OCS exchange is that the empirical field data is incomplete (Table 1, Figure 2). Some ecosystems have nearly no data: published literature about the Arctic tundra mentions only two, unreported observations (Hines & Morrison, 1992). Other ecosystems have

Table 3

Parameters for Soil Carbonyl Sulfide (OCS) Uptake Calculated by Fitting Equations 3 and 4 to Available Field and Laboratory Data After Subtracting Soil Production Term Calculated in Section 2.1

Biome	Estimated θ_{opt} (%VWC)	F_{opt} with temperature ($^{\circ}C$) at θ_{opt} (OCS pmol $m^{-2} s^{-1}$)	θ_g (%VWC)	F_g with temperature ($^{\circ}C$) at θ_g (OCS pmol $m^{-2} s^{-1}$)
Grassland	12.5 ± 1.9	F_{opt} : -4.5 ± 0.5 F_{Tg} : -1.5 ± 0.2 T_{opt} : 10.9 ± 1.8 T_g : 25 ± 1.0	26.9 ± 0.3	F_{opt} : -2.3 ± 0.4 F_{Tg} : -1.3 ± 0.5 T_{opt} : 14.8 ± 2.7 T_g : 25 ± 1.0
Forest—temperate or Broadleaf	24.6 ± 0.6	-12.6 ± 1.0	51 ± 21.6	-0.18T + 0.48 (r^2 of 0.9 with 4 data points)
Forest—boreal or needleleaf	12.5 ± 1.3	F_{opt} : -18 ± 2.3 F_{Tg} : -12 ± 6.8 T_{opt} : 28 ± 2.5 T_g : 35 ± 2.5	19.3 ± 0.6	F_{opt} : -5.9 ± 1.1 F_{Tg} : -3.8 ± 2.5 T_{opt} : 28 ± 3.5 T_g : 35 ± 3.5
Tropical forest	24.6 ± 0.6*	-2.7 ± 0.1	31.0 ± 1.0	-0.86 ± 0.74
Agricultural	17.7 ± 2.1	-9.7 ± 1.8	22 ± 1.1	-5.36 ± 0.78
Tundra	n.d.	n.d.	n.d.	n.d.

Note. *Because of lack of data, the optimum uptake for tropical soils is assumed to be identical to temperate forests. More detail on calculations for individual biomes are provided in Text S1 of Supporting Information S1.

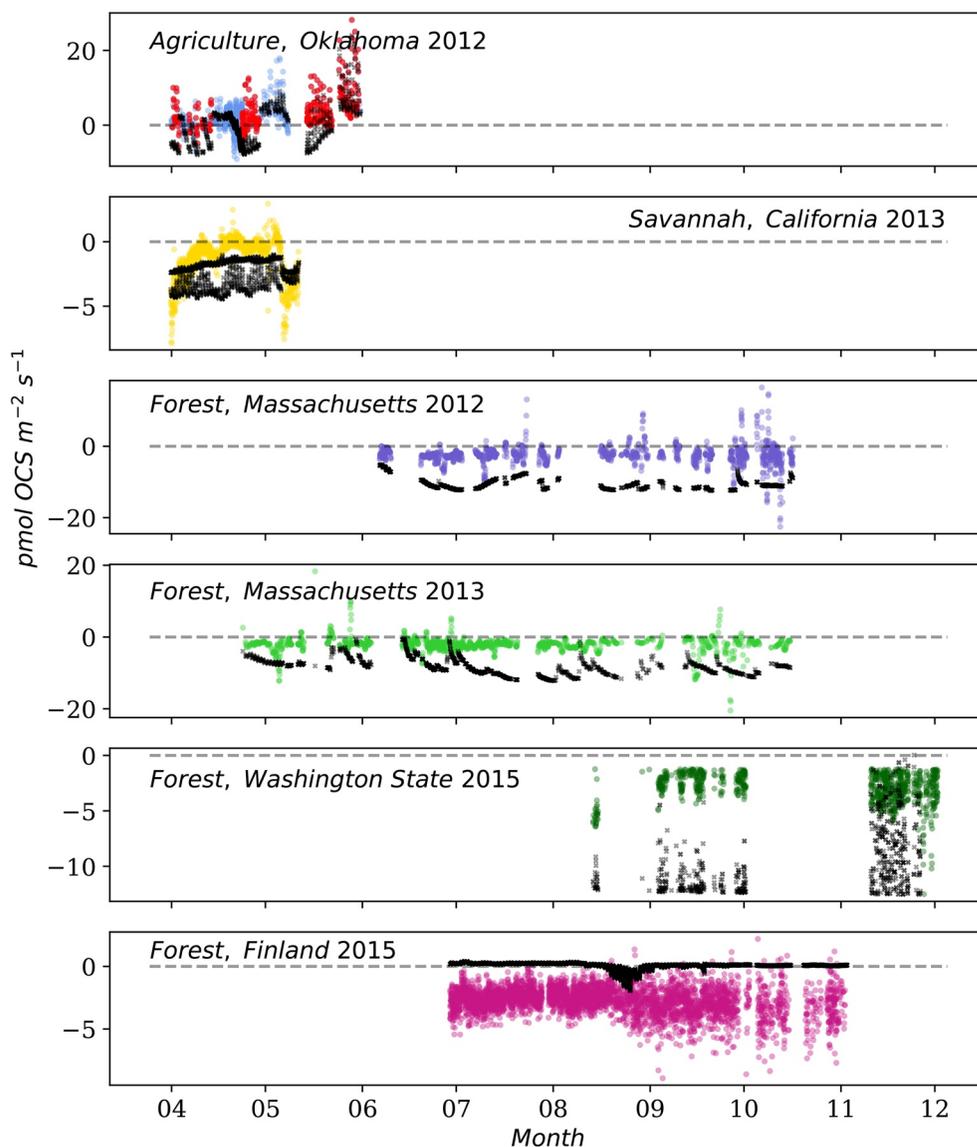


Figure 2. Field observations used in this analysis, flux of carbonyl sulfide (OCS) by time of year: Oklahoma (Maseyk et al., 2014), California (Sun et al., 2016), Massachusetts (Wehr et al., 2017), Washington State (Rastogi, Berkelhammer, Wharton, Whelan, Itter, et al., 2018), and Finland (Sun et al., 2018). Estimates from this model are in black; observations are in other colors. The red markers on the top panel indicate data that were used in the formulation of the empirical model.

published datasets from soil lab incubations only, for example, tropical rainforest soils (Whelan et al., 2016). This approach clarifies where there might be significant knowledge gaps while creating a data set that allows us to test the sensitivity of the global OCS budget to soil OCS exchange. Here an empirically-derived set of response curves (Tables 2 and 3) was used to estimate soil OCS fluxes for individual sites (Figure 2) and on global scales (Figure 4). We then address small scale variation in OCS emissions from cultivated land (Figure 5). To explore the potential variability of biomes where we have little data, we apply two different empirical treatments for tundra regions (Figure 6) and compare a model based on a saline environment to a model based on freshwater observations.

3.1. Comparing the Soil OCS Empirical Model With Field Observations

We compared estimates from our empirical model to dedicated observations of ecosystem ground surface OCS fluxes from several campaigns (Figure 2) and calculated their residuals (Figure 3). We calculated the root mean

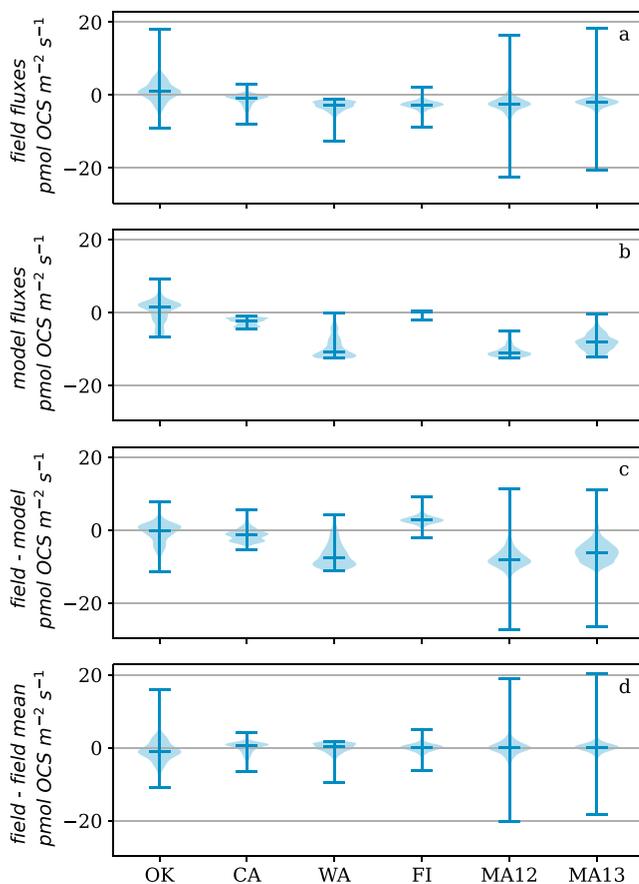


Figure 3. (a) A violin plot of the median and standard deviation of field observations, excluding those used to formulate the model (red markers in Figure 2). The field sites are OK for an agricultural site (Maseyk et al., 2014), CA for a savannah site (Sun et al., 2016), MA12 and MA13 for a temperate forest site in 2012 and 2013, respectively (Wehr et al., 2017), WA for a temperate forest site (Rastogi, Berkelhammer, Wharton, Whelan, Iiter, et al., 2018), and FI for a boreal forest site (Sun et al., 2018). (b) The model estimates of carbonyl sulfide (OCS) soil fluxes using observed soil moisture and soil temperature. (c) The model-data mismatch, with individual model estimates (b) subtracted by individual field observations (a). (d) For comparison, the difference between individual field observations and the mean of field observations for each site.

square error (RMSE, Table 5) and found in many cases the error was larger than the total variability of the observations. Supporting this idea, we also calculated modeling efficiency (MEF, Table 5), which was less than 0 at all sites, suggesting the variability of the observations exceeds the variability of the model.

3.2. Comparing Oxidic Fluxes in SOCSEM and Process-Based Models

We compared the output of SOCSEM to two other approaches that have been used in the past: scaling OCS uptake to soil respiration (Berry et al., 2013) and a process-based model that takes into account multiple soil layers (Ogée et al., 2015) (Figure 4). We chose to leave out a third method used in Kettle et al. (2002): the model essentially reflects the same idea used in SOCSEM with fewer available observations and no oxidic production terms. The respiration-based model (Figure 4c) also leaves out oxidic production and has less variability in uptake compared to the other two methods. The process-based model and SOCSEM both have production in South Asia and the Sahel, but the production magnitude is smaller in SOCSEM (see Figure 4d). We first assume that soils in tundra will behave either like grassland soils (as in Figure 4a) or like the floor of a temperate forest so that we can calculate fluxes globally. Using soil temperature and soil moisture from the top 9 cm of ORCHIDEE runs, the average global exchange from our empirical model from 2009 to 2016 is $-187 \text{ Gg S yr}^{-1}$ when tundra regions (defined in ORCHIDEE and SOCSEM in Table 4) are assumed to act similarly to a temperate forest floor and $-142 \text{ Gg S yr}^{-1}$ when tundra regions act similarly to grasslands, compared to $-126 \text{ Gg S yr}^{-1}$ from the process-based model (Abadie et al., 2022).

3.3. Estimates Using ECOSTRESS Remote Sensing Data

In agricultural regions where fields are harvested or not yet planted, surface emissivity-based remote sensing product can capture the soil surface temperature. We used cloud free observations from LANDSAT to link our hotspots with likely bare soil areas (Figure 5d). Surface temperature and soil moisture in Figures 5a and 5b were averaged over the study area ($\sim 32 \times 32 \text{ km}$), then used to calculate the soil OCS flux with our empirical model, resulting in an average flux of $+4 \text{ pmol OCS m}^2 \text{ s}^{-1}$. In contrast, using output computed at $70 \times 70 \text{ m}$ resolution, we found emissions of $+6 \text{ pmol OCS m}^2 \text{ s}^{-1}$ (Figure 5c). The uncertainty introduced by using lower resolution data

can cause errors in anticipated soil OCS fluxes from agricultural areas when soils are expected to be hot and dry in a patchwork.

3.4. Effect of Unknown Biome Ground Surface Behavior

More observations are needed to clarify the role of soils in OCS fluxes at the poles, the equator, and the coasts. To explore the influence of tundra dynamics, we put forth scenarios to understand the possible impact of soil fluxes on the total OCS budget.

Ice-covered regions and tundra have no available data. We expect ice-covered areas to have low OCS exchange due cold temperatures and lack of atmospheric access to organic matter precursors, though widespread algae on ice may play a role (Yallop et al., 2012). In tundra, we expect that OCS uptake and emissions are affected by the dynamics of soil organic carbon and water availability. Tundra has both large stocks of soil organic matter and can contain layers that are permanently or seasonally frozen, creating unique hydrological conditions (Street et al., 2016). Tundra could respond like a grassland as it is characterized in the ORCHIDEE land classification

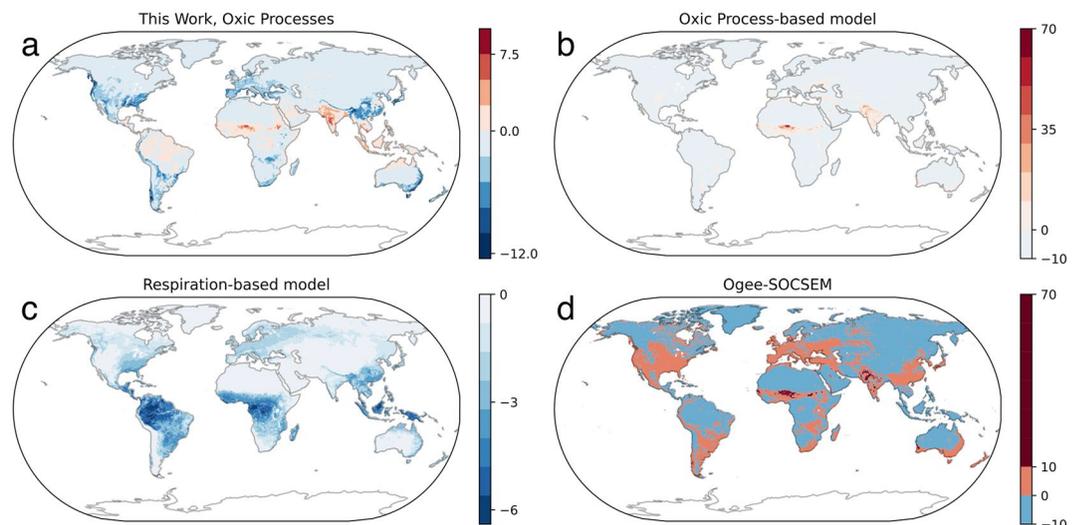


Figure 4. (a) The average soil carbonyl sulfide (OCS) flux over 2009–2016 using non-Stomatal OCS exchange Empirical Model and the top 9 cm averaged soil temperature and soil volumetric water content from ORCHIDEE. (b) Output from the process-based model in Abadie et al. (2022) integrated into ORCHIDEE. (c) The approach used in Berry et al. (2013) scaling OCS soil uptake to soil respiration in ORCHIDEE from Abadie et al. (2022). (d) The difference between panel (a) and b.

scheme, or like the understory of a wet temperate forest, as in the Pacific Northwest US (Rastogi, Berkelhammer, Wharton, Whelan, Itter, et al., 2018). The effect of using these different schemes is presented in Figure 6.

To compare the influence of these two scenarios (tundra as grassland vs. tundra as forest floor) on the global OCS budget, we ran our empirical soil model for the entire globe with different biomes defined by ORCHIDEE (see Table 4) and using the soil moisture and soil temperature averaged over the top 9 cm of the soil profile over the years 2010–2019 (Figure 6). Cold northern hemisphere temperatures yield low global soil OCS uptake during the northern hemisphere winter months. However, in the northern hemisphere summer, the tundra-as-temperate forest scenario serves to increase the global soil OCS uptake by 30%.

Table 4
Biomes Defined in ORCHIDEE Presented in the Left Column Are Re-Classified in the Right Column to Apply Non-Stomatal OCS Exchange Empirical Model (SOCSEM) Globally

Biome in ORCHIDEE	Biome for SOCSEM
1 Bare soil	Desert
2 Tropical broad-leaved evergreen	Tropical forest
3 Tropical broad-leaved raingreen	
4 Temperate needleleaf evergreen	Temperate forest
5 Temperate broad-leaved evergreen	
6 Temperate broad-leaved summergreen	
7 Boreal needleleaf evergreen	Boreal forest
8 Boreal broad-leaved summergreen	
9 Boreal needleleaf summergreen	
10 C3 grass	Grassland
11 C4 grass	
12 C3 agriculture	Agriculture
13 C4 agriculture	
14 Tropical natural grassland (C3)	Grassland
15 Boreal natural grassland (C3)	Tundra (grassland or temperate forest)

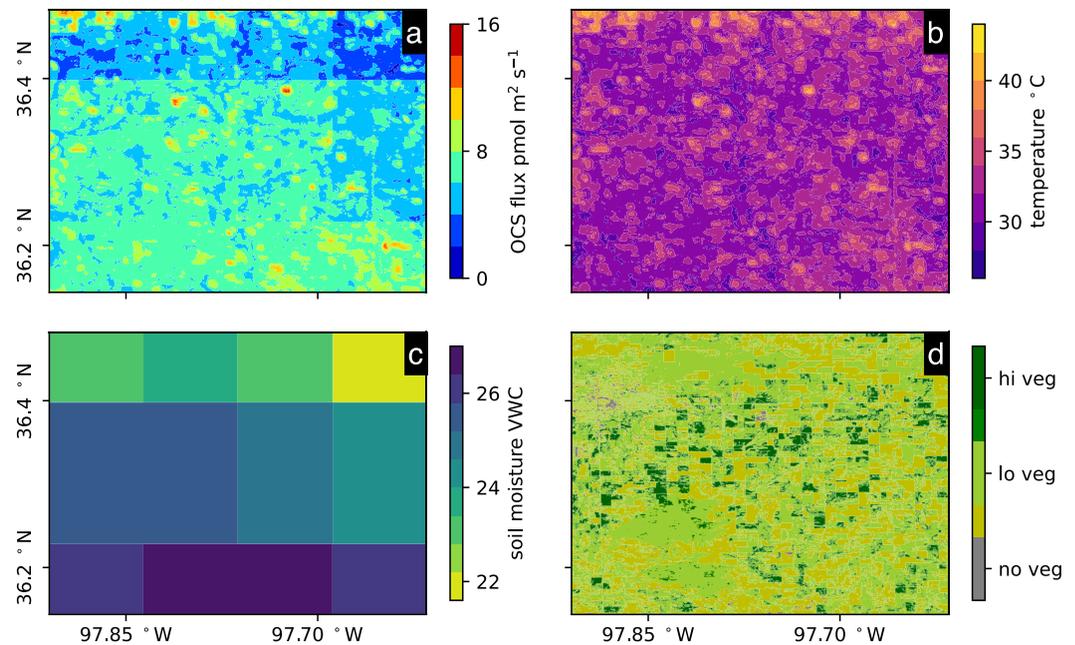


Figure 5. Remotely sensed data and calculated carbonyl sulfide (OCS) fluxes over an agricultural area in Oklahoma near the site investigated in Maseyk et al. (2014) in May 2020. (a) Calculated OCS fluxes using the empirical model presented here with data input shown in the (b and c). (b) Surface temperature from ECOSTRESS Land Surface Temperature and Emissivity Daily L2 (Hook & Hulley, 2019) from 29 May 2020 at 21:42 UTC. (c) Soil moisture data from soil moisture active passive Enhanced L3 Radiometer Global Daily 9 km EASE-Grid Soil Moisture, Version 4 (O'Neill et al., 2020), averaged between 28 May and 30 May 2020 to achieve full coverage of high quality data. (d) NDVI calculated from a clear LANDSAT scene on 5 May 2020.

While wetlands are perhaps the best studied ecosystem for OCS surface fluxes (Whelan et al., 2018), it is difficult to directly address the factors that control OCS fluxes on a global scale. It is unclear if saline wetlands produce more observed OCS because of salinity, tidal influences, or other biogeochemical cycling effects. Here

we contrast the Q10-based model used by Abadie et al. (2022) that restricted individual plots to no more than $10 \text{ pmol m}^{-2} \text{ s}^{-1}$, with our empirical model based on field observations in a salt marsh (Whelan et al., 2013) (Figure 7). For our empirical model, we emphasize the high emissions found in saline environments (Whelan et al., 2018) yielding an average annual emission of 400 Gg S as OCS per year, contrasting the Q10 model that is influenced more by freshwater environments (Abadie et al., 2022) which estimated an average of 96 Gg S emitted from wetlands as OCS per year.

4. Discussion: Implications of SOCSEM Model Results on Global and Finer Scales

4.1. Global Soil OCS Production in the Atmospheric OCS Budget

Both anoxic and oxic OCS production pose problems for anticipating the balance of soil OCS exchange. Wetlands cover only a small portion of the Earth's surface but can contribute to regional fluxes, as was possibly observed during the ACT-America observations of OCS near coastal Texas (Parazoo et al., 2021). Where restricting OCS production to $10 \text{ pmol m}^{-2} \text{ s}^{-1}$ as in Abadie et al. (2022) will not capture the high emissions from saltmarshes, instead anticipating that all wetlands will emit large amounts of OCS like in saline environments, as we have done here, is likely erring in the opposite direction. New observations capturing the transition from saline to freshwater

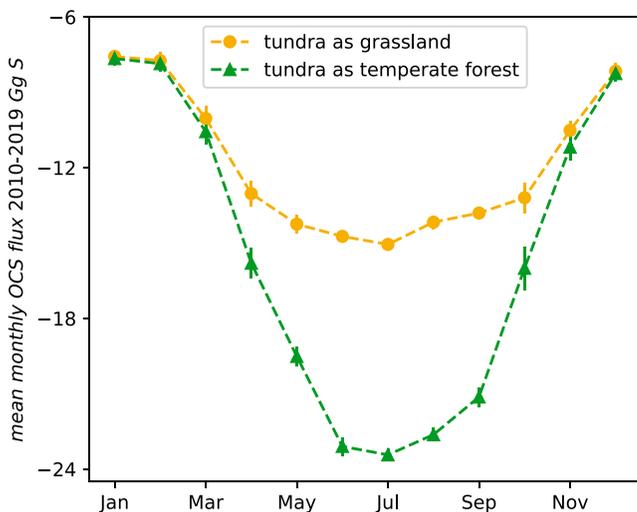


Figure 6. A comparison of two possible scenarios for tundra carbonyl sulfide (OCS) exchange: *tundra as temperate forest*, where we apply the empirical relationships found from temperate forest soils versus *tundra as grassland*, where we apply the empirical relationships observed for grassland ecosystems.

Table 5
The Root Mean Square Error (RMSE) and Model Efficiency (MEF) of Modeled Versus Observed OCS Soil Fluxes

Site	RMSE	MEF
OK	2.4	-0.07
CA	2.1	-0.8
MA12	6.9	-24
MA13	2.6	-6.9
WA	8.6	-7.9
FI	6.6	-8.5

wetlands would be useful in constraining this component of the global OCS budget.

Using the empirical model developed here and environmental variable output from ORCHIDEE at $0.5^\circ \times 0.5^\circ$ resolution, we anticipated OCS soil fluxes to estimate global fluxes using two scenarios for unknown tundra fluxes (Figure 6). In both cases, our model anticipates small OCS uptake (-191 and -174 GgS yr^{-1} for *tundra as forest* and *tundra as grassland*, respectively) compared to modeled biosphere uptake (e.g., -753 GgS yr^{-1} , Kooijmans et al., 2021). While the difference between the two scenarios appears small, it is impossible to determine what model might be the most appropriate for a region where we have no observations.

Tropical regions (e.g., the Amazon rainforest) are associated with emissions due to high temperatures, though observations are also sparse for this region.

Tropical forest soil is qualitatively different than temperate forest soil, where most observations have been made (Whelan et al., 2018, Figure 3). Tropical forests tend to have a much higher soil organic matter turnover. The observations used here are based on incubating soil samples from the Peruvian Amazon which showed low OCS production and consumption rates. While some data is preferable to an entire absence of data, the variability of tropical rainforests is likely not captured by a single site.

Some areas (e.g., South Asia, central US) are associated with OCS emissions, typically where there are grid cells partially containing agricultural activity with a high average temperature for the entire pixel. Accurately representing soil OCS exchange in agricultural regions is of particular importance for making estimates of GPP, especially over North America where GPP is highest in summer over cultivated lands (Hilton et al., 2017). Irrigated agricultural fields can experience hot and dry conditions in a patchwork, with associated large OCS soil emissions (Figure 5c). Soil moisture variability increases in fields that are intermittently irrigated or when irrigation stops after harvest. We found that SMAP data at a resolution of 9 km did not capture heterogeneity in the area (Figures 5a and 5c). The modeled OCS fluxes were driven primarily by the variation in temperature revealed by ECOSTRESS surface temperature with a resolution of 70 m (Figure 5b). Scaling remotely sensed data is challenging because data availability is intermittent and temperature is interpolated, generally with lower resolution remote sensing products.

4.2. Dynamics Not Included in Current Models

Multiple observed phenomena are absent from this treatment and other models: OCS exchange dynamics with non-vascular plants, the quick changes in soil OCS fluxes after an abrupt shift in water availability, leaf litter OCS exchange, photodegradation of soil organic matter, and heterogeneity of the soil environment. These and other processes likely explain model-data mismatch presented in Figure 3 and Table 5. While the observation-based approach presented here omits significant complexities, empirical data gaps currently pose an even greater challenge to process-based models.

Bryophytes (e.g., mosses) and lichen contain OCS-destroying carbonic anhydrase, but do not regulate gas exchange with stomata. As expected, isolated bryophytes and lichen take up OCS in both dark and light conditions, with water availability explaining much of the variability (Gimeno et al., 2017; Kuhn & Kesselmeier, 2000). Based on a laboratory study, Gimeno et al. (2017) concluded that moss-dominated ecosystems may have OCS uptake that is not directly related to photosynthesis, confounded further by OCS emissions with higher temperatures. Further observations of bryophyte OCS exchange are included in the Supplement (Text S2 in Supporting Information S1). OCS emissions from tundra soils may be generated from two distinct sets of processes. In oxic environments OCS production can occur through the thermal or photodegradation of soil organic matter (Whelan & Rhew, 2015). OCS emissions from anoxic environments develop

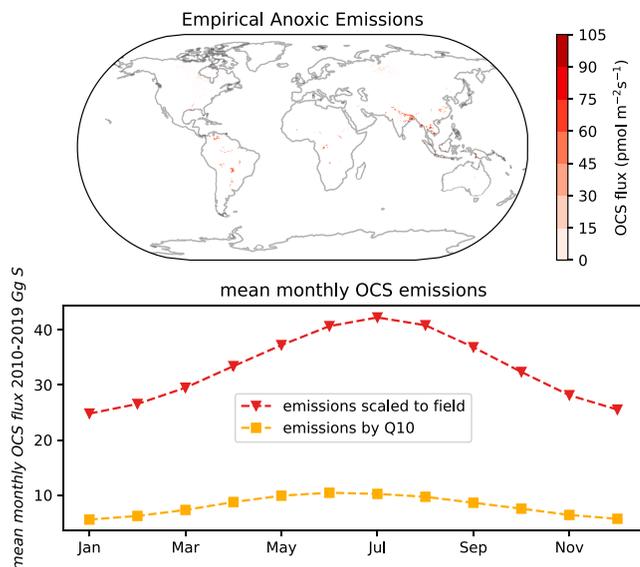


Figure 7. Anoxic soil carbonyl sulfide (OCS) production in wetlands. The top panel shows the emissions anticipated if all grid cells containing wetlands mapped in Tootchi et al. (2018) exhibited the same behavior as a saltmarsh (Figure 1b). The bottom panel shows the mean monthly (2010–2019) OCS flux in Gg S using soil temperature from the ORCHIDEE land surface model for our empirical model and the Q10-based model used by Abadie et al. (2022).

through redox transformations of sulfur compounds which can be transported to the atmosphere via plant stems, circumventing uptake (Whelan et al., 2013).

OCS uptake is driven by carbonic anhydrase (Whelan et al., 2018), contained in the moss and lichen that blanket much of the Arctic tundra (Schoor et al., 2007). The only analog OCS observations we have to this type of surface is the lichen and moss-covered understory of the Pacific Northwest forest (Rastogi, Berkelhammer, Wharton, Whelan, Iiter, et al., 2018). We do not understand the dynamics of bryophyte OCS exchange completely (Gimeno et al., 2017); however, because of the prevalence of tundra mosses, something similar may be happening in tundra regions.

Sudden changes in ground surface water content can also cause large swings in OCS uptake. This was observed in two seasonally dry ecosystems, a grassland (Whelan & Rhew, 2016) and an oak savannah (Sun et al., 2016) both in California. Whelan and Rhew (2016) suggested that this was analogous to the Birch Effect (Birch, 1958), where wetting causes a microbial community change and a simultaneous increase in respiration. The Birch effect proves difficult to characterize even for a well-studied gas like CO₂ (e.g., Manzoni et al., 2020) and is likely to exhibit similar complexity for OCS.

Sun et al. (2016) uncovered the importance of the litter layer in trace gas exchange dynamics, where a rainfall event caused changes in OCS fluxes in opposite directions for soil chamber observations with and without an intact litter layer (Figure S3 in Supporting Information S1). While Sun et al. (2016) was able to reproduce the effect of litter fluxes in a process-based model, more information is needed to capture global litter dynamics.

The photodegradation of soil organic matter has been shown to cause OCS emissions (Kitz et al., 2017; Whelan & Rhew, 2015); however, in one grassland with little exposed soil, the difference between a light and dark measurement of OCS exchange was minimal (Whelan & Rhew, 2016). Most of the observations shown in Figure 2 are taken with dark chambers. Light will certainly play a role in OCS production, though we do not have enough data to explain this relationship in a robust way.

5. Conclusions

Observations of soil OCS fluxes in the Tropics and Arctic are obviously needed. Several groups have already applied the OCS tracer to the Arctic with compelling results (e.g., Hu et al., 2021), but no in situ observations have been published to confirm the underpinnings of the studies. If our empirical model of OCS soil exchange generates reasonable values, the global OCS-associated sulfur exchanged by soils calculated at low resolution is not large enough to explain the missing source of hundreds of Gg S yr⁻¹ in the atmospheric OCS budget (Whelan et al., 2018). However, discovering areas where soils might produce much more OCS, that is, agricultural “hot spots” using remote sensing data, will reveal new sources of OCS that should be taken into account on the global and regional scales. The patchwork of agricultural OCS sources (Figure 5) underscores the importance of using finer surface data to estimate trace gas exchanges that are sensitive to temperature (e.g., Figure 1). Further complication arises from non-stomatal sources and sinks of OCS in ecosystems aside from soil.

Data Availability Statement

ECOSTRESS and SMAP data for Figure 3 were accessed via AppEEARS (<https://lpdaacsvc.cr.usgs.gov/appeears/>): land surface temperature with data quality (SDS_LST, SDS_LST_err, and SDS_QC (ECO2L-STE.001)) and soil moisture with data quality (Soil_Moisture_Retrieval_Data_PM_soil_moisture_pm, Soil_Moisture_Retrieval_Data_PM_soil_moisture_error_pm, and Soil_Moisture_Retrieval_Data_PM_retrieval_qual_flag_pm (SPL3SMP_E.003)) for May 28-20, 2021. Red and infrared reflectance bands used to calculate NDVI from Landsat Collection 2 data was accessed via USGS EarthExplorer for 5 May 2020. Version 8.0 of the Soil OCS Empirical Model (SOCSEM) described in this manuscript is preserved via Zenodo (<https://doi.org/10.5281/zenodo.5752450>) available via the MIT license and developed openly with Python 3.7. Please cite this manuscript for use.

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