SiB4 Modeled 0.5-degree Carbonyl Sulfide Vegetation and Soil Fluxes, 2000-2020

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Dataset Version: 1

Summary

This dataset provides outputs from the Simple Biosphere Model (v 4.2). Products include hourly 0.5-degree gridded fluxes of gross primary productivity (GPP), respiration, carbonyl sulfide (COS) uptake by vegetation and soil, along with conductance of COS (apparent mesophyll and total), stomatal conductance of water and partial pressure of CO2 in the canopy air space, leaf surface, interior and chloroplast. The data are separated by plant functional type (PFT). Fluxes have dimensions of latitude, longitude, time, and plant functional type. Model output spans 53N to 90N latitude and 180W to 180E longitude over years 2000 to 2020. The data are provided in NetCDF version 4 format.

There are 7,671 data files in NetCDF version 4 format (.nc4) with this dataset: one file for each day of the year for the years 2000 through 2020.

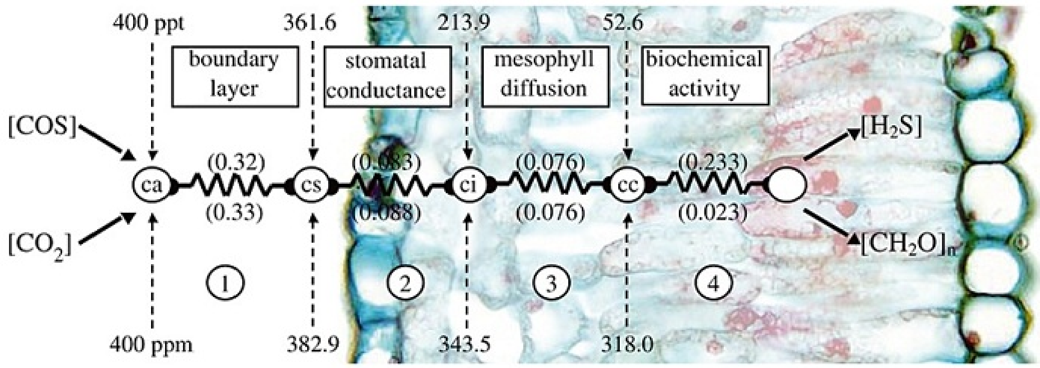

Figure 1. SiB4 COS Uptake-Resistance Model. Numbers in parentheses are conductance values corresponding to the processes in the square boxes: (1) Boundary layer conductance, (2) Stomatal conductance, (3) Mesophyll conductance, and (4) Biochemical rate constant. For COS, we take steps 3 and 4 together to produce an apparent COS mesophyll conductance (variable cosgm in dataset). This figure was taken from Berry et al. (2013).

Citation

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1. Dataset Overview

This dataset provides outputs from the Simple Biosphere Model (v 4.2) using a modified methodology from Haynes et al. (2021). Products include hourly 0.5-degree gridded fluxes of gross primary productivity (GPP), respiration, carbonyl sulfide (COS) uptake by vegetation and soil, along with conductance of COS (apparent mesophyll and total), stomatal conductance of water and partial pressure of CO2 in the canopy air space, leaf surface, interior and chloroplast. The data are separated by plant functional type (PFT). Fluxes have dimensions of latitude, longitude,

longitude, time, and plant functional type. Model output spans 53N to 90N latitude and 180W to 180E longitude over years 2000 to 2020.

Project: ABoVE

The Arctic-Boreal Vulnerability Experiment (ABoVE) is a NASA Terrestrial Ecology Program field campaign being conducted in Alaska and western Canada, for 8 to 10 years, starting in 2015. Research for ABoVE links field-based, process-level studies with geospatial data products derived from airborne and satellite sensors, providing a foundation for improving the analysis, and modeling capabilities needed to understand and predict ecosystem responses to, and societal implications of, climate change in the Arctic and Boreal regions.

Related Dataset

Haynes, K.D., I.T. Baker, and A.S. Denning. 2021. SiB4 Modeled Global 0.5-Degree Monthly Carbon Fluxes and Pools, 2000-2018. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1848

- The methodology employed was taken from this dataset with modifications: After performing an equilibrium spin-up, a varying CO_2 boundary condition was employed during the simulation period. This was implemented using NOAA data to distribute monthly mean CO_2 values across a global grid as part of the forcing data.

Acknowledgments

This study was funded by the NASA ABoVE Program (grant 80NSSC19M0105). SiB4 development was also supported in part by funding from the NOAA Climate Program Office Atmospheric Chemistry Carbon Cycle and Climate program.

2. Data Characteristics

Spatial Coverage: Circumpolar, latitudes > 53 degrees north

Spatial Resolution: 0.5 degree

Temporal Coverage: 2000-01-01 to 2020-12-31

Temporal Resolution: Daily files with hourly data

Study Area: Latitude and longitude are given in decimal degrees.

Site	Westernmost Longitude	Easternmost Longitude	Northernmost Latitude	Southernmost Latitude
Pan-arctic	-180	180	90	53

Data File Information

There are 7,671 data files in NetCDF version 4 format (.nc4) with this dataset: one file for each day of the year for the years 2000 through 2020. Each data file contains both modeled variables and input variables, as described in Tables 1 and 2. Plant functional types (PFT) are listed in Table 3.

The files are named *sib4-hourly-<YYYY-MM-DD>.nc4*, where *<YYYY-MM-DD>* is each day of all months for the period 2000-01-01 to 2020-12-31.

Example file name: *sib4-hourly-2000-01-26.nc4*

Table 1. Modeled variables.

Variable	Dimensions	Units	Description
assim	lon, lat, npft, time	µmole m^{-2} s^{-1}	Assimilation (or Gross Primary Productivity)
cos_assim	lon, lat, npft, time	pmole m^{-2} s^{-1}	Carbonyl Sulfide (COS) Vegetation Assimilation
cos_grnd	lon, lat, npft, time	pmole m^{-2} s^{-1}	COS Soil Uptake
cosgm	lon, lat, npft, time	mole m^{-2} s^{-1}	Apparent mesophyll conductance of COS
cosgt	lon, lat, npft, time	mole m^{-2} s^{-1}	Total conductance of COS
gsh2o	lon, lat, npft, time	mole m^{-2} s^{-1}	Stomatal conductance of water (H2O)
resp_auto	lon, lat, npft, time	µmole m^{-2} s^{-1}	Autotrophic Respiration
resp_het	lon, lat, npft, time	µmole m^{-2} s^{-1}	Heterotrophic Respiration
pco2cas	lon, lat, npft, time	Pa	Canopy Air Space CO_2 partial pressure
pco2s	lon, lat, npft, time	Pa	Leaf Surface CO_2 partial pressure
pco2i	lon, lat, npft, time	Pa	Leaf Internal CO_2 partial pressure
pco2c	lon, lat, npft, time	Pa	Leaf Chloroplast CO_2 partial pressure

Table 2. Input variable descriptions.

Variable	Dimensions	Units	Description
crs	-	-	The Coordinate Reference System, WGS84 (EPSG:4326)

lat	lat	degrees north	Latitude
lon	lon	degrees east	Longitude
pft_area	lon, lat, npft	1	Fractional areal coverage of PFT in each grid cell
pft_names	npft, clen	-	Names of 15 plant functional types (PFT); three-character string abbreviations (*clen*) defined in Table 3. Output variables are partitioned by PFT and indexed by the *npft* dimension.
time	time	d	Timestep in hours since the beginning of 2000-01-01
time_bnds	time, bnds	d	Timestep in hours since the beginning of 2000-01-01 (*bnds*=2)

Table 3. Plant functional types (PFT) from Haynes et al. (2020). **npft** and **clen** are dimensions of variable *pft_names* (Table 2).

npft value	clen value	Plant Functional Type
1	DBG	Desert and Bare Ground
2	ENF	Evergreen Needleleaf Forest
3	DNF	Deciduous Needleleaf Forest
4	EBF	Evergreen Broadleaf Forest
5	DBF	Deciduous Broadleaf Forest
6	SHB	Shrubs (Non-Tundra)
7	SHA	Tundra Shrubs
8	C3A	Tundra Grassland
9	C3G	C3 Grassland
10	C4G	C4 Grassland
11	C3C	C3 Generic Crop
12	C4C	C4 Generic Crop
13	MZE	Maize
14	SOY	Soybeans
15	WWT	Winter Wheat

3. Application and Derivation

CO_2 fluxes are used to study terrestrial ecosystem changes in response to climate warming. COS fluxes are used in the carbon cycle community as a proxy for gross plant uptake and for plant stomatal conductance. The output variables were used for calculating the seasonal cycle trends and results explored in the submitted manuscript.

4. Quality Assessment

The model was run once with a fixed set of parameters. This study does not include uncertainty based on parameter selection. Annual GPP values included in this dataset were found to be reasonable compared to other datasets when tested with the ILAMB framework (unpublished). Previous SiB4 datasets published on the ORNL DAAC have included more extensive comparisons with other datasets (e.g. see QA section in the ORNL DAAC related dataset https://doi.org/10.3334/ORNLDAAC/1848).

5. Data Acquisition, Materials, and Methods

This dataset is output from a Simple Biosphere Model (SiB4) simulation, following SiB4 methodology described in Haynes et al. (2019, 2021). SiB4 OCS simulations are described in Section 7 of the SiB4 Tech note (Haynes et al., 2020), and the methodology is summarized below. CO_2 simulations were performed following the methodology described in Haynes et al. (2021). The only modification is that after performing an equilibrium spin-up, a varying CO_2 boundary condition was employed during the simulation period. This was implemented using NOAA data to distribute monthly mean CO_2 values across a global grid as part of the forcing data.

Carbonyl sulfide (COS) is an atmospheric trace gas analog of carbon dioxide (CO_2). While CO_2 is both taken up and emitted during interactions with plants (through photosynthesis and respiration, respectively), COS is irreversibly hydrolyzed inside the leaf once it is taken up. In recent years, COS has been used as a proxy for plant carbon uptake. While there are other sources and sinks that potentially complicate this relationship, they are generally small compared to the magnitude of plant uptake (Whelan et al., 2018). COS has thus been used as a tracer for gross plant uptake and stomatal conductance at site and regional scales (e.g., Seibt et al. (2010), Montzka et al. (2007), Wehr et al. (2017), Hilton et al. (2017), Hu et al. (2021), Kooijmans et al. (2021)).

The implementation of COS plant uptake in SiB4 is based on the mechanistic and empirical descriptions of leaf uptake described in Berry et al. (2013). Atmospheric COS is taken up by plants and consumed inside leaf chloroplasts by the enzyme carbonic anhydrase (CA). Since COS takes the same pathway as CO_2, the series of resistances is similar and this is illustrated in Figure 1.

Relative to water (H_2O), the greater mass and larger cross-section of COS results in diffusion restriction by a factor of 1.94 in the stomata and 1.56 in the laminar boundary layer. Once inside the leaf cell, COS hydrolysis is catalyzed by CA at a rate proportional to the internal partial pressure of COS. The combined mesophyll conductance and biochemical CA activity ('apparent mesophyll conductance', or gm_{cos}) scales with photosynthetic capacity V_{max} such that: $gm_{cos} = \alpha * V_{max}$, where α is a parameter that is calibrated to observations (Stimler et al., 2012). Using this simplified framework, COS uptake by plants ($assim_{cos}$) is written as:

$$assim_{cos} = cos_{CAS} * gt_{cos}$$
$$gt_{cos} = [1.56/g_{bh2o} + 1.94/g_{sh2o} + 1.0/gm_{cos}]^{-1}$$
$$gm_{cos} = 1400 * V_{max} * (1.0 + 5.33 * C4) * APAR_{KK} * RSTFAC_2 * (P/P0_{sfc}) * (T_{can}/T_{ice})$$

,

where COS_{CAS} is the canopy air space COS mole fraction, gt_{cos} is calculated from the respective water vapor conductances to boundary layer (g_{bh2o}) and stomata (g_{sh2o}), $C4$ is a one or zero respectively depending on whether or not the plant is C4 or C3. $APAR_{kk}$ is the scaling factor for leaf radiation, $RSTFAC_2$ is the root zone water potential, P is the pressure, $P0_{sfc}$ is the reference surface pressure (10,000 Pa), T_{can} is the canopy temperature, and T_{ice} is the freezing temperature of water (273.15 K).

In addition to plant uptake, COS is also taken up by soils. Soil COS exchange is modeled in SiB4 following the mechanistic soil model described in Kooijmans et al. (2021). Briefly, field and laboratory experiments have shown that soil both takes up and emits COS, and that emission due to abiotic thermal degradation and photodegradation of soil organic matter can be particularly pronounced in agricultural soils (Meredith et al., 2018). A new mechanistic model describes the uptake and production pathways together in the soil column (Ogée et al., 2016). Due to recent efforts, parameter values are now available for a range of biomes and land cover types. The COS soil flux calculation is as follows:

$$F_{COS,soil} = \sqrt{kB\theta D}\left(C_a - \frac{z_1^2 P}{D}\left(1 - \exp\left(\frac{z_p}{z_1}\right)\right)\right),$$

where k is the CA reaction rate (s^{-1}), B is the solubility of COS in water (cubic meters of water per cubic meter of air), θ is the soil water content ($m^3\ m^{-3}$), D is the soil COS diffusivity (cubic meters of air per meter of soil per second), C_a is the canopy air space COS mole fraction, z_1^2 is D / ($kB\theta$), and P is the uniform COS production rate over depth z_p (here assumed to be 1.0 m). Soil COS diffusivity further depends on (a) soil porosity (calculated from sand fractions following Lawrence and Slater (2008)), (b) the layer used for soil temperature and soil moisture (taken from the top 5-cm layer, where most of the OCS uptake and emissions are assumed to take place), and (c) tortuosity functions (using Deepagoda et al. (2011) for air and Millington and Quirk (1961) for water). Uptake through hydrolysis in soil water depends on soil CA enzyme activity. Following Meredith et al. (2019), this is expressed as:

$$k = f_{CA} k_{uncat} \frac{x_{CA}(T)}{x_{CA}(T_{ref})},$$

where f_{CA} is the CA enhancement factor, k_{uncat} varies with soil pH following Elliott et al. (1989), and $x_{CA}(T)$ and $x_{CA}(T_{ref})$ are temperature response functions from Ogée et al. (2016). Biome-averaged f_{CA} from Meredith et al. (2019) was used to calculate COS uptake for different PFTs.

COS production (P_{cos}) is a temperature-dependent response function modulated by soil redox potential. Following Meredith et al. (2018), this exponential temperature model was used with biome-averaged values for constants a and b.

The COS parameters used in the calculations described are listed in Figure 2.

	Production parameters		Uptake parameter
	$a \pm SD$ (pmol $m^{-3}\ s^{-1}$)	$b \pm SD$ ($1°C^{-1}$)	f_{CA}
Grass	2.20 ± 0.5	0.096 ± 0.005	17000
Evergreen Forest	4.86 ± 2.7	0.101 ± 0.015	32000
Deciduous Forest	4.94 ± 0.7	0.107 ± 0.002	32000
Agriculture	9.59 ± 7.3	0.104 ± 0.004	6500
Desert/bare soil	5.60 ± 5.1	0.050 ± 0.010	13000

Figure 2. Biome-averaged uptake and production parameters used to simulate OCS in SiB4.

6. Data Access

These data are available through the Oak Ridge National Laboratory (ORNL) Distributed Active Archive Center (DAAC).

SiB4 Modeled 0.5-degree Carbonyl Sulfide Vegetation and Soil Fluxes, 2000-2020

Contact for Data Center Access Information:

- E-mail: uso@daac.ornl.gov
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