



**Jet Propulsion Laboratory**  
California Institute of Technology

# Uncertainty Quantification and Traceability for Remote Sensing of the Carbon Cycle

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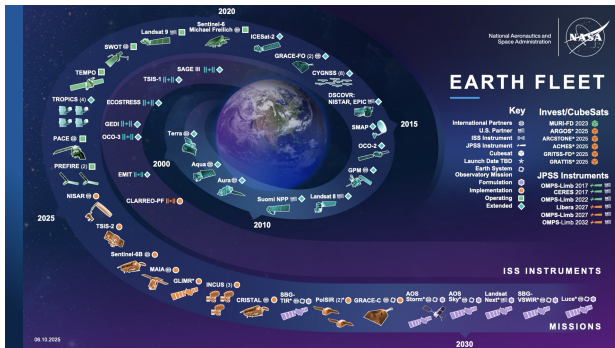
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# Outline

## Outline

- NASA Earth Science and Traceability
- Level 2 Inverse Problem
- Simulation-Based UQ
- Higher Level Products

# NASA Earth Science



- Satellite assets are managed as *missions*
- Mission design is informed by science objectives
- Development spans multiple phases across years
- Earth science missions deliver publicly available science data products

<https://science.nasa.gov/earth-science/earth-missions>

See also: NASA's Eyes on the Earth

SBG rescoped as EAGLE

AOS rescoped as FALCON

# Science Traceability

- A mission is proposed with a science traceability matrix (STM), linking science goals and objectives to design and delivery requirements
- Science goals are broad, often motivated from community consensus
- Objectives are specific and capable of being validated

## Science Traceability Matrix

National Aeronautics and  
Space Administration



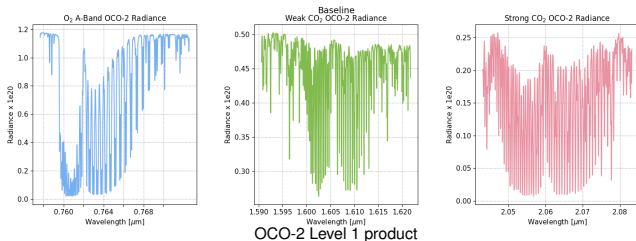
Science Goal	Measurement Objective	Measurement Requirement	Instrument	Instrument Requirement	Data Product	Mission Requirement
<i>The specific science questions the mission intends to answer.</i>	<i>What would need to happen during the mission to accomplish the measurement objective (and therefore the science objective)</i>	<i>What the measurement must include in terms of content, precision, quality.</i>	<i>What instrument would be needed to carry out the measurement.</i>	<i>How and how well the instrument would need to perform.</i>	<i>What will be the output (the product) of this measurement (for example, a map or a spectrum)</i>	<i>What would need to happen during the mission to accomplish the measurement objective (and therefore the science objective)</i>

Science traceability matrix (<https://science.nasa.gov/mission/psyche/>, Weiss et al., 2005)

# Data Products

## Earth System Data Record (ESDR) pipeline for NASA Earth-observing satellites

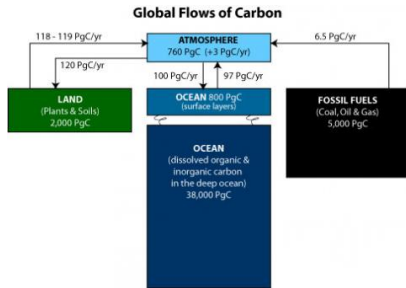
- Level 1: Instrument data (radiance spectra) that have been processed to sensor units
- Level 2: Derived geophysical variables at the same resolution and location as Level 1 source data.
- Level 3: Variables mapped on uniform space-time grid scales, usually with some completeness and consistency.
- Level 4: Model output or results from analyses of lower-level data



# Carbon Cycle

Remote sensing data and carbon cycle science, overview in Cressie (2018)

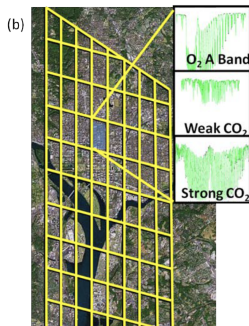
1. Level 1: Radiances  $\mathbf{Y}(A, t)$  at satellite footprint resolution
2. Level 2: Retrievals  $\hat{\mathbf{X}}(A, t)$  of atmospheric  $\text{CO}_2$  concentration (ppm)
3. Level 3: Aggregated, gap-filled retrievals  $\tilde{\mathbf{X}}(s, t)$  at coarse resolution
4. Level 4: Flux estimates  $\hat{W}(s, t)$  as mass of carbon per unit area per unit time ( $\text{g C m}^{-2}\text{yr}^{-1}$ )



<https://science.nasa.gov/earth-science>

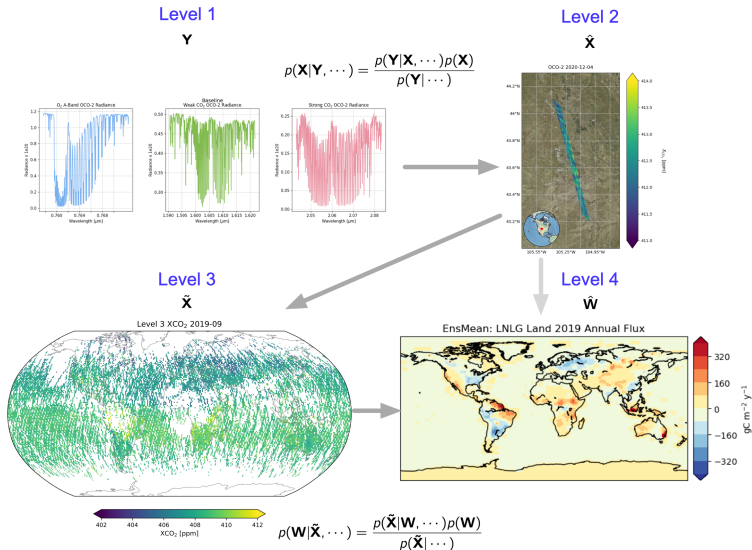
# OCO-2/3

- Satellite-based estimates of carbon dioxide ( $\text{CO}_2$ ) from a collection of satellites, including NASA's Orbiting Carbon Observatory-2 and -3 (OCO-2/3), can provide a more comprehensive constraint on the *carbon cycle*.
- Science goals focused on precision of global and regional fluxes
- Traceability for OCO-2/3 focused on atmospheric vertical average  $\text{CO}_2$  concentration:  $\text{XCO}_2$  (Miller et al., 2007)
- Remote sensing data and carbon cycle science, statistical overview in Cressie (2018)
- Long-term: Will (are) oceans and land biosphere maintain(ing) rate of uptake from perturbations to global carbon cycle?



<http://ocov2.jpl.nasa.gov>

# Carbon Cycle Product Pipeline



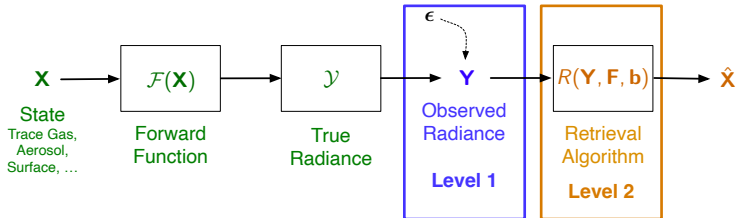
# Level 2 Inverse Problem

## Level 2 Inverse Problem

- Data products are actually inferences
- Retrieval: Level 1  $\rightarrow$  Level 2

# Retrieval Inverse Problem

- General objective: infer unknown surface and/or atmosphere states from remote sensing observations of radiation:  $[X|Y]$ 
  - Combine scientific knowledge with statistical and computational tools
- Probabilistic formulation provides guidance on inference
  - General knowledge of state distribution  $[X]$
  - Forward function informs  $[Y|X]$



#### Aleatoric Uncertainty

State vector variability  
Measurement noise

#### Epistemic Uncertainty

State vector structure  
Forward model structure  
Forward model parameters  
Retrieval prior distribution  
Lower level inputs  
Computational artifacts

# Retrieval

- For OCO-2/3, the state vector  $\mathbf{X}$  includes vertical profile of  $\text{CO}_2$ , along with other atmosphere, surface, and instrument unknowns
- Operational *working* statistical model (Rodgers, 2000)

$$\mathbf{X}^{(w)} \sim \text{MVN}(\mathbf{X}_a, \mathbf{S}_a)$$

$$\mathbf{Y}_{\text{OBS}} \sim \text{MVN}(\mathbf{F}^{(w)}(\mathbf{X}^{(w)}, \mathbf{B}^{(w)}), \mathbf{S}_\epsilon)$$

- $\mathbf{S}_a$  is the a priori covariance matrix, and  $\mathbf{X}_a$  is the a priori state (prior mean).
- Optimization with nonlinear least squares algorithm, denote converged state  $\hat{\mathbf{X}}^{\text{raw}}$
- Raw retrieved column average,  $\widehat{XCO}_2^{\text{raw}} = \mathbf{h}^T \hat{\mathbf{X}}^{\text{raw}}$

# Bias Correction

- $\widehat{XCO_2}^{raw}$  exhibits patterns of systematic bias, due to multiple epistemic sources
- Algorithm and validation teams implement post-retrieval bias correction (Payne et al., 2023)

$$\widehat{XCO_2}^{bc} = \widehat{XCO_2}^{raw} + g(\hat{X}^{raw})$$

- Provides traceability to ground-based observation standards from the Total Carbon Column Observing Network (TCCON)
- Operational uncertainty quantification is incomplete

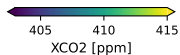
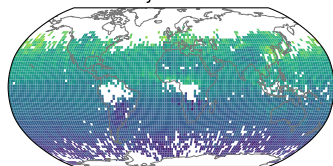


TCCON validation sites for OCO-2/3

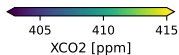
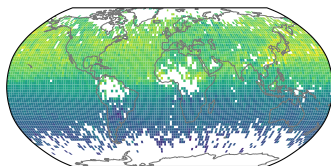
# Seasonal XCO<sub>2</sub>

OCO-2 2019 QF Good

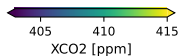
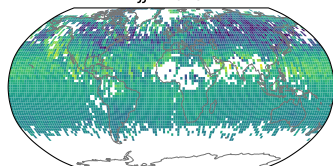
DJF 2018



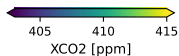
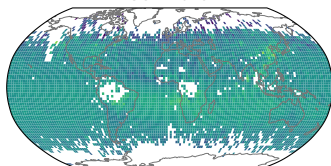
MAM 2019



JJA 2019



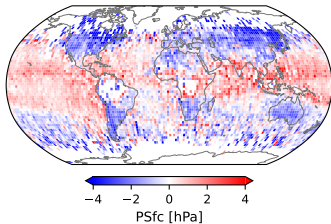
SON 2019



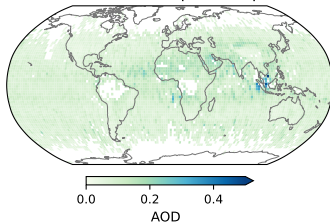
# State Vector Elements

OCO-2 SON 2019 QF Good

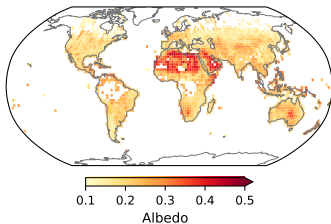
Surface Pressure



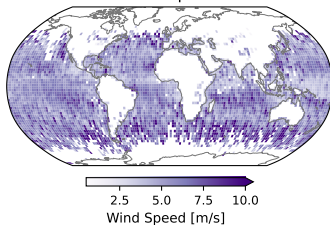
Total Aerosol Optical Depth



Albedo

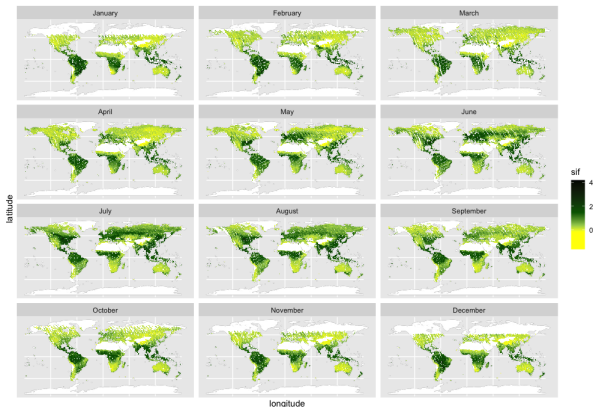


Wind Speed



# Solar-Induced Fluorescence

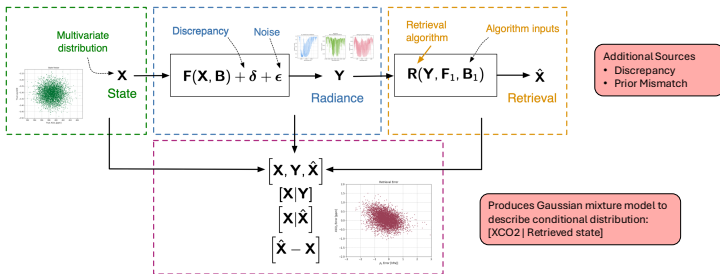
- Science opportunities evolve over mission lifetimes
- OCO-2/3 also estimate solar-induced fluorescence (SIF)
- Additional information for biospheric role in carbon cycle (Jacobson et al., 2025)



OCO-2 monthly SIF (Johny et al., 2025)

# Simulation-Based UQ

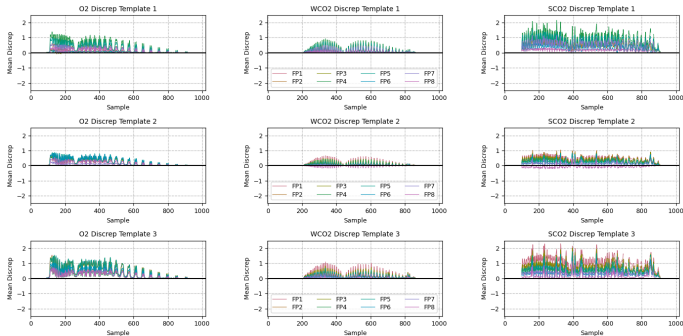
- Simulation-based UQ (SBUQ) incorporates nonzero mean, correlated model discrepancy in simulating retrieval pipeline
- Framework targets *total variability* in retrieval error



# Model Discrepancy

- Approaches for incorporating model discrepancy
  - Alternative forward model and/or parameters, e.g. McGarragh et al., 2024
  - Construct empirical specification from mission data, e.g. Braverman et al., 2021

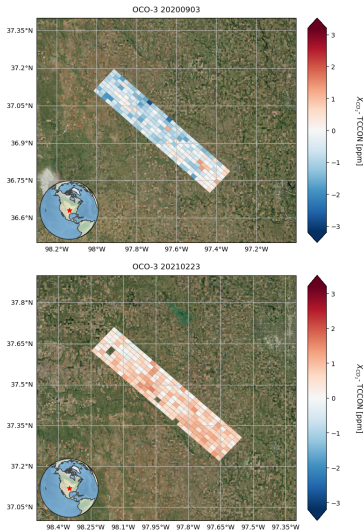
V11 Discrepancy Mean 202005



Distribution of model discrepancy for OCO-2 clusters.

# Partitioning Variability

- Higher-level aggregate products consider inference for an *areal unit* containing many footprints
- Indicators of common epistemic sources
  - Partitioning variability for validation (Yadav et al., 2025)
  - Variation in aggregates for OCO-2/3 coincident observations (Taylor et al., 2023)
  - Prior misspecification and spatially correlated states (Patil et al. 2022, Nguyen et al. 2019)
  - Shared forward-model parameter errors (Connor et al. 2016, Hobbs et al. 2020)
- Random effects approach (Zhang et al. 2019, Hobbs et al. 2026+) to partition sources



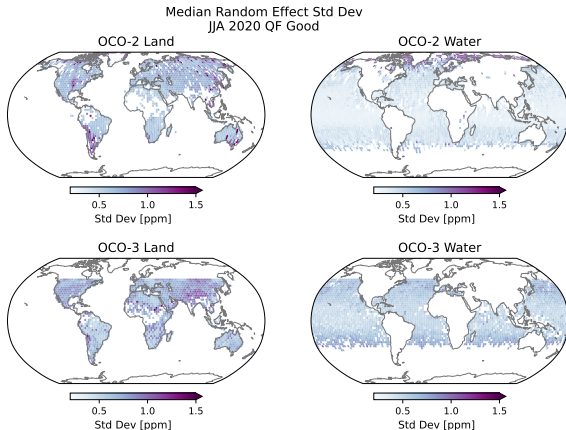
Difference between OCO-3  $X_{CO_2}$  and TCCON at  
Lamont, OK for two overpasses

# Epistemic Uncertainty

- Epistemic uncertainty contributes random effect for small areas:

$$\hat{X}_{i,j}^{(bc)} - X_{i,j} = \alpha_j + \gamma_{i,j}$$

- $Var(\alpha_j)$  critical for higher-level products and traceability



Grid scale random effect standard deviation for JJA 2020

# Higher-Level Products

## Higher-Level Products

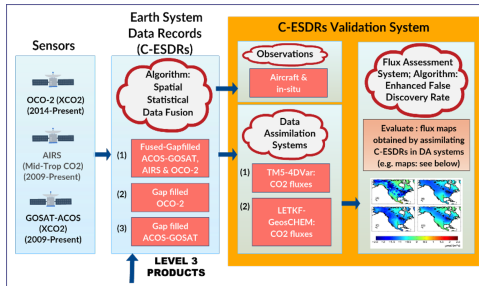
- Level 3 incorporates data fusion methods
- Flux inversion: Level 2, 3 → Level 4

# Level 3 Products

- Aggregated products offer manageable data volume for long records
- Probabilistic framework for multi-instrument fusion and continuity

$$\begin{aligned} & [\text{Product 1} | \text{Target Quantity}] \times \\ & [\text{Product 2} | \text{Target Quantity}] \times \\ & \dots, \\ & [\text{Product K} | \text{Target Quantity}] \times \\ & \quad [\text{Target Quantity}] \end{aligned}$$

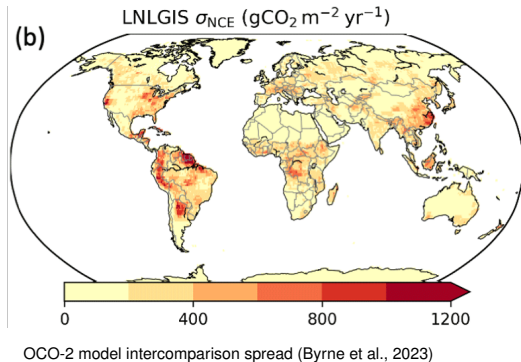
- Level 3 products from recent MEaSUREs effort (Yadav et al., 2025)



Fused XCO<sub>2</sub> products, described in Yadav et al., 2025

# Flux Uncertainty

- Key uncertainty sources in flux inversions
  - Atmospheric transport
  - Inversion system prior assumptions (Stanley et al., 2024)
  - Satellite data products
- Added value information for multi-model ensembles
  - Within-inversion posterior uncertainties
  - Approaches for consensus flux estimates (Cressie et al., 2022)



# Discussion

- Traceability and extended mission data records
  - Science traceability storylines evolve for extended missions
  - Continuity of data record across changing satellite constellation
- Carbon cycle challenges
  - Interactions with other Earth system processes
  - Fine spatial and temporal scales, including diurnal, interannual
- UQ research opportunities
  - Hierarchical treatment of discrepancy/forward model error
  - Joint UQ for multiple footprints

Questions?  
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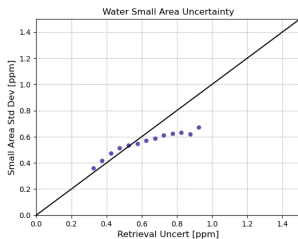
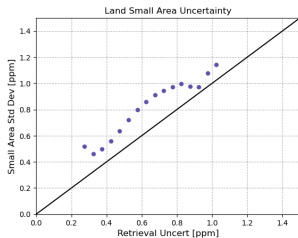
# Backup

## Backup

### Level 2 Uncertainty Estimates and Error Partitioning

# Uncertainty Estimates

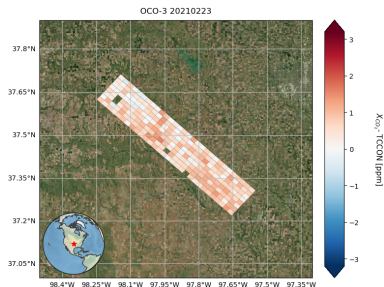
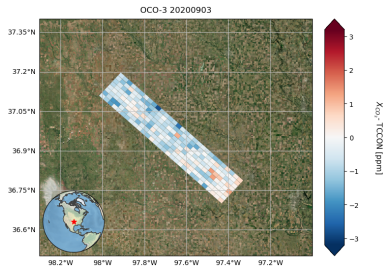
- OCO-2/3 reported  $XCO_2$  uncertainty from L2 retrieval, assumes *working model*
- Captures some but not all contributions to retrieval error variability
  - Profile smoothing error
  - Interference error due to cross-correlation
  - Retrieval sensitivity to radiance measurement noise
- Demonstrated relationship to scatter in small areas (Worden et al. 2017, Taylor et al. 2023)
- Suggests meaningful contribution to error from measurement noise (Hobbs et al. 2017, Mitchell et al. 2023)



OCO-2  $XCO_2$  retrieval scatter in small areas, binned by reported uncertainty.

# Partitioning Variability

- Higher-level aggregate products (Peiro et al. 2022, Yadav et al. 2025+) consider inference for an *areal unit*, e.g. small area, containing many footprints
- Indicators of common epistemic sources contribute to uncertainty in the aggregate estimate
  - Partitioning variability for TCCON coincidences (Yadav et al., 2025+)
  - Variation in aggregates for OCO-2/3 coincident observations (Taylor et al., 2023)
  - Retrieval sensitivity studies
  - Simulation-based UQ with model discrepancy
- Random effects approach (e.g. Zhang et al., 2019)



Difference between OCO-3  $X_{CO_2}$  and TCCON at  
Lamont, OK for two overpasses

# Partitioning Variability

- Statistical model for small area  $j$

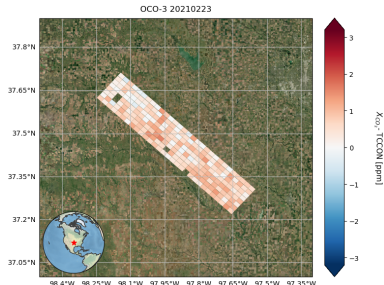
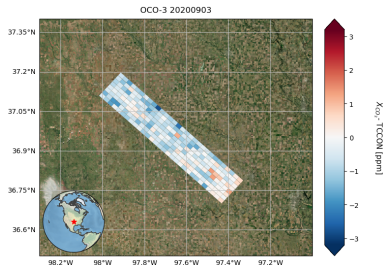
$$\hat{X}_{i,j}^{(bc)} = \mu_j + \alpha_j + \gamma_{i,j}$$

$$\text{Var}(\alpha_j) = \sigma_{\alpha,j}^2$$

$$\text{Cor}(\gamma_{i,j}, \gamma_{i',j}) = \rho_{i,j}^{|f(i,j) - f(i',j)|}$$

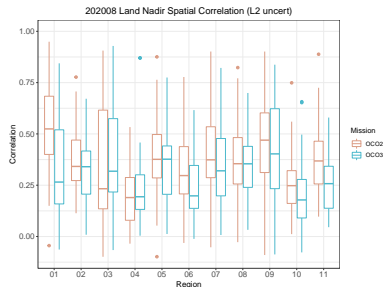
- Multi-level framework for collection of soundings (Kulawik et al. 2016, Zhang et al. 2019, Yadav et al. 2025+)

- Area-wide common error  $\alpha_j$
- Total error variability bound with simulation-based UQ
- Sounding-specific random errors, leverage small area scatter skill
- Local-scale spatial correlation (Torres et al. 2019, Mitchell et al., 2023)



# Spatial Correlation

- Combination of variability of  $\alpha_j$  (Yadav et al., 2025+) and fine-scale spatial correlation in  $\gamma_{i,j}$  (Mitchell et al., 2023) impact uncertainty in aggregated estimates
- Multiple retrieval mechanisms can induce these correlations
  - Prior misspecification and spatially correlated states (Patil et al. 2022, Nguyen et al. 2019)
  - Shared forward-model parameter errors (Connor et al. 2016, Hobbs et al. 2020)



**Table 4**  
Spatially Coherent Fine-Scale Variability ( $c_s$ )<sup>1/2</sup>, Random Variability ( $c_r$ )<sup>1/2</sup>, and Geostatistical Range ( $a_{space}$ ) by Biome

Region	( $c_s$ ) <sup>1/2</sup> (ppm)	( $c_r$ ) <sup>1/2</sup> (ppm)	( $a_{space}$ ) (km)
N. A. Boreal	1.11	0.27	12
N Pacific Temperate	0.52	0.21	16
W Pacific Tropical	0.46	0.24	21
E Pacific Tropical	0.54	0.22	20
N.A. Temperate	0.76	0.35	15
Northern Ocean	0.67	0.17	14
N Atlantic Temperate	0.49	0.23	18
Atlantic Tropical	0.48	0.22	21
N Tropical S.A.	0.72	0.26	17
All	0.66	0.24	16

Table 4 from Mitchell et al. (2023)