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GOSAT-2 Level 4 CH_4 Algorithm Theoretical Basis Document

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National Institute for Environmental Studies
GOSAT-2 Project

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Revision History

Version	Revised	Page	Description
00	Dec. 2025	-	-

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1 Introduction

1.1 Objective

This document describes the algorithm and processing method for the Greenhouse gases Observing SATellite-2 (GOSAT-2) Level 4 (L4) methane (CH_4) Product and provides an overview of the initial version (01.01). The algorithm is intended to estimate the global surface CH_4 flux based on the GOSAT-2 Thermal And Near infrared Sensor for carbon Observation-Fourier Transform Spectrometer-2 (TANSO-FTS-2) short wavelength infrared (SWIR) Level 2 (L2) Column-averaged Dry-air Mole Fraction Product, as well as the global CH_4 distribution. The system consists of an atmospheric tracer transport model, an inverse analysis scheme, and *a priori* information. This document provides a description and references for each of these components.

1.2 Product revision history

Table 1. Revision history

Version	Date	Author	Description
01.01	25 December 2025	M. Saito	Initial version

2 GOSAT-2 observations

GOSAT-2 is a satellite dedicated to greenhouse gas observations of carbon dioxide (CO_2) and CH_4. The satellite carries a Fourier transform spectrometer (TANSO-FTS-2) and a push-broom imaging radiometer TANSO Cloud and Aerosol Imager-2 (TANSO-CAI-2). TANSO-FTS-2 measures SWIR sunlight reflected from Earth's surface and thermal infrared (TIR) radiation emitted from the ground and Earth's atmosphere. TANSO-FTS-2 has a high spectral resolution of 0.2 cm^{-1} and operates in five spectral bands: three in the SWIR spectral range (0.75–0.77, 1.56–1.69, and 1.92–2.33 μm; bands 1, 2, and 3, respectively), and two in the TIR spectral range (5.5–8.4 and 8.4–14.3 μm; bands 4 and 5, respectively). Column-averaged dry-air mole fractions of CO_2 and CH_4 (denoted as XCO_2 and XCH_4, respectively) are retrieved using the 1.6 and 2.0 μm bands for CO_2 and the 1.6 and 2.3 μm bands for CH_4. TANSO-FTS-2 spectral data can also resolve carbon monoxide (CO) using the 2.3 μm band, in addition to XCO_2 and XCH_4. Spectral radiance in the two TIR bands is used to obtain information on vertical profiles of atmospheric concentrations of CO_2 and CH_4. TANSO-FTS-2 has an intelligent pointing mechanism that immediately identifies cloud positions in the field of view using an onboard camera and points to a cloud-free location. The camera has a spatial resolution of ~0.1 km with 608 × 1024 pixels over 30 km in the along-track field and 50 km in the cross-track field.

TANSO-CAI-2 has five observation bands for forward viewing at 343, 443, 674, 869, and 1630 nm, and backward viewing at 380, 550, 674, 869, and 1630 nm. It provides data for identifying clouds and aerosol conditions in the cross-track field over a distance of 1000 km.

The instruments on GOSAT-2 have been described in detail by *Suto et al.* (2021).

GOSAT-2 flies in a sun-synchronous orbit at an altitude of 613 km. The equator-crossing local time of the descending node is 13:00 with a repeat cycle of 6 days (inclination angle of 98.0° ± 0.1°). The pointing mechanism for TANSO-FTS-2 covers a range of ±40° in the along-track direction and ±35° in the cross-track direction. The observation interval of TANSO-FTS-2 is 4.024 s, with a nominal turnaround time of 0.65 s required for changing the pointing location, taking an image, identifying cloud locations in the image, and repointing to a cloud-free location. The field of view of TANSO-FTS-2 is 15.8 mrad for all bands, and the instantaneous ground field of view is a circle with diameter 9.6 km.

3 Product design

The GOSAT-2 mission is designed to enhance the space-borne measurements of major greenhouse gases that began with GOSAT observations, and to monitor the impacts of climate change and human activities on the carbon cycle. GOSAT observations have improved the accuracy of single shot measurements of greenhouse gases (*Yokota et al.*, 2009) relative to former satellite missions, providing confidence in the use of XCO_2 and XCH_4 data from space to constrain models that generate global flux estimates using atmospheric inversions (e.g., *Maksyutov et al.*, 2013). However, GOSAT observations provide sparse coverage as a trade-off for the high data quality, resulting in difficulties in quantifying regional fluxes using satellite observations alone. This limited observational coverage, together with the need to minimize the computational cost of atmospheric inversion, means that flux estimates from GOSAT data are resolved on a sub-continental scale (64 regions over the globe) using the National Institute for Environmental Studies (NIES) atmospheric tracer transport model (NIES-TM) and a fixed-lag Kalman smoother with ground-based observations and GOSAT XCO_2 and XCH_4 observations (*Maksyutov et al.*, 2013). This combined application of ground-based and satellite observations to atmospheric inversion allows more accurate inverse estimation of sub-continental fluxes; however, it does not allow a quantitative assessment of the degree to which satellite observations contribute to filling the gaps in greenhouse gas observations for carbon flux estimates at regional and even national scales.

TANSO-FTS-2 measures XCO_2 and XCH_4 over land with better sampling (more than twice the sampling rate) than TANSO-FTS, the main sensor aboard GOSAT, using an intelligent pointing mechanism. In addition, TANSO-FTS-2 has wider pointing angles than those of TANSO-FTS, especially in the along-track direction, allowing wider coverage of observation locations, which contributes to an increase in the available sun glint points over the ocean. Observations by GOSAT-2, which is equipped with enhanced versions of the instruments aboard GOSAT, are expected to facilitate the use of satellite observations in carbon cycle assessments and further improve the spatial resolution of flux estimates to better understand regional sources and sinks. The improvement in satellite observations afforded by GOSAT-2 is illustrated by the fact that using GOSAT-2 observations alone, the GOSAT-2 L4 Product estimates global surface CO_2 and CH_4 fluxes with a higher spatial resolution than those estimated by GOSAT. The atmospheric transport model and inverse scheme used for the GOSAT-2 L4 Product represent an upgraded version of the model system used in the GOSAT mission (NIES-TM with a fixed-lag Kalman smoother). The new model system, which is the Non-hydrostatic Icosahedral Atmospheric Model (NICAM)-based Inverse Simulation for Monitoring CH_4 (NISMON-CH_4), as described by *Niwa et al.* (2025), improves the spatial resolution of flux estimates. The NISMON-CH_4 consists of a NICAM-based transport model (NICAM-TM; *Niwa et al.*, 2011) for forward simulation and an atmospheric inversion using the four-dimensional variational (4D-Var) method (*Niwa et al.*, 2017a, b). The NISMON-CH_4 is operated on an icosahedral grid obtained by five iterations of recursive division (glevel-5, horizontal spatial resolution of ~223 km) and 40 vertical layers with a time step of 20 min. Information on the GOSAT-2 L4 Product plays an important role in assessing the robustness of GOSAT-2 measurements and the contribution of GOSAT-2 observations to the identification of regional sources and sinks.

4 Algorithm description

4.1 Overview

The GOSAT-2 L4 Product consists of global surface CO_2 and CH_4 flux estimates from GOSAT-2 XCO_2 and XCH_4 data, and three-dimensional fields of atmospheric CO_2 and CH_4 concentrations that are simulated using the estimated surface fluxes. The GOSAT-2 L4 product is provided by simulation frameworks that make up the GOSAT-2 L4 computational system.

The global surface CH_4 flux is estimated using NISMON-CH_4 in the context of Bayesian inference. The Bayesian least-squares estimate is obtained by minimizing the cost function as follows:

$$J = \frac{1}{2}(\mathbf{x} - \mathbf{x}_{\mathrm{pri}})^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_{\mathrm{pri}}) + \frac{1}{2}(\mathbf{M}\mathbf{x} - \mathbf{y})^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{M}\mathbf{x} - \mathbf{y}), \tag{1}$$

where $\mathbf{x}$ and $\mathbf{x}_{\mathrm{pri}}$ are vectors for modeled and *a priori* source and sink strengths, respectively; $\mathbf{M}$ is a matrix of a linear forward transport model used to obtain estimates of concentrations at each measurement; $\mathbf{y}$ is a vector of observed concentrations; and $\mathbf{B}$ and $\mathbf{R}$ are error covariance matrices for the *a priori* flux estimates and the misfit of concentrations between observations and model predictions, respectively. The superscript T denotes the transpose operator. In practical operation of NISMON-CH_4, Eq. (1) is replaced with $\delta\mathbf{x} = \mathbf{x} - \mathbf{x}_{\mathrm{pri}}$ as follows:

$$J = \frac{1}{2}\delta\mathbf{x}^{\mathrm{T}}\mathbf{B}^{-1}\delta\mathbf{x} + \frac{1}{2}(\mathbf{M}\delta\mathbf{x} - \mathbf{d})^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{M}\delta\mathbf{x} - \mathbf{d}), \tag{2}$$

where $\mathbf{d} = \mathbf{y} - \mathbf{M}\mathbf{x}_{\mathrm{pri}}$.

In the inversion, GOSAT-2 XCH_4 data serve as the primary observations ($\mathbf{y}$) for estimating global surface CH_4 fluxes ($\mathbf{x}$). The *a priori* fluxes ($\mathbf{x}_{\mathrm{pri}}$), as used in the GOSAT-2 Level 4 system, include ten categories: five annual anthropogenic sources (coal mining, oil and gas exploitation and use, landfill and waste, biofuel, and enteric fermentation and manure management), monthly rice paddy flux, monthly wetland flux, monthly soil oxidation, monthly biomass burning flux, and climatological natural fluxes (ocean, termite, and geological emissions).

These fluxes are optimized using two parameters: scaling factors ($\Delta\alpha$) and flux deviations (Δf). Scaling factors adjust flux magnitudes without changing spatial patterns, expressed as $\big(1 + \Delta\alpha_i(a,t)\big)\mathbf{x}_{\mathrm{pri},i}(a,t)$, where a and t denote location and time. This constraint reflects the difficulty of resolving fine-scale distributions due to atmospheric mixing. In contrast, flux deviations modify both magnitude and spatial distribution, represented as $\mathbf{x}_{\mathrm{pri},i}(a,t) + \Delta f_i(a,t)$. Anthropogenic, biomass burning, and natural fluxes are adjusted using scaling factors, whereas rice paddy, wetland, and soil oxidation fluxes are optimized through flux deviations.

In version 01.01, to evaluate the ability of the GOSAT-2 XCH_4 data to deduce the global surface CH_4 fluxes, $\mathbf{R}$ is represented using a uniform value ($\mathbf{R}$ = 20 ppb) for all retrieved concentrations. For the error covariance matrix $\mathbf{B}$, prior uncertainties are set at 50% for anthropogenic emissions and 100% for biomass burning and natural fluxes, assuming no spatiotemporal correlation. For rice paddy, wetland, and soil oxidation fluxes, prior errors and covariances are derived from ensembles based on a 120-year terrestrial biosphere model simulation (1901–2020), where each year represents one member. Variances and covariances are spatially localized using a Gaussian function to suppress unrealistic long-range correlations, and temporal correlations are ignored.

In the GOSAT-2 L4 CH_4 computational system, monthly averaged global surface CH_4 fluxes are estimated at a spatial resolution of 1.0°. Based on these *a posteriori* flux estimates, 6-hourly atmospheric CH_4 concentrations are simulated on a three-dimensional grid with the horizontal resolution of 2.5° and 17 vertical pressure levels, plus a near-surface level. These grids are derived by interpolating from the original model resolution (glevel-5 and 40 vertical layers). These outputs are provided as the GOSAT-2 L4A Global CH_4 Flux Product and the GOSAT-2 L4B Global CH_4 Distribution Product, respectively.

4.2 Processing outline

The GOSAT-2 L4 computational system was constructed on the NEC SX-Aurora TSUBASA A511-64 supercomputer at NIES, which features a maximum of 256 nodes, each with eight cores; the vector processor has a peak performance of up to 622.8 teraflops. The HPE Apollo2000 scalar computer with a peak performance of 86.0 teraflops at NIES is also used for preprocessing to convert the input information to the model grid data.

The process of deducing the global surface CH_4 flux from GOSAT-2 XCH_4 data begins with the assembly of various input data that are required for operation of the system. The input data are reanalyzed meteorological fields, *a priori* CH_4 sources and sinks, and observations of atmospheric CH_4. In the simulation of atmospheric transport, horizontal winds of the model are nudged toward those of the reanalysis to reproduce past and current atmospheric transport fields. In the operation of the GOSAT-2 L4 computational system, an atmospheric tracer transport simulation is first performed with nudging to generate and archive three-dimensional transport fields (air mass density, air mass flux, vertical diffusion coefficient, water substances, temperature, and cumulus base mass flux). The instantaneous values of these fields are archived every hour for the cumulus base mass flux and every 3 h for other variables, excluding the air mass flux. For the air mass flux, the variables are averaged every 3 h to maintain better consistency with continuity (CWC). The archive data are then used as input for an iterative operation of the atmospheric tracer transport model to deduce the surface fluxes using a four-dimensional variational (4D-Var) method (*Niwa et al.*, 2017a, b; see Section 4.4).

The *a priori* CH_4 source and sink data are prepared for a given analysis period and interpolated onto the model grid of the atmospheric tracer transport model. GOSAT-2 XCH_4 data are used as the atmospheric observational data to drive the GOSAT-2 L4 CH_4 computational system for calculating the monthly global surface CH_4 fluxes and their three-dimensional variability in the atmosphere over the analysis period. The forward and backward simulations of atmospheric CH_4 are performed for a duration of 2 months before the analysis period and 2 months after.

4.3 Input data

4.3.1 Meteorological reanalysis data

Horizontal winds in the atmospheric tracer transport model are nudged using the Japanese Reanalysis for Three Quarters of a Century data (JRA-3Q; *Kobayashi et al.*, 2024). Reanalysis data are used in our model system for the u- and v-components of wind ("anl mdl ugrd" and "anl mdl vgrd"; m s^{-1}) in the Quasi-regular Gaussian latitude/longitude grid field with 100 hybrid vertical levels. The JRA-3Q horizontal winds are provided on a 6 h time step at 0000, 0600, 1200, and 1800 UTC. As 40 vertical layers are implemented in the atmospheric tracer transport model used in our system, the vertical coordinate system in the JRA-3Q horizontal wind data is interpolated to that of the atmospheric tracer transport model; subsequently, the horizontal winds of the model simulation are nudged every 6 h to the wind fields in JRA-3Q.

4.3.2 *A priori* fluxes

Anthropogenic emissions are prescribed using the Emissions Database for Global Atmospheric Research (EDGAR version 6.0; *Crippa et al.*, 2021; *Monforti-Ferrario et al.*, 2021). Annual emission data are used because their temporal variability is much smaller than that of other fluxes. Monthly CH_4 flux components associated with the terrestrial biosphere (i.e., rice paddy, wetland, and soil oxidation) are derived from a prognostic biosphere model, the Vegetation Integrative SImulator for Trace gases (VISIT; *Ito and Inatomi*, 2012). CH_4 emissions from wetlands and rice paddies in VISIT are estimated using two schemes: *Cao et al.* (1996) and *Walter and Heimann* (2000). The GOSAT-2 L4 CH_4 computational system applies the *Cao et al.* (1996) scheme. Monthly biomass burning CH_4 flux is provided using a bottom-up approach with a burned area method; i.e., the Global Biomass Burning Emissions Inventory (GBEI version "2022a"; *Shiraishi et al.*, 2021; *Saito et al.*, 2022). GBEI provides data products for CO_2, CH_4, and CO emissions at 1-km and 1° grid resolutions with a monthly time step. The 1° resolution data are used as monthly biomass burning CH_4 emissions in our system. Natural fluxes are taken from *Weber et al.* (2019) for ocean, *Ito* (2023) for termite, and *Etiope et al.* (2019) for geological emissions, with the latter scaled to a global total of 23 Tg following *Canadell et al.* (2021). Because their interannual variability is highly uncertain and their contributions are small compared to other fluxes, both fluxes and scaling factors are kept constant throughout the analysis period. Table 2 lists the *a priori* fluxes and their data sources with respective references.

Table 2. List of *a priori* fluxes used in the GOSAT-2 L4 CH_4 computational system.

Prior	Model/Product	Reference	Temporal
Anthropogenic*	EDGAR	*Crippa et al.* (2021); *Monforti-Ferrario et al.* (2021)	annual
Rice paddy	VISIT	*Ito and Inatomi* (2012)	monthly
Wetland	VISIT	*Ito and Inatomi* (2012)	monthly
Soil oxidation	VISIT	*Ito and Inatomi* (2012)	monthly
Biomass burning	GBEI	*Shiraishi et al.* (2021); *Saito et al.* (2022)	monthly
Natural†	-	*Weber et al.* (2019); *Ito* (2023); *Etiope et al.* (2019)	climatology

* Anthropogenic emissions include five sources: coal mining, oil and gas exploitation and use, landfill and waste, biofuel, and enteric fermentation and manure management.

† Natural fluxes are the sum of ocean, termite and geological components.

4.3.3 Atmospheric observational data

The estimation of global surface CH_4 flux using the inverse scheme requires atmospheric concentration data to infer the spatial distribution of surface fluxes. The primary information on atmospheric observations used in our system is GOSAT-2 XCH_4 data retrieved from the SWIR spectra acquired by TANSO-FTS-2 (*Yoshida and Oshio*, 2022). GOSAT-2 XCH_4 products ver. 01.04 and ver. 01.07 were released in November 2020 and December 2021, respectively. Subsequent updates, ver. 02.00 and ver. 02.10, were released in August 2022 and February 2025. Revision details between ver. 02.00 and ver. 02.10 are provided by *Yoshida and Oshio* (2025). The main changes are summarized below:

- Corrected an error in the prior specification of aerosol optical thickness.
- Upgraded the TANSO-FTS-2 L1B input product and revised the CO_2 covariance matrix applied in the retrieval algorithm.
- Modified the conditions for quality control.

NIES GOSAT-2 Project (2022, 2025) reported comparison results of XCH_4 data between GOSAT-2 and the Total Carbon Column Observing Network (TCCON; *Wunch et al.*, 2011). This comparison uses GOSAT-2 XCH_4 data (ver. 02.00 for August 2019–July 2020 and ver. 02.10 for March 2019–January 2024), analyzed within radii of ±0.1°, ±1°, ±2°, and ±5° around TCCON sites. As shown in Table 3, mean biases (ppb) over land improved in GOSAT-2 XCH_4 ver. 02.10 compared to ver. 02.00, with absolute bias reductions of 7–75%, although standard deviations slightly increased. However, mean biases over ocean increased within ±2° and ±5° areas.

Table 3. Comparison of XCH_4 (over land and ocean) between GOSAT-2 and TCCON using *NIES GOSAT-2 Project* (2025). Distance indicates the target area for comparison, N is the number of comparison data, Bias is the mean bias (ppb), and STDEV is the standard deviation (ppb).

Data	Distance	Land			Ocean		
		N	Bias (ppb)	STDEV (ppb)	N	Bias (ppb)	STDEV (ppb)
Ver. 02.00	±0.1°	429	−2.10	8.79	0	-	-
	±1°	1741	−4.11	10.78	67	1.12	24.10
	±2°	2537	−2.96	12.29	172	−0.57	20.44
	±5°	5464	−3.08	14.66	872	−4.15	23.00
Ver. 02.10	±0.1°	2370	−1.57	9.45	0	-	-
	±1°	12905	−0.28	11.83	135	0.70	14.15
	±2°	16605	0.62	12.65	333	−2.20	16.57
	±5°	32882	−0.68	14.44	2220	−7.71	17.42

4.4 Atmospheric simulation and flux estimate

We use the NICAM-TM to simulate the transport of atmospheric CH_4. NICAM uses a quasi-homogeneous distribution of hexagonal or pentagonal grid cells derived from recursive division of an icosahedron to perform global simulations with high spatiotemporal resolution (*Tomita and Satoh*, 2004). The dynamic core of the model involves the use of nonhydrostatic equations expressed with finite volume methods, which can implement the CWC for tracer transport in the model. The NICAM-TM ensures strict mass conservation to produce realistic simulations of atmospheric tracer transport (*Niwa et al.*, 2011). CH_4 chemical reactions in the atmosphere are calculated in the NICAM-TM using prescribed chemical data from the TransCom-CH_4 experiment (*Patra et al.*, 2011). Tropospheric OH concentrations are reduced by 8% relative to the three-dimensional climatological fields (*Spivakovsky et al.*, 2000), and stratospheric reactions with Cl and O(^{1}D) are represented by parameterized loss rates (*Velders*, 1995).

The solution of $\delta\mathbf{x}$ that minimizes Eq. (2) is given by the gradient of the objective function, $\mathbf{g} = \partial\mathbf{J}/\partial\delta\mathbf{x}$, so that

$$\mathbf{g} = \mathbf{B}^{-1}\delta\mathbf{x} + \mathbf{M}^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{M}\delta\mathbf{x} - \mathbf{d}). \tag{3}$$

The second term on the right-hand side in Eq. (3) denotes that a vector of model–observation misfit, $\mathbf{M}\delta\mathbf{x} - \mathbf{d}$, is integrated backward in time by an adjoint operator, $\mathbf{M}^{\mathrm{T}}$. The optimized vector of $\delta\mathbf{x}$ is deduced by minimizing the gradient $\mathbf{g}$ using the 4D-Var method with the iterative operation of a forward model and its backward integration that is represented using an adjoint model.

The adjoint calculation requires program codes to step backward in time for integrating sensitivities to source components, as shown in the second term of Eq. (3). The adjoint model in NISMON-CH_4 implements the backward integration by reading in reverse order the meteorological variables that are archived for forward simulations with NICAM-TM. In the model, adjoint codes for vertical diffusion and cumulus convection are written based on a so-called discrete approach, and the expression for advection is given by both the discrete and continuous approaches (*Niwa et al.*, 2017a). In the GOSAT-2 L4 computational system, the continuous approach is used to calculate advection processes.

In the estimates of global surface fluxes using NISMON-CH_4, the POpULar scheme (*Fujii*, 2005), based on a quasi-Newton method, is applied to obtain the $\delta\mathbf{x}$ that minimizes the cost function J (*Niwa et al.*, 2017b). The POpULar scheme uses the Broyden–Fletcher–Goldfarb–Shanno algorithm (BFGS) to estimate the inverse Hessian of J, which gives the approximate Newton's direction $\mathbf{d}_{\mathrm{k}} = -\mathbf{H}_{\mathrm{k}}\mathbf{g}_{\mathrm{k}}$, where $\mathbf{H}_{\mathrm{k}}$ is the approximated inverse Hessian matrix of $\mathbf{J}$, and $\mathbf{g}_{\mathrm{k}}$ is the gradient shown in Eq. (3) at the *k*-th iteration. The approximate Newton's direction $\mathbf{d}_{\mathrm{k}}$ is then used to find the next point of the vector $\mathbf{x}$ with step size α_k in the direction $\mathbf{x}_{\mathrm{k+1}} = \mathbf{x}_{\mathrm{k}} + \alpha_k\mathbf{d}_{\mathrm{k}}$. Practical algorithms of POpULar for the iterative solution to obtain $\delta\mathbf{x}$ have been described by *Fujii* (2005) and *Niwa et al.* (2017b).

Initial atmospheric CH_4 concentration fields were derived from in situ observations archived at the World Data Centre for Greenhouse Gases (WDCGG) under the WMO Global Atmospheric Watch (GAW) program. The GOSAT-2 Level 4 system applies the grid conversion scheme of *Niwa et al.* (2022) to compute *a posteriori* fluxes at 1.0° spatial resolution from NICAM icosahedral grids (glevel-5). The scheme represents $\mathbf{M}$ in Eq. (3) as

$$\mathbf{M} = \mathbf{H}\ \mathbf{M}'\ \mathbf{G}, \tag{4}$$

where $\mathbf{H}$ and $\mathbf{G}$ denote spatiotemporal interpolation and flux data conversion, respectively. The matrix $\mathbf{M}'$ performs the integral calculation of atmospheric transport. The operator $\mathbf{G}$ arranges the flux data contained in $\delta\mathbf{x}$ onto latitude–longitude grids, enabling optimization in that space rather than in the model grid space. In practice, the scheme first subdivides the original latitude–longitude grid into a finer-scale grid. Each finer grid cell is then mapped to a hexagonal cell whose boundaries are defined trigonometrically in latitude–longitude coordinates. Because each finer grid cell is uniquely assigned to one of the surrounding icosahedral grids, global data integrity is preserved. This grid conversion scheme is entirely linear and thus represented by the matrix $\mathbf{G}$ in Eq. (4). This property facilitates development of the adjoint code represented by $\mathbf{G}^{\mathrm{T}}$:

$$\mathbf{M}^{\mathrm{T}} = \mathbf{G}^{\mathrm{T}}\ \mathbf{M}'^{\mathrm{T}}\ \mathbf{H}^{\mathrm{T}}. \tag{5}$$

By introducing $\mathbf{G}$ and $\mathbf{G}^{\mathrm{T}}$ into the model operator and its adjoint, respectively, the control variables can be arrayed in latitude–longitude grids.

The scaling factors or flux deviations optimized through inversion may lead to unrealistic negative fluxes. To prevent such artifacts, the GOSAT-2 Level 4 system applies the scheme of *Niwa et al.* (2025), which adopts the exterior penalty function method (*Sawada and Honda*, 2021) to introduce an additional constraint—a "penalty term J_p"—into the cost function. Specifically, a combined form $J + J_p$ is used as the cost function in the 4D-Var iterative calculation instead of J in Eq. (2).

The sensitivity of the remote sensing measurements to the atmosphere is generally not uniform with altitude. Therefore, an accurate representation of vertical atmospheric profiles retrieved from TANSO-FTS-2 measurements in the model simulation results is essential for comparison between GOSAT-2 XCH_4 data and the simulations. We apply the averaging kernel matrix $\mathbf{A}$ with *a priori* information used in the retrieval to the atmospheric inversion of simulated atmospheric concentrations, as follows:

$$x_s = x_a + \mathbf{a}^{\mathrm{T}}(\mathbf{x}_{\mathrm{s}} - \mathbf{x}_{\mathrm{a}}), \tag{6}$$

where x is the column-averaged dry-air mole fraction, and $\mathbf{a}$ and $\mathbf{x}$ are vectors for the column averaging kernel of the dry-air mole fraction and the vertical profile of atmospheric concentrations, respectively. Subscripts a and s refer to *a priori* and simulated atmospheric concentrations, respectively. Here, the entire depth of the atmosphere is divided into 15 vertical layers in the retrieval of the GOSAT-2 TANSO-FTS-2 SWIR Level 2 Column-averaged Dry-air Mole Fraction.

The *a priori* column-averaged dry-air mole fraction is given by

$$x_a = \mathbf{h}^{\mathrm{T}}\mathbf{x}_{\mathrm{a}}, \tag{7}$$

where $\mathbf{h}$ is a pressure weighting function, which is expressed using a vector of the partial column amount of dry air ω:

$$\mathbf{h}_i = \frac{\omega_{i,j}}{\sum_j \omega_{i,j}}, \tag{8}$$

where i refers to a discrete observation point and j is the vertical level. The total column averaging kernel $\mathbf{a}$ is determined as follows using $\mathbf{h}$ and the averaging kernel matrix $\mathbf{A}$:

$$\mathbf{a} = \mathbf{h}^{\mathrm{T}}\mathbf{A}. \tag{9}$$

We applied the variables $\mathbf{x}_{\mathrm{a}}$, ω, $\mathbf{A}$, pressures in the vertical layers, and surface pressure (hPa) derived from the GOSAT-2 SWIR L2 CH_4 product to Eqs. (6)–(9). The pressures and surface pressure were used to adjust the vertical profile of partial column amount given by $\mathbf{x}_{\mathrm{s}}$ to that of $\mathbf{x}_{\mathrm{a}}$.

5 Level 4A and Level 4B Products

The GOSAT-2 L4 CH_4 Product consists of the L4A Global CH_4 Flux Product and the L4B Global CH_4 Distribution Product. The L4A Product is created by gridding the *a posteriori* CH_4 fluxes to a 1.0° latitude/longitude grid on a monthly timescale, and the L4B Product provides global distributions for instantaneous values of atmospheric CH_4 concentrations every 6 h at 17 fixed atmospheric pressure levels (975, 925, 900, 850, 700, 600, 500, 400, 300, 250, 200, 150, 100, 70, 50, 30, and 10 hPa) and near the surface on a 2.5° latitude/longitude grid. The L4B Product is produced by performing forward simulation using the atmospheric tracer transport model with the *a posteriori* CH_4 fluxes.

The GOSAT-2 L4 Product is stored in NetCDF format data files (Conventions CF-1.6). In the L4A Product, *a priori* fluxes for six types of source and sink strengths and *a posteriori* flux for total fluxes (mg CH_4 m^{-2} day^{-1}). The L4B Product provides three-dimensional atmospheric CH_4 concentration fields (mmol mol^{-1}) and surface pressures derived from the atmospheric simulations. For comparison of the GOSAT-2 XCH_4 data, column concentrations of the L4B Product can be estimated using variables stored in the product, and some additional parameters may be obtained from the GOSAT-2 SWIR L2 CH_4 product, as described in Section 4.4.

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