



1 **Signal-Domain Guided Deep Learning for Gap-Filling of** 2 **XCO and XCH₄: A Masked Spatio-Temporal Fusion of** 3 **TROPOMI and GEOS-Chem (2019–2023)**

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12 **Abstract**

13 Long-term, high-resolution monitoring of carbon monoxide (CO) and methane (CH₄) is
14 essential for understanding their spatiotemporal variability and guiding climate mitigation strategies.
15 However, satellite observations like TROPOMI are often incomplete, and existing fusion methods
16 have limitations in accuracy and continuity. This study proposes a signal-domain fusion approach
17 combining 3D discrete cosine transform (DCT) and singular value decomposition (SVD) to
18 integrate TROPOMI data with GEOS-Chem simulations. A lightweight residual U-Net is employed
19 to refine the initial reconstruction by learning the residual field using meteorological drivers and
20 model outputs, guided by a masked loss. The method produces global 0.25° and China-specific
21 0.05° daily gap-free XCO and XCH₄ datasets from 2019 to 2023. The fused results outperform
22 GEOS-Chem and are comparable or superior to TROPOMI, with R² values of 0.92 for XCO and
23 0.85 for XCH₄. Trend analysis reveals regional patterns such as XCO increases in North America
24 and declines in Eastern China, and widespread CH₄ growth. High-resolution data captures
25 enhancements during the 2022 Chongqing wildfires, with average increases of 17.1 ppb in XCO
26 and 24.5 ppb in XCH₄, and reveals lower XCH₄ increases over rice-growing areas compared to



27 TROPOMI, with overestimation reduced by 17–26%, and stronger XCO reductions, with satellite
28 underestimations up to 38%. These results highlight agricultural contributions and policy impacts.
29 This approach effectively reconstructs missing observations and enhances the utility of satellite–
30 model data for atmospheric research and emission assessments. The generated daily gap-free
31 datasets are publicly available at <https://doi.org/10.5281/zenodo.17936461>.
32 **Keywords:** CO; CH₄; TROPOMI; GEOS-Chem; Signal Domain Fusion; Deep Learning;
33 Spatiotemporal Reconstruction

34 1. Introduction

35 Carbon monoxide (CO) and methane (CH₄) are two critical atmospheric gases that play a key
36 role in air quality monitoring and climate change research. CO is primarily produced through
37 incomplete combustion of fossil fuels and biomass, as well as the oxidation of methane and other
38 hydrocarbons. Its main sink is the reaction with hydroxyl radicals (OH), which contributes to the
39 formation of tropospheric ozone (O₃) and greenhouse gases such as carbon dioxide (CO₂) (Lelieveld
40 et al., 2016; Spivakovsky et al., 2000). Due to its atmospheric lifetime of weeks to months, CO
41 serves as an effective tracer for pollutant transport, facilitating the study of both horizontal and
42 vertical atmospheric movements (Heald et al., 2003). Methane (CH₄) is a powerful greenhouse gas
43 with a significantly longer atmospheric lifespan—around ten years—and a greater global warming
44 potential compared to numerous other gases (Filonchyk et al., 2024; Heilig, 1994). It originates
45 from both natural sources, such as wetlands, permafrost, and wildfires, and anthropogenic activities,
46 including agriculture, livestock digestion, landfills, and fossil fuel extraction (Chai et al., 2016;
47 Jackson et al., 2020). CH₄ plays a crucial role in atmospheric chemistry, influencing the oxidative
48 capacity of the atmosphere and contributing to tropospheric ozone formation. Its rising
49 concentration is a major driver of climate change.

50 CO provides valuable insights into pollution transport and atmospheric chemistry, while CH₄
51 monitoring is critical for assessing greenhouse gas emissions and climate impacts. Both CO and
52 CH₄ are essential targets for monitoring efforts due to their distinct roles in atmospheric processes.
53 A comprehensive understanding of these gases is fundamental to improving air quality predictions
54 and formulating climate mitigation policies. The spatial distribution of CO and CH₄ in the



55 atmosphere is now routinely determined through remote sensing observations. The source, transport,
 56 and removal processes of pollutants can be effectively tracked and analyzed through global-scale
 57 monitoring through satellite platforms. At present, a number of satellite instruments are equipped
 58 with the ability to observe CO and CH₄, including the Measurement of Pollutants in the Troposphere
 59 (MOPITT) (Deeter et al., 2003), Atmospheric Infrared Sounder (AIRS) (McMillan et al., 2005),
 60 Tropospheric Emission Spectrometer (TES) (Rinsland et al., 2006), and Interferometer for the
 61 Exploration of the Atmosphere in the Infrared (IASI) (Turquety et al., 2004). These instruments
 62 offer critical data support for the global distribution of CO and CH₄ in the atmosphere.

63 The TROPOMI instrument of the Sentinel-5P mission of the European Space Agency (ESA)
 64 provides a greater degree of daily global coverage and spatial resolution than previous observing
 65 missions. TROPOMI has been able to monitor the total atmospheric XCO and XCH₄ (column
 66 concentrations of atmospheric CO and CH₄, respectively) through spectroscopic measurements in
 67 the ultraviolet (UV) to short-wave infrared (SWIR) bands, with a spatial resolution of approximately
 68 7×7 km and high radiometric precision, since its successful launch on October 13, 2017.
 69 TROPOMI has already been employed in numerous pertinent applications for XCO and XCH₄
 70 investigations, including the calculation of emissions from biomass combustion (Goudar et al., 2023;
 71 Griffin et al., 2024). Nevertheless, the TROPOMI observations of XCO and XCH₄ at the surface
 72 and in the atmosphere are impeded by the ability of clouds and atmospheric aerosols to block or
 73 deflect reflected sunlight observed by satellite sensors. Observations may be incomplete,
 74 particularly in regions with elevated levels of air pollution or overcast skies.

75 The continuous coverage of XCO and XCH₄ products for TROPOMI has been the subject of
 76 numerous efforts, which primarily fall into three categories. On one hand, machine learning-based
 77 interpolation methods (X. Chen et al., 2022; Hu et al., 2022; Valerio et al., 2025; Wei et al., 2025)
 78 can effectively address data gaps. However, their precision is contingent upon the quality and
 79 diversity of the training data, and inaccurate predictions may arise from insufficient or unbalanced
 80 datasets. In addition to these approaches, model fusion methods have been developed to leverage
 81 the complementary strengths of different data sources or modeling frameworks. For instance,
 82 statistical data assimilation and hybrid modeling schemes combine outputs from chemical transport
 83 models (Fritz et al., 2022; Schneising et al., 2023; Sicard et al., 2021) with satellite retrievals to
 84 generate more spatially consistent and temporally continuous products. By integrating physical



85 model constraints with empirical corrections, these methods can effectively reduce retrieval bias
 86 and improve gap-filling robustness(Inness et al., 2022; Wang et al., 2023). However, their
 87 performance often depends on the accuracy of prior model simulations and the representativeness
 88 of assimilated observations. On the other hand, enhanced spectral fitting algorithms (Borsdorff et al.,
 89 2019; Guanter et al., 2015; Schneising et al., 2023; Wang et al., 2020) offer an alternative approach.
 90 These algorithms can mitigate bias from fluctuations in spectral reflectance by increasing the order
 91 of the polynomial fit. Nevertheless, this heightened complexity often demands greater
 92 computational resources and leads to longer processing times.

93 This study aims to develop a robust framework for generating daily global and regional
 94 continuous XCO and XCH₄ products over the period 2019–2023, at a spatial resolution of 0.25°
 95 globally and 0.05° over China. The core objective is to address the frequent data gaps in satellite
 96 observations, especially those caused by cloud coverage and retrieval errors in the TROPOMI sensor,
 97 by leveraging complementary information from chemical transport modeling and frequency-domain
 98 representations.

99 To achieve this, we propose a signal-domain guided spatio-temporal fusion method that
 100 integrates GEOS-Chem simulations with TROPOMI observations. Our approach consists of two
 101 stages: (1) a low-rank signal-domain reconstruction using 3D Discrete Cosine Transform (DCT)
 102 (Rao and Yip, 2014) and Singular Value Decomposition (SVD) (Wall et al., 2003), which exploits
 103 the shared spatio-temporal structure between model and satellite data to approximate missing values,
 104 and (2) a learning-based refinement module that employs a lightweight residual U-Net to predict
 105 pixel-level corrections based on GEOS-Chem output, reconstructed fields, and meteorological
 106 variables(Ronneberger et al., 2015; Tang, n.d.).

107 Instead of using the TROPOMI data mask as a direct input, we apply it as a spatial constraint
 108 during model training to focus learning only on valid observations(Wei et al., 2022). This masked
 109 learning strategy improves generalization while preserving physical consistency.

110 By fusing model-driven priors and observational constraints in both frequency and spatial
 111 domains, our method significantly improves the completeness and accuracy of XCO and XCH₄
 112 datasets. Validation against held-out TROPOMI data shows that the fused outputs outperform
 113 GEOS-Chem alone and remain comparable to or better than TROPOMI retrievals in cloud-covered
 114 regions. The proposed framework provides an efficient and interpretable solution for large-scale



115 trace gas monitoring and offers new opportunities for atmospheric data assimilation and long-term
 116 climate analysis.

117 **2. Measurement and materials**

118 **2.1. Data description**

119 *2.1.1. TROPOMI XCO and XCH₄ product*

120 This study employs TROPOMI Level-2 data products of column-averaged CO (XCO) and CH₄
 121 (XCH₄). Mounted on the Sentinel-5 Precursor (S5P) satellite, the TROPospheric Monitoring
 122 Instrument (TROPOMI) functions in a polar sun-synchronous orbit. The Sentinel-5 Precursor (S5P)
 123 satellite is equipped with the TROPOMI, which operates in a polar sun-synchronous orbit.
 124 TROPOMI provides daily global XCO measurements at 13:30 local solar time, thereby facilitating
 125 daily global coverage. The pixel resolution of TROPOMI's XCO and XCH₄ data has been enhanced
 126 from $7.0 \times 7.0 \text{ km}^2$ to $7.0 \times 5.5 \text{ km}^2$ as of June 2019.

127 By measuring the Earth's radiation in the short-wave infrared (SWIR) spectral range (2305-
 128 2385 nm), TROPOMI inverts XCO and XCH₄. TROPOMI exhibits a high sensitivity to the
 129 tropospheric boundary layer for XCO in clear-sky conditions, but this sensitivity is subject to
 130 variation based on the optical path in overcast conditions. TROPOMI employs absorption
 131 information in the oxygen-A band (760 nm) and the SWIR spectral range (2305-2385 nm) for
 132 inversion of XCH₄.

133 In order to guarantee the quality of the data, we implemented rigorous data selection criteria
 134 and exclusively selected data points with a Quality Value (QV) greater than 0.5 for analysis (Kawka
 135 et al., 2021). The data were obtained from a secondary offline and reprocessed product provided by
 136 NASA (<https://tropomi.gesdisc.eosdis.nasa.gov/data/>) for the period 2019–2023. The data regarding
 137 XCO and XCH₄ are presented in the form of column-averaged dry air mole fractions in parts per
 138 billion (ppb) in this study.

139 *2.1.2. GEOS-Chem Chemical Transport Model*

140 This investigation employs the GEOS-Chem model, a three-dimensional global atmospheric
 141 chemistry model that is comprehensive and employs Goddard Earth Observation System (GEOS)
 142 meteorological data supplied by the NASA Global Modelling and Assimilation Office (GMAO).



143 Global Observation System (GEOS) meteorological data supplied by the NASA Global Modelling
 144 and Assimilation Office (GMAO). We employed version 14.1.1
 145 (<http://acmg.seas.harvard.edu/geos/>), which is powered by GEOS-FP meteorological data. The most
 146 recent GEOS-5 meteorological data product to be provided by NASA/GMAO is GEOS-FP
 147 ("forward processing") (<http://gmao.com/gmao.html>). This product has a native horizontal
 148 resolution of 0.25° latitude \times 0.3125° longitude and a temporal resolution of hourly data and 3-
 149 hourly data.

150 To reduce computational overhead, we employed a $2^\circ \times 2.5^\circ$ GEOS-Chem horizontal grid for
 151 the global XCO and XCH₄ simulations and a $0.25^\circ \times 0.3125^\circ$ GEOS-Chem horizontal grid for the
 152 XCO and XCH₄ simulations for the China region in order to achieve more precise results. The model
 153 calculates the concentrations of CO and CH₄ by integrating emission inventories from various
 154 regions, which are based on surface emissions and chemical reactions.

155 The following are specific emission inventories: The Air Pollutant Emission Inventory (APEI)
 156 v2016 was used to obtain Canadian anthropogenic emissions data, while the National Emission
 157 Inventory (NEI) v2015-03 was used to obtain North American regional emissions data. The Diffuse
 158 and Inefficient Combustion Emissions in Africa (DICE-Africa) inventory was used to obtain
 159 anthropogenic emissions data for the Africa region (Marais and Wiedinmyer, 2016). The MIX v1.1
 160 inventory was used to obtain regional emissions data in Asia (Li et al., 2017) and HTAP. The
 161 Community Emissions Data System (CEDS) inventory was used to derive global aircraft and ship
 162 emissions data (Hoesly et al., 2018). The Quick Fire Emissions Dataset (QFED): Documentation of
 163 Versions 2.1, 2.2, and 2.4 was used to acquire carbon monoxide emissions data from biomass
 164 combustion.

165 The time step for convective and advective transport in the simulation is 300 seconds, while
 166 the time step for chemical processes is 600 seconds. The distribution of XCO and XCH₄
 167 concentrations and their alterations from 2019 to 2023 can be efficiently and accurately simulated
 168 using the aforementioned setup.

169 2.1.3. Total Carbon Column Observing Network (TCCON) Measurements

170 TCCON employs a Fourier Transform Infrared Spectrometer (FTS) to measure direct solar
 171 light in order to determine the total column concentrations of greenhouse gases in the atmosphere,
 172 including carbon dioxide (CO₂), methane (CH₄), carbon monoxide (CO), and others (Buschmann et



173 al., 2016; Kiel et al., 2016; Sha et al., 2019; Yang et al., 2020). These data are extensively utilized
174 to validate satellite remote sensing data (e.g., G. Chander et al., 2013; Imasu et al., 2023; Lin et al.,
175 2024; Loew et al., 2017; Wu et al., 2019; etc.) and to evaluate the performance of climate models.
176 They are rigorously calibrated and validated with high accuracy and reliability. TCCON's observing
177 stations are situated in numerous regions worldwide, providing a comprehensive understanding of
178 the global greenhouse gas distribution. These stations are capable of observing a diverse array of
179 climates and ecosystems. Harmonized processing is implemented for each site's data. In order to
180 guarantee data consistency and comparability, the data from each station is processed in a consistent
181 manner. TCCON's XCO and XCH₄ Dry Air Mole Fraction (Xgas) in ppb are employed in this
182 investigation. Site-specific and time-scale data are accessible through the official website of
183 TCCON (<https://tccon.ornl.gov/>), and users may select the data that is most relevant to their research
184 requirements. The validation of XCO and XCH₄ products from TROPOMI and GEOS-Chem is
185 frequently conducted using TCCON (Borsdorff et al., 2019; Cogan et al., 2012; Inness et al., 2022;
186 Schneising et al., 2019). Figure 1 illustrates the global TCCON site location map, which comprises
187 operational, prospective, and former sites, accordingly. The TCCON data version GGG2020
188 (Laughner et al., 2023) was employed in this experiment. Table 1 provides a list of the sites that
189 were utilized and are cross-correlated with the time frames in our experiment.



190
191 Fig. 1 Map showing global TCCON site locations, including operating sites, potential sites, and past
192 sites, respectively.



194

195 Table 1. Details of the TCCON sites used in this study, No. is the serial number.

No.	Site name	Latitude	Longitude	Location	Start date	End date
1	bremen01	53.104	8.85	Bremen, Germany	2009/1/6	2021/6/24
2	burgos01	18.5325	120.6496	Burgos, Philippines	2017/3/3	2023/6/23
3	darwin01	-12.425	130.891	Darwin, Australia	2013/1/1	2022/12/27
4	easttroutlake01	54.354	-104.987	East Trout Lake, Canada	2016/10/3	2024/2/15
5	edwards01	34.9599	-117.881	AFRC, Edwards, CA, USA	2013/7/20	2024/2/22
6	garmisch01	47.476	11.063	Garmisch, Germany	2007/7/18	2023/5/4
7	hefei01	31.91	117.17	Hefei, China	2015/11/2	2023/12/25
8	izana01	28.31	-16.5	Izana, Tenerife, Spain	2014/1/2	2023/8/30
9	karlsruhe01	49.103	8.44	Karlsruhe, Germany	2014/1/15	2023/6/26
10	lamont01	36.604	-97.486	Lamont, Oklahoma, USA	2011/4/16	2024/2/25
11	lauder03	-45.038	169.684	Lauder, New Zealand	2018/10/2	2023/12/28
12	nicosia01	35.141	33.381	Nicosia, Cyprus	2019/9/1	2023/5/10
13	orleans01	47.97	2.113	Orleans, France	2009/9/6	2023/6/23
14	parkfalls01	45.945	-90.273	Park Falls, Wisconsin, USA	2004/6/2	2024/2/25
15	pasadena01	34.136	-118.127	Pasadena, California, USA	2012/9/20	2024/2/25
16	reunion01	-20.901	55.485	Reunion Island, France	2015/3/1	2020/7/18
17	rikubetsu01	43.4567	143.7661	Rikubetsu, Hokkaido, Japan	2014/6/24	2021/6/30
18	sodankyla01	67.367	26.631	Sodankylä, Finland	2009/5/16	2023/5/30
19	tsukuba02	36.0513	140.1215	Tsukuba, Ibaraki, Japan, 125HR	2014/3/28	2021/3/31
20	wollongong01	-34.406	150.891	Wollongong, Australia	2013/1/4	2023/6/27
21	xianghe01	39.8	116.96	Xianghe, China	2018/6/14	2023/5/29

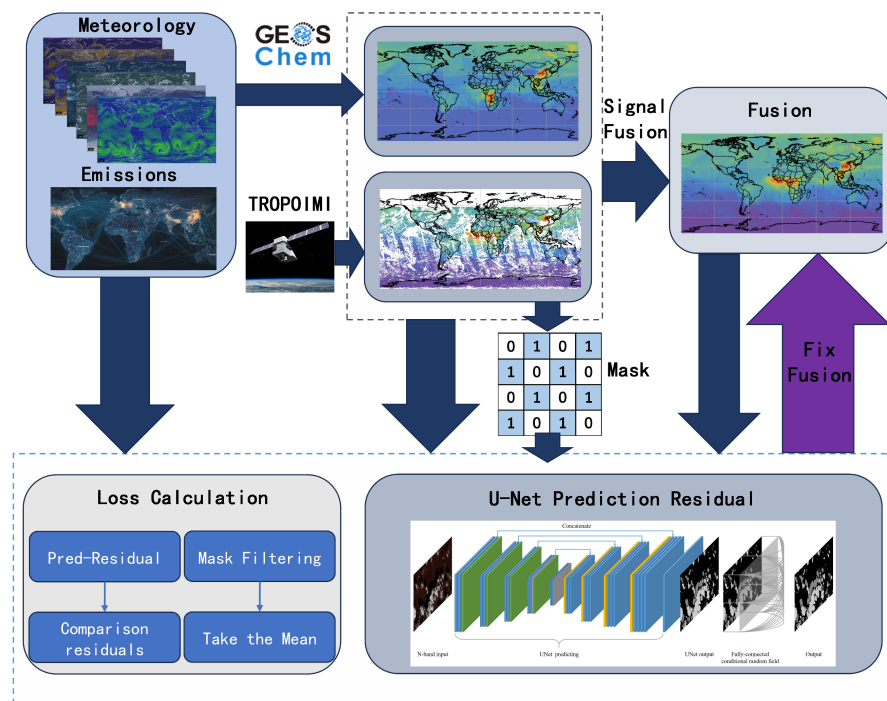
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197 2.2. Methodology

198 In this study, we propose a two-stage fusion framework that integrates physical modeling,
 199 signal-domain reconstruction, and deep learning-based residual correction to achieve continuous
 200 and accurate global mapping of atmospheric trace gases. The overall workflow is illustrated in
 201 Figure 2, which presents the main components and their interconnections. In the first stage, a signal-
 202 domain spatio-temporal reconstruction is employed to exploit the low-frequency consistency and
 203 spatio-temporal correlations between the TROPOMI observations and GEOS-Chem simulations,
 204 effectively filling missing data regions caused by cloud cover or instrument limitations. In the
 205 second stage, a residual learning network based on a lightweight residual U-Net is introduced to
 206 refine the fused results by learning nonlinear and region-specific discrepancies between the



207 preliminary reconstruction and the true satellite observations.



208
 209 Fig. 2. Overview of the proposed fusion framework combining physical modeling, signal-domain
 210 reconstruction, and deep learning-based residual correction. The process includes data
 211 preprocessing, DCT&SVD-based spatio-temporal fusion, and residual refinement via a lightweight
 212 residual U-Net architecture. Arrows indicate the information flow across different modules.

214 2.2.1. Data Preprocessing

215 Data preprocessing is a critical component in guaranteeing the reliability and rationality of the
 216 fusion results. In this investigation, values with data quality less than 0.5 in XCO and XCH₄ in
 217 TROPOMI are discarded to eliminate inaccurate data and are subsequently aligned to a global
 218 coverage of 720 x 1440 (0.25°) horizontal grid through area-weighted aggregation (Wang et al.,
 219 2018). The global-scale data from GEOS-Chem simulations should be aligned to the same 0.25°
 220 horizontal grid by inverse distance-weighted interpolation, and the TROPOMI data should be
 221 maintained at the same resolving power as GEOS-Chem (Setianto and Triandini, 2013). Global-
 222 scale data were simulated by GEOS-Chem and aligned to the same 0.25° horizontal grid.



223 To reconcile the heterogeneous spatial supports of satellite retrievals and model simulations,
 224 the TROPOMI XCO and XCH₄ data are first filtered by discarding pixels with a quality flag below
 225 0.5 and then regridded to a global 0.25°×0.25° grid (720×1440) using area-weighted aggregation
 226 (Wang et al., 2018). The GEOS-Chem outputs are interpolated onto the same 0.25° grid via inverse
 227 distance weighting to ensure spatial compatibility between the datasets (Setianto and Triandini,
 228 2013). The choice of 0.25° represents a widely adopted trade-off: it is fine enough to preserve
 229 mesoscale spatial gradients without excessively increasing data volume or the computational burden
 230 for multi-year global fusion analyses (Hu et al., 2024; Wang et al., 2023).

231 2.2.2. Spatio-Temporal Data Fusion Method Based on Signal Domain Reconstruction

232 The accuracy of the inventory typically results in an underestimation of GEOS-Chem
 233 simulation data, as demonstrated by previous research (Hu et al., 2018; Liang et al., 2023). However,
 234 the spatio-temporal consistency of the GEOS-Chem simulation data with TROPOMI data is still
 235 satisfactory (i.e., similar increase–decrease patterns over time). The spatio-temporal correlation
 236 between GEOS-Chem simulation data and TROPOMI data can be thoroughly leveraged to derive
 237 continuous coverage data through data fusion (J. Chen et al., 2022; He et al., 2022; Wang et al.,
 238 2021).

239 We will assume that a spatio-temporal relationship function exists between XCO and XCH₄
 240 for GEOS-Chem and TROPOMI, as shown below:

$$241 \quad XT = f(XG, \text{Lat}, \text{Lon}, \text{Date}) \quad (1)$$

242 Where Lat, Lon, and Date denote latitude, longitude, and time series, respectively, and XG is
 243 the GEOS-Chem XCO and XCH₄ concentration value. That is, the TROPOMI value at a given
 244 spatial and temporal coordinate can be determined by taking the modeled concentration value and
 245 the spatial and temporal coordinates to which it pertains.

246 In order to simplify the resolution of this issue, we convert the aforementioned equation to the
 247 form of a scalar product of XG with a spacetime transformation matrix M, as follows:

$$248 \quad XT = XG * \rho \quad (2)$$

249 The parameter relationships corresponding to GEOS-Chem and TROPOMI are established at
 250 each spatio-temporal coordinate in ρ , a spatio-temporal three-dimensional matrix with the same
 251 scale as XT and XG. ρ is a smoothed three-dimensional parameter matrix, inspired by previous work
 252 on filling in the vacant values in the spatio-temporal data and enhancing the smoothing of the data



using the multidimensional discrete cosine transform (Elharar et al., 2007; Garcia, 2010, 2010; J. Robinson and V. Kecman, 2003; Okolie and Smit, 2022; Peng et al., 2005; Rao and Yip, 2014; Wang et al., 2023). The majority of the known parameters in ρ can be obtained from the valid values in GEOS-Chem and TROPOMI. We suggest a spatio-temporal 3D matrix smoothing algorithm that is based on Singular Value Decomposition (SVD) and Discrete Cosine Transform (DCT) to enhance the smoothness of the data and fill unoccupied values in spatio-temporal data. This algorithm is designed to suit our data. The method effectively manages spatio-temporal data with missing values while maintaining the spatio-temporal correlation of the data by combining spatio-temporal nearest-neighbor interpolation and regularized optimization techniques.

We find the spatio-temporal 3D matrix $\hat{\rho}$ that minimizes Eq. (3) by means of the 3D discrete cosine transform method, as a way to obtain the best estimate of the vacancy value, including the residual term on the left-hand side and the smoothing term on the right-hand side.

$$E(\hat{\rho}) = \left\| \omega^{\frac{1}{2}} * (\hat{\rho} - \rho) \right\|^2 + \varepsilon \left\| \nabla^2 \hat{\rho} \right\|^2 \quad (3)$$

where $\| \cdot \|$ denotes the Euclidean paradigm, ω is a binary mask indicating the availability of a parameter corresponding to the spatio-temporal location of ρ , ε denotes the smoothing parameter, and ∇^2 denotes the Laplace operator. This satisfied condition $\hat{\rho}$ can be solved by iteration of Eq. (4).

$$\hat{\rho} = \alpha \text{IDCT}_3 \left(\Gamma^3 * \text{DCT}_3 (\omega * (\rho - \hat{\rho}) + \hat{\rho}) \right) + (1 - \alpha) \hat{\rho} \quad (4)$$

where α is a parametric factor for accelerating convergence, Γ^3 denotes the 3D spatio-temporal filtering matrix associated with the smoothing term, which can be obtained through Eq. (5), and DCT_3 and IDCT_3 denote the 3D discrete cosine signal transform and its inverse transform, respectively, with Eqs. (6) and (7) as their transformation rules.

$$\Gamma_{i_1, i_2, i_3}^3 = \frac{1}{1 + \varepsilon \sum_{k=1}^3 2 \left[1 - \cos \frac{(i_k - 1)\pi}{n_k} \right]} \quad (5)$$

Here, i_k denotes the i th value along the k th dimension and n_k denotes the size of ρ along the k th dimension. This means that the value at each position of this three-dimensional spatio-temporal filtering matrix is completely determined by its position, and the closer its position is to the element of the matrix at position (1, 1, 1), the larger (the closer it is to 1) the value is, and vice versa the smaller it is. The value at position (1, 1, 1) is 1. Since the low frequencies of the discrete cosine transformed signal matrix are mainly located close to position (1, 1, 1), with this filtering matrix, it



is possible to search for ρ that is suitable for smoothing. In this study, the total number of iterations is empirically set to 100, α is set to 0.75, and ε takes values in the middle of the range from 10^3 to 10^{-1} .

$$F(u, v, w) = \frac{2}{\sqrt{NMP}} \sum_{x=0}^{N-1} \sum_{y=0}^{M-1} \sum_{z=0}^{P-1} f(x, y, z) \cos\left(\frac{\pi(2x+1)u}{2N}\right) \cos\left(\frac{\pi(2y+1)v}{2M}\right) \cos\left(\frac{\pi(2z+1)w}{2P}\right) \quad (6)$$

Three-dimensional discrete cosine signal transform (DCT₃) rule, where $u=0, 1, 2, \dots, N-1$, $v=0, 1, 2, \dots, M-1$, $w=0, 1, 2, \dots, P-1$. N , M , and P represent the magnitude of the signal in each of the three dimensions.

$$f(x, y, z) = \frac{2}{\sqrt{NMP}} \sum_{u=0}^{N-1} \sum_{v=0}^{M-1} \sum_{w=0}^{P-1} F(u, v, w) \cos\left(\frac{\pi(2x+1)u}{2N}\right) \cos\left(\frac{\pi(2y+1)v}{2M}\right) \cos\left(\frac{\pi(2z+1)w}{2P}\right) \quad (7)$$

Three-dimensional discrete cosine inverse transform (IDCT₃) rule, where $x=0, 1, 2, \dots, N-1$, $y=0, 1, 2, \dots, M-1$, and $z=0, 1, 2, \dots, P-1$. N , M , and P represent the magnitude of the signal in each of the three dimensions.

Furthermore, the 3D discrete cosine transform is provided with a complete 3D matrix for signal conversion. Consequently, we interpolate ρ with missing values using the spatio-temporal autocorrelation property of ρ . Subsequently, we employ singular value decomposition (SVD) to retain 80% of the singular value energy, thereby enabling data downscaling and compression. The rules of the singular value decomposition (SVD) are illustrated in Eq. (8) as a method of preserving the primary ρ components for the iteration of Eq. (4).

$$A = U\Sigma V^T \quad (8)$$

where the matrices $A \in \mathbb{R}^{m \times n}$, $U \in \mathbb{R}^{m \times m}$ are orthogonal matrices whose column vectors are called left singular vectors; $\Sigma \in \mathbb{R}^{m \times n}$ is a diagonal matrix whose diagonal elements are the singular values $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r \geq 0$ (r is the rank of the matrix A). $V \in \mathbb{R}^{n \times n}$ is an orthogonal matrix whose column vectors are called right singular vectors.

Calculate the total energy of the singular values $E_{\text{total}} = \sum_{i=1}^r \sigma_i^2$, and find the smallest k such that the first k singular values account for at least 80% of the total energy, i.e., $(\sum_{i=1}^k \sigma_i^2) / E_{\text{total}} \geq 0.8$. Setting the last $r - k$ smaller singular values in Σ to zero yields the truncated diagonal matrix $\Sigma_k = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_k, 0, \dots, 0)$, and reconstructing the approximation matrix using the truncated singular value matrix $A_k = U\Sigma_k V^T$.

2.2.3. Deep Residual Refinement via Learning-Based Mask Reconstruction



To further enhance the reconstruction quality, we introduce a residual learning module based on a deep neural network to refine the fused product. To evaluate the effectiveness of the residual learning module, we conducted a site-based validation experiment across all TCCON stations, using data from the year 2021, to provide a rigorous comparison of the five reconstruction methods: (1) only DCT fusion(Garcia, 2010), (2) DCT and SVD mixed-signal reconstruction(M. Bengherabi et al., 2008; Majhi and Pal, 2021), (3) residual CNN(Y. Jiang et al., 2024), (4) residual U-Net(Ronneberger et al., 2015; Yan et al., 2022), and (5) residual XGBoost(Naseem et al., 2024). The performance was assessed using the coefficient of determination (R^2), root mean square error (RMSE), and mean bias (μ).

As shown in Tables S1 and S2, the residual U-Net consistently outperforms other methods for both XCO and XCH₄. Specifically, R^2 increased from 0.8227 (only DCT) to 0.845 for XCO and from 0.7056 to 0.7598 for XCH₄, while RMSE decreased correspondingly. These results demonstrate a improvement in the quality of the reconstructed data.

Residual Learning Objective

Let X_{DCT} denote the preliminary fused XCO/XCH₄ field obtained from the DCT/SVD-based reconstruction, and $X_{TROPOMI}$ be the valid observational values from the satellite. The residual between the fusion estimate and the true value (only available at observed locations) is defined as:

$$\Delta X_{true} = X_{TROPOMI} - X_{DCT}, \text{ where } M = 1 \quad (9)$$

Here, $M \in \{0,1\}^{H \times W}$ is a binary mask indicating the presence (1) or absence (0) of valid satellite data. The goal is to train a model $\mathcal{F}_\theta(\cdot)$ parameterized by θ to predict the residual ΔX_{pred} across the entire domain:

$$\Delta X_{pred} = \mathcal{F}_\theta(X_G, X_{DCT}, \mathbf{A}) \quad (10)$$

Where X_G denotes the GEOS-Chem full-coverage simulation data; X_{DCT} denotes the DCT/SVD-reconstructed preliminary fusion; \mathbf{A} denotes the auxiliary information such as meteorological fields and emission inventories. Precursor meteorological data simulated by GEOS-Chem and emission inventory were used in this study. The final fused product is obtained by correcting the DCT/SVD estimate with the predicted residual:

$$X_{fused} = X_{DCT} + \Delta X_{pred} \quad (11)$$

Loss Function Design



The model is trained using only the valid observations, i.e., locations where $M=1$. The loss function is designed to minimize the residual error at these observed locations:

$$\mathcal{L}(\theta) = \frac{1}{\sum M_{i,j}} \sum_{i,j} M_{i,j} \cdot \left(\Delta X_{\text{pred}}^{(i,j)} - \Delta X_{\text{true}}^{(i,j)} \right)^2 \quad (12)$$

This masked mean squared error ensures that the learning focuses on valid regions, while generalization to unobserved regions is achieved through the spatial context and auxiliary inputs.

Model Architecture and Training

In this study, we employ a lightweight residual U-Net architecture to predict the full-domain residual field ΔX_{pred} , which represents the correction from the DCT/SVD reconstruction to the expected TROPOMI observation. The network inputs include the GEOS-Chem simulation, the DCT/SVD reconstruction output, and auxiliary meteorological variables (Wang et al., 2025). The TROPOMI mask is not used as an input but is instead applied during the loss computation to focus learning only on valid pixels.

The residual U-Net consists of an encoder-decoder structure with skip connections and lightweight residual blocks to enhance gradient flow and convergence speed. The input and output spatial dimensions remain unchanged (i.e., 720×1440 at 0.25° resolution), enabling pixel-wise learning of spatial residuals. The training data comprises daily global maps from 2019 to 2023.

To ensure stable training and prevent overfitting, we implemented standard regularization strategies by incorporating early stopping, dropout layers ($p = 0.3$), and input normalization (mean = 0, std = 1). The final output is truncated to avoid physically implausible corrections, by enforcing:

$$|\Delta X_{\text{pred}}| < \gamma \cdot \sigma_{\text{TROPOMI}}, \gamma \in [2,3] \quad (13)$$

where σ_{TROPOMI} denotes the standard deviation of observed valid values, and γ is a hyperparameter controlling confidence bounds.

2.2.4. Evaluation Schem

Our study's evaluation methodology encompasses ground station validation and the assessment of geographical dispersion alongside relevant applications. The ground site validation entails the assessment of GEOS-Chem simulations, TROPOMI, and the fusion-generated XCO and XCH₄ data against TCCON measurements. This process encompasses the validation of overall results across all sites in comparison to individual site evaluations, utilizing the coefficient of determination (R^2), root mean square error (RMSE), mean bias (μ), and standard deviation of the bias (σ) (Karunasingha,



2022; Kobayashi and Salam, 2000; Wang et al., 2023). The aforementioned measures were computed using a significant threshold of $p < 0.01$ (Walsh et al., 2014). The assessment of geographical distribution includes the analysis of GEOS-Chem simulations, TROPOMI, and integrated XCO and XCH₄ data over several temporal scales, including multi-year averages, seasonal variations, and yearly metrics. Relevant applications include the evaluation of TROPOMI data acquisition, the integration of XCO and XCH₄ data at extremes, and the comparative analysis of multi-year column concentration increase rates across various geographies.

3. Results and discussion

3.1. TCCON Site Validation

The TCCON sites are uniformly spread worldwide, and the TROPOMI satellite traverses the region at around 13:30 local time; hence, we use the average column concentrations from the TCCON sites at $13:30 \pm 1\text{h}$ local time as the validation data for the ground stations. The GEOS-Chem simulation, TROPOMI, and the integrated data are then collected within a 2° radius surrounding each location as the corresponding validation outcomes. Only those cases in which the satellite data exhibit a missing rate exceeding 0.5 at the site are retained for comparison.

Figure 3 and 4 illustrate the time series of daily GEOS-Chem, TROPOMI, fusion data, and TCCON's XCO and XCH₄ data for several different ground stations, respectively. Figure 3 presents a time series plot of carbon monoxide column concentrations from three stations: easttroutlake01, lamont01, and parkfalls01. Figure 4 illustrates a daily time series plot of methane column concentrations, exemplified by edwards01, nicosia01, and pasadena01. In comparison to TCCON, both GEOS-Chem simulated XCO and XCH₄ data exhibit underestimation; nonetheless, they maintain time-varying consistency (i.e., similar increase–decrease patterns over time) with the TCCON site data, suggesting that the model simulation may serve as a reference for temporal and geographic fluctuations in the fused data. The temporal trend of TROPOMI and integrated XCO and XCH₄ data aligns with that of TCCON. The amalgamated data exhibit reduced biases μ (−0.79, −3.58, −1.08 ppb for XCO; −5.43, −2.49, −4.34 ppb for XCH₄) and diminished standard deviations σ (9.93, 4.26, 5.73 ppb for XCO; 5.99, 6.87, 6.77 ppb for XCH₄) in comparison to the TROPOMI data.

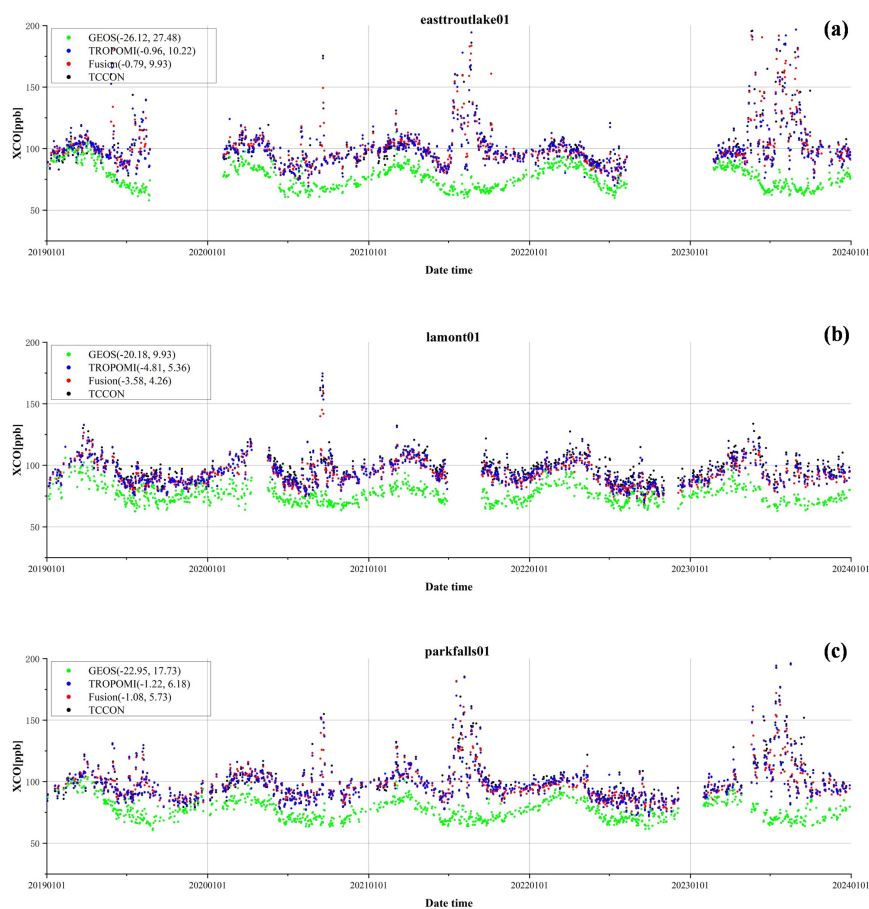


Fig. 3 (a)(b)(c) Time-series scatter plots of daily GEOS-Chem, TROPOMI, fusion data, and TCCON on XCO at three sites, easttroutlake01, lamont01, and parkfalls01, respectively. The first and second numbers in parentheses indicate the deviation (μ) and standard deviation (σ), respectively, both in parts per billion (ppb).

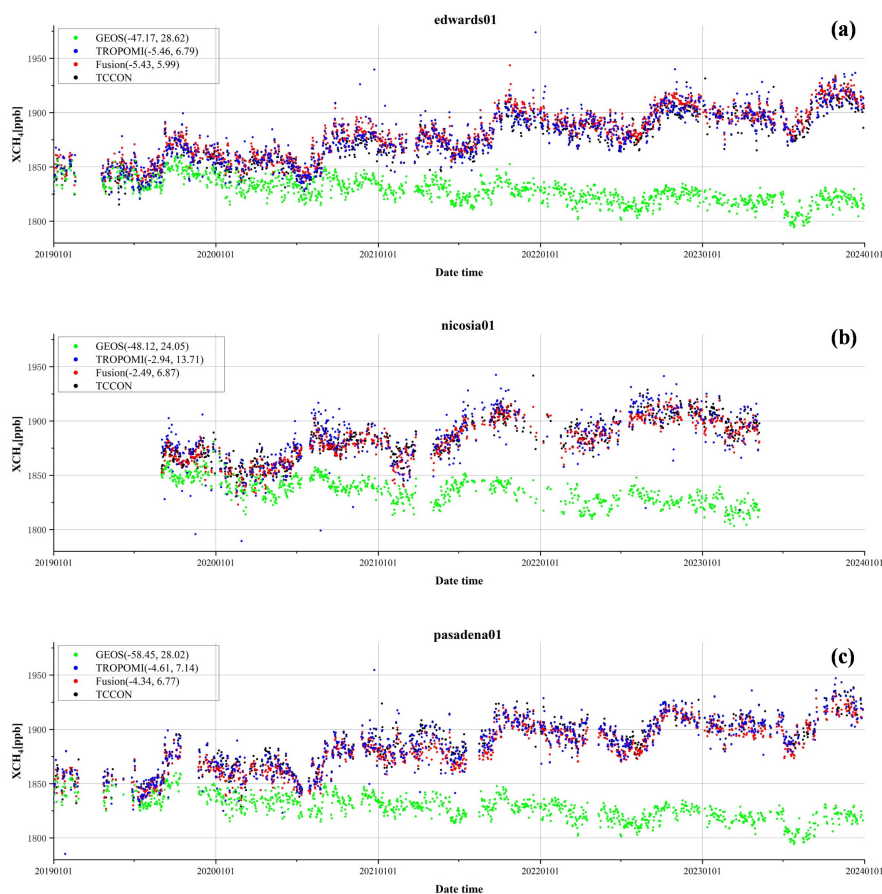


Fig. 4 (a)(b)(c) Scatterplots of daily time series of GEOS-Chem, TROPOMI, fusion data, and TCCON on XCH_4 for the three sites edwards01, nicosia01, and pasadena01, respectively. The first and second numbers in parentheses indicate the deviation (μ) and standard deviation (σ), respectively, both in parts per billion (ppb).

The systematic underestimation of GEOS-Chem model simulations may introduce bias in the correlation analysis when directly compared with TCCON observations. The average bias of the GEOS-Chem simulation data was corrected using a manual correction method, which more accurately reflects the relationship with TCCON observation data, thereby enhancing the reliability of the correlation analysis. This study further enhances scientific validity and relevance by screening TROPOMI satellite observation data samples with a missing rate exceeding 50% at the stations, and comparing these with TCCON data for validation. This screening method effectively addresses uncertainty arising from insufficient data coverage while concentrating on the incremental aspects



414 of the study, thereby enhancing the scientific basis for model optimization and satellite data
 415 validation.

416 Representative sites were selected based on data completeness to ensure statistical validity.
 417 Specifically, for each TCCON station, we computed the fraction of TROPOMI retrievals with a
 418 quality flag ≥ 0.5 within the $13:30 \pm 1$ h local-time window. Stations with the highest
 419 availability ratios were retained for analysis. Three sites, burgos01, izana01, and nicosia01, were
 420 utilized for XCO validation (refer to Figure 5). The findings indicate that the fused datasets at the
 421 burgos01 and izana01 sites demonstrate notable superiority compared to the GEOS-Chem
 422 simulation results and TROPOMI satellite observations, as evidenced by higher coefficients of
 423 determination (R^2), reduced root-mean-square error (RMSE), diminished bias (μ), and lower
 424 standard deviation (σ). This suggests that the fusion methods effectively enhance data accuracy and
 425 consistency. The fusion results on the nicosia01 site do not significantly exceed those of TROPOMI,
 426 yet they demonstrate comparable performance, thereby further validating the robustness of the
 427 fusion method. To validate XCH₄, we examine three sites: burgos01, rikubetsu01, and xianghe01
 428 (refer to Figure 6). The analysis indicates that at the burgos01 and xianghe01 sites, the fused dataset
 429 markedly outperforms GEOS-Chem and shows modest but consistent improvements over
 430 TROPOMI across key evaluation metrics, including the coefficient of determination (R^2), root mean
 431 square error (RMSE), bias (μ), and standard deviation (σ). This finding suggests that the fusion
 432 method significantly enhances the quality of XCH₄ data. The fusion results on the rikubetsu01 site
 433 do not significantly exceed those of TROPOMI, yet they remain comparable, further illustrating the
 434 wide applicability and reliability of the fusion method. Table S3 and Table S4 present the validation
 435 results for each valid individual site for XCO and XCH₄, respectively. The fusion results
 436 demonstrate superior performance compared to the TROPOMI results at a minimum of 70% of the
 437 sites examined.

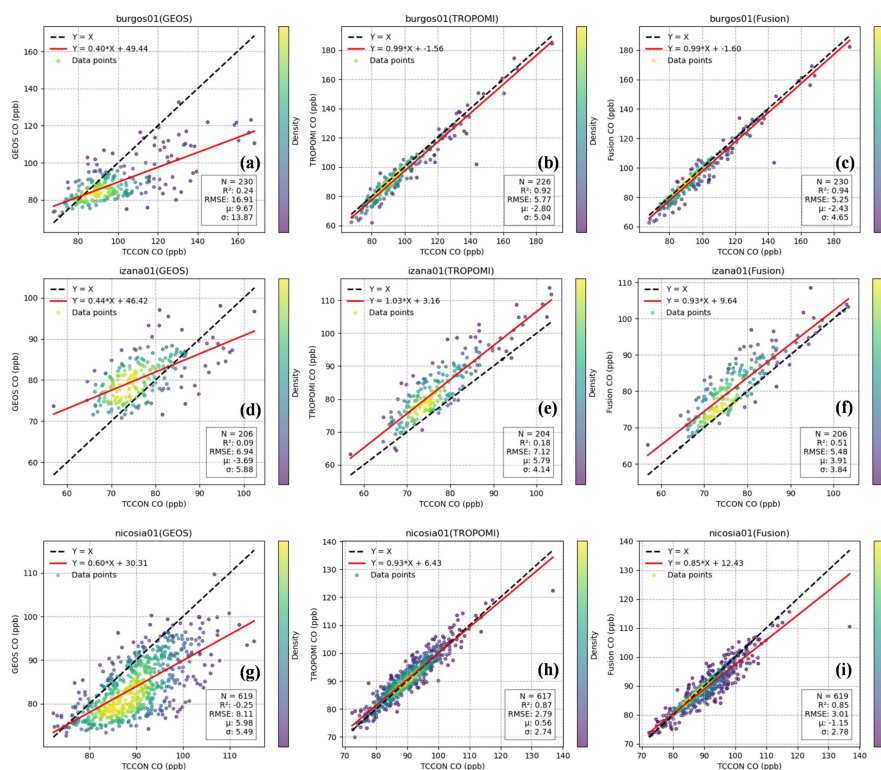
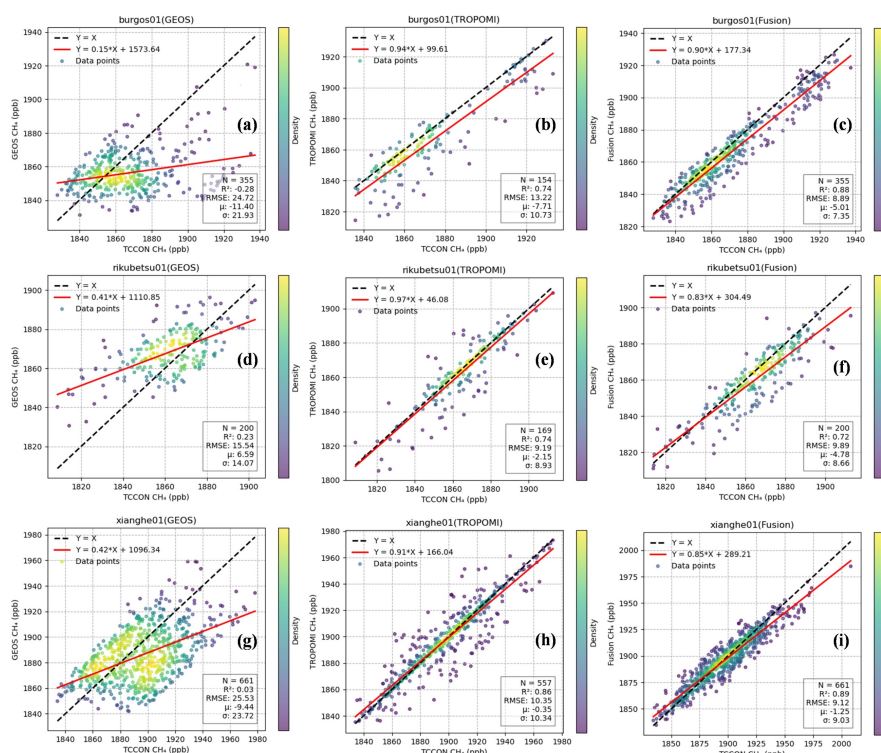


Fig. 5 (a, d, g) Scatterplots of the results of the independent validation of the (a, d, g) GEOS-Chem, (b, e, h) TROPOMI, and (c, f, i) fused XCO data at the burgos01, izana01, and nicosia01 sites, respectively. Black dashed lines and red realizations represent 1:1 and fitted lines, respectively. The x-axis is TCCON data, and the y-axis is GEOS-Chem, TROPOMI, and fusion data, all in parts per billion (ppb).



444

445 Fig. 6 (a, d, g) Scatterplots of the results of the independent validation of the (a, d, g) GEOS-Chem,
 446 (b, e, h) TROPOMI, and (c, f, i) fused XCH₄ data at the burgos01, rikubetsu01, and xianghe01 sites,
 447 respectively. Black dashed lines and red realizations represent 1:1 and fitted lines, respectively. The
 448 x-axis is TCCON data, and the y-axis is GEOS-Chem, TROPOMI, and fusion data, all in parts per
 449 billion (ppb).

450 Figure 7 illustrates the findings of the comprehensive correlation validation between XCO and
 451 XCH₄ across all verified locations. For XCO, the integrated dataset markedly surpasses the GEOS-
 452 Chem simulations for data quality and exceeds the TROPOMI satellite observations across
 453 numerous critical criteria. The fused data exhibit a coefficient of determination (R²) of 0.92,
 454 markedly surpassing that of TROPOMI, thereby demonstrating superior capacity to encapsulate
 455 observational variability. The root mean square error (RMSE) is 4.85 ppb, and the standard deviation
 456 (σ) is 4.70 ppb, both of which outperform the corresponding metrics of TROPOMI, further
 457 substantiating the enhanced accuracy and consistency of the fused data. Moreover, the fused data
 458 exhibit a deviation (μ) index comparable to TROPOMI, indicating that systematic errors have been



efficiently managed and the overall performance is more resilient. The fused dataset for XCH₄ demonstrates notable advantages, exhibiting a coefficient of determination (R^2) of 0.85, surpassing that of TROPOMI, thereby indicating superior interpretative capability; additionally, it presents a standard deviation (σ) of 12.59 ppb, which is more favorable than TROPOMI's, further substantiating the efficacy of the fused data in minimizing dispersion. While the fused data exhibits comparable performance to TROPOMI for root mean square error (RMSE) and bias (μ) parameters, its overall efficacy reflects a significant level of stability and consistency, particularly in complex contexts. This illustrates the favorable outcomes attained by the aforementioned fusion approach.

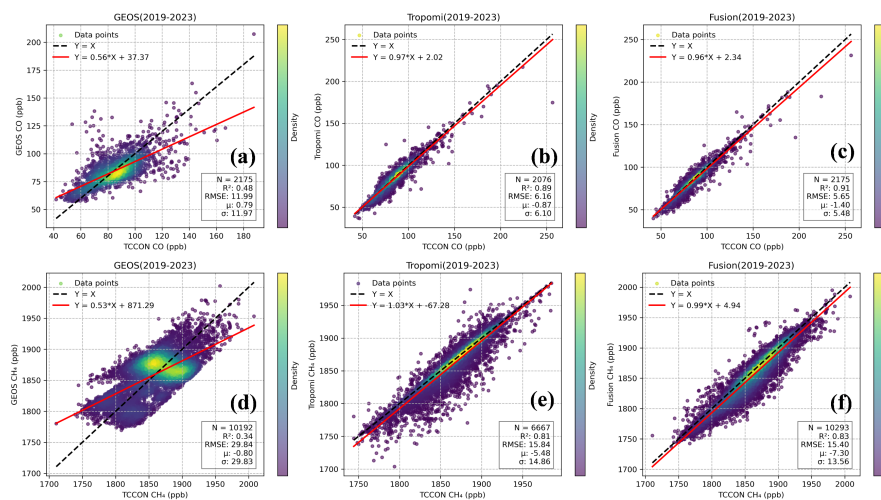


Fig. 7 Scatterplots of the results of the overall validation of (a, d) GEOS-Chem, (b, e) TROPOMI, and (c, f) fused XCO vs. XCH₄ data at all respective validated sites. Black dashed lines and red realizations represent 1:1 and fitted lines, respectively. The x-axis is TCCON data, and the y-axis is GEOS-Chem, TROPOMI, and fusion data, all in parts per billion (ppb).

3.2. Multi-Scale Spatio-Temporal Analysis

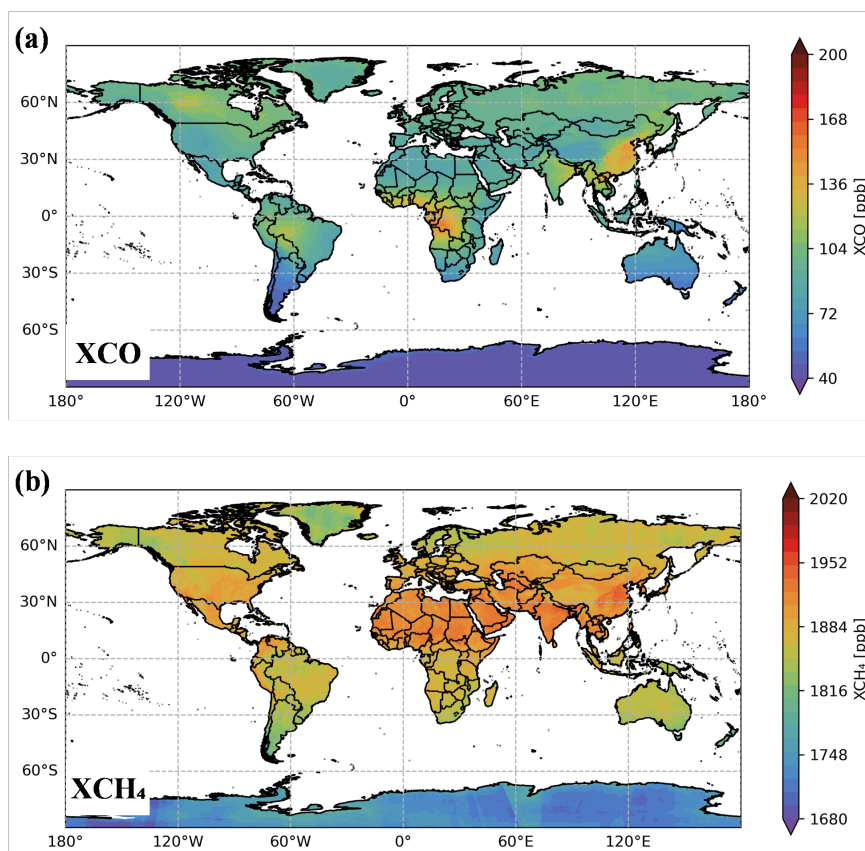
Figure S1 illustrates the comparison of worldwide yearly GEOS-Chem, TROPOMI, fused XCO, and XCH₄ for the years 2020 and 2022. The fused data exhibit a similar geographical distribution with TROPOMI. Despite a substantial underestimation of GEOS-Chem, it retains a



477 robust geographic distribution alignment with TROPOMI, providing a critical reference for data
478 fusion, and this underestimation is markedly altered post-fusion.

479 Figure S2 illustrates the global distribution of fused XCO and XCH₄ for three representative
480 days in 2020 and 2022, respectively. The fusion findings, as seen in the image, offer comprehensive
481 information on atmospheric CO and CH₄, distinctly revealing their worldwide geographical
482 distribution. For comparison, Figure S3 illustrates the global distribution of XCO and XCH₄
483 observed by TROPOMI on these corresponding days. Meteorological factors have resulted in
484 several gaps in the satellite observations, particularly evident in the XCH₄ data, when compared to
485 Figure S2. Figure S2 illustrates that the integrated data addresses the deficiencies in geographical
486 and temporal information, so improving data continuity while preserving the integrity of the satellite
487 observations.

488 Figure 8 illustrates the global multi-year average distributions of fused XCO and XCH₄ for the
489 period 2019–2023. Elevated concentrations of both gases are predominantly observed across Asia,
490 particularly over China and India. For XCO, distinct high-value regions are also evident in Central
491 Africa and northern South America. Figures S4 and S5 illustrate the seasonal averages of the fused
492 global XCO and XCH₄ data from 2019 to 2023. The seasonal variations in the geographical
493 distribution are distinctly captured by the fusion results. Notably, XCO exhibits more pronounced
494 spatiotemporal variability compared to XCH₄. Specifically, CO tends to be spatially concentrated in
495 certain regions, whereas CH₄ displays a relatively more uniform global distribution.



496
 497 Fig. 8 (a) Global concentration distribution of fused XCO data averaged over multiple years from
 498 2019 to 2023; (b) Global concentration distribution of fused XCH₄ data averaged over multiple
 499 years from 2019 to 2023. The color bars indicate the concentrations of XCO and XCH₄ in parts per
 500 billion (ppb).

501 Figures S6 and S7 illustrate the annual trends of global XCO and XCH₄ from 2019 to 2023,
 502 alongside their respective regional trajectories. Figure S6 indicates that XCO levels in North
 503 America showed a consistent increase from 2019 to 2023, while Central Africa and Eastern China
 504 exhibited a declining trend. Global XCH₄ levels demonstrated a steady increase over this period,
 505 with a notably higher growth rate observed in Central Africa (Figure S7).



3.3. Local High-Resolution Data Analysis

To enhance the refinement capability of our fused data, we employed GEOS-Chem to simulate 0.25x0.3125 nested gridded data for the Chinese region. Utilizing the same methodology, we refined the fused data for this region, achieving a grid accuracy of 0.05°, which served as the basis for our analysis of the local area in China.

Figure S8 and S9 illustrate the fluctuations of XCO and XCH₄ in the TROPOMI and fusion datasets, respectively, during the late August 2022 hill fire in Chongqing. This encompasses a comparative analysis of the TROPOMI and fusion data over three days during the fire, along with a histogram depicting the daily variations in mean XCO and XCH₄ concentrations within the fire-affected area during the mid to late months of the event. The Figure demonstrate that the fused data preserves local observational details from the satellite, thereby enhancing the comprehensiveness of the satellite data to a certain degree. The histograms reveal that the fused data reflects an upward trend in XCO and XCH₄ concentrations during the hill fires, with average increases of 17.1 ppb and 24.5 ppb, respectively, during the hill fire period compared to the non-hill fire period at midday.

Figure 9 and 10 depict the fluctuations in XCO and XCH₄ recorded by TROPOMI and integrated data in rice cultivation areas of Northeast and Southeast China, respectively. XCH₄ exhibits a steady increase in both satellite and fused data across these areas. In contrast to the fused data, the yearly growth rate obtained from satellite XCH₄ demonstrates an overestimation in both regions, with discrepancies of 17% and 26% for the Southeast and Northeast, respectively.

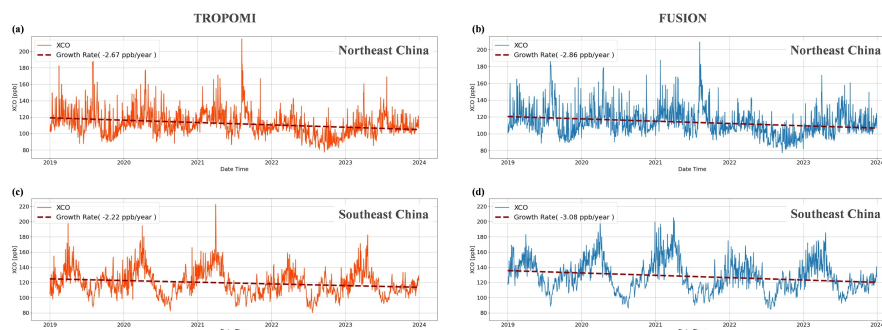


Fig. 9 (a, c) Line plots of daily changes in parts per billion (ppb) for TROPOMI and (b, d) fused XCO data over rice-growing regions of northeastern China and southeastern China, respectively; the red dashed line is the fitted line of annual growth rate, and the annual growth rate is shown in



parentheses, in parts per billion per year (ppb/year).

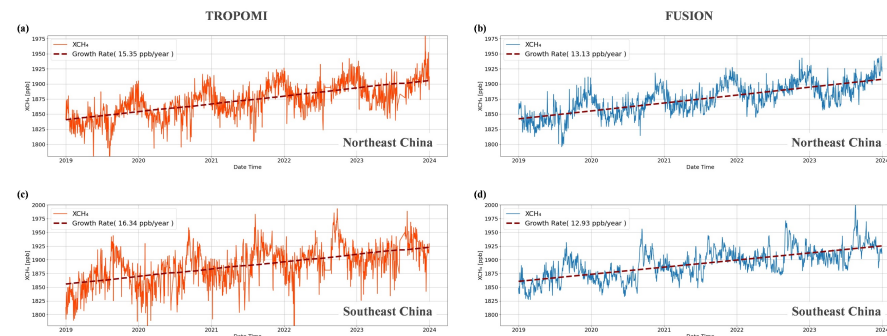


Fig. 10 (a, c) Line plots of daily changes in parts per billion (ppb) for TROPOMI and (b, d) fused XCH₄ data over rice-growing regions in northeastern China versus southeastern China, respectively; red dashed line is the fitted line of the annual growth rate, and in parentheses is the annual growth rate in parts per billion per year (ppb/year).

XCO exhibits a downward trajectory in both satellite and fused data across rice cultivation areas of Northeast and Southeast China. Nonetheless, the annual decline rate of satellite XCO is underestimated relative to the fused data, with discrepancies of 7% and 38% for the Southeast and Northeast regions, respectively. This variance results from absent values in the satellite data, which omit specific low-concentration areas from the computations, thereby inflating the estimation of concentration changes. In contrast, the fused data somewhat alleviate the intensity of these fluctuations.

Rice paddies, as a major source of methane emissions, exhibit a robust association between their increasing cultivation area and the persistent growth in methane emissions. The expansion of rice farming has resulted in a proportional increase in methane emissions, underscoring the considerable influence of agricultural practices on greenhouse gas output (Shen et al., 2024). Straw burning is a key source of carbon monoxide, and the enforcement of pertinent control laws has markedly reduced CO emissions, leading to a steady decline in carbon monoxide levels in both regions (Huang et al., 2021).



551 4. Conclusions

552 This study introduces a two-stage spatio-temporal fusion approach that integrates GEOS-Chem
553 model outputs with TROPOMI satellite data. The method initially performs a signal-domain
554 reconstruction using three-dimensional discrete cosine transform (DCT) and singular value
555 decomposition (SVD), followed by a residual refinement step based on a lightweight convolutional
556 neural network, enabling accurate gap-filling and spatial smoothing. This method successfully
557 produces global daily continuous coverage of XCO and XCH₄ products at a resolution of 0.25° for
558 the years 2019-2023, achieving high-resolution data fusion at 0.05°. The findings indicate that the
559 fused data surpass the GEOS-Chem simulation results in accuracy and consistency and are
560 comparable to or exceed the TROPOMI satellite observations across numerous critical criteria. The
561 integrated data provide notable improvements in the coefficient of determination (R^2), root mean
562 square error (RMSE), bias (μ), and standard deviation (σ) globally, particularly in addressing
563 missing areas and enhancing smoothness. This study effectively addressed the systematic
564 underestimation issue of the GEOS-Chem model, attributed to inaccuracies in emission inventories,
565 through data fusion, enabling the fused data to more accurately represent the long-term spatial and
566 temporal distributions and seasonal variations of global XCO and XCH₄.

567 The fused data offer a definitive overview of the geographical distribution patterns of XCO
568 and XCH₄, together with their temporal trends. In regions like Asia, Africa, and North America, the
569 fusion data effectively captured pronounced spatiotemporal variations and regional patterns. The
570 fusion data demonstrates a robust capacity to detect extreme events (e.g., wildfires) and accurately
571 represent short-term significant fluctuations in XCO and XCH₄ concentrations, serving as an
572 excellent instrument for monitoring severe weather and pollution occurrences. This study elucidates
573 the atmospheric distribution and alterations in specific locations of China using high-resolution data
574 fusion. Particularly in the examination of methane emissions from the mountain fire incident and
575 rice cultivation region in Chongqing, the integrated data exhibit elevated spatial resolution and
576 temporal continuity, thereby offering significant data support for regional air quality monitoring and
577 climate change research. All created fusion data may be obtained upon request from the authors for
578 academics and policymakers.



579 This study has yielded significant outcomes in data fusion and product production; nonetheless,
580 several deficiencies require more enhancement and optimization in further research. The GEOS-
581 Chem model exhibits systematic bias in simulating XCO and XCH₄. While the data fusion approach
582 has largely mitigated this issue, additional optimization of the emission inventories and chemical
583 reaction processes is necessary to enhance simulation accuracy. This work primarily utilizes
584 TROPOMI and GEOS-Chem data; however, the incorporation of additional satellite observation
585 data (e.g., GOSAT, OCO-2) and ground observation data in the future might enhance the diversity
586 and precision of data fusion.

587 This work effectively produced high-resolution XCO and XCH₄ products for global and
588 Chinese areas by employing multi-source data fusion and spatio-temporal distribution analysis
589 methodologies, therefore offering significant data assistance for climate change and air quality
590 monitoring. In the future, as model accuracy improves, data fusion methods are optimized, and
591 multi-source data is introduced, the methodologies and findings of this study are anticipated to have
592 a more significant impact across a broader array of application situations. Data Availability
593 Statement The global (0.25°) and China-specific (0.05°) daily gap-free XCO and XCH₄ datasets
594 (2019–2023) generated in this study are openly available in the Zenodo repository at
595 <https://doi.org/10.5281/zenodo.17936461>.

596 Declaration of competing interest

597 The authors declare that they have no known competing financial interests or personal
598 relationships that could have appeared to influence the work reported in this paper.

599 Data availability

600 The primary dataset generated in this work is available at Zenodo via
601 <https://doi.org/10.5281/zenodo.17936461> (Li et al., 2025).



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