1	The role of OCO-3 XCO ₂ retrievals in estimating global ter-
2	restrial net ecosystem exchanges
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24 Abstract

25 Satellite-based column-averaged dry air CO₂ mole fraction (XCO₂) retrievals are frequently used to 26 improve the estimates of terrestrial net carbon exchanges (NEE). The Orbiting Carbon Observatory 3 27 (OCO-3) satellite, launched in May 2019, was designed to address important questions about the dis-28 tribution of carbon fluxes on Earth, but its role in estimating global terrestrial NEE remains unclear. Here, using the Global Carbon Assimilation System, version 2, we investigate the impact of OCO-3 29 30 XCO₂ on the estimation of global NEE by assimilating the OCO-3 XCO₂ retrievals alone and in combination with the OCO-2 XCO₂ retrievals. The results show that when only the OCO-3 XCO₂ is as-31 32 similated (Exp OCO3), the estimated global land sink is significantly lower than that from the OCO-33 2 experiment (Exp OCO2). The estimate from the joint assimilation of OCO-3 and OCO-2 34 (Exp OCO3&2) is comparable on a global scale to that of Exp OCO2. However, there are significant 35 regional differences. Compared to the observed global annual CO₂ growth rate, Exp OCO3 has the largest bias, and Exp OCO3&2 shows the best performance. Furthermore, validation with independent 36 37 CO₂ observations shows that the biases of the Exp OCO3 are significantly larger than those of 38 Exp OCO2 and Exp OCO3&2 at mid and high latitudes. The reasons for the poor performance of assimilating OCO-3 XCO₂ alone include the lack of observations beyond 52°S and 52°N, the large 39 40 fluctuations in the data amount, and its varied observation time. Our study indicates that assimilating 41 OCO-3 XCO₂ retrievals alone leads to an underestimation of land sinks at high latitudes, and that a joint assimilation of OCO-2 XCO₂ and the OCO-3 XCO₂ retrievals observed in the afternoon is re-42 43 quired for a better estimation of global terrestrial NEE.

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51 **1 Introduction**

52 The rising of the carbon dioxide (CO_2) concentration in the Earth's atmosphere in recent decades, 53 which is mainly caused by human activities, such as the burning of fossil fuels, deforestation and land-54 use change, has become a global concern (Hansen et al., 2013). Terrestrial ecosystems and oceans 55 together absorb about 56 % of anthropogenic CO₂ emissions (Friedlingstein et al., 2023). Among them, 56 terrestrial ecosystems play a crucial role in regulating the atmospheric CO₂ concentration. However, the carbon uptake capacity of terrestrial ecosystems varies considerably globally and regionally 57 58 (Bousquet et al., 2000; Takahashi et al., 2009; Piao et al., 2020). Therefore, accurate quantification of 59 global and regional terrestrial net ecosystem exchange (NEE) is very important to understand their role 60 and potential in regulating changes in the atmospheric CO₂ concentration.

61 Atmospheric inversion is a major method for estimating surface carbon fluxes from observations 62 of atmospheric CO₂ concentration (Enting and Newsam, 1990; Gurney et al., 2002; Thompson et al., 2016; Jiang et al., 2021), but it is more effective at the global scale than at the regional scale. A large 63 64 number of previous studies have shown that different atmospheric inversion models can produce relatively consistent global estimates of carbon fluxes, but their performance at regional scales is variable. 65 66 In regions such as the tropics, southern hemisphere oceans, and most continental interiors (South 67 America, Africa and boreal Asia), the reliability of atmospheric inversions varies considerably due to 68 the heterogeneous distribution of in-situ observations, leading to an increase in the uncertainty of car-69 bon flux estimates (Peylin et al., 2013; Wang et al., 2019). The use of satellite observations to constrain 70 atmospheric inversions can be effective in improving carbon flux estimates because of their better 71 spatial coverage (Basu et al., 2013; Byrne et al., 2020; Jiang et al., 2021; Wang et al., 2022; He et al., 72 2023a). The National Aeronautics and Space Administration (NASA) launched the Orbiting Carbon 73 Observatory 2 (OCO-2) satellite in 2014 (Crisp et al., 2017; Eldering et al., 2012, 2017), followed by 74 the Orbiting Carbon Observatory 3 (OCO-3) satellite in 2019 (Taylor et al., 2023). The OCO satellites 75 have a high sensitivity to column-averaged dry air CO2 mole fraction (XCO₂), a fine footprint, and 76 good spatial coverage, and can therefore be used to better constrain surface carbon flux estimates. In 77 previous studies, many atmospheric inversion models have used the XCO₂ from the OCO-2 satellites 78 to estimate global (e.g., Crowell et al., 2019; Peiro et al., 2022; Byrne et al., 2023) and regional (e.g.,

79 Palmer et al., 2019; Byrne et al., 2021; Philip et al., 2022; He et al., 2022; He et al., 2023a) surface 80 carbon fluxes. For example, Miller et al. (2018) evaluated the effectiveness of OCO-2 observations in 81 constraining regional biospheric CO₂ fluxes. Their findings indicate that OCO-2 observations are most 82 effective at continental and hemispheric scales. Byrne et al. (2022) utilised OCO-2 data to fill a gap in 83 station observations at high latitudes. Their study confirmed the presence of significant and widely 84 distributed early cold-season CO₂ emissions in the northeastern region of Eurasia. Furthermore, several 85 studies have utilised OCO-2 XCO₂ data to investigate the impact of climate extremes on terrestrial 86 NEE, such as El Niño (e.g., Liu et al., 2017) and droughts (He et al., 2023 b; Chen et al., 2024). OCO-87 3 introduces new technologies and observational methods to monitor CO₂ on Earth, offering the same 88 spatial resolution as OCO-2. It is aimed at detecting mid-latitude regions where human CO₂ emissions 89 are concentrated. However, few studies have used the OCO-3 XCO₂ retrievals to constrain global and 90 regional surface carbon fluxes until now. Therefore, it is important to investigate the impact of assim-91 ilating OCO-3 observations on the estimates of global and terrestrial carbon sinks.

In this study, we used both OCO-2 and OCO-3 XCO₂ retrievals to invert global and regional carbon fluxes for the period of 2020-2022 with the Global Carbon Assimilation System, version 2 (GCASv2) (Jiang et al., 2021). The XCO₂ retrievals from OCO-2 and OCO-3 were assimilated separately and together in order to disentangle the effect of OCO-3 XCO₂ retrievals on the estimates of global and regional terrestrial carbon sinks.

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98 2 Methods and data

99 **2.1 Inversion method**

The Global Carbon Assimilation System, version 2 (GCASv2) (Jiang et al., 2021; Wang et al., 2021) designed primarily for assimilating satellite XCO₂ retrievals was adopted in this study to invert surface carbon fluxes. The system uses the Model for Ozone and Related Chemical Tracers, version 4 (MOZART-4; Emmons et al., 2010) to simulate three-dimensional atmospheric CO₂ concentrations, and an ensemble square root filter (EnSRF; Whitaker and Hamill, 2002) to implement the inversion of surface fluxes. MOZART-4 is an offline global chemical transport model developed in the National Center for Atmospheric Research (NCAR). It can be driven by essentially any meteorological data set 107 and with any emissions inventory, so there is not a unique standard simulation (Emmons et al., 2010). 108 We turned off all gas-phase, heterogeneous chemical reactions, aerosol and deposition processes in the 109 MOZART4 model and added a corresponding number of CO2 tracers according to the ensemble num-110 ber in GCASv2, in order to allow the model to run more quickly. EnSRF assimilates observations in a 111 sequential way, and obviates the need to perturb the observations. It shows good performance as long 112 as the observation errors are uncorrelated (Houtekamer and Mitchell, 2001). GCASv2 is an upgrade 113 from the GCAS (Zhang et al., 2015) that was established in 2015. The main upgrades include: 1) the 114 addition of an assimilation module for satellite observations; 2) a change in the assimilation algorithm 115 (i.e., EnSRF); 3) a change in the operational flow of the assimilation system; 4) the addition of a 'super-116 observation' scheme; 5) inversion of fluxes at the grid scale; and 6) an improvement in the localization 117 scheme.

118 GCASv2 runs cyclically, with a two-step optimization strategy in each assimilation window (1 119 week). In the first step, the prior fluxes (X_0^b) in each grid are independently perturbed with a random 120 number (δ_i) drawn from a Gaussian distribution with mean of 0 and standard deviation of 1, and a 121 scaling factor (λ) that represents the uncertainty of each prior flux (Eq. 1).

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$$\boldsymbol{X_i^b} = \boldsymbol{X_0^b} + \lambda \times \delta_i \times \boldsymbol{X_0^b} \quad , i = 1, 2, \dots, N$$
 (1)

Then, the perturbed fluxes are put into the MOZART-4 model to simulate ensembles of CO₂ concentrations. The CO₂ profiles are sampled according to the locations and times of XCO₂ observations and converted to the simulated ensembles of $XCO_2(XCO_{2,i}^m)$ according to prior $XCO_2(XCO_2^a)$, prior XCO_2 profiles $(y_{a,j})$, pressure weighting function (h_j) , and averaging kernel (a_j) of the XCO_2 retrievals (Eq. 2).

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$$XCO_{2,i}^{m} = XCO_{2}^{a} + \sum_{j} h_{j}a_{j}(A(CO_{2,i}) - y_{a,j})$$
(2)

Subsequently, the perturbed fluxes (X_i^b) , the simulated XCO₂ ensembles and the observed XCO₂ (y)are used in EnSRF to optimize the carbon fluxes $(\overline{X^a})$ (Eqs. 3-5). The background error covariance matrix (P^b) is calculated based on X_i^b according to Eq. (3), where \overline{X}^b is the mean of X_i^b . The posterior flux $(\overline{X^a})$ is a correction to the prior flux using the bias between simulated and observed XCO₂ $(\mathbf{y} - H\overline{X^b})$ and the Kalman gain matrix (K) (Eq. 4). And K is calculated according to Eq. (5), which is 134 a function of model-data mismatch error covariance matrix (\mathbf{R}) and the background error covariance 135 matrix.

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$$\boldsymbol{P}^{\boldsymbol{b}} = \frac{1}{n-1} \sum_{i=1}^{n} (\boldsymbol{X}_{i}^{\boldsymbol{b}} - \overline{\boldsymbol{X}}^{\boldsymbol{b}}) (\boldsymbol{X}_{i}^{\boldsymbol{b}} - \overline{\boldsymbol{X}}^{\boldsymbol{b}})^{T}$$
(3)

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$$\overline{X^a} = \overline{X^b} + \mathbf{K}(\mathbf{y} - H\overline{X^b})$$
(4)

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$$\mathbf{K} = \mathbf{P}^{\mathbf{b}} \mathbf{H}^{T} (\mathbf{H} \mathbf{P}^{\mathbf{b}} \mathbf{H}^{T} + \mathbf{R})^{-1}$$
(5)

In the second step, the optimized carbon fluxes are put into the MOZART-4 model to obtain the initial field of the next assimilation window. This scheme allows compensation of inversion results between neighboring windows and mass conservation between flux adjustments and concentration changes.

In order to reduce the effects of horizontal observation error correlation and representativeness error, based on the optimal estimation theory (Miyazaki et al., 2012), the system also performs a "super-observation" scheme, which combines multiple observations located within a same model grid into a single high-precision "super-observation". In this method, it first calculates the simulated XCO₂ corresponding to each observed XCO₂ based on the observation time and location, and then, it performs a retrieval error-weighted average for all the simulated and observed XCO₂ falling within the same model grid in the DA window, respectively.

150 There are inevitably spurious correlations in the EnKF method, to reduce the effect of spurious 151 correlations, a two-layer localization scale was adopted in GCASv2, which is used to select which observations can be used for the flux analysis for each grid. The localization technique is based on the 152 correlation coefficient between the simulated XCO_2 ensembles $(XCO_{2,i}^m)$ in each observation location 153 and the perturbed fluxes (X_i^b) in current model grids and their distances. The observations will be 154 155 accepted for assimilation if the distance is less than 500 km and the correlation coefficient is greater 156 than 0; and if the distance is greater than or equal to 500 km and less than 3000 km and the correlation 157 coefficient should be significant (p < 0.05). Otherwise, the observations are not accepted. The reason 158 for this scheme is that considering the atmospheric horizontal diffusion, we believe that there must be a correlation between the flux of one grid and the concentrations in its neighbouring grids, and therefore observations are accepted as long as this correlation coefficient is greater than zero. In contrast, at distant locations (>500 km), where the effect of atmospheric horizontal diffusion is essentially negligible, the relationship between source and receptor is mainly due to atmospheric transport, and in order to minimize spurious correlations we require that such correlations must be significant. More details of the system can be found in Jiang et al (2021).

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2.2 OCO-2 and OCO-3 XCO₂ retrievals

166 In July 2014, the Orbiting Carbon Observatory (OCO) -2 satellite was launched by NASA with 167 the primary objective of providing accurate space-based measurements to quantify changes in XCO₂. The satellite is equipped with three high-resolution spectrometers that can detect two near-infrared 168 169 wavelength bands (1.61µm and 2.06 µm) of sunlight reflectance spectra to observe CO₂. In May 2019, 170 NASA launched OCO-3 to the International Space Station (ISS) to detect CO₂ in mid-latitudes, where 171 human emissions are more concentrated. OCO-3 operates in a low-inclination orbit from 52°S to 52°N 172 and is equipped with three high-resolution spectrometers, providing the same spatial resolutions and 173 similar observation mode as the OCO-2 satellite (Taylor et al., 2023). However, since OCO-3 is 174 mounted on the ISS, its observation time and frequency for the same place is different from the OCO-175 2.

The XCO₂ data from OCO-3 and OCO-2 used in this study are bias-corrected products from 176 177 August 2019 to December 2022 at the image element level. The data are sourced from Version 10.4r 178 Level 2 Lite and Version 11.1r Level 2 Lite, respectively. Before using them in our inversion system, 179 it is essential to pre-process the data. First, both the land (Land Nadir + Land Glint, LNLG) and ocean 180 (Ocean Glint, OG) retrievals were adopted, and they were filtered using the parameter of XCO₂ qual-181 ity flag, which indicates the quality of the data. Only data with XCO₂ quality flag=0 was selected for 182 assimilation in this study. Then, the LNLG and OG retrievals and their corresponding retrieval parameters (namely XCO_2^a , $y_{a,i}$, h_i , and a_i in Eq. 2) were re-gridded to a spatial resolution of $1^\circ \times 1^\circ$ and 183 $5^{\circ} \times 5^{\circ}$ using the arithmetic averaging method, respectively. For the OG data, we used a coarser re-184 185 gridding resolution, that is because the distribution of XCO₂ is more homogeneous on sea than on land. 186 Finally, both OCO-3 and OCO-2 XCO₂ retrievals were converted to the X2019 scale of the World 187 Meteorological Organization (WMO) following Hall et al., (2021). Figure 1a and c display the distri-188 bution and coverage of screened OCO-3 and OCO-2 XCO₂ retrievals from 2020 to 2022. Compared 189 to OCO-2, OCO-3 has more observational data in the mid-latitudes of the northern and southern hem-190 ispheres, especially in arid and semi-arid regions.

191 Following Jiang et al. (2022), the model-data mismatch errors were amplified by a factor on top 192 of the XCO₂ posterior errors, but with the minimum observation error setting to 1 ppm. It needs to be 193 noted that in the OCO-3 and OCO-2 products, the XCO₂ posterior errors of OG retrievals (0.48 ± 0.11 194 and 0.51±0.15 ppm in 2020 for OCO-2 and OCO-3, respectively) are smaller than LNLG (0.54±0.12 195 and 0.64±0.18 ppm in 2020 for OCO-2 and OCO-3, respectively), but in fact, the observational error 196 should be greater at sea than on land (Peiro et al., 2022). Therefore, before multiplying by a uniform 197 factor, we increased the XCO₂ posterior errors of OG retrievals by 0.2 ppm. Taylor et al. (2023) re-198 ported that the mean of the uncertainties for the OCO-2 and OCO-3 quality-filtered and bias-corrected 199 XCO₂ are 1.0 and 1.3 ppm, respectively. Considering that the global atmospheric transport model may 200 have an uncertainty of about 1.0 ppm (Lauvaux et al., 2009), thus in this study, we set the amplification 201 factor to be 3.5. Through this treatment, the mean model-data mismatch errors of LNLG and OG are about 1.9 and 2.4 ppm for OCO-2, and 2.3 and 2.5 ppm for OCO-3, respectively. 202



Figure 1. Data amount (the sum of 2020-2022) of XCO_2 in each grid cell ($1^{\circ} \times 1^{\circ}$) and at each latitude used in this study (a, b, OCO-3; c, d, OCO-2)

206 **2.3 Prior carbon fluxes**

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207 There are 4 prior carbon fluxes used in this study, which are terrestrial NEE, ocean-atmosphere 208 (OCN) carbon exchanges, fossil fuel and cement production (FOSSIL) carbon emissions, and biomass 209 combustion (FIRE) carbon emissions. The NEE were simulated using the BEPS model (Chen et al., 210 2019). The OCN fluxes were derived from the mean of the JMA Ocean CO₂ Map (Iida et al., 2021), which contains a global product with 1°×1° resolution (Globe, v2022) and another product for the 211 212 Northwest Pacific region with a resolution of 0.25°×0.25° (The western North Pacific, v2023). These 213 two products were integrated before they are used in this study. The FOSSIL carbon emissions were 214 obtained from GCP-GridFEDv2023.1 (Jones et al., 2021), which contains monthly global carbon emissions from fossil fuels, cement production, and cement product weathering carbon sequestration at a 215

spatial resolution of $0.1^{\circ} \times 0.1^{\circ}$. The FIRE carbon emissions were obtained directly from the Global Fire Emissions Database, Version 4.1(GFED4.1s; Randerson et al., 2017). All 4 prior fluxes cover the entire time period of this study (i.e., August 2019 to December 2022) and they were re-grided to a unified spatial resolution of $1^{\circ} \times 1^{\circ}$ before used in the GCASv2 system.

220 **2.4 Evaluation data and methods**

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221 Due to the significant spatial scale discrepancy between the inverted fluxes and the in-situ ob-222 served fluxes, direct validation of the posterior Net Ecosystem Exchange (NEE) using observed data 223 is typically unattainable. However, we are able to indirectly evaluate the posterior fluxes by comparing 224 the atmospheric CO_2 concentrations, simulated with the posterior fluxes, against independent CO_2 measurements. (e.g., Jin et al., 2018; Wang et al., 2019; Feng et al., 2020; Jiang et al., 2021). In this 225 226 study, we used surface flask observations at 66 sites from the ObsPack dataset (ObsPack v9.1, Schuldt 227 et al., 2023) to independently assess the posterior fluxes. The screening of the 66 sites followed the 228 methodology of Jiang et al. (2022). The distribution of the 66 flask sites is shown in Figure 2. The 229 specific metrics assessed were the statistics of mean bias (BIAS), absolute bias (MAE), and root mean 230 square error (RMSE). We calculated annual BIAS, MAE, and RMSE globally, for different latitudinal 231 zones, and for different land areas.



Figure2. Distributions of the observation sites used for independent evaluation in this study and the 11 TransCom-3 regions on land defined in Botta et al. (2012).

235 **3 Inversion experiments**

236 The GCASv2 system was run from 1 August 2019 to 31 December 2022. The initial five months 237 were designated as the spin-up stage, and the results from January 2020 to December 2022 were ana-238 lyzed in this study. Three inversion experiments were conducted: (1) assimilation of OCO-3 XCO₂ (all inversion experiments use OG+LNLG data) retrievals alone (Exp OCO3); (2) assimilation of OCO-2 239 XCO₂ retrievals alone (Exp OCO₂); and (3) simultaneous assimilation of OCO-3 and OCO-2 XCO₂ 240 retrievals (Exp OCO3&2). In each experiment, the methodology employed was consistent with that 241 242 of previous studies (Peters et al., 2007; Jiang et al., 2021, 2022), only the NEE and OCN fluxes were optimized, and the FIRE and FOSSIL emissions are prescribed. According to Eq. (1), the prior NEE 243 244 and OCN fluxes were perturbed using Eq. (6).

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$$X_{i}^{b} = \lambda_{NEE} \times \delta_{i,NEE} \times X_{NEE}^{b} + \lambda_{ocn} \times \delta_{i,ocn} \times X_{OCN}^{b} + X_{Fire}^{b} + X_{Fossil}^{b}, i = 1, 2, ..., N$$
(6)

where X_{NEE}^{b} , X_{OCN}^{b} , X_{Fire}^{b} , and X_{Fossil}^{b} represent the prior fluxes of NEE, OCN, FIRE, and FOSSIL, respectively; δ_{i} is random perturbation samples, which is independent between grids; λ_{NEE} and λ_{ocn} are the scaling factors for prior NEE and OCN fluxes, which were set to be 6 and 10 in this study, respectively. As described above, the prior fluxes have a spatial resolution of $1^{\circ} \times 1^{\circ}$, for $\delta_{i,NEE}$ and $\delta_{i,ocn}$, we adopted a spatial resolution of $3^{\circ} \times 3^{\circ}$, and the outputs of the posterior fluxes have the same spatial resolution with the prior fluxes, that means in each $3^{\circ} \times 3^{\circ}$ grid, the prior fluxes were adjusted with a same factor.

Additionally, two forward simulations were conducted to obtain the prior and posterior CO_2 concentrations, which were then compared with the independent CO_2 observations to assess the posterior carbon fluxes. Following Jiang et al. (2022), MOZART-4 is driven by the $1.9^{\circ} \times 2.5^{\circ}$ grids version of the GEOS5 Global Atmosphere Forcing Data (Tilmes, 2016). It has a vertical level of 72 layers, and MOZART-4 uses the lowest 56 vertical levels of GEOS-5 and the same spatial resolution with GEOS-5 data.

259 4 Results and discussion

260 **4.1 Global carbon budget**

Table 1 presents the prior and the posterior annual global carbon budgets from the 3 inversion

262	experiments during 2020-2022. The global terrestrial NEEs obtained from the Exp_OCO3,
263	Exp_OCO2, and Exp_OCO3&2 experiments are -3.41±0.65, -4.17±0.60, and -4.14±0.57 PgC yr ⁻¹ ,
264	respectively. The global NEE inferred from the Exp_OCO3 is significantly weaker than those from
265	Exp_OCO2 and Exp_OCO3&2, and the latter two are comparable. For the OCN carbon sink,
266	Exp_OCO3 has the strongest sink but is closest to the a priori result, while Exp_OCO2 and
267	Exp_OCO3&2 have essentially the same sink. Combined with the FOSSIL and FIRE carbon emissions
268	the global net carbon fluxes are 4.74 \pm 0.77, 5.55 \pm 0.67, 4.90 \pm 0.63, and 4.93 \pm 0.60 PgC yr ⁻¹ for the a
269	priori, Exp_OCO3, Exp_OCO2, and Exp_OCO3&2, respectively. In comparison with the average at-
270	mospheric CO_2 growth rate of 4.93 PgC yr ⁻¹ for 2020-2022 given by the Global Carbon Budget 2023
271	(Friedlingstein et al., 2023), the results of Exp_OCO3&2 are the closest, with a mean bias of 0.0 PgC
272	yr ⁻¹ , whereas Exp_OCO3 has the largest bias, with a deviation of 0.62 PgC yr ⁻¹ . This indicates that the
273	carbon sinks in Exp_OCO3 may be significantly underestimated, and joint assimilation of OCO-2 and
274	OCO-3 XCO ₂ retrievals gives the best performance on a global scale.

	Prior	Exp_OCO3	Exp_OCO2	Exp_OCO3&2
FOSSIL emissions	9.71			
FIRE emissions	1.97			
NEE	-4.10±0.75	-3.41±0.65	-4.17±0.60	-4.14±0.57
OCN fluxes	-2.84 ± 0.17	-2.71±0.17	-2.61±0.17	-2.61±0.17
Global net carbon fluxes	4.74±0.77	5.55±0.67	4.90±0.63	4.93±0.60
Observed global CO ₂ growth rates			4.93	

275 **Table 1.** Global carbon budget estimated in the 3 inversion experiments (PgC yr⁻¹).

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277 4.2 Regional NEE

Figure 3 shows the spatial distribution of annual mean posterior terrestrial fluxes and oceanic fluxes from the Exp_OCO3, Exp_OCO2, Exp_OCO3&2 and their differences against the a priori fluxes. Overall, the spatial distribution of carbon sources and sinks in terrestrial ecosystems obtained from different experiments is basically the same, with sources in western North America (N. America), 282 eastern Amazonia, parts of Siberia, parts of Northwest China, central and western Australia, and the 283 Sahel region and eastern parts of Africa, while other areas are carbon sinks. However, the carbon 284 sources/sinks obtained from Exp OCO3 exhibit a markedly different strength compared to those de-285 rived from the other two experiments. Compared with the prior flux, the terrestrial carbon sinks in 286 northeastern China, most of Europe, northern Siberia, the central and northeastern United States (US), 287 and southern Africa increased significantly in all the 3 experiments. However, the increase in terrestrial 288 carbon sinks in regions other than northeastern China in the Exp OCO2 and Exp OCO3&2 was 289 greater than that in the Exp OCO3. Meanwhile, in southern Canada, western and southern US, eastern 290 Brazil and northern South America (S. America), the Sahel region and eastern parts of Africa, all the 291 3 inversion experiments show a significant decrease in the terrestrial carbon sink. The degree of change 292 in the inversion results is more pronounced in the Exp OCO2 and Exp OCO3&2 than in the 293 Exp OCO3. Figure 3 also show the distribution of terrestrial carbon fluxes along latitudes. The poste-294 rior and prior fluxes have a similar distribution trend along the latitude, with a significant peak of 295 carbon sink near 60°N, and the strongest sinks of Exp OCO2 and Exp OCO3&2 are comparable, 296 which are significantly stronger than the a priori, while Exp OCO3 has the weakest peak of carbon 297 sink and that is close to the a priori. In addition, it also could be found that the terrestrial carbon sinks 298 obtained from Exp OCO3 are also significantly smaller than those from Exp OCO2 and 299 Exp OCO3&2 near 30°S.

300 In order to better understand and compare the differences among different inversion experiments, 301 we have aggregated the prior and the posterior NEEs into the 11 TransCom-3 land regions (Figure 2), 302 as shown in Table 2. It is clearly that almost all terrestrial regions behave as carbon sinks, both prior 303 and posterior fluxes. Among the experiments, only the terrestrial NEE in northern Africa obtained by 304 Exp OCO3&2 shows a weak carbon source. There is relatively good agreement between all the inver-305 sion experiments on whether the land carbon flux is a source or sink, but there is significant difference 306 in the NEE values. In all regions except temperate N. America, northern Africa, temperate Asia, and 307 Australia, Exp OCO3 shows a weaker carbon sink than Exp OCO2. Comparing Exp OCO3 with 308 Exp OCO3&2, Exp OCO3&2 shows stronger carbon sinks in temperate N. America, southern Africa, 309 Australia, and Europe; and weaker sinks in tropical S. America, northern Africa, and boreal Asia; and



310 elsewhere Exp OCO3&2 shows sinks intermediate to the other two experiments.

Figure 3. Spatial distribution of annual mean posterior terrestrial and oceanic carbon fluxes from 2020 to 2022,
the difference between posterior and prior fluxes, and the distribution of terrestrial NEEs at different latitudes.
(a, b, c, Exp_OCO3; d, e, f, Exp_OCO2; g, h, i, Exp_OCO3&2)

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316 The regions with more pronounced differences among experiments are temperate S. America and 317 Europe. In Europe, the posterior fluxes of each inversion experiment show a pronounced carbon sink, which is significantly larger than the prior flux, but the results of different experiments vary to some 318 319 extent, with NEEs ranging from -0.88 ± 0.24 to -1.18 ± 0.21 PgC yr⁻¹ (Table 2), with Exp OCO3&2 320 having the largest sink. In the temperate S. America, Exp OCO3 exhibits a very weak carbon sink, 321 whereas both Exp OCO2 and Exp OCO3&2 show a moderate carbon sink. One potential explanation 322 for this discrepancy is that the XCO₂ concentration observed by OCO-3 in the temperate South Amer-323 ica is higher than that observed by OCO-2 for the duration of the study period (by ~0.55 ppm). Con-324 sequently, in that assimilating the OCO-3 observations yields a weaker carbon sink. Compared with 325 the prior flux, the posterior NEE in the tropical S. America shows a significant discrepancy, the prior flux show a very strong carbon sink of -0.78±0.23 PgC yr⁻¹, whereas the subsequent application of 326

327 constraints from satellite observations resulted in a reduction of the carbon sinks by approximately 2 328 to 3 times, with values ranging from -0.21 ± 0.19 to -0.41 ± 0.20 PgC yr⁻¹.

Following the imposition of constraints derived from satellite observations, the carbon sinks on 329 the Northern Hemisphere land are all enhanced, with the largest enhancement of 0.59 PgC yr⁻¹ in 330 Exp OCO3&2, followed by 0.19 and 0.36 PgC yr⁻¹ in Exp OCO3 and Exp OCO2, respectively. 331 332 While in the tropics, the carbon sinks were all weakened, with Exp OCO3 being weakened most, by 0.67 PgC yr⁻¹, and the Exp OCO2 and Exp OCO3&2 being weakened by 0.37 and 0.59 PgC yr⁻¹, 333 respectively; on Southern Hemisphere land, in Exp_OCO3, the sinks were weakened by 0.2 PgC yr⁻¹, 334 whereas in Exp OCO2 and Exp OCO3&2, they were enhanced by 0.08 and 0.05 PgC yr⁻¹, respec-335 336 tively.

Table 2. Annual mean terrestrial fluxes (PgC yr⁻¹) in 2020-2022 for 11 TransCom-3 land regions, as well as for
 Northern Hemisphere land, Tropical land and Southern Hemisphere land. Includes the prior flux and the posterior fluxes from three inversion experiments.

Regions	Prior	Exp_OCO3	Exp_OCO2	Exp_OCO3&2
Boreal North America	-0.32±0.16	-0.26 ± 0.14	-0.38±0.13	-0.32 ± 0.13
Temperate North America	-0.19±0.30	-0.25 ± 0.25	-0.12±0.25	-0.35 ± 0.21
Tropical South America	-0.78±0.23	-0.31±0.21	-0.41±0.20	-0.21 ± 0.19
Temperate South America	-0.28±0.22	-0.03 ± 0.17	-0.40±0.16	-0.27 ± 0.14
Northern Africa	-0.17±0.28	-0.06 ± 0.24	-0.02 ± 0.23	0.03 ± 0.20
Southern Africa	-0.30±0.24	-0.30±0.19	-0.49 ± 0.17	-0.54 ± 0.16
Boreal Asia	-0.56±0.26	-0.37 ± 0.24	-0.52 ± 0.21	-0.34 ± 0.23
Temperate Asia	-0.42±0.23	-0.33 ± 0.20	-0.22±0.19	-0.30 ± 0.18
Tropical Asia	-0.37±0.13	-0.31±0.12	-0.39±0.11	-0.35 ± 0.11
Australia	-0.15±0.09	-0.20 ± 0.08	-0.11±0.08	-0.21 ± 0.07
Europe	-0.40±0.26	-0.88 ± 0.24	-1.01±0.19	-1.18 ± 0.21
Northern Hemisphere lands	-1.89±0.56	-2.08 ± 0.49	-2.25 ± 0.44	-2.48 ± 0.44
Tropical lands	-1.65 ± 0.45	-0.98 ± 0.38	-1.28 ± 0.37	-1.06 ± 0.34
Southern Hemisphere lands	-0.43 ± 0.24	-0.23±0.18	-0.51±0.17	-0.48 ± 0.15

340

341 4.3 Seasonal cycle of NEE

342 Figure 4 illustrates the seasonal cycle of NEE for each TransCom-3 region. The posterior NEEs 343 of different experiments are in good agreement on the seasonal cycle in most regions. In the Northern 344 Hemisphere, the seasonal cycles of NEE in boreal N. America, temperate N. America, boreal Asia, 345 temperate Asia, and Europe show relatively consistent trends. Carbon sinks in these regions generally 346 occur from May to September and carbon sources from October to April. Large differences are evi-347 dent in the strength of the carbon sinks observed in different regions, with different months in which 348 the strongest carbon sinks occur. Boreal N. America, temperate N. America, and boreal Asia have the 349 strongest carbon sinks in July, temperate Asia has the peak in July or August, and Europe has the 350 strongest sinks in June. In the Southern Hemisphere, the southern Africa and temperate S. America 351 have more consistent seasonal cycles, with their carbon sources occurring roughly from July to De-352 cember and sinks from January to June. The strongest carbon sources all occur in October, and the 353 strongest sinks occur around March. In Australia, carbon sinks occur mainly from March to October, 354 with the peak occurring in August. In the tropics, southern Africa shows a seasonal cycle opposite to 355 that of northern Africa, and carbon sinks occur from January to July with the strongest carbon sinks 356 occurring near March. Tropical Asia shows a carbon sink in most months, with the strongest sink in 357 September. The seasonal cycle in tropical S. America is more complex, with the strongest carbon 358 source in October. In general, seasonal amplitudes are small in the tropics and large in the northern 359 regions. The averaged seasonal amplitudes of the three inversion experiments in the boreal Asia, Europe, and temperate N. America are 1.17, 0.97, and 0.72 PgC yr⁻¹, respectively, while the seasonal 360 361 amplitudes in tropical Asia and S. America are about 0.10 PgC yr⁻¹.

The regions where the difference between the prior and posterior NEEs is particularly pronounced are tropical S. America, southern Africa, Australia, and Europe. In the tropical S. America, the prior NEE is a significant sink from May to July, but after constraints from satellite observations, the carbon sink decreases significantly, even approaching neutral in June and July, and furthermore, in September and October, the sink also decreases significantly compared to the a priori. In southern Africa, the carbon sink is significantly stronger from January to March compared to the a priori, and conversely, the carbon source is significantly stronger in October and November. In Australia, the carbon sink is 369 significantly increased from January to August and decreased in October and November compared to 370 the a priori. In Europe, there is a significant increase in the carbon sinks from May to June compared 371 to the a priori.

372 As described in Section 4.2 that in temperate N. America, northern Africa, temperate Asia, and Australia, Exp OCO3 shows a stronger sink than Exp OCO2 which mainly occurs in May and June 373 374 in temperate N. America, in August and September in northern Africa, from April to September in 375 temperate Asia, and in Australia except for July. In other regions, Exp OCO3 has weaker sinks than Exp OCO2. In the high latitudinal regions, on the one hand, the carbon sinks in June and July of the 376 377 Exp OCO3 are generally smaller than those of Exp OCO2, and on the other hand, the carbon source 378 in October is significantly higher than that of Exp OCO2, while in the tropics, the carbon sink is lower 379 than that of Exp OCO2 almost all year round. Compared to Exp OCO3, Exp OCO3&2 shows 380 stronger carbon sinks in temperate N. America, southern Africa, Australia, and Europe, mainly in sum-381 mer; and weaker sinks in tropical S. America, northern Africa, and boreal Asia, mainly in autumn. 382 Elsewhere Exp OCO3&2 shows carbon sinks intermediate to the other two experiments.



Figure 4. Averaged prior and posterior seasonal cycle of NEE in different TransCom-3 regions during 2020–
2022; (a) boreal N. America, (b) temperate N. America, (c) tropical S. America, (d) temperate S. America, (e)

northern Africa, (f) southern Africa, (g) boreal Asia, (h) temperate Asia, (i) tropical Asia, (j) Australia, (k) Europe.

387 4.4 Evaluation against independent observations

388 As shown in Figure 5, observations from 66 surface flask sites were used to evaluate the posterior 389 fluxes. The prior and posterior CO₂ concentrations were simulated by the MOZART-4 model using the 390 corresponding prior and posterior fluxes, as described in Section 3. The overall assessment results of 391 the individual inversion experiments on a global scale are shown in Table 3. The results show that the 392 mean BIAS, MAE, and RMSE between the prior CO₂ concentrations and surface flask observations are -1.82, 3.27, and 5.01 ppm, respectively. The prior BIAS shows a pronounced negative bias, which 393 394 can be attributed to the fact that the prior NEE in 2019 (generated by the spin-up stage) was, on average, 395 approximately 3.5 PgC less than the posterior NEE. This part of the NEE has an impact on the sub-396 sequent inversion. After constraints using the XCO₂ retrievals, the biases of the three experiments are 397 reduced significantly compared to the a priori, indicating that the surface carbon fluxes have been 398 improved. A comparison of the three inversion experiments reveals that Exp OCO3 exhibits the largest 399 BIAS, while Exp OCO3&2 exhibits the lowest MAE and RMSE.

401		BIAS	MAE	RMSE
402	Prior	-1.82	3.27	5.01
403	Exp_OCO3	0.32	2.44	4.56
404	Exp_OCO2	0.02	2.42	4.49
405	Exp_OCO3&2	0.05	2.34	4.47
406				

400 **Table 3.** Error statistics between the simulated CO₂ concentrations and surface flask observations (ppm).

Figure 5a and 5b illustrate the BIAS of the individual inversion experiments at different latitudinal zones and in different TransCom-3 land regions. In all latitudinal bands and all land regions, the CO₂ concentrations modelled by the a priori fluxes have the largest negative BIAS, which is greater than -1.2 ppm in all cases. Across latitudinal zones, in the Southern Hemisphere, and south of 30°N latitude, the Exp OCO3 had the smallest BIAS, which is smaller than the Exp OCO2 and comparable to the 412 results of the Exp OCO3&2. However, in the mid to high latitudes of the Northern Hemisphere, the 413 BIAS of the Exp OCO3 is higher than those of the Exp OCO2 and Exp OCO3&2. Especially in the 414 region north of 60°N latitude, the Exp OCO3 exhibits a significant positive BIAS, while the 415 Exp OCO2 and Exp OCO3&2 both exhibit small negative BIAS. This suggests that the carbon sinks at mid to high latitudes were underestimated. We also find that the OCO-3 retrievals help with the lack 416 of space-based XCO₂ observations in the tropics compared to OCO-2. The BIAS of Exp OCO3&2 is 417 418 smaller than Exp OCO2 in the region from 30°S to 30°N. Meanwhile, the BIAS of Exp OCO3&2 is 419 also smaller than Exp OCO2 in southern Africa, northern Africa and tropical Asia. Furthermore, we 420 can find that the BIAS can be further reduced in the mid to high latitudes of the Northern Hemisphere 421 after the addition of assimilated OCO-3 observations compared to the Exp OCO2. In different Trans-422 Com-3 land regions, the BIAS of the three inversion experiments is less than ± 0.6 ppm, except in the 423 temperate Asia. In Africa, temperate S. America, tropical Asia, and Australia, the Exp OCO3 had the 424 smallest BIAS, while the BIAS of Exp OCO3&2 was between those of Exp OCO3 and Exp OCO2. 425 However, in temperate N. America and Europe, the Exp OCO3 has the largest BIAS, followed by the 426 Exp OCO2, while the Exp OCO3&2 has the smallest BIAS.



427

Figure 5. The prior and posterior CO₂ BIAS(a) at different latitudinal zones and (b) in different land
 regions.

430 4.5 Discussion

In most of the previous studies that used OCO-2 XCO_2 to invert surface carbon fluxes, the OG data were not used (e.g., Peiro et al., 2022; Byrne et al., 2023), the reason is that the OG XCO_2 may have larger uncertainties, inversions assimilating OCO-2 OG retrievals produced unrealistic results of annual global ocean sinks (Peiro et al., 2022). In addition to its large uncertainties, we believe that another reason for the poor assimilation performance of OG is the relatively homogeneous distribution of XCO_2 on ocean, causing a large correlation of the model-data biases among different XCO_2 observations within a same region, which leads to observations at the same region having the same direction 438 of adjustment for surface fluxes, and thus leads to a significant overestimated or underestimated 439 ofocean carbon sink. Because of this, some assimilation algorithms (e.g., EnSRF) can only achieve 440 better assimilation results when the model-data biases between observations have relatively small correlation or are uncorrelated. Therefore, in this study, we set the OG data with larger uncertainties than 441 the LNLG data, and re-grided it at a coarser spatial resolution of $5^{\circ} \times 5^{\circ}$. The results show that 442 under this scheme, the inverted ocean sink is reasonable, with value of -2.6 PgC yr⁻¹ (Table 1). In 443 addition, in order to compare the scheme that we have adopted in this study with the previous scheme 444 445 that do not assimilate the OG, we added three additional inversion experiments, in which only the 446 LNLG data were assimilated (Table S1). It could be found that all the three inversion experiments 447 without OG observations place smaller constraints on the ocean fluxes compared to the original exper-448 iments, with the posterior ocean fluxes remaining almost identical to the prior ocean fluxes. Corre-449 spondingly, the inverted global land sink as well as the sinks in most regions show a slight decrease 450 (Tables S2 and S3). Evaluations in comparison with *in-situ* observations showed that there are some 451 increases in the a posteriori concentration biases for all three experiments after removing OG. For example, for the experiments assimilating OCO-2 data, the mean bias increased from 0.02 to 0.14 ppm 452 (Table S4). This suggests that assimilating OG data with our method can improve the inversions some-453 454 what compared to removing OG.

455 Since OCO-3 has similar observation uncertainties of XCO_2 with OCO-2 (Taylor et al., 2023), the 456 poor performance of assimilating OCO-3 XCO₂ retrievals (Exp OCO3) may be related to that 1) 457 OCO-3 lacks observations beyond 52° North and South latitudes (Figure 1a); 2) the observation time 458 different from OCO-2; and 3) its spatial coverage between 52°S and 52°N. We first examined weekly 459 changes in the data amount of OCO-3 using the re-grided data as described in Section 2.3, and found 460 that there are very significant cyclical fluctuations in the data amount from OCO-3 (Figure S4a). Every 461 8 weeks or so, there is a trough in the data amount. There is a difference of about 5 times between the 462 weeks with the highest and the lowest data amount, and in the weeks with least data amount, there 463 were essentially no observations in the northern hemisphere (Figure S4b). This implies that the surface

carbon fluxes are largely unconstrained in the Northern Hemisphere, especially at mid- to high-lati-464 465 tudes, during the weeks with low observational data, resulting in poorer assimilation performance than 466 for OCO-2. For the observation time, all observations of OCO-2 were at 1:30 p.m. local time (LST), 467 whereas that of OCO-3 were variable, with only about 14% of the observations near 13:30 p.m. LST 468 and about 54% in the morning or after 4:00 p.m. LST (Figure S1). For reasons such as coarser model 469 resolution, the global atmospheric chemical transport models generally simulate atmospheric concen-470 trations better only in the afternoon, when boundary layer heights are at their highest and atmospheric 471 mixing is at its best, so assimilating these observations in the morning and after 4 p.m. LST may result 472 in poorer inversions due to the greater simulation bias of the atmospheric transport models at these 473 times of day.

474 In order to quantify these effects, we added another 3 additional inversion experiments, which 475 were named as Exp OCO2r, Exp OCO3tc, and Exp OCO2ts (Table S1). In Exp OCO2r, only the 476 OCO-2 XCO₂ retrievals located between 52°S and 52°N retrievals were assimilated, in Exp OCO3tc, 477 all the observation times of the OCO-3 XCO₂ retrievals were changed to 1.30 p.m. LST, and in 478 Exp OCO3ts, only OCO-3 data with observation times between 12 and 3 p.m. LST were assimilated. 479 When the OCO-2 data beyond 52° North and South latitudes were also removed (Exp OCO2r), the 480 NEE estimates, both globally and for individual regions, are close to those of the Exp OCO3 experi-481 ment, especially in the high latitude region of Europe and boreal North America, the inverted NEEs 482 are almost identical to those of the Exp OCO3 experiment (Table S2 and S3), and the bias of a poste-483 riori concentrations from observations at high latitudes is close to that of the OCO-3 experiment (Fig-484 ure S3). However, globally, compared to the OCO-3 experiment, the Exp OCO2r experiment still has 485 smaller the deviation between the global net flux and the observed annual growth rate (Table S2), and 486 smaller the global mean bias of the posterior concentrations (Table S4). This suggests that the lack of 487 observations of OCO-3 beyond 52° North and South latitudes does have a significant impact on the 488 inversion results. In addition, it can also be noted that at mid-latitudes, the bias of Exp OCO2r is also 489 smaller than the OCO-3 experiment, which may be caused by the significant fluctuations in the data 490 amount of OCO-3 (Figure S4). When we changed all the observation times of the OCO-3 XCO₂ re-491 trievals to 1.30 p.m. LST (Exp OCO3tc), although we are not actually able to do so, the inversion does 492 show a significant improvement compared to Exp OCO3. However, if we only select the data with 493 observation time between 12:00 and 3:00 p.m. LST (Exp OCO3ts), the deviation between the global 494 net flux and the observed annual growth rate, and the mean biases of the posterior concentrations at 495 most latitudes are larger than those of Exp OCO3 (Table S2 and Figure S3), indicating a poorer per-496 formance than Exp OCO3. The probably reason is that the data number of observations is substantially 497 reduced at this time (Figure S2), which leads to a substantial weakening of the observational constraints 498 on surface carbon fluxes (Figure S5).

499

500 **5 Summary and Conclusion**

In this study, we constrained terrestrial NEEs for the period from 1 August 2019 to 31 December 2022 using the OCO-2 and OCO-3 XCO₂ retrievals and the GCASv2 system, and analyzed the inversion results from 2020 to 2022. We conducted three inversion experiments for separately and jointly assimilating the OCO-2 and OCO-3 XCO₂ retrievals, to explore the impact of the OCO-3 XCO₂ retrievals on the constraints of global terrestrial NEEs. The prior and posterior CO_2 mixing ratios obtained from forward simulations using the prior and posterior fluxes are analysed in comparison with observations from 66 surface flask sites.

508 Globally, the terrestrial carbon sink from the Exp OCO3 is smaller than the prior, while the ter-509 restrial carbon sinks from the other two inversion experiments are slightly larger than the prior, but the 510 difference is small. The global net carbon flux from the Exp OCO3&2 is very close to the observed 511 atmospheric CO₂ growth rate. Regionally, the posterior NEEs for most terrestrial regions show a car-512 bon sink, with Europe showing a very strong sink and North Africa close to carbon neutrality. In the 513 Northern Hemisphere, the carbon sinks are enhanced, with the Exp OCO3&2 being the most enhanced by 0.59 PgC yr⁻¹ and the Exp OCO3 and Exp OCO2 by 0.19 and 0.36 PgC yr⁻¹, respectively. In the 514 515 tropics, the carbon sinks are weakened, with the Exp OCO3 being the most weakened by 0.67 PgC yr⁻¹, and the Exp OCO2 and Exp OCO3&2 sinks being weakened by 0.37 and 0.59 PgC yr⁻¹, respec-516 tively; in the southern land, the sink inverted in Exp OCO3 is weakened by 0.2 PgC yr⁻¹, whereas 517

those in the Exp_OCO2 and Exp_OCO3&2 are enhanced, by 0.08 and 0.05 PgC yr⁻¹, respectively.

519 On a global scale, the BIAS between the prior CO₂ concentrations and surface flask observations 520 is -1.82 ppm, with a MAE of 3.27 ppm and a RMSE of 5.01 ppm. The deviations between the posterior 521 CO₂ concentrations and surface flask observations for all three inversions are reduced to different degrees from the prior, especially for the BIAS, which decreased to 0.32, 0.02, and 0.05 ppm by 522 523 Exp OCO3, Exp OCO2, and Exp OCO3&2, respectively. The reasons for the poor performance of 524 assimilating OCO-3 XCO₂ alone are, on the one hand, the fact that it is only available between 52° S and 52°N, which leads to a lack of observational constraints on the carbon sinks at high latitudes, and 525 526 the large fluctuations in the amount of observational data, which leads to significant differences in 527 observational constraints at mid-latitudes at different times; on the other hand, its varied observation 528 time also affect the inversions, but even choosing afternoon observations does not improve the inver-529 sions because the amount of observed data drops significantly. Therefore, a better option for the future would be to jointly assimilate the OCO-2 XCO₂ data and the OCO-3 XCO₂ retrievals observed in the 530 531 afternoon (12:00 to 16:00 LST).

532

533 Code availability. The code of the GCASv2 system is available to the community and can be accessed
534 upon request from Fei Jiang(jiangf@nju.edu.cn) at Nanjing University.

535 **Data availability.** The OCO-2 and OCO-3 data used in this study is available at https://wwww.earthdata.nasa.gov. The FOSSIL carbon emissions of GCP-GridFEDv2023.1 is available at https://doi.org/10.5281/zenodo.8386803. The FIRE carbon emissions GFED 4.1s is available at https://doi.org/10.5281/zenodo.8386803. The FIRE carbon emissions GFED 4.1s is available at https://daac.ornl.gov/VEGETATION/guides/fire emissions v4 R1.html. The results of three in version experiments and evaluation are publicly available at https://doi.org/10.5281/zenodo.112 https

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542	Author contributions. XW and FJ designed the research. XW ran the model, analyzed the results		
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559			
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