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# Spatio-Temporal Mapping of Multi-Satellite Observed Column Atmospheric CO<sub>2</sub> Using Precision-Weighted Kriging Method

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**Abstract:** Column-averaged dry air mole fraction of atmospheric CO<sub>2</sub> (XCO<sub>2</sub>), obtained by multiple satellite observations since 2003 such as ENVISAT/SCIAMACHY, GOSAT, and OCO-2 satellite, is valuable for understanding the spatio-temporal variations of atmospheric CO<sub>2</sub> concentrations which are related to carbon uptake and emissions. In order to construct long-term spatio-temporal continuous XCO<sub>2</sub> from multiple satellites with different temporal and spatial periods of observations, we developed a precision-weighted spatio-temporal kriging method for integrating and mapping multi-satellite observed XCO<sub>2</sub>. The approach integrated XCO<sub>2</sub> from different sensors considering differences in vertical sensitivity, overpass time, the field of view, repeat cycle and measurement precision. We produced globally mapped XCO<sub>2</sub> (GM-XCO<sub>2</sub>) with spatial/temporal resolution of 1 × 1 degree every eight days from 2003 to 2016 with corresponding data precision and interpolation uncertainty in each grid. The predicted GM-XCO<sub>2</sub> precision improved in most grids compared with conventional spatio-temporal kriging results, especially during the satellites overlapping period (0.3–0.5 ppm). The method showed good reliability with R<sup>2</sup> of 0.97 from cross-validation. GM-XCO<sub>2</sub> showed good accuracy with a standard deviation of bias from total carbon column observing network (TCCON) measurements of 1.05 ppm. This method has potential applications for integrating and mapping XCO<sub>2</sub> or other similar datasets observed from multiple satellite sensors. The resulting GM-XCO<sub>2</sub> product may be also used in different carbon cycle research applications with different precision requirements.

**Keywords:** XCO<sub>2</sub>; multi-satellites; precision weighting; spatio-temporal kriging; mapping

## 1. Introduction

Spatio-temporal variation of atmospheric CO<sub>2</sub> concentration reflects the balance between anthropogenic carbon emissions and terrestrial and oceanic carbon uptake or emissions [1]. Increased fossil fuel emissions after the start of the Industrial Revolution contribute to the continuous growth of atmospheric CO<sub>2</sub> concentrations [2] from 277 parts per million (ppm) in 1750 [3] to 407.4 ± 0.1 ppm in 2018 [4]. The growth rate of CO<sub>2</sub> concentrations in the atmosphere is smaller than the rate

of CO<sub>2</sub> emitted by human activities because nearly 45% of the emissions are absorbed by oceans and the terrestrial biosphere each year [5]. The seasonal variations of terrestrial carbon uptake and emission contribute most to the seasonal cycle in atmospheric CO<sub>2</sub> [6], which varies spatially due to non-uniform land-biosphere CO<sub>2</sub> exchange [7]. In addition, there is spatial-temporal variability of atmospheric CO<sub>2</sub> concentrations that can be used to study changes in regional land biosphere net CO<sub>2</sub> fluxes, for example, seasonal cycle amplitude increase [8,9] and regional effects of extreme weather patterns like droughts [10,11]. Atmospheric CO<sub>2</sub> concentrations have also been used for carbon flux or to estimate carbon uptake/emission changes using atmospheric inversion models [12,13] and a data-driven method [14]. The spatio-temporal variability of CO<sub>2</sub> and related carbon sources/sinks distribution are still not fully understood [15,16]. A long time series of comparable global CO<sub>2</sub> concentration datasets has the potential to improve our understanding of land-biosphere interactions and our ability to evaluate trends in regional terrestrial CO<sub>2</sub> absorption capacity.

There are several methods to measure atmospheric CO<sub>2</sub> concentrations, including surface measurements and satellite observations and approaches to estimate concentrations from model simulations. A network of surface CO<sub>2</sub> monitoring station observations has been organized into the popular GLOBALVIEW-CO<sub>2</sub> product and provides in situ measurements but is limited by station sparseness and the inherent spatial inhomogeneity of the surface atmosphere. Model simulations can provide continuous maps of CO<sub>2</sub> using estimated surface fluxes and atmospheric mixing transport in addition to the previously noted sparse validation stations [17]. Satellite observations of atmospheric CO<sub>2</sub> have the advantage of global coverage and high measurement density and can complement the surface network to advance our understandings of the carbon cycle and its changes [18,19]. With the development of remote sensing technology, there are several satellites used for atmospheric CO<sub>2</sub> concentration observations [20,21]. Leveraging all available XCO<sub>2</sub> datasets to construct a long time series, continuous, and comparable global CO<sub>2</sub> concentrations would be useful.

Satellite-observed column-averaged dry air mole fraction of CO<sub>2</sub> (XCO<sub>2</sub>) have been widely used for carbon cycle studies, including CO<sub>2</sub> enhancement detection induced by anthropogenic emissions [22,23], constraining model simulations of carbon fluxes [24,25], investigating carbon cycle responses to weather extremes [11,26], and improving understanding of vegetation uptake [27]. Satellites measuring XCO<sub>2</sub> are the SCanning Imaging Absorption spectrometer for Atmospheric CHartographY (SCIAMACHY) onboard the Environmental Satellite (ENVISAT) [28], Greenhouse Gases Observing Satellite (GOSAT) [29], and Orbiting Carbon Observatory-2 (OCO-2) [30]. They observe XCO<sub>2</sub> but with different spatial/temporal resolution, prior vertical profile estimates, local overpass time, data precision, and observing gaps. As a result, there is an opportunity to generate a long time series of global XCO<sub>2</sub> dataset starting from 2003 using XCO<sub>2</sub> retrievals from these satellites with careful integration and gap-filling.

Gap-filling satellite-observed XCO<sub>2</sub> has been investigated in several studies from different perspectives [31–33]. Geostatistical approaches, especially kriging, were widely used for GOSAT observed XCO<sub>2</sub> Level 3 product production [17,34,35]. Spatial-only geostatistical methods do not take into account the temporal correlation structure of CO<sub>2</sub> data [19], which may provide extra information. In order to make full use of spatio-temporal correlation of atmospheric CO<sub>2</sub>, a new spatio-temporal kriging method was developed for the global mapping of XCO<sub>2</sub> [19,36]. Because these methods were previously used for observations from a single satellite, measurement error could be assumed to be uniform and not interfere with the kriging approach. In order to produce high spatio-temporal resolution and a long time series of XCO<sub>2</sub> from multiple satellite observations, the precision of different datasets should be considered in this geostatistical method.

In this study, to create the longest possible time series of XCO<sub>2</sub> and leverage multiple measurements to improve precision when possible, we developed a precision-weighted spatio-temporal kriging method for gap filling of integrated XCO<sub>2</sub> from multiple satellite observations. Datasets used in this study and data preprocessing are described in Section 2. XCO<sub>2</sub> integration methods and global mapping can be found in Section 3. Results of global mapped XCO<sub>2</sub> and its validation are shown in

Section 4 and data quality considerations are discussed in Section 5. Finally, conclusions are presented in Section 6.

## 2. Dataset

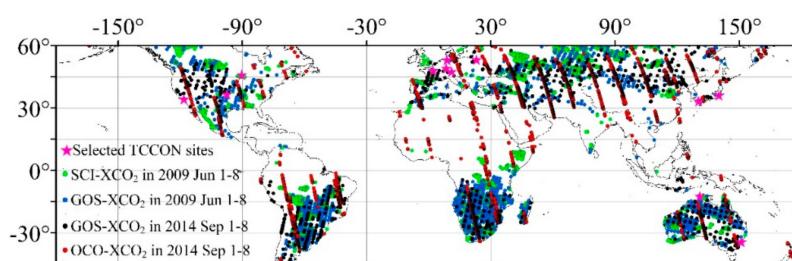
In this study, we collected atmospheric CO<sub>2</sub> concentration datasets from multiple satellite-observations to produce a long time series of spatio-temporal continuous XCO<sub>2</sub> from satellite observations, which was then evaluated by XCO<sub>2</sub> from surface measurements and model simulations.

### 2.1. XCO<sub>2</sub> from Multi-Satellite Observations

Atmospheric CO<sub>2</sub> concentrations used here were the released Level 2 products that contain the full-physics retrievals of column-averaged CO<sub>2</sub> in units of dry air mole fraction (XCO<sub>2</sub>). Satellite observations of XCO<sub>2</sub> used here are from ENVISAT/SCIAMACHY, GOSAT, and OCO-2, which span from 2003 to 2016. XCO<sub>2</sub> from SCIAMACHY onboard the European ENVISAT are obtained by the full-physics based Bremen Optimal Estimation–DOAS (BESD) algorithm (v02.01.01) [37], which span from January 2003 to March 2012 with a spatial/temporal resolution of 30x60 km every 35 days. XCO<sub>2</sub> from GOSAT is produced by the algorithm of the Atmospheric CO<sub>2</sub> Observations from Space (ACOS) team (v7.3 lite) [38], which span from June 2009 to May 2016 with spatial/temporal resolution of a diameter of 10.5 km every three days. XCO<sub>2</sub> from OCO-2 is produced by the ACOS team (r9 lite) [39], which span from September 2014 to December 2016 with spatial/temporal resolution of 2.25 × 1.25 km every 16 days. Data quality was maximized by filtering XCO<sub>2</sub> product by screening criteria specified by the corresponding user guides. Specifications of the three satellites that observed XCO<sub>2</sub> are shown in Table 1. These satellites follow different orbits and have different gaps as shown in Figure 1. XCO<sub>2</sub> retrievals from each satellite also have different data precision for different sensors, observation conditions, and retrieval methods. Therefore, we use different XCO<sub>2</sub> precisions in time and space in the XCO<sub>2</sub> integration and mapping with the spatio-temporal kriging method.

**Table 1.** Specifications of multiple satellites that observed XCO<sub>2</sub>.

Attributes\Satellites	ENVISAT/SCIAMACHY	GOSAT	OCO-2
Period of selected data	January 2003–March 2012	June 2009–May 2016	September 2014–December 2016
Repeat cycle (days)	35	3	16
Field of view (km)	30 × 60	Diameter of 10.5	2.25 × 1.25
Overpass local time version	10:00 BESD v02.01.01	13:00 ACOS v7.3	13:36 OCO2 r9
Profile layers number	10	20	20
Criteria of data screening	XCO <sub>2</sub> _quality_flag=0;	XCO <sub>2</sub> _quality_flag=0; gain=H; land_fraction>90; warn_level<10	XCO <sub>2</sub> _quality_flag=0; gain=H; land_fraction>90
Name referred hereafter Reference	SCI-XCO <sub>2</sub> [37]	GOS-XCO <sub>2</sub> [38]	OCO-XCO <sub>2</sub> [39]



**Figure 1.** Example of XCO<sub>2</sub> from SCIAMACHY, GOSAT, and OCO-2. Green and blue points represent SCI-XCO<sub>2</sub> and GOS-XCO<sub>2</sub> from 1–8 June 2009. Black and red points are GOS-XCO<sub>2</sub> and OCO-XCO<sub>2</sub> from 1–8 September 2014. Total carbon column observing network (TCCON) sites used for validation are shown with a pink star.

## 2.2. The Total Carbon Column Observing Network

The total carbon column observing network (TCCON) are upward-looking terrestrial Fourier transform spectrometers established for measuring atmospheric XCO<sub>2</sub> and other trace gases from the surface [40]. The instruments have high accuracy with approximately 0.25% error in XCO<sub>2</sub> retrievals, which has been extensively used for validation of satellite observations [21,40,41]. In this study, we selected 12 TCCON sites within the mapping area as shown in Figure 1, with at least five years of coincidental measurements in the period from January 2003 to December 2016 for validating combined XCO<sub>2</sub> products.

## 2.3. XCO<sub>2</sub> from Model Simulation

CarbonTracker (CT) is a modeling system that assimilates global atmospheric CO<sub>2</sub> observations from the ground, tall tower, and aircraft, coupled with an atmospheric transport model for simulating global distributions of atmospheric CO<sub>2</sub> and tracking CO<sub>2</sub> sources and sinks. Model-simulated atmospheric CO<sub>2</sub> from CarbonTracker 2017 [42] was used in three steps of the integration and mapping method, primarily to normalize differences in altitude sensitivity and overpass time. First, we used CarbonTracker CO<sub>2</sub> profiles in a grid of  $2^\circ \times 3^\circ$  (latitude  $\times$  longitude) in 3-hour intervals as the common profile to align the a priori CO<sub>2</sub> profiles and averaging kernels of multi-satellite observations. Second, we adopted diurnal patterns of CO<sub>2</sub> concentrations in different pressure layers from CarbonTracker to unify the CO<sub>2</sub> from satellite observations to 13:00 local time. XCO<sub>2</sub> from CarbonTracker (CT-XCO<sub>2</sub>) was calculated from the model CO<sub>2</sub> profile data with 25 layers at the local time 13:00 by using a pressure weighting average method [43]. Third, we used the CT-XCO<sub>2</sub> for comparing with our new globally mapped XCO<sub>2</sub> product.

## 3. Method

In this study, we developed a method for spatio-temporal integration and mapping of multi-satellite observed XCO<sub>2</sub> considering variable data precision for producing globally mapped continuous XCO<sub>2</sub> with spatial/temporal resolution of  $1^\circ \times 1^\circ$  every eight days from 2003 to 2016. We present the flow chart of global mapped XCO<sub>2</sub> production and the precision weighted spatio-temporal kriging method in Figure 2. First, we adjusted a priori vertical CO<sub>2</sub> profiles and averaging kernels of multiple satellite-observed XCO<sub>2</sub> products to a common profile. Second, we corrected to a common local time and regularizing spatio-temporal scales of XCO<sub>2</sub> from multiple satellites. Third, we used a modeled continuous XCO<sub>2</sub> spatio-temporal random field for interpolation. Fourth, we developed a precision-weighted spatio-temporal kriging method for producing global maps of XCO<sub>2</sub>. Finally, we validated the new global mapped XCO<sub>2</sub>. We present details on developing the precision-weighted spatio-temporal kriging method including: (1) conventional spatio-temporal kriging method; (2) optimization of spatio-temporal correlation structure; (3) XCO<sub>2</sub> prediction through integrating data precision, and; (4) uncertainty and precision of mapped XCO<sub>2</sub>.

### 3.1. Preprocessing

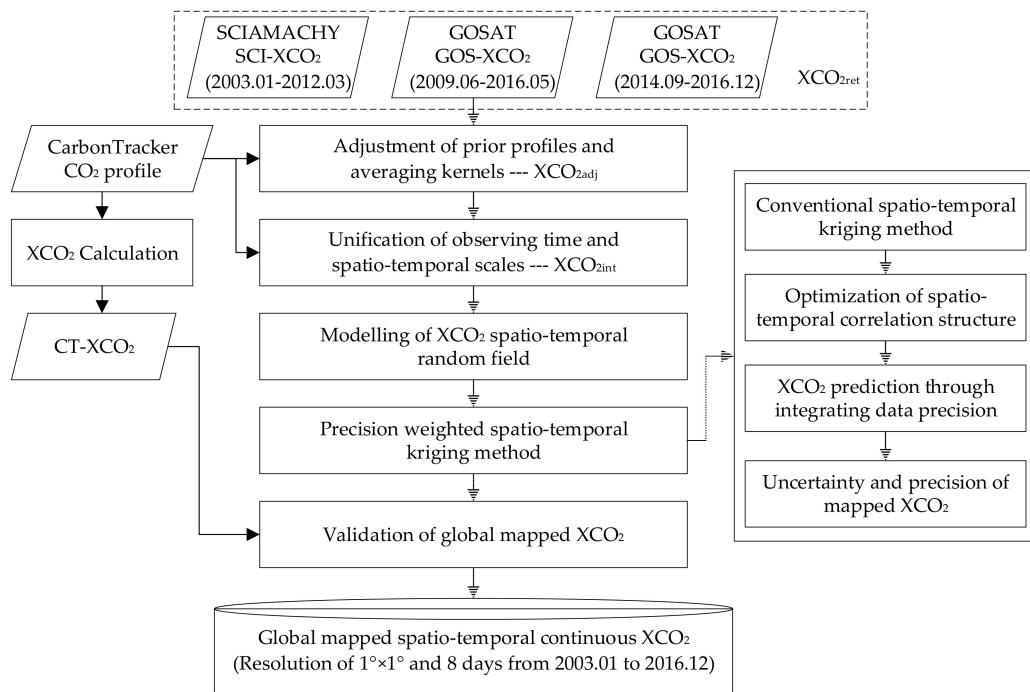
#### 3.1.1. Adjustment of a Priori Vertical Profiles and Averaging Kernels

Each satellite has different measurement sensitivity at different altitudes through the atmospheric column and, therefore, they use different averaging kernels based on a priori assumptions of vertical CO<sub>2</sub> profiles to account for sensor sensitivities in XCO<sub>2</sub> retrieval algorithms. The corrections are based on prior vertical profile layers as shown in Table 1. The a priori profiles from different satellite retrievals should be adjusted to a common profile when comparing XCO<sub>2</sub> from different instruments. Additionally, the smoothing effect of the retrievals should be considered by applying the averaging kernels [44] to reduce the effects from different instruments on XCO<sub>2</sub> retrievals [37,45]. In this study,

we introduce a common a priori  $\text{XCO}_2$  profile from CT to integrate  $\text{XCO}_2$  retrievals from ENVISAT/SCIAMACHY, GOSAT, and OCO-2 by using Equation (1).

$$\text{XCO}_{2\text{adj},t} = \text{XCO}_{2\text{ret},t} + \mathbf{h}^T \cdot (\mathbf{I} - \mathbf{A}) \cdot (\mathbf{X}_{M,t} - \mathbf{X}_{a,t}) \quad (1)$$

where  $\text{XCO}_{2\text{adj},t}$  is the adjusted  $\text{XCO}_{2\text{ret}}$  at observation time  $t$ ,  $\text{XCO}_{2\text{ret},t}$  is the original  $\text{XCO}_2$  retrievals from satellites,  $\mathbf{h}$  is a pressure-weighting vector,  $\mathbf{A}$  is column-averaging kernels in the  $\text{XCO}_2$  retrieval algorithm,  $\mathbf{I}$  is an identity matrix,  $\mathbf{X}_{M,t}$  is a set of common a priori  $\text{CO}_2$  profiles from CT, and  $\mathbf{X}_{a,t}$  is a set of a priori  $\text{CO}_2$  profiles used in  $\text{XCO}_2$  original satellite-specific retrieval algorithms. A priori  $\text{CO}_2$  profiles of each satellite, as shown in Table 1, were interpolated into the same 25 pressure layers of the CT model.



**Figure 2.** Workflow chart of spatio-temporal integration of multi-satellite observed  $\text{XCO}_2$  using a precision-weighted kriging method.

### 3.1.2. Unification of Observing Time and Spatio-Temporal Scales

The three satellites have different local overpass times: SCIAMACHY at 10:00, GOSAT at 13:00, and OCO-2 at 13:36 (Table 1). In order to reduce the effect of atmospheric  $\text{CO}_2$  concentrations diurnal variation [46,47], we introduce a correction coefficient to normalize the satellite observations local time to 13:00 based on diurnal variation of CT model simulations using Equation (2).

$$\text{XCO}_{2\text{con},rt} = \frac{\mathbf{h}^T \mathbf{X}_{M,rt}}{\mathbf{h}^T \mathbf{X}_{M,t}} \cdot \text{XCO}_{2\text{adj},t} \quad (2)$$

where  $\text{XCO}_{2\text{con},rt}$  is the converted  $\text{XCO}_{2\text{adj}}$  at the reference time ( $rt$ , 13:00 local time);  $\text{XCO}_{2\text{adj},t}$  is the adjusted  $\text{XCO}_2$  derived from Equation (1) at satellite overpass time  $t$ ;  $\mathbf{X}_{M,rt}$  and  $\mathbf{X}_{M,t}$  are  $\text{CO}_2$  profiles from CT at times of  $rt$  and  $t$ , respectively; and  $\mathbf{h}$  is the pressure-weighting vector.

Moreover,  $\text{XCO}_2$  is affected by the different fields of view and observing dates as shown in Table 1. In order to reduce this effect, we integrate spatial and temporal scales of  $\text{XCO}_2$  retrievals using precision weighted averaging of  $\text{XCO}_{2\text{con},rt}$  within 30 km by 30 km every 8 days using Equations (3-1) and (3-2). This unification also reduces computational complexity and preserves local spatiotemporal patterns. A temporal resolution of 8 days is also well-suited for biosphere-atmosphere interaction analysis

with other 8-day resolution datasets like vegetation indices from the Moderate Resolution Imaging Spectroradiometer (MODIS). An integrated XCO<sub>2</sub> dataset at 30 km resolution every 8 days from 2003 to 2016 (integrated-XCO<sub>2</sub>) was generated.

$$\text{XCO}_{2\text{int,rt}} = \sum_{i=1}^n p_i \cdot \text{XCO}_{2\text{con,rt}_i} \quad (3-1)$$

$$\sum_{i=1}^n p_i = \sum_{i=1}^n \frac{\mu^2}{m_i^2} = 1 \quad (3-2)$$

where XCO<sub>2int,rt</sub> is the integrated combination of XCO<sub>2con</sub> datasets, n is the number of observations in one unit, XCO<sub>2con,rt<sub>i</sub></sub> is converted satellite observed XCO<sub>2</sub>, p<sub>i</sub> is the weighting factor, which is determined by m<sub>i</sub> (data precision of XCO<sub>2con,rt<sub>i</sub></sub>). μ is an arbitrary constant used for normalizing the data precision weighting factor. We adopted the data precision from these satellites observed XCO<sub>2</sub> Level 2 product. The data precision in ACOS-GOSAT and OCO-2 is XCO<sub>2</sub> posterior error, and that in BESD-SCIAMACHY is 1-sigma uncertainty of the retrieved XCO<sub>2</sub>.

### 3.2. Modeling XCO<sub>2</sub> Spatio-Temporal Random Field for use in Kriging

XCO<sub>2</sub> increases from year-to-year varies by latitude and has a significant seasonal cycle in most locations [48,49]. In order to interpret spatio-temporal geostatistics, we need to construct a second-order stationary random field represented by the stochastic residual component after removing inter-annual, latitudinal, and seasonal trends mentioned above, termed the deterministic mean. In this study, we adopted a fitting method for decomposing [50] the deterministic spatiotemporal mean and stochastic residual component of latitude-zonal XCO<sub>2</sub>. The fitting method is a combination of a linear function to fit the long-term increase and annual periodic function as shown in Equation (4).

$$m(s, t) = a_0(s) + a_t(s) + \sum_{i=1}^4 (\beta_i(s) \cdot \sin(i\omega t) + \gamma_i(s) \cdot \cos(i\omega t)) + R(s, t) \quad (4)$$

where  $\omega = 2\pi/T$  and T is the period of 46 time-units, t is the time in the time-unit, s represents the latitudinal zone, and a<sub>0</sub>, β<sub>1-4</sub> and γ<sub>1-4</sub> are parameters to be estimated. a<sub>t</sub> is the cumulative annual increase for each time-unit determined by the Earth System Research Laboratory (ESRL) global annual CO<sub>2</sub> growth rate [4]. The harmonic functions fit the annual cycle, semi-annual oscillation, seasonal variation and monthly variation of XCO<sub>2</sub> [19]. R(s, t) represents the spatio-temporal residual component of satellite observed integrated XCO<sub>2</sub>, which will be used for interpretation.

### 3.3. Precision Weighted Spatio-Temporal Kriging

In the ordinary kriging method, a predicted value at an arbitrary target point is estimated by considering the statistical properties of a set of observed data. As a result, the predicted value (Z(s<sub>0</sub>)) at point s<sub>0</sub> can be expressed as a weighted sum of the observational data as shown in Equation (5).

$$Z(s_0) = \sum_{i=1}^n \omega_i \cdot Z(s_i) \quad (5)$$

where ω<sub>i</sub> is the weighting factor at the observation point s<sub>i</sub>, n is the total number of observational points to be used, and Z(s<sub>i</sub>) is the observed value at each point s<sub>i</sub>. The following subsections describe the precision-weighted spatio-temporal kriging method. Different kriging models were developed by adjusting the number of points 'n' and the weighting factor 'ω<sub>i</sub>'.

### 3.3.1. Conventional Spatio-Temporal Kriging

In spatio-temporal geostatistical analysis of XCO<sub>2</sub>, kriging prediction of Z(s<sub>0</sub>, t<sub>0</sub>) at a point (s<sub>0</sub>, t<sub>0</sub>) can be calculated as the linear weighted sum of the XCO<sub>2</sub> values that minimizes the mean squared prediction error [19]. Weights of observations used for interpolation are determined by the geometry of observations and the spatio-temporal correlation structure of the data. Spatial and temporal information would be used for variogram modeling of the correlation structure [19,31] as shown in Equation (6).

$$\hat{\gamma}_{ST}(h_s, h_t) = \frac{1}{2N(h_s, h_t)} \sum_{i=1}^{N(h_s, h_t)} [Z(s_i + h_s, t_i + h_t) - Z(s_i, t_i)]^2 \quad (6)$$

where  $\hat{\gamma}_{ST}(h_s, h_t)$  is an empirical variogram value at the lag (h<sub>s</sub>, h<sub>t</sub>). Z(s<sub>i</sub>, t<sub>i</sub>) is the observational data. N(h<sub>s</sub>, h<sub>t</sub>) is the number of data pairs within a distance of (h<sub>s</sub>, h<sub>t</sub>). Once the empirical variogram has been constructed, we need to select a spatio-temporal variogram model to fit it. As shown in Zeng et al. [19,31], the spatio-temporal variogram model adopted here (Equation (7)) is a combination of the product-sum model [51,52] and an extra global nugget model to capture the nugget effect [53] (last term in Equation (7)).

$$\gamma_{ST}(h_s, h_t; \theta_s, \theta_t, \kappa, N_{ST}) = \gamma_S(h_s; \theta_s) + \gamma_T(h_t; \theta_t) - \kappa \cdot \gamma_S(h_s; \theta_s) \cdot \gamma_T(h_t; \theta_t) + N_{ST} \cdot \gamma_0(h_s; h_t) \quad (7)$$

We selected the exponential model for the marginal variogram model  $\gamma_S(h_s)$  and  $\gamma_T(h_t)$  as shown in Equation (8).

$$\gamma(h; \theta = [C, a]) = \begin{cases} 0, & h = 0 \\ C \cdot (1 - e^{-\frac{h}{a}}), & h \neq 0 \end{cases} \quad (8)$$

where  $\gamma_S(h_s; \theta_s)$  and  $\gamma_T(h_t; \theta_t)$  are the marginal spatial and temporal variograms,  $[\theta_s, \theta_t, \kappa, N_{ST}] = [C_s, a_s, C_t, a_t, \kappa, N_{ST}]$  are parameters to be estimated, and  $N_{ST}$ , C, and a are all greater than or equal to zero. In the exponential model, a, C and  $N_{ST}$  represent the influence range, partial sill, and nugget effects, respectively.

As a result, an arbitrary target point ( $\hat{Z}(s_0, t_0)$ ) to be estimated by using the spatio-temporal kriging method can be expressed as Equation (9).

$$\hat{Z}(s_0, t_0) = \sum_{i=1}^n \omega_i(s_0, t_0) \cdot Z(s_i, t_i) \text{ with } \sum_{i=1}^n \omega_i(s_0, t_0) = 1 \quad (9)$$

where  $\omega_i(s_0, t_0)$  is the weight assigned to a known observation Z(s<sub>i</sub>, t<sub>i</sub>) so as to minimize the prediction error variance while maintaining an unbiased prediction. The prediction error variance, which is a measurement of prediction uncertainty, is given by

$$\sigma^2 = \gamma_0^T \Gamma^{-1} \gamma_0 - \frac{(\mathbf{1}^T \Gamma^{-1} \gamma_0 - 1)^2}{\mathbf{1}^T \Gamma^{-1} \mathbf{1}} \quad (10)$$

where  $\Gamma(i, j) = \gamma(|s_i - s_j|, |t_i - t_j|)$ ,  $\gamma_0(i, 1) = \gamma(|s_i - s_0|, |t_i - t_0|)$ , and  $\mathbf{1}$  is the  $n \times 1$  unit vector.

### 3.3.2. Optimization of Spatio-Temporal Correlation Structure

In a conventional spatio-temporal geostatistical analysis, all data pairs were used for spatio-temporal correlation structure using equal weight. XCO<sub>2</sub> observations from different satellites/sensors, observing conditions and inversion methods have different data precision. So, the

varying data precision should be considered in building the loss function for optimizing spatio-temporal correlation structure with precision weighting factor as shown in Equation (11).

$$\delta = \sum_{i=1}^m \lambda_i \cdot (\gamma_{ST} - \hat{\gamma}_{ST})^2 = \sum_{i=1}^m \lambda_i \cdot (\gamma_s(h_s) + \gamma_T(h_t) - \kappa \cdot \gamma_s(h_s) \cdot \gamma_T(h_t) + N_{ST} - \hat{\gamma}(h_s, h_t))^2 \quad (11-1)$$

$$\sum_{i=1}^n \lambda_i = \sum_{i=1}^n \frac{\mu_1^2}{m_i^2} = 1 \quad (11-2)$$

where  $\lambda_i$  represents different weighting factors for data with different precisions.  $\gamma_{ST}$  is the spatio-temporal variogram model shown in Equation (7).  $\hat{\gamma}_{ST}$  is the empirical variogram shown in Equation (6).  $m_i$  and  $\mu_1$  represent data precision and a normalization term.

The gradient descent method was used to calculate the optimal parameters. The partial derivative parameters ( $\delta'_{C_s^*}, \delta'_{a_s^*}, \delta'_{C_t^*}, \delta'_{a_t^*}, \delta'_{\kappa^*}, \delta'_{N_{ST}^*}$ ) that need to be estimated are shown in Equations (12-1)–(12-6).

$$\delta'_{C_s^*} = 2 \cdot \sum_{i=1}^m \{\lambda_i \cdot (\gamma_{ST}(h_s, h_t) - \hat{\gamma}(h_s, h_t))\} \cdot \left(1 - e^{-\frac{\|h_s\|}{a_s^*}}\right) \quad (12-1)$$

$$\delta'_{a_s^*} = 2 \cdot \sum_{i=1}^m \{\lambda_i \cdot (\gamma_{ST}(h_s, h_t) - \hat{\gamma}(h_s, h_t))\} \cdot \left(-C_s^* \cdot e^{-\frac{\|h_s\|}{a_s^*}}\right) \cdot (\|h_s\| \cdot a_s^{*-2}) \quad (12-2)$$

$$\delta'_{C_t^*} = 2 \cdot \sum_{i=1}^m \{\lambda_i \cdot (\gamma_{ST}(h_s, h_t) - \hat{\gamma}(h_s, h_t))\} \cdot \left(1 - e^{-\frac{\|h_t\|}{a_t^*}}\right) \quad (12-3)$$

$$\delta'_{a_t^*} = 2 \cdot \sum_{i=1}^m \{\lambda_i \cdot (\gamma_{ST}(h_s, h_t) - \hat{\gamma}(h_s, h_t))\} \cdot \left(-C_t^* \cdot e^{-\frac{\|h_t\|}{a_t^*}}\right) \cdot (\|h_t\| \cdot a_t^{*-2}) \quad (12-4)$$

$$\delta'_{\kappa^*} = 2 \cdot \sum_{i=1}^m \{\lambda_i \cdot (\gamma_{ST}(h_s, h_t) - \hat{\gamma}(h_s, h_t))\} \cdot (\gamma_s(h_s; \theta_s^*) \cdot \gamma_T(h_t; \theta_t^*)) \quad (12-5)$$

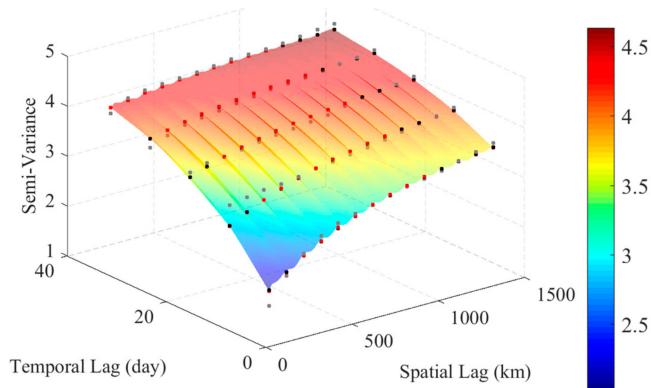
$$\delta'_{N_{ST}^*} = 2 \cdot \sum_{i=1}^m \{\lambda_i \cdot (\gamma_{ST}(h_s, h_t) - \hat{\gamma}(h_s, h_t))\} \quad (12-6)$$

where  $C_s^*, a_s^*, C_t^*, a_t^*, \kappa^*$  and  $N_{ST}^*$  are parameters waiting to be optimized. Parameters,  $\lambda_i$ ,  $\gamma_{ST}$ ,  $\gamma$  and  $\hat{\gamma}$  are the weighting factors (Equation (11-2)), exponential models (Equation (7) and Equation (8)) and empirical variogram values (Equation (6)), respectively.

We optimized the structure through minimizing  $\delta$ . Initial parameters  $\beta_0 = (C_{s0}, a_{s0}, C_{t0}, a_{t0}, \kappa_0, N_{ST0})$  were obtained by using a least-squares approximation in the conventional spatio-temporal kriging method. Then, parameters were determined by a learning rate and partial derivative as shown in Equation (13).

$$\beta_i = \beta_{i-1} + \alpha \cdot \delta'_{i-1} \quad (13)$$

where  $\beta$  represents  $(C_s^*, a_s^*, C_t^*, a_t^*, \kappa^*, N_{ST}^*)$ .  $\alpha$  is the learning rate, usually in the range of  $(10^{-4} \sim 10^{-2})$ .  $\delta'$  is the partial derivative parameter. We set the operating condition as a current change of less than 1% of all the changes in this adjustment. As a result, one example of optimized spatio-temporal semi-variogram surface is shown in Figure 3.



**Figure 3.** One example of the optimized spatio-temporal semi-variogram surface (Zone 1: Latitude center: 55°N). Grey, black, and red points represent spatio-temporal semi-variogram that was calculated from experimental data, fitted models of the conventional and optimized correlation structure.

### 3.3.3. Integrating XCO<sub>2</sub> Using Variable Data Precision

We estimated XCO<sub>2</sub> in unobserved points using observational data and weighting factors from spatio-temporal correlation structure and data precision as shown in Equation (14).

$$Z(s_0, t_0) = \sum_{i=1}^n \omega_{1i} \cdot \omega_{2i} \cdot Z(s_i, t_i) \quad (14)$$

where  $\omega_{1i}$  is the weighting factor from the spatio-temporal correlation structure and  $\omega_{2i}$  is from data precision.  $Z(s_i, t_i)$  is observed XCO<sub>2</sub> used for  $Z(s_0, t_0)$  estimation. These two weighting factors were calculated by Equations (15-1) and (15-2).

$$\begin{aligned} \sum_{i=1}^s \omega_{1i} \cdot \gamma(h_{1i}) + \varepsilon &= \gamma(h_{10}) \\ \sum_{i=1}^s \omega_{1i} \cdot \gamma(h_{2i}) + \varepsilon &= \gamma(h_{20}) \\ &\dots \\ \sum_{i=1}^s \omega_{1i} \cdot \gamma(h_{si}) + \varepsilon &= \gamma(h_{s0}) \end{aligned} \quad (15-1)$$

$$\sum_{i=1}^s \omega_{1i} \cdot \omega_{2i} = 1 \quad (15-2)$$

where  $\omega_{1i}$  and  $\omega_{2i}$  are weighting factors in Equation (14). Equation (15-2) was used to control unbiased estimation.  $\gamma(h_{1i}) \dots \gamma(h_{si})$  and  $\gamma(h_{10}) \dots \gamma(h_{s0})$  are spatio-temporal variograms for observations used for estimation of  $Z(s_0, t_0)$ .  $\varepsilon$  is the polynomial residuals.  $\omega_{2i}$  can be achieved by Equation (16).

$$\sum_{i=1}^s \omega_{2i} = \sum_{i=1}^s \frac{\mu_2^2}{m_i^2} = s \quad (16)$$

where  $m_i$ ,  $\mu_2$  and  $s$  are data precision, arbitrary constant and the number of used observational data.

We applied this method for global mapping of XCO<sub>2</sub> (GM-XCO<sub>2</sub>), which provides a long time series of spatio-temporal continuous XCO<sub>2</sub> dataset for global carbon cycle research.

### 3.3.4. Uncertainty and Precision of Mapped XCO<sub>2</sub>

We calculated data uncertainty and precision of the mapped XCO<sub>2</sub> by using precision-weighted kriging. Uncertainty of predicted data from the spatio-temporal kriging method is shown in Equation (17)

$$\sigma_0^2 = \sum_{i=1}^s w_{1i} \cdot \gamma(h_{i0}) + \varepsilon \quad (17)$$

where  $\sigma_0^2$  presents the prediction uncertainty,  $w_{1i}$ ,  $\gamma(h_{i0})$  and  $\varepsilon$  are the estimated weighting factor, spatio-temporal variograms, and polynomial residuals, respectively as shown in Equation (15).

In addition, the precision of GM-XCO<sub>2</sub> integrated from the observed data is shown in Equation (18), according to the error transfer equation.

$$\varepsilon_0 = \sqrt{\sum_{i=1}^s \varepsilon_i^2 \cdot w_{1i}^2 \cdot w_{2i}^2} \quad (18)$$

As a result, these two sources of uncertainty can be used for data screening in GM-XCO<sub>2</sub> application.

### 3.4. Validation of Global Mapped XCO<sub>2</sub>

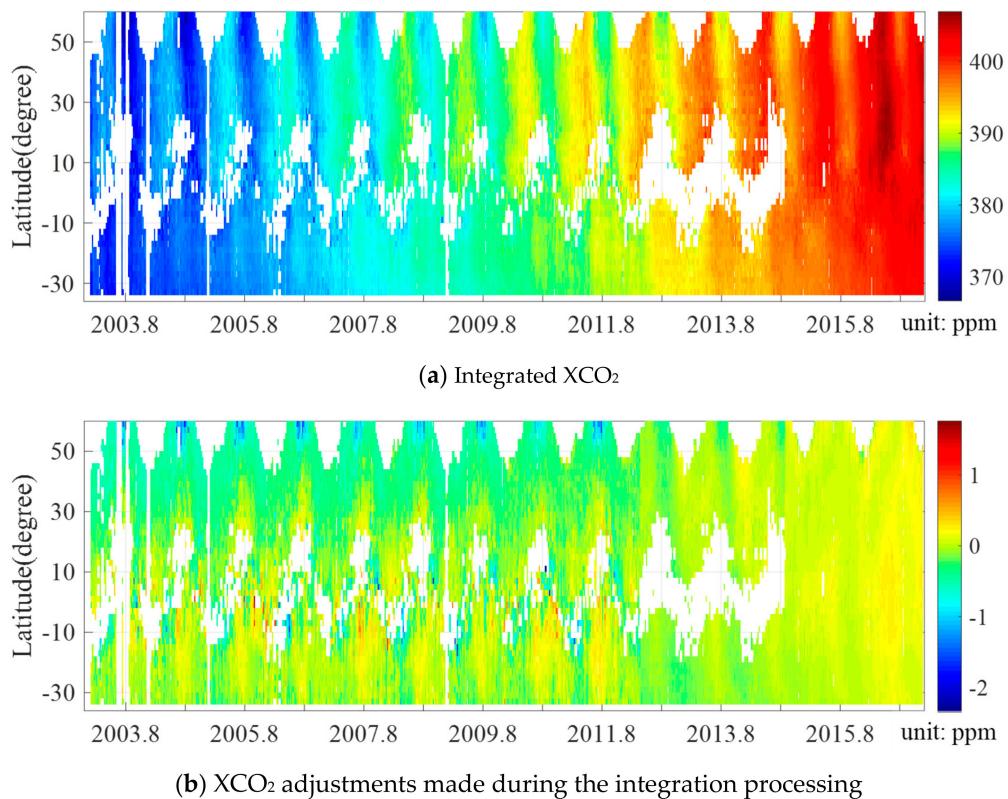
We validated the mapped GM-XCO<sub>2</sub> product using cross-validation, compared to TCCON measurements and model simulation. Cross-validation has been used in accuracy assessments for spatio-temporal kriging methods [19,54]. In this study, we adopted cross-validation based on the Monte Carlo sampling method used in Zeng et al. [19]. As above, we used the satellite-observed integrated XCO<sub>2</sub> dataset (XCO<sub>2,int</sub>) for interpolation to GM-XCO<sub>2</sub>. The cross-validation was conducted by repeatedly (100 times) reserving 5% of the XCO<sub>2,int</sub> data for validation. Predicted GM-XCO<sub>2</sub> was compared with the 5% reserved XCO<sub>2,int</sub> data in those corresponding spatio-temporal locations. We selected three statistical parameters for results evaluation: (1) the coefficient of determination ( $r^2$ ), (2) the root mean square error (RMSE), and (3) the percentage of estimation bias less than 1 or 2 times of data precision.

We compared GM-XCO<sub>2</sub> with the XCO<sub>2</sub> measured from TCCON (TCCON-XCO<sub>2</sub>) in 12 sites with more than 5 years of observation. TCCON-XCO<sub>2</sub> was calculated with the pressure-averaged method [43] and data observed at a local time of 11:00 to 15:00. In addition, we did a comparison between GM-XCO<sub>2</sub> and XCO<sub>2</sub> from the CT model simulation in the spatio-temporal change over the global area.

## 4. Results

### 4.1. Integrated-XCO<sub>2</sub> from Three Satellites

Here we presented latitudinal and temporal variability of the integrated XCO<sub>2</sub> (top panel) and the difference between the integrated product and the original retrieval XCO<sub>2</sub> values (bottom panel) from SCIAMACHY, GOSAT, and OCO-2 (Figure 4). The top panel shows XCO<sub>2</sub> increased more than 30 ppm from 2003 to 2016 over most latitudes. Especially high XCO<sub>2</sub> values occurred during the start of 2016 in the northern hemisphere (dark red). The bottom panel shows XCO<sub>2</sub> adjustments, integrated XCO<sub>2</sub> (XCO<sub>2,int</sub>) minus original XCO<sub>2</sub> (XCO<sub>2,ret</sub>) were mainly within -2.0 to 1.0 ppm and include seasonality, with high adjustment values in summer and low adjustment values in winter, except for some scattered grids in high or low latitudes. This could be caused by seasonal changes of the XCO<sub>2</sub> averaging kernel (Appendix A: Figure A1) that was adopted for XCO<sub>2</sub> adjustment in Equation (1). In addition, the adjustments decreased sharply in 2012 and 2016, with stability improvements of the newer satellite sensors.



**Figure 4.** Latitudinal-temporal change of integrated  $\text{XCO}_2$  (a) and  $\text{XCO}_2$  adjustments made during the integration processing, integrated  $\text{XCO}_2$  ( $\text{XCO}_{2\text{int}}$ ) minus original  $\text{XCO}_2$  ( $\text{XCO}_{2\text{ret}}$ ) (b) from SCIAMACHY, GOSAT, and OCO-2.

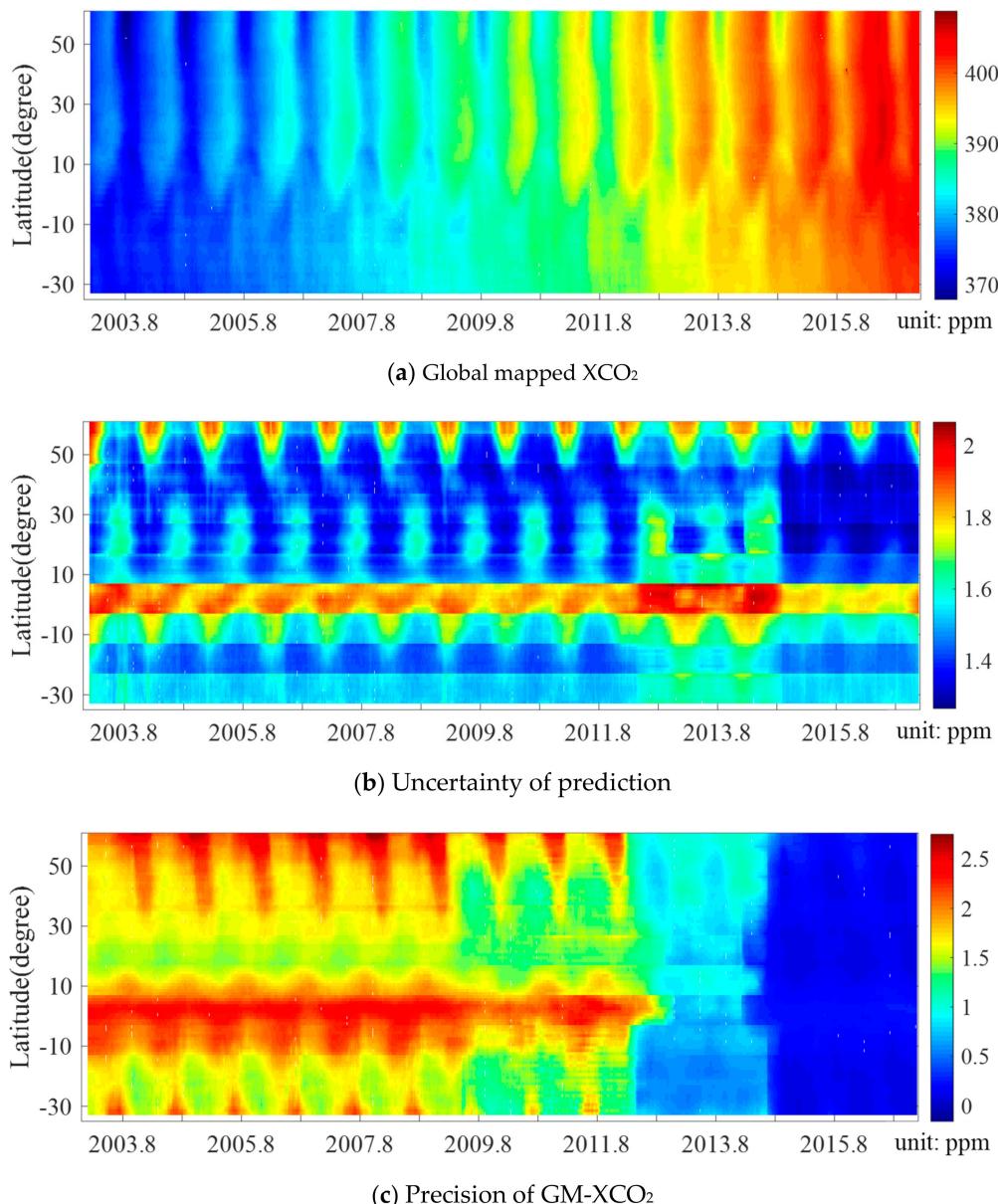
#### 4.2. Globally-Mapped $\text{XCO}_2$

##### 4.2.1. Latitudinal and Temporal Variability of Globally Mapped $\text{XCO}_2$

The latitudinal and temporal variability of globally mapped  $\text{XCO}_2$  (GM- $\text{XCO}_2$ ) and its prediction uncertainty and precision are shown in Figure 5. Comparing Figure 5a to gaps in Figure 4a show missing observations have been reasonably filled. GM- $\text{XCO}_2$  also shows the yearly increase and seasonal variation from 2003 to 2016. GM- $\text{XCO}_2$  is higher in the northern hemisphere compared to the southern hemisphere, and the annual maximum GM- $\text{XCO}_2$  lasts longer in mid-latitudes than high/low latitudes.

In the middle panel, kriging standard deviations (square root of  $\sigma_0^2$  in Equation 17) of the predicted GM- $\text{XCO}_2$  represents the prediction uncertainty, which is determined by the available data around gaps. Higher uncertainty is shown in the tropic and high latitudes because of low numbers of robust observations in these latitudes corresponding to gaps in Figure 4a. The uncertainty also shows seasonal variation for different latitudes. In mid-high latitudes ( $35\text{--}60^\circ\text{N}$ ), the uncertainty is high in winter for the observations affected by snow cover. In mid-low latitudes (extratropics within  $35^\circ\text{N/S}$ ), uncertainty is high in summer likely due to cloud contamination during the monsoon season.

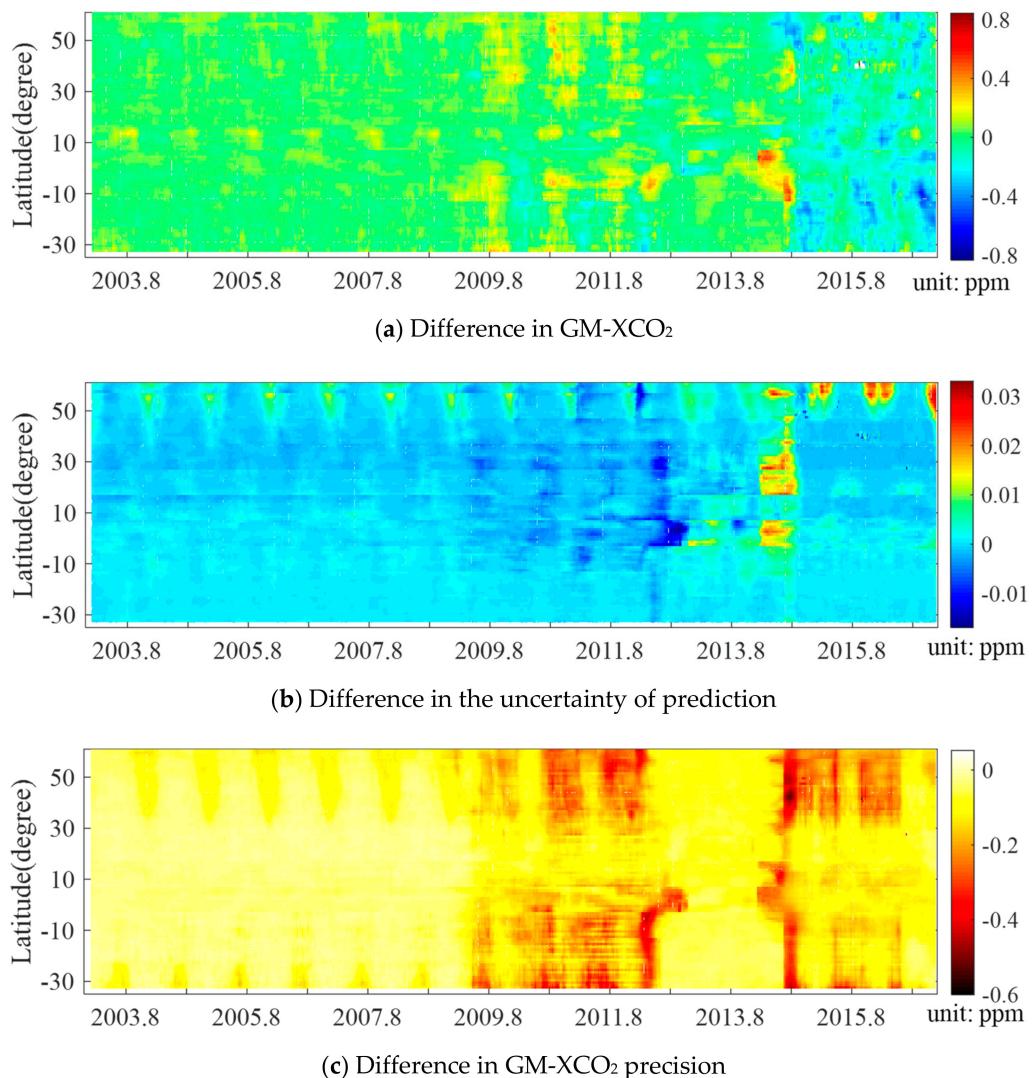
In the bottom panel, GM- $\text{XCO}_2$  precision is calculated from integrated  $\text{XCO}_2$  ( $\text{XCO}_{2\text{int}}$ ) precision. The precision is significantly improved from the middle of 2009 and 2014. It was 1.5 to 2.5 ppm before 2009, 0.5 to 1.5 from 2009 to 2014, and below 0.5 after 2014. That is because of the observing precision improvement of the newer sensors. Generally, the observed GM- $\text{XCO}_2$  precision is better in mid-latitudes.



**Figure 5.** Latitudinal and temporal variability of global mapped XCO<sub>2</sub> (GM-XCO<sub>2</sub>, top panel), the uncertainty of the prediction (standard deviation, middle panel), and precision (bottom panel).

#### 4.2.2. Comparison with Conventional Spatio-Temporal Kriging Results

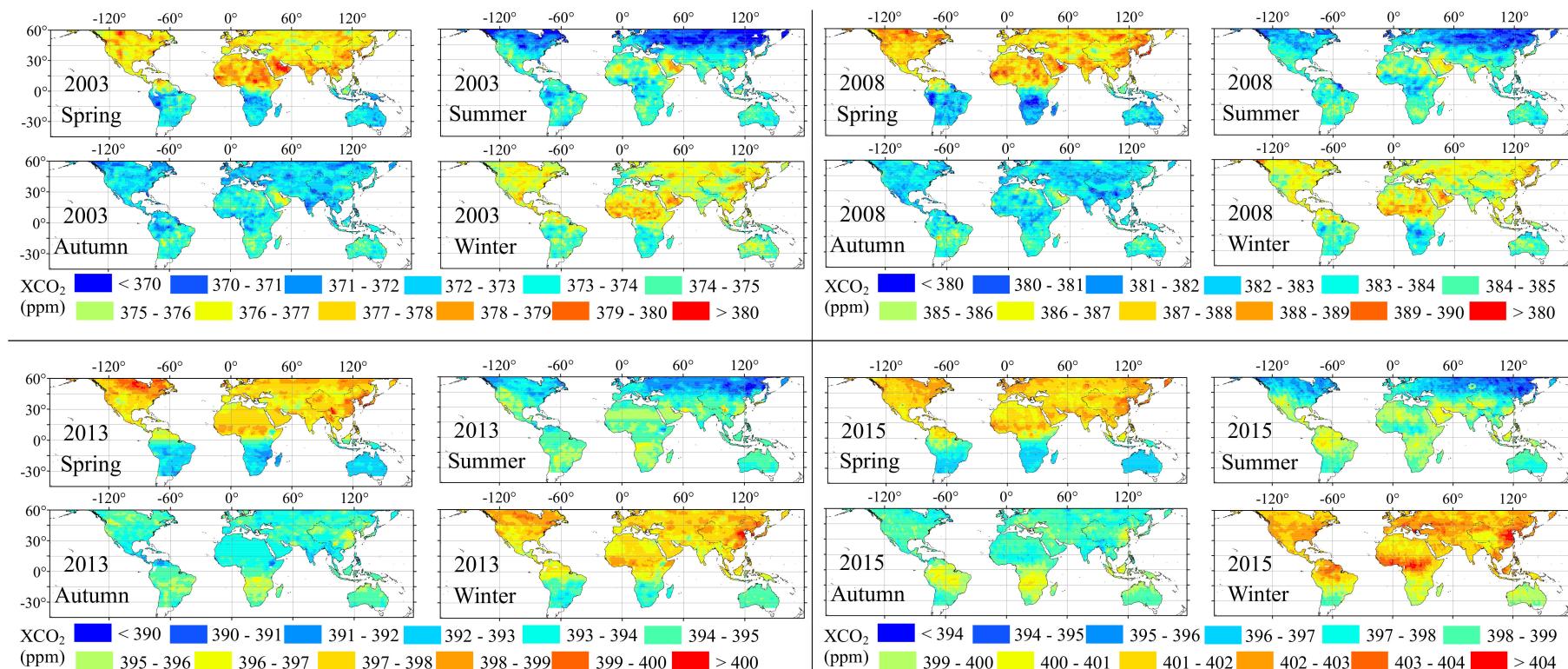
The latitudinal and temporal differences between the results from the precision-weighted (this study) and conventional spatio-temporal kriging methods are shown in Figure 6. Precision (Figure 6c) of GM-XCO<sub>2</sub> from precision weighted spatio-temporal kriging is improved for most of the predictions, especially for the SCIAMACHY and GOSAT overlapping periods (June 2009–March 2012) or GOSAT and OCO-2 overlaps (September 2014–May 2016). The precision improved by 0.3–0.5 ppm over latitudes with overlapping observations. GM-XCO<sub>2</sub> (Figure 6a) is enhanced by 0.1–0.2 ppm for the summer of 2009 to 2011 and reduced by 0.2–0.3 for the summer of 2014 to 2016. Differences in the uncertainty of prediction (Figure 6b) are small for both kriging results (conventional and precision-weighted) because they are based on the same observations (XCO<sub>2,int</sub>), which results in a similar spatio-temporal correlation structure as shown in Figure 3.



**Figure 6.** Latitudinal and temporal difference between results from precision-weighted and conventional spatio-temporal kriging methods for global mapped XCO<sub>2</sub> (GM-XCO<sub>2</sub>, top panel), the difference in the uncertainty of the prediction (standard deviation, middle panel) and the difference in GM-XCO<sub>2</sub> precision (bottom panel). Positive values indicate precision-weighted results are higher and vice versa.

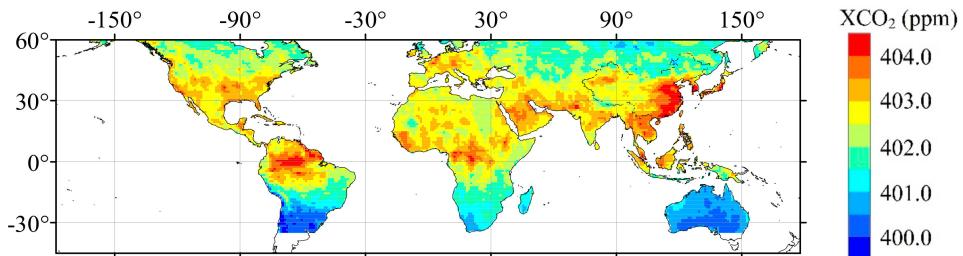
#### 4.2.3. Spatial Distribution of GM-XCO<sub>2</sub>

GM-XCO<sub>2</sub> provides important information about the mean spatial distribution and localized anomalies which could relate to local carbon uptake and emission. We present the spatial-temporal distribution of GM-XCO<sub>2</sub> during different seasons in 2003, 2008, 2013, and 2015 (Figure 7). Seasonal patterns of GM-XCO<sub>2</sub> were similar with an annual increase of approximately around 2.0 ppm. In spring, high GM-XCO<sub>2</sub> appeared in northern Canada, the North China Plain, and the Arabian Peninsula. In summer, extremely low GM-XCO<sub>2</sub> occurred in mid-high latitudes in the northern hemisphere. In autumn, the north-south hemispheric GM-XCO<sub>2</sub> gradient relaxes. In winter, high XCO<sub>2</sub> returns over the North China Plain and Central Africa.



**Figure 7.** Spatial-temporal distribution of mean seasonal globally-mapped XCO<sub>2</sub> (GM-CO<sub>2</sub>) during spring (March, April, May), summer (June, July, August), autumn (September, October, November) and winter (December, January, February) of 2003 (top-left), 2008 (top-right), 2013 (bottom-left), and 2015 (bottom-right). Color bars for different years assume an annual increase of 2 ppm.

In addition, we give out the global spatial distribution of mean XCO<sub>2</sub> in 2016 shown in Figure 8. We can find that the main high XCO<sub>2</sub> of 2016 is distributed in Eastern China, Southeast Asian regions, Amazon forest regions, African forest regions, south of the United States, the Arabian Peninsula, and India. These regions could be related to three main conditions, including (1) an industrial development zone inhabited by human beings; (2) a large area of tropical/subtropical rainforest area; (3) large agricultural regions.

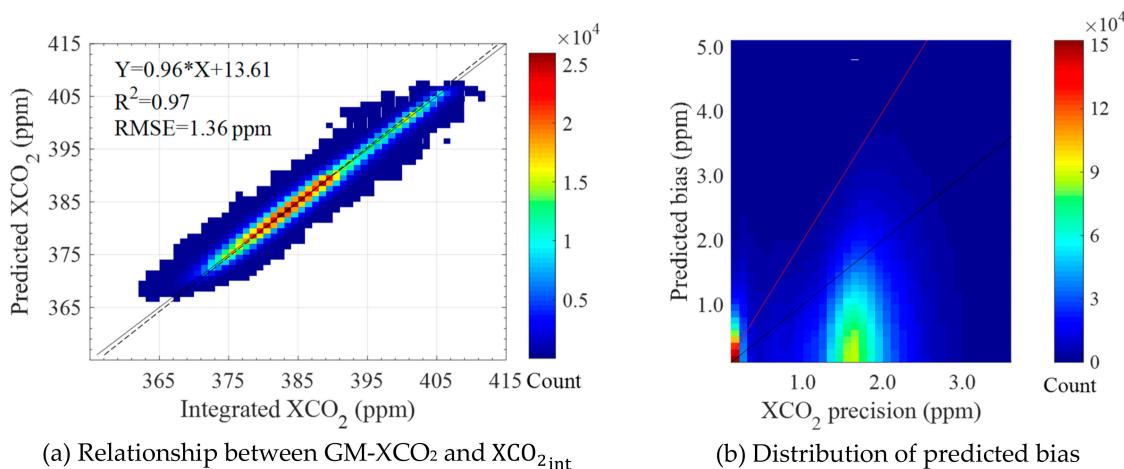


**Figure 8.** Spatial-temporal distribution of mean GM-XCO<sub>2</sub> in 2016.

#### 4.3. GM-XCO<sub>2</sub> Validation

##### 4.3.1. Evaluation Using Cross-Validation

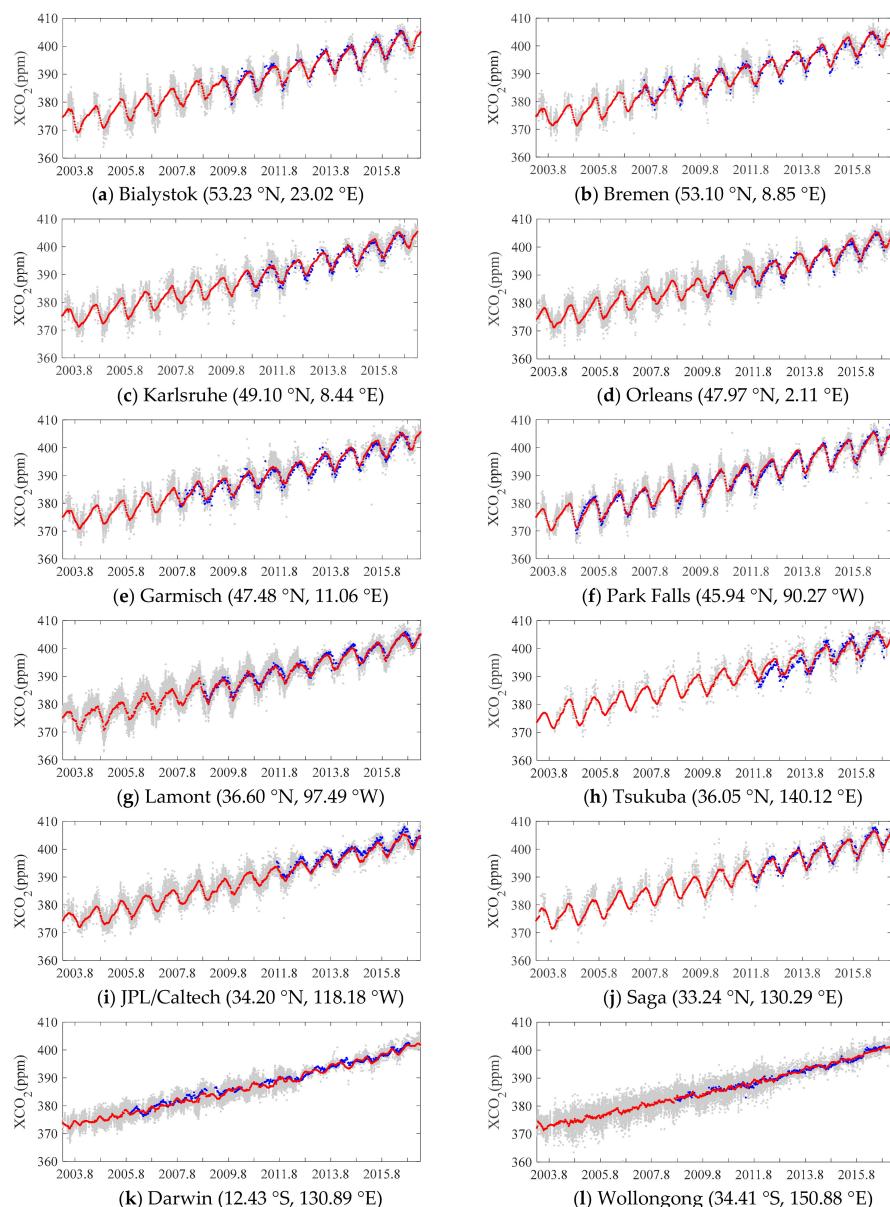
Results of cross-validation using the precision-weighted spatio-temporal kriging method are shown in Figure 9. Predicted XCO<sub>2</sub> (GM-XCO<sub>2</sub>) agreed well with integrated XCO<sub>2</sub> (XCO<sub>2,int</sub>) with a high R<sup>2</sup> of 0.97, showing the interpolation method retains much of the input signal. Total RMSE (root mean square error) between predicted GM-XCO<sub>2</sub> and integrated XCO<sub>2</sub> (XCO<sub>2,int</sub>) is 1.36 ppm, which indicates good stability and the high precision of this method. Most of the predicted bias is within 1.0 ppm, except for some XCO<sub>2</sub> data precision which is larger than 1.5 ppm (right panel). Specifically, 61% of the prediction bias is less than 1.0 ppm. Additionally, 70% and 80% of the predicted bias is within 1 and 2 times of XCO<sub>2</sub> precision, respectively. Results from cross-validation suggest that this mapping method is effective and precise in gap-filling of multi-satellites observed XCO<sub>2</sub>, which could also be affected by original data precision.



**Figure 9.** Results of cross-validation using the precision-weighted spatio-temporal kriging method. The relationship between predicted XCO<sub>2</sub> (GM-XCO<sub>2</sub>) and reserved integrated XCO<sub>2</sub> (XCO<sub>2,int</sub>) is shown in the left panel. The distribution of predicted bias (absolute difference between GM-XCO<sub>2</sub> and reserved XCO<sub>2,int</sub>) and XCO<sub>2,int</sub> precision is shown in the right panel. The black and red lines in the right panel represent the slope of 1 and 2.

#### 4.3.2. Validation of GM-XCO<sub>2</sub> with TCCON Measurements

High accuracy and continuous time series of XCO<sub>2</sub> from TCCON measurements were used for validation of GM-XCO<sub>2</sub> derived from satellite observations. In this study, we selected 12 sites with measurements for more than five years from 2003 to 2016 for comparison with GM-XCO<sub>2</sub>. XCO<sub>2,int</sub> and GM-XCO<sub>2</sub> data within 500 km of each TCCON site was used for this comparison (Figure 10). GM-XCO<sub>2</sub> retained information from satellite observations, which captured the annual increase and seasonal variation of XCO<sub>2</sub> well. The temporal variation of GM-XCO<sub>2</sub> is consistent with TCCON XCO<sub>2</sub>. Comparison statistics between GM-XCO<sub>2</sub> and TCCON XCO<sub>2</sub> are shown in Table 2. If we assume TCCON measurements are accurate, the accuracy of GM-XCO<sub>2</sub> performs well with the total averaged bias of 0.01 ppm across 303 data pairs. The precision of GM-XCO<sub>2</sub> in most TCCON sites (9/12) is within 1.0 ppm with an averaged absolute bias of 0.92 ppm. The mean value of the standard deviation of the bias over 12 sites is 1.05 ppm.



**Figure 10.** Temporal variation comparison of GM-XCO<sub>2</sub> at 12 TCCON sites. Grey, red, and blue points represent XCO<sub>2,int</sub>, GM-XCO<sub>2</sub>, and XCO<sub>2</sub> from TCCON measurements, respectively. XCO<sub>2,int</sub> was retrieved within 500 km of TCCON sites. TCCON measurements from 11:00 to 15:00 local time were selected for comparison.

**Table 2.** Comparison statistics between GM-XCO<sub>2</sub> and TCCON XCO<sub>2</sub>. Bias is calculated using GM-XCO<sub>2</sub> minus TCCON XCO<sub>2</sub> for each coincident data pair and averaged for each site.

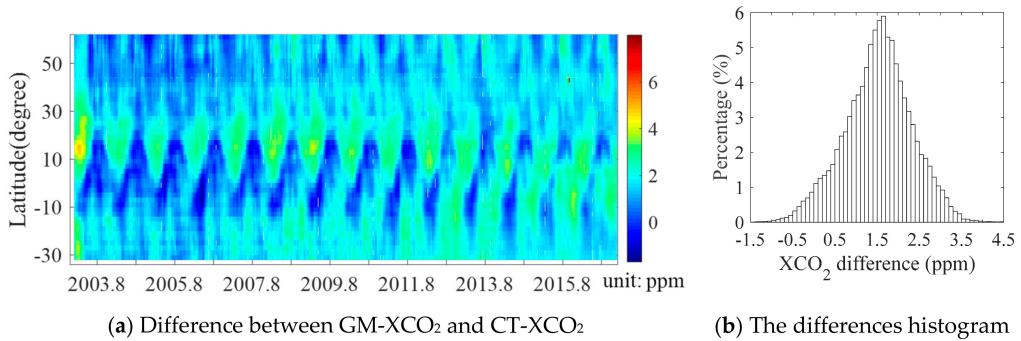
Sites	Location (Latitude, Longitude)	Coincident Data Pairs	Averaged Bias (ppm)	Averaged Absolute Bias (ppm)	Standard Deviation (ppm)
Bialystok	(53.23°N, 23.02°E)	249	-0.19	0.73	0.92
Bremen	(53.10°N, 8.85°E)	260	0.21	0.97	1.25
Karlsruhe	(49.10°N, 8.44°E)	226	0.51	0.90	0.98
Orleans	(47.97°N, 2.11°E)	232	0.34	0.71	0.85
Garmisch	(47.48°N, 11.06°E)	361	0.62	1.05	1.16
Park Falls	(45.94°N, 90.27°W)	499	0.00	0.74	0.96
Lamont	(36.60°N, 97.49°W)	381	-0.45	0.77	0.92
Tsukuba	(36.05°N, 140.12°E)	210	0.73	1.70	1.89
JPL/Caltech	(34.20°N, 118.18°W)	243	-1.06	1.19	0.97
Saga	(33.24°N, 130.29°E)	204	-0.33	0.76	0.91
Darwin	(12.43°S, 130.89°E)	434	-0.47	0.89	1.00
Wollongong	(34.41°S, 150.88°E)	341	0.09	0.58	0.75
Overall	-	303	0.01	0.92	1.05

#### 4.4. Comparison between GM-XCO<sub>2</sub> and CarbonTracker Simulated XCO<sub>2</sub>

GM-XCO<sub>2</sub>, the spatial-temporal continuous XCO<sub>2</sub> from satellite observations, can provide a detailed distribution of XCO<sub>2</sub> over global or regional land areas. In order to explore the advantages and disadvantages of GM-XCO<sub>2</sub>, we present the latitudinal-temporal change comparison between GM-XCO<sub>2</sub> with CT-XCO<sub>2</sub> and their local temporal change comparison in the northern hemisphere.

##### 4.4.1. Comparison with Latitudinal and Temporal Variability of CT-XCO<sub>2</sub>

The latitudinal and temporal variability of the difference between GM-XCO<sub>2</sub> (Figure 5) and CT-XCO<sub>2</sub> (Appendix A: Figure A2) and statistical summary are shown in Figure 11. The mean difference is  $1.53 \pm 0.80$  ppm. XCO<sub>2</sub> difference in the mid-latitudes showed better consistency with the mean value than that in low/high latitudes. The difference in high latitudes is smaller, especially for data before March 2012. In low latitudes, the difference varied with time, with lower values in summer and higher values in winter. The differences decreased with the satellite observations precision improvement from 2009 to 2016.

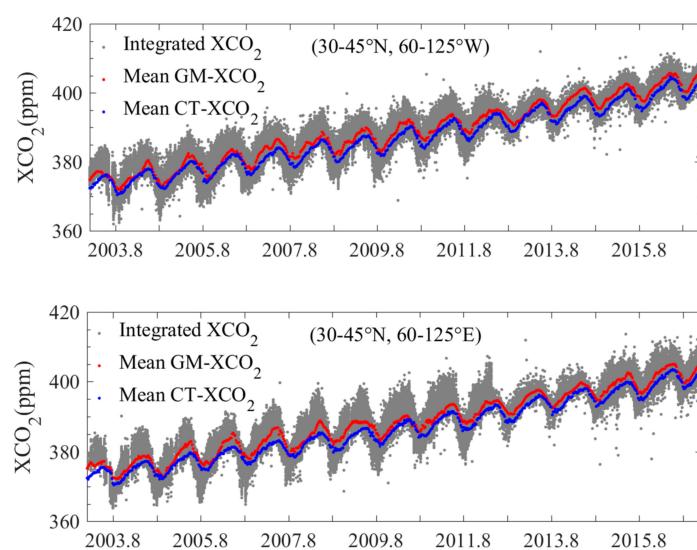


**Figure 11.** Latitudinal and temporal variability of the difference between GM-XCO<sub>2</sub> and CT-XCO<sub>2</sub> (a): GM-XCO<sub>2</sub> minus CT-XCO<sub>2</sub>) and a histogram of the differences (b).

XCO<sub>2</sub> from low/high latitudes, especially for data before March 2012, shows the largest differences between GM-XCO<sub>2</sub> and CT-XCO<sub>2</sub>. The potential reasons for this are: (1) Sparse satellite observation in high/low latitudes limited the accuracy of GM-XCO<sub>2</sub>; (2) Limited precision of XCO<sub>2</sub> from SCIAMCHY contributed to large differences compared to CT-XCO<sub>2</sub>; (3) Lacking or limited surface measurements in low/high latitudes constrained the CT model and affected the simulation of accurate XCO<sub>2</sub>. GM-XCO<sub>2</sub> provided spatial-temporal continuous XCO<sub>2</sub> based on satellite observations that are different from the model simulation.

#### 4.4.2. Temporal Variability of GM-XCO<sub>2</sub> and CT-XCO<sub>2</sub> in Mid-Latitudes

GM-XCO<sub>2</sub> may provide insights into local carbon uptake and emission. We present the temporal variability of XCO<sub>2,int</sub>, GM-XCO<sub>2</sub>, and XCO<sub>2</sub> from CarbonTracker (CT-XCO<sub>2</sub>) from 2003 to 2016 over mid-latitudes of North America and Eastern Asia (Figure 12). Mean GM-XCO<sub>2</sub> kept the original XCO<sub>2</sub> information from the satellites observation by kriging the XCO<sub>2,int</sub>. However, GM-XCO<sub>2</sub> presented sharp changes in XCO<sub>2</sub> during the peak and minimum of XCO<sub>2</sub> in each year, which is not as smooth as that of CT-XCO<sub>2</sub>. In addition, the temporal variability of GM-XCO<sub>2</sub> was more consistent with CT-XCO<sub>2</sub> in Northern America than that of Eastern Asia. That could be attributed to the contribution from more surface measurements to constrain the models. As a result, GM-XCO<sub>2</sub> might provide more information for areas with limited surface measurements, such as China.



**Figure 12.** Temporal variation of XCO<sub>2</sub> from integrated and global mapped results (grey and red points) and CarbonTracker (blue points) over latitude in the range of 30 to 45°N and longitude of 60 to 125°W and 60 to 125°E.

## 5. Discussion

There are some advantages of GM-XCO<sub>2</sub> used in global carbon cycle studies. GM-XCO<sub>2</sub> provided spatial-temporal continuous XCO<sub>2</sub> data from 2003 to 2016 which filled the gaps in observation as shown in Figure 1. It improved the data precision compared with XCO<sub>2</sub> from conventional spatio-temporal kriging, especially for data in the satellites overlapping period. As a result, GM-XCO<sub>2</sub> could help us understand the temporal and spatial changes in the global distribution of CO<sub>2</sub> [17]. Because GM-XCO<sub>2</sub> is from instantaneous satellite observations, it could capture detailed and abnormal XCO<sub>2</sub> change which could be related to local carbon uptake and emission [10,55]. It could also be an important dataset for biosphere-atmosphere interactions by relating its changes to local biosphere parameter variations [7,11]. In addition, we provide XCO<sub>2</sub> precision and interpolation uncertainty for each XCO<sub>2</sub>. Users can select different temporal and spatial segments of GM-XCO<sub>2</sub> data for their specific application. As it was discussed that space-based XCO<sub>2</sub> with precision (no bias) of 2.5 ppm could be used for matching ground-based network and precision within 1.0 ppm, it could help reduce inferred CO<sub>2</sub> flux uncertainties significantly [56]. For anthropogenic CO<sub>2</sub> monitoring, a precision requirement of GM-XCO<sub>2</sub> must be better than 0.7 ppm [57].

However, there are also some challenges that need to be discussed. Prediction of GM-XCO<sub>2</sub> in regions with little observations could have low precision and high interpolation uncertainty. GM-XCO<sub>2</sub> in the tropical rainforest area and the winter in high latitudes should be used carefully as a few observations were limited by observing conditions [58,59]. The interpolation method might not describe the process of atmospheric transport perfectly, especially for regions with a complex climate like the Tibetan area. In addition, GM-XCO<sub>2</sub> over a desert like the Sahara with an influence from high brightness reflection and complex dust for satellite observations inversion should also be used carefully [60].

## 6. Conclusions

In this study, we developed a precision-weighted spatio-temporal kriging interpolation method of multiple satellite observed XCO<sub>2</sub>. It not only used the spatio-temporal variability of XCO<sub>2</sub>, but also the precision of each observation for gap filling. The spatio-temporal correlation structure was optimized and the weighting of XCO<sub>2</sub> with high precision was improved. The precision of predictions improved in most of the grids, especially for the satellites overlapping period (0.3–0.5 ppm). It would be useful for gap-filling of increasing satellite observations not only in XCO<sub>2</sub> but also for other data observed by multiply satellites with different precision.

We also produced a spatial-temporal continuous XCO<sub>2</sub> product, which provides the data precision and interpolation uncertainty of each grid. It is spatio-temporal continuous XCO<sub>2</sub> from satellite observations which could capture the detailed change of XCO<sub>2</sub>. It could be an available dataset for global carbon cycle studies like biosphere-atmosphere interaction.

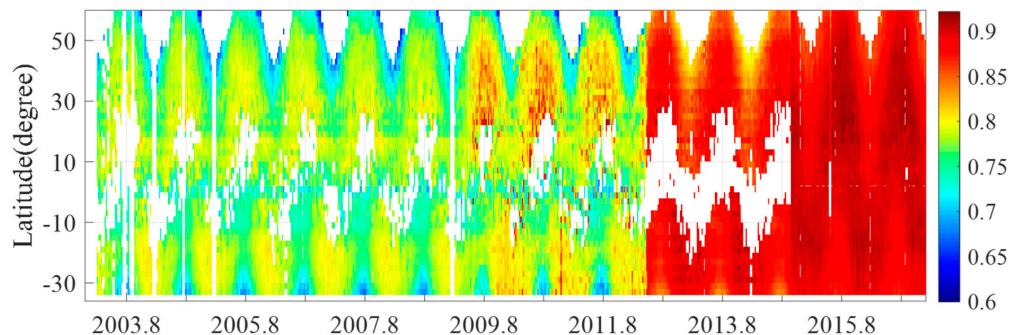
**Author Contributions:** L.L., and Z.H. conceived and designed the experiments; Z.H. performed the experiments; L.R.W., Z.H., and L.L. analyzed the data; C.W., M.S., Y.Z., L.L. and Z.-C.Z. contributed analysis tools; Z.H., and L.R.W. wrote the paper. All authors have read and agreed to the published version of the manuscript.

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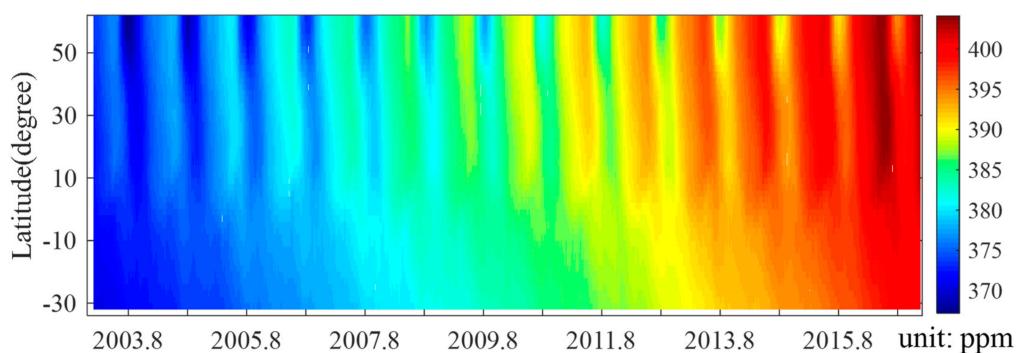
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**Conflicts of Interest:** No conflict.

## Appendix A



**Figure A1.** Latitudinal-temporal change of mean  $\text{XCO}_2$  averaging kernel from SCIAMACHY (January–March 2003), GOSAT (June 2009–May 2014), and OCO-2 (September 2014.09–December 2016).



**Figure A2.** Latitudinal-temporal change of CT- $\text{XCO}_2$  from 2003 to 2016

## Acronyms

Acronyms	Full Names
$\text{XCO}_2$	Column-averaged dry air mole fraction of atmospheric $\text{CO}_2$
$\text{XCO}_{2\text{ret}}$	Original $\text{XCO}_2$ retrievals from satellites
$\text{XCO}_{2\text{adj}}$	Adjusted $\text{XCO}_{2\text{ret}}$
$\text{XCO}_{2\text{con}}$	Converted $\text{XCO}_{2\text{adj}}$
$\text{XCO}_{2\text{int}}$	Integrated combination of $\text{XCO}_{2\text{con}}$
GM- $\text{XCO}_2$	Global mapped $\text{XCO}_2$
ENVISAT	Environmental Satellite
SCIAMACHY	SCanning Imaging Absorption spectrometer for Atmospheric CHartographY
GOSAT	Greenhouse Gases Observing Satellite
OCO-2	Orbiting Carbon Observatory-2
BESD	Bremen Optimal Estimation–DOAS
ACOS	Atmospheric $\text{CO}_2$ Observations from Space
TCCON	The total carbon column observing network
CT	CarbonTracker
$r^2$	the coefficient of determination
RMSE	the root mean square error
ESRL	Earth System Research Laboratory

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