



# A full-coverage daily XCO<sub>2</sub> dataset in China from 2015 to 2020 based on DSC-DF-LGB

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**Abstract.** Carbon dioxide (CO<sub>2</sub>), as a major greenhouse gas, is one of the important causes of global warming. In recent years, the atmospheric CO<sub>2</sub> concentration in China has been increasing year by year. Satellite observation is the main means  
10 of obtaining atmospheric CO<sub>2</sub> concentration. However, the current onboard sensors used for measuring atmospheric CO<sub>2</sub> have a narrow observation range and cannot obtain spatiotemporal continuous atmospheric CO<sub>2</sub> concentrations. Therefore, this paper proposes a daily full-coverage XCO<sub>2</sub> dataset generation method based on the DSC-DF-LGB (Deep Separable  
15 Convolutional Neural Network and Deep Forest concatenated with LightGBM) model to obtain the spatiotemporal distribution of atmospheric CO<sub>2</sub> in China. The DSC-DF-LGB model was established to train the mapping relationship between OCO-2 XCO<sub>2</sub> retrieval and related variables (reanalysis XCO<sub>2</sub>, vegetation parameters, human factors, elevation,  
20 and meteorological parameters). The model was used to generate a daily 0.1° full-coverage XCO<sub>2</sub> dataset for China from 2015 to 2020. The cross validation (CV) result indicates that the model has strong performance in estimating XCO<sub>2</sub>, with R<sup>2</sup> and RMSE of 0.9633 and 0.9761 ppm. The TCCON independent site validation result indicates that the estimated XCO<sub>2</sub> has high consistency with in-situ measurements, with R<sup>2</sup> and RMSE of 0.8786 and 1.5452 ppm. The full-coverage and high-resolution XCO<sub>2</sub> dataset can provide data support for research on carbon sources and sinks. The dataset is available at  
<https://zenodo.org/doi/10.5281/zenodo.12696674> (Huang, 2024).

## 1 Introduction

The increase in the amount of CO<sub>2</sub> is generally considered the main cause of climate change (Kump, 2000). Since the Industrial Revolution, global carbon dioxide concentration has been continuously increasing. At present, the global CO<sub>2</sub>  
25 concentration has increased from 280 ppm in the pre-industrial to 419.31 ppm in 2023 (Lan et al., 2024; Petit and Raynaud, 2020). Under this background, nearly 200 countries and regions signed the Paris Climate Agreement in 2016, making the goal of controlling temperatures by 1.5°C possible (IPCC, 2018; Voigt, 2016). Subsequently, at the 75th United Nations General Assembly, the Chinese government announced that it will strive to peak carbon dioxide emissions before 2030 and achieve carbon neutrality target before 2060. In order to achieve the "dual carbon" target, it is urgent to carry out



30 spatiotemporal continuous CO<sub>2</sub> concentration mapping to understand the spatiotemporal variation pattern of CO<sub>2</sub> concentration in China.

So far, the atmospheric CO<sub>2</sub> concentration mainly measured by in situ stations, aircraft flights and satellite instruments (Yang et al., 2020). However, the spatial distributions of in situ measurements and aerial measurements are sparse, making it impossible to obtain the distribution of CO<sub>2</sub> concentration over a large-scale region (He et al., 2023). Satellite-based observations have made up for this deficiency. Even though satellite-based observations have low temporal resolution, their coverage is wide which makes them the most effective way to measure regional and global atmospheric CO<sub>2</sub> (Mustafa et al., 2021; Wang et al., 2021). Satellite-based observations use near-infrared (NIR) and shortwave infrared (SWIR) spectra to monitor atmospheric CO<sub>2</sub> from space, which can provide high-precision global distribution of CO<sub>2</sub> and help improve our understanding of CO<sub>2</sub> flux (Liu et al., 2018; Yue et al., 2016). The current carbon satellites in orbit mainly include Japanese Greenhouse gases Observing Satellites (GOSAT) (Yoshida et al., 2011), the United States' the Orbiting Carbon Observatory-2 (OCO-2)/Orbiting Carbon Observatory-3 (OCO-3) (Miller et al., 2014), and Chinese Carbon Dioxide Observation Satellite (TanSat) (Ran and Li, 2019). The GOSAT satellite was launched into space by Japan in 2009, which is the first satellite in the world specifically designed to measure the distribution of greenhouse gas concentrations. OCO-2 satellite was launched by NASA in 2014, which is dedicated to monitor carbon dioxide emissions. And Tansat is the first global atmospheric CO<sub>2</sub> observation satellite developed by China, which was successfully launched in 2016. The XCO<sub>2</sub> products retrieved by GOSAT and OCO-2 have been widely used in various studies. These satellites can all provide XCO<sub>2</sub> products. However, due to the presence of clouds and aerosols, and the narrow satellite orbiting tracks, the retrieved atmospheric CO<sub>2</sub> concentration data is not spatially continuous. Besides, the satellites have long revisiting intervals, which results in satellite data not being temporally continuous. The spatiotemporal discontinuity limits our research on regional carbon sources and sinks. Therefore, it is of great significance to map spatiotemporally continuous XCO<sub>2</sub> concentration in China.

At present, three kinds of methods for obtaining spatiotemporal continuous XCO<sub>2</sub> concentration dataset have been developed (He et al., 2022a), which include spatial interpolation (He et al., 2020), chemical transport model simulation (Fu et al., 2019) and multi-source data fusion (Liang et al., 2023; Wang et al., 2023). Spatial interpolation is a geostatistical method. The method cannot consider factors affecting XCO<sub>2</sub> concentration and capture the spatial gradients (Zhang and Liu, 2023). And the generated XCO<sub>2</sub> data through chemical transport model simulation has a low spatial resolution, making it difficult to gather some detailed information (Zhang et al., 2017). In recent years, with the increasing popularity of machine learning, various machine learning models have gradually been applied to multi-source data fusion. Although machine learning lacks interpretability, it can establish relationship models between multiple input variables and output variables. It allows us to train models and estimate atmospheric CO<sub>2</sub> concentrations by combining multiple relevant factors. More and more researches have proven its effectiveness in collaborative fusion of multi-source data. A 500 m spatially continuous normalized microwave reflection index (NMRI) product was obtained by integrating site data with other VWC-related products using Random Forest (RF) (Yuan et al., 2019). Various machine learning methods such as Extremely Randomized Trees (ERT) (Wei et al., 2020), RF (Tang et al., 2023; Yang et al., 2022; Zhao et al., 2019), and Deep Belief Network (DBN)



(Li et al., 2017) have been used to fuse AOD satellite data, meteorological data, and model data, obtaining spatiotemporal continuous PM<sub>2.5</sub> datasets. Besides, the DBN was utilized to downscale the 9 km SMAP SSM and 0.1° ERA5-Land SSM to 1 km (Huang et al., 2022). RF have also been used to plot the global distribution of XCH<sub>4</sub> concentrations, which has a higher accuracy and computing efficiency than the operational full-physics retrieval algorithms (Li et al., 2024). Zhang et al. (2024) generated a 1km high spatial resolution dataset of monthly moisture index collection in China by the light gradient boosting model (LightGBM).

As for CO<sub>2</sub>, various neural networks and ensemble models based on decision tree have been widely used to generate global or regional atmospheric CO<sub>2</sub> concentration datasets. A common means is to use model to establish the relationship between ancillary factors and XCO<sub>2</sub> retrievals, and subsequently estimate full-coverage XCO<sub>2</sub> data (Li et al., 2023). To evaluate the spatial distribution of CO<sub>2</sub> concentration during the growing season in Iran in 2015, the XCO<sub>2</sub> data belonging to OCO-2 and eight environmental variables data were modeled by multi-layer perceptron (MLP) (Siabi et al., 2019). Wang et al. (2022) used RF to generate daily XCO<sub>2</sub> concentrations in the Beijing Tianjin Hebei region from 2015 to 2019. Li et al. (2022) proposed a reconstruction method using ERT to generate a spatiotemporally continuous CO<sub>2</sub> concentration dataset with high-spatiotemporal resolution based on satellite CO<sub>2</sub> retrievals and environmental factors. In addition, the improved ANN and GRWN also achieved good results in generating CO<sub>2</sub> concentration datasets in China (Zhang et al., 2022; Zhang and Liu, 2023).

Based on previous research, the decision tree based ensemble model has been proven to perform well in estimating atmospheric CO<sub>2</sub> concentration (He et al., 2023). Deep Forest (DF) is an advanced ensemble model that has demonstrated efficient performance in multi-source data fusion research in fields such as PM<sub>2.5</sub> (Song et al., 2022a; Song et al., 2022b), CO (Wang et al., 2022), O<sub>3</sub> (Chen et al., 2023), surface soil moisture (Li et al., 2024). Therefore, the DF-LGB model was developed to generate high-precision and spatiotemporal continuous daily XCO<sub>2</sub> datasets with a resolution of 0.1° in China from 2015 to 2020. The concentration of XCO<sub>2</sub> is not only influenced by the local geographical environment, but also closely related to the surrounding carbon sources and sinks (Cui et al., 2024; He et al., 2022b). However, unlike Convolutional Neural Networks (CNN), general machine learning models cannot provide local receptive fields and simulate the impact of the surrounding environment on local CO<sub>2</sub> concentration. To address this problem, DSC is introduced to capture local features of vegetation parameters and anthropogenic factors. In addition, the inverse distance weighting (IDW) was used to preprocess OCO-2 XCO<sub>2</sub> retrievals to optimize the output dataset. After establishing the DSC-DF-LGB model, we conducted 10-fold cross validation (CV) and in situ site validation, and evaluated the ability of this model to generate earlier and latest datasets. Finally, the 0.1°×0.1° daily XCO<sub>2</sub> dataset from 2015 to 2020 was generated, and the spatiotemporal distribution pattern of XCO<sub>2</sub> in China was analyzed using the generated dataset.



## 2 Materials and methods

### 95 2.1 Datasets and preprocessing

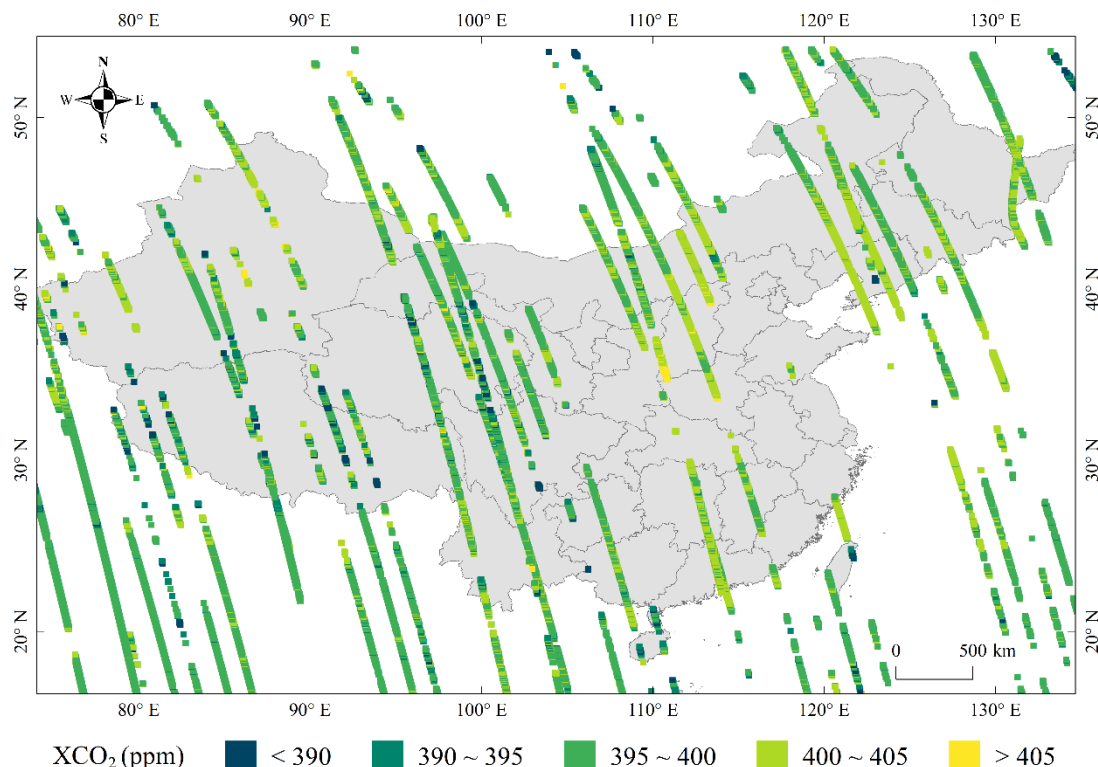
The data used in this study includes satellite XCO<sub>2</sub> data, reanalyzed XCO<sub>2</sub> data, Leaf Area Index (LAI), Fractional Vegetation Coverage (FVC), CO<sub>2</sub> emissions (Emi), population (Pop), Digital Elevation Model (DEM), temperature (T), relative humidity (Rh), surface pressure (Sp), total precipitation (Tp), boundary layer height (Blh), and in situ XCO<sub>2</sub> data from 2015 to 2020. Table 1 summarizes the basic information of these data.

100 **Table 1** Summary of research data

Source	Variable	Spatial resolution	Temporal resolution
OCO-2	XCO <sub>2</sub>	2.25km×1.29km	16-daily
CAMS	XCO <sub>2</sub>	0.75°×0.75°	3-hourly
GLASS	LAI	0.05°×0.05°	8-daily
	FVC		
ODIAC	CO <sub>2</sub> emissions	1km×1km	Monthly
LandScan	Population	1km×1km	Yearly
SRTM15	DEM	500m×500m	\
Era5	Temperature	0.25°×0.25°	Hourly
	Relative humidity		
	Surface pressure		
	Total precipitation		
	Boundary layer height		
TCCON	XCO <sub>2</sub>	\	2min

#### 2.1.1 Satellite XCO<sub>2</sub> retrievals

105 Satellite XCO<sub>2</sub> retrievals were sourced from OCO-2. The OCO mission made the global, space-based measurements of atmospheric CO<sub>2</sub> with the precision, resolution, and coverage needed to characterize CO<sub>2</sub> sources and sinks on regional scales (Crisp et al., 2004). The OCO-2 satellite was launched in July 2014 to measure reflected solar radiation in specific narrow spectral bands in the NIR and SWIR regions with high spectral resolution. Subsequently, the measured spectra are converted into estimated XCO<sub>2</sub> values through various physics-based algorithms and sources of prior information (Taylor et al., 2023). This study selected OCO-2 L2 XCO<sub>2</sub> retrieval from 2015 to 2020 as the data source for the target dataset of the model, which can be accessed at <https://disc.gsfc.nasa.gov>. The data has a spatial resolution of 2.25km × 1.29 km and a revisiting interval of 16 days. Fig. 1 shows the coverage of OCO-2 retrieval in one revisiting interval.



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**Fig. 1.** Spatial distribution of OCO-2 XCO<sub>2</sub> retrievals from January 1 to January 16, 2015 (a revisiting interval) in China.

### 2.1.2 Reanalyzed XCO<sub>2</sub> data

Reanalyzed XCO<sub>2</sub> data was sourced from Copernicus Atmospheric Monitoring Service (CAMS) global greenhouse gas reanalysis (EGG4). European Centre for Medium-Range Weather Forecasts (ECMWF) combines model data with various observations (Such as GOSAT XCO<sub>2</sub> products) using 4D-Var data assimilation method to generate a global CAMS XCO<sub>2</sub> reanalysis dataset (Engelen et al., 2009; Massart et al., 2016). Reanalysis does not require timely release of data, so there is more time to improve data quality. In this study, the CAMS reanalyzed XCO<sub>2</sub> data were collected as the main input data for model with a spatial resolution of 0.75°×0.75° and a temporal resolution of 3 hours. The data can be accessed at <https://ads.atmosphere.copernicus.eu/>.

### 120 2.1.3 Vegetation parameters

Terrestrial vegetation growth is the dominant driver of the seasonality of the concentration of atmospheric CO<sub>2</sub> (Tiwari et al., 2013; Yuan et al., 2018). There is a certain correlation between vegetation growth and seasonal cycle of CO<sub>2</sub> concentration. This study selected LAI and FVC as vegetation parameters to be involved in modeling.

LAI and FVC was obtained from The Global Land Surface Satellite (GLASS) products. GLASS LAI product use



125 generalized regression neural networks (GRNNs) to generate real LAI. This generalized regression neural network combines satellite LAI data and MODIS surface reflectance data (Liang et al., 2021). Considering the low computational efficiency of GRNNs, the multivariate adaptive regression splines (MARS) model was proposed for generating GLASS FVC products from MODIS data (Yang et al., 2016). In this study, the LAI and FVC products has a spatial resolution of  $0.05^{\circ} \times 0.05^{\circ}$  and a temporal resolution of 8 days. The products can be accessed at <http://www.glass.umd.edu/>.

#### 130 **2.1.4 Anthropogenic factors**

There is a close relationship between atmospheric CO<sub>2</sub> concentration and human activities (Fang et al., 2011). To characterize the impact of human activities on atmospheric CO<sub>2</sub> concentration, carbon emissions and population density were added as anthropogenic factors to the input variables of the model.

The Open-source Data Inventory for Anthropogenic CO<sub>2</sub> (ODIAC) is a global high spatial resolution gridded emissions data product that distributes CO<sub>2</sub> emissions from fossil fuel combustion (Oda et al., 2018). ODIAC carbon emissions data product is generated from national emission estimates through spatiotemporal disaggregation. Carbon emission data product was obtained with a spatial resolution of  $1\text{km} \times 1\text{km}$  and a temporal resolution of one month from the ODIAC fossil fuel emission dataset ([https://db.cger.nies.go.jp/dataset/ODIAC/DL\\_odiad2022.html](https://db.cger.nies.go.jp/dataset/ODIAC/DL_odiad2022.html)).

Landscan data is a global population distribution dataset developed by Oak Ridge National Laboratory (ORNL). It is the only global and annually updated population dataset since 2000 which has been widely used in various studies (Calka and Bielecka, 2019). In this study, the population dataset from Landscan had a spatial resolution of  $1\text{km} \times 1\text{km}$  and a temporal resolution of one year, which can be accessed at <https://landscan.ornl.gov/>.

#### **2.1.5 DEM and meteorological parameters**

Due to the higher density of CO<sub>2</sub> compared to air, the concentration of CO<sub>2</sub> is influenced by elevation. And population distribution is closely related to terrain as well. Therefore, in this study, DEM with a spatial resolution of  $500\text{m} \times 500\text{m}$  obtained from SRTM15 was introduced in the model input as a geographic covariate (Tozer et al., 2019).

Besides, it has been proven that meteorological parameters such as precipitation and temperature have a correlation with atmospheric CO<sub>2</sub> concentration (Golkar et al., 2020; Perez et al., 2018; Royer, 2006). The meteorological parameters used in this study were derived from the ERA5 reanalysis dataset, which used the same assimilation scheme as CAMS (Hersbach et al., 2020). These meteorological parameter data include relative humidity, temperature, boundary layer height, surface pressure, and total precipitation, all of which had a spatial resolution of  $0.25^{\circ} \times 0.25^{\circ}$  and a temporal resolution of one hour. Considering that OCO-2 satellite measures XCO<sub>2</sub> at a local overpass time of approximately 13:30, only CAMS and ERA5 reanalysis data with time of 6:00 UTC was used in this study. The meteorological parameters data can be accessed at <https://cds.climate.copernicus.eu/>.



## 155 2.1.6 In situ measurement

TCCON is a global network of ground-based Fourier transform spectrometers with 34 globally dispersed sites, including 27 operational sites, 3 future sites and 4 previous sites. Column abundances of CO<sub>2</sub>, CO, CH<sub>4</sub>, N<sub>2</sub>O and other molecules that absorb in the near-infrared are remotely measured by the network, which can be directly comparable with the near-infrared total column measurements from space-based instruments (Wunch et al., 2011). In this study, the measurements from Hefei  
160 site and Xianghe site was used for model accuracy verification. Table B1 shows the basic information of the sites. And the measurements can be accessed at <https://tccodata.org/>.

## 2.1.7 Data preprocessing

To ensure the reliability of the data, high-quality XCO<sub>2</sub> retrievals were acquired through quality control (xco2\_quality\_flag=0). With the grid center as the interpolated point, IDW was used for XCO<sub>2</sub> retrievals in each grid  
165 (0.1°×0.1°) to obtain the CO<sub>2</sub> concentration representing the grid. As for the input data of the model, XCO<sub>2</sub> reanalysis, LAI, FVC, DEM and five meteorological parameter data from the ERA5 dataset were resampled using bilinear interpolation to a spatial resolution of 0.1°×0.1°. Population data and CO<sub>2</sub> emission data are also aggregated into a spatial resolution of 0.1°×0.1°. We assume that LAI and FVC remain unchanged for 8 days, population remains unchanged for a year, while the monthly CO<sub>2</sub> emission data is evenly distributed to each day in month. In addition, due to OCO-2 satellite measuring XCO<sub>2</sub>  
170 at a local overpass time of approximately 13:30, XCO<sub>2</sub> measurements between 12:00 and 15:00 daily were screened from TCCON in situ measurement for model validation.

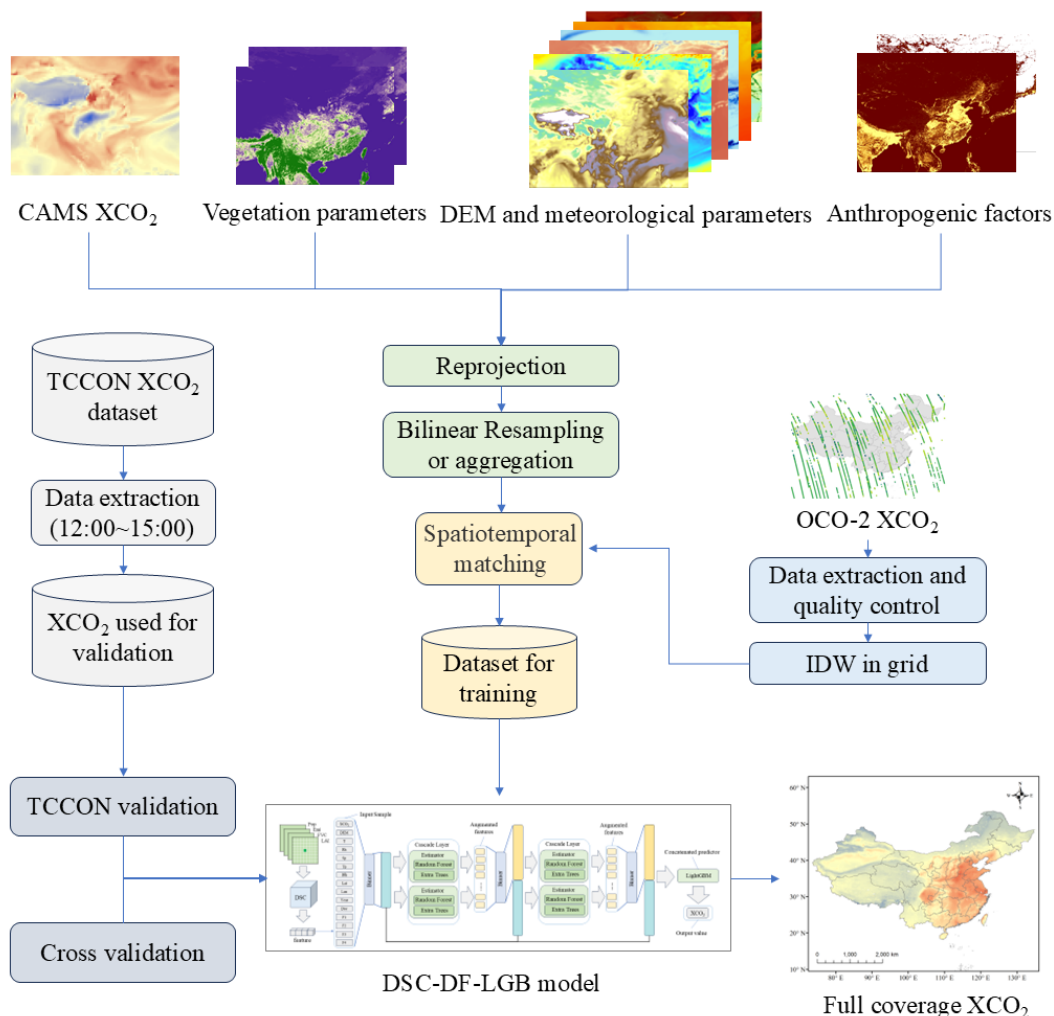
## 2.2 Method

### 2.2.1 The framework for generating XCO<sub>2</sub> dataset

Fig. 2 presents the workflow for generation of atmospheric CO<sub>2</sub> concentration dataset in this study. In order to generate full-  
175 coverage and high-resolution daily XCO<sub>2</sub> in China, CAMS XCO<sub>2</sub> reanalysis, vegetation parameter data, anthropogenic factors data, DEM data, meteorological parameters, and OCO-2 XCO<sub>2</sub> data were collected for DSC-DF-LGB model training, while TCCON data was collected for validation. Then, the input data (i.e. data other than OCO-2 XCO<sub>2</sub> and TCCON) was reprojected and the spatial resolution was adjusted to 0.1°×0.1° using bilinear resampling or aggregation. After that, the OCO-2 XCO<sub>2</sub> data from 2015 to 2020 was extracted and quality control was performed through xco2\_quality\_flag=0. For  
180 OCO-2 XCO<sub>2</sub> located in the same grid (0.1°×0.1°), calculated the XCO<sub>2</sub> value of that grid using IDW. Subsequently, the processed OCO-2 XCO<sub>2</sub> data (target XCO<sub>2</sub>) was spatiotemporally matched with the processed input data to construct a dataset for model training. In addition, XCO<sub>2</sub> measurements from 12:00 to 15:00 at the Hefei and Xianghe TCCON sites were extracted for model accuracy validation. When training the DSC-DF-LGB model, the coefficient of determination (R<sup>2</sup>), mean absolute error (MAE), root mean square error (RMSE), and mean absolute percentage error (MAPE) were used as  
185 evaluation indicators for the model. Firstly, the model estimation performance was assessed based on 10-fold cross



validation and then used the TCCON sites to further verify the accuracy of model estimation. Finally, the trained DSC-DF-LGB model was used to generate full-coverage and high-resolution daily XCO<sub>2</sub> concentration in China from 2015 to 2020.



**Fig. 2.** The workflow for generation of atmospheric CO<sub>2</sub> concentration dataset

## 190 2.2.2 Model description

In this study, DSC-DF-LGB was used to generate atmospheric CO<sub>2</sub> datasets. The model structure is shown in Fig. 3. This model consisted of a Deep Separable Convolutional Neural Network and a deep forest concatenated with LightGBM. Given that each variable is independent, DSC (Fig. A1) is used to capture the local features of each variable instead of CNN. Deep Forest (Zhou and Feng, 2019) had 2 cascaded layers, each with 2 estimators (each estimator includes 1 RF and 1 ERT). The

195 cascaded layers were mainly used to generate augmented features. These augmented features and input variables were fed





together into LightGBM for calculating and outputting estimated  $XCO_2$ . The general form of the estimation model is shown in Eq. (1).

$$estimated\ XCO_{2j} = f_j \left( XCO_{2j}, DEM_j, T_j, RH_j, Sp_j, Tp_j, Blh_j, Lat_j, Lon_j, Year_j, Doy_j, F1_j, F2_j, F3_j, F4_j \right) \quad (1)$$

Where  $j$  is a specific grid, estimated  $XCO_2$  represents the value calculated through DSC-DF-LGB model,  $f_j$  is the function of the DF-LGB model at the grid position, and  $XCO_{2j}$ ,  $DEM_j$ , etc. are the various input features described in the second section. Besides, longitude (Lon), latitude (Lat), year, and day of year (Doy) are added to the input data to represent spatiotemporal information. F1, F2, F3 and F4 represent the feature values extracted by DSC.

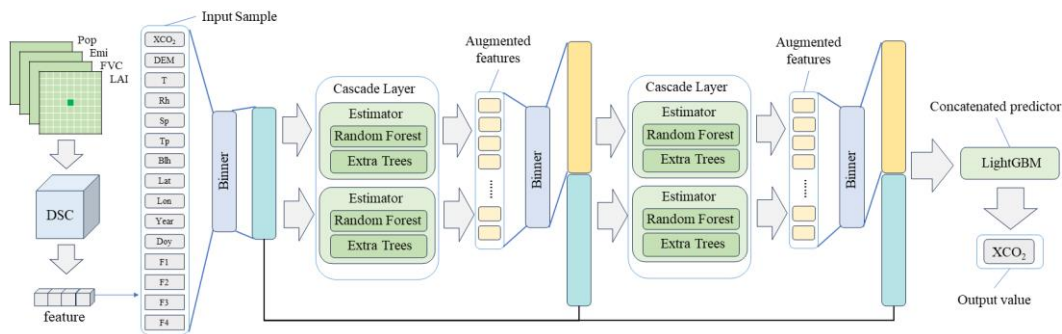


Fig. 3. The structure of the DSC-DF-LGB model.

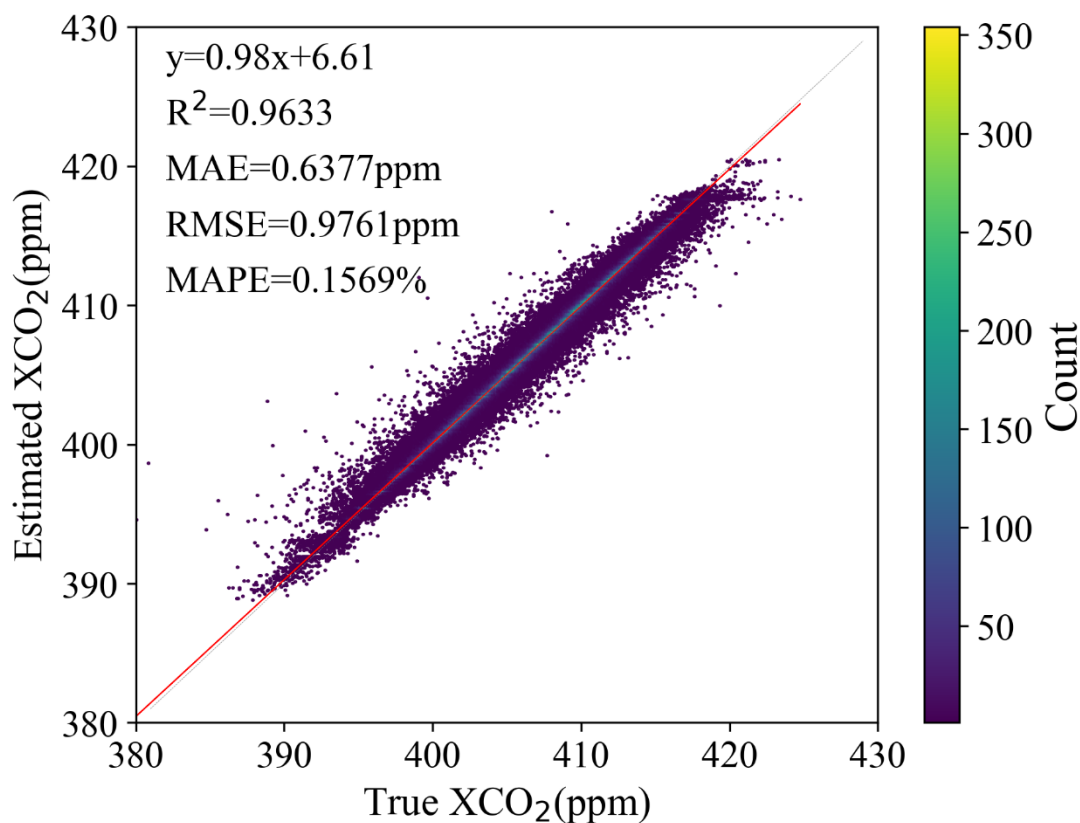
## 205 3 Results and Discussions

### 3.1 Model performance evaluation

Firstly, the overall performance of the DSC-DF-LGB model was evaluated based on 10-fold CV. Fig. 4 reveals the estimation performance of the model through comparison between  $XCO_2$  estimated by model and true  $XCO_2$ . The CV result showed that  $R^2$  reached 0.9633, while MAE, RMSE, and MAPE were as low as 0.6377, 0.9761, and 0.1569%, indicating that DSC-DF-LGB has excellent estimation performance. However, when estimating  $XCO_2$ , there is a tendency to overestimate low values and underestimate high values. This is due to the robustness of the model itself, which can identify and suppress numerical anomalies. Next, TCCON measurements were used for independent data validation of the model. Fig. 5 illustrates the validation result of  $XCO_2$  estimated by DSC-DF-LGB, and compares the result with CAMS  $XCO_2$  and OCO-2  $XCO_2$ . The estimated  $XCO_2$  have high consistency with TCCON, and the  $R^2$ , MAE, RMSE, and MAPE are 0.8786, 1.1956 ppm, 1.5452 ppm, and 0.2910%, respectively. Compared with the validation results of CAMS  $XCO_2$  with  $R^2$  and RMSE of 0.7005, 2.4267 ppm, the estimated  $XCO_2$  accuracy has been significantly improved. Surprisingly, the estimated  $XCO_2$  accuracy is also higher than OCO-2  $XCO_2$ . due to the small amount of OCO-2  $XCO_2$  used for validation and most of the data being located in Xianghe. Table 2 presents the validation results for estimating  $XCO_2$ , CAMS  $XCO_2$ , and OCO-2  $XCO_2$  at each site. At both sites, the validation results for estimating  $XCO_2$  were superior to CAMS  $XCO_2$ . At the Xianghe site, the validation results of CAMS  $XCO_2$  and OCO-2  $XCO_2$  were not satisfactory, with  $R^2$  less than 0.5. On the contrary,

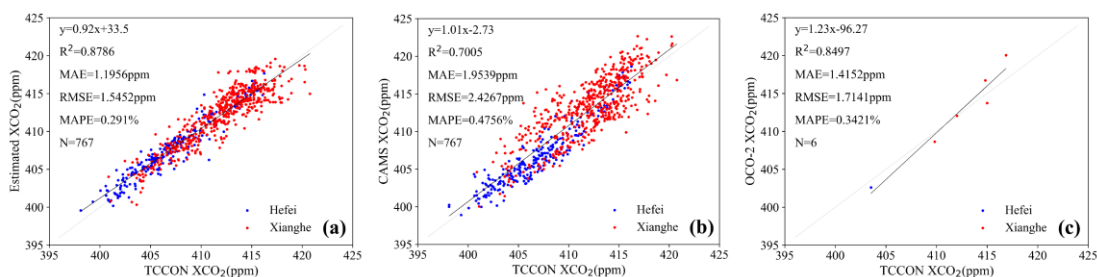


the estimated XCO<sub>2</sub> at Xianghe site showed quite good validation results, with R<sup>2</sup> close to 0.8. This excellent validation result demonstrates the strong spatial generalization ability of the model and further proved the feasibility of generating full-coverage and high spatiotemporal resolution XCO<sub>2</sub> data through the DSC-DF-LGB model.



225

**Fig. 4.** Comparison between XCO<sub>2</sub> estimated by DSC-DF-LGB model and true XCO<sub>2</sub>



**Fig. 5.** Comparison of TCCON sites verification results. (a)-(c) represent the validation results of the estimated XCO<sub>2</sub>, CAMS XCO<sub>2</sub>, and OCO-2 XCO<sub>2</sub>

230



**Table 2** Verification accuracy for each TCCON site

Data source	Hefei				Xianghe			
	R <sup>2</sup>	MAE (ppm)	RMSE (ppm)	MAPE (%)	R <sup>2</sup>	MAE (ppm)	RMSE (ppm)	MAPE (%)
Estimated XCO <sub>2</sub>	0.9092	0.9881	1.2137	0.2429	0.7949	1.2941	1.6799	0.3138
CAMS XCO <sub>2</sub>	0.8793	1.0833	1.3993	0.2659	0.4364	2.3674	2.7849	0.5752
OCO-2 XCO <sub>2</sub>	\	0.9257	0.9257	0.2294	0.4573	1.5131	1.8315	0.3647

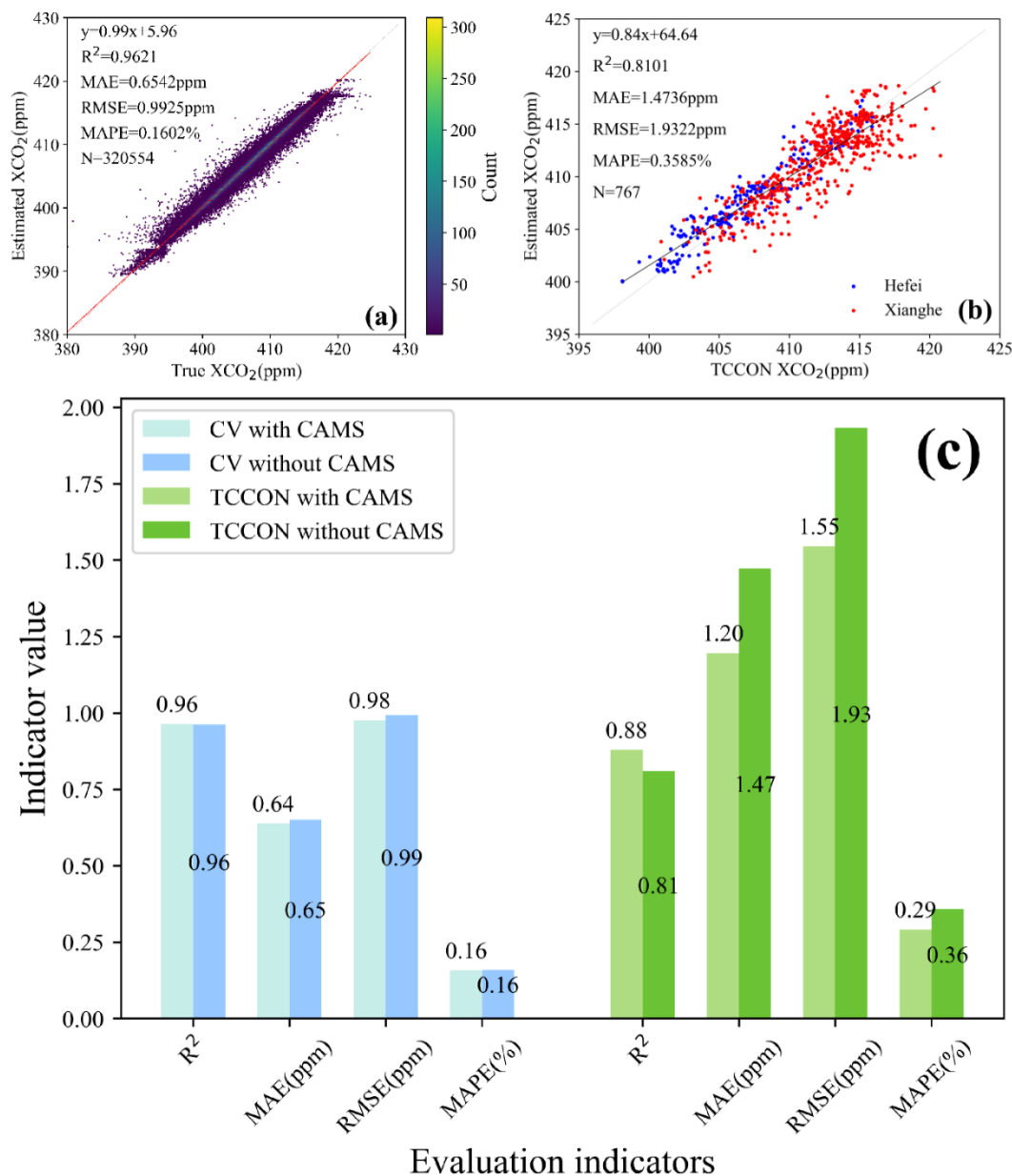
### 3.2 The ability of the model to generate earlier and later datasets

Due to the limitation of OCO-2 XCO<sub>2</sub> retrievals, DSC-DF-LGB model can only train data after 2015. In order to understand the model's ability to estimate past XCO<sub>2</sub>, only data from 2016 to 2020 was used for model training, and 10-fold CV was used to evaluate model performance. Then the generalization of the model was tested using dataset in 2015 as an independent test set. As shown in Table 3, the CV result was good, with R<sup>2</sup>, MAE, RMSE, and MAPE of 0.9478, 0.6395 ppm, 0.9798 ppm, and 0.1568%, respectively. However, during independent dataset testing, there is no linear relationship between input and output data, with an R<sup>2</sup> of -0.1767. It indicates that the model has weak temporal generalization ability and cannot estimate past XCO<sub>2</sub>. This is mainly due to the inherent shortcomings of decision tree based models and their inability to capture the trend of XCO<sub>2</sub> in 2015 without training.

**Table 3** Model validation results for estimating past XCO<sub>2</sub>

Verification method	R <sup>2</sup>	MAE (ppm)	RMSE (ppm)	MAPE (%)
CV	0.9478	0.6395	0.9798	0.1568
Independent dataset testing	-0.1767	2.5324	2.8644	0.6352

Actually, most variables have data from 2020 onwards, but the time range of the generated XCO<sub>2</sub> dataset is limited by CAMS to 2020. Therefore, we attempted to remove CAMS variables and use the remained ones to train the DSC-DF-LGB model. Similar to section 3.1, CV and independent site validation are used to evaluate model performance. As shown in Fig. 6, the model performed well in cross validation, with R<sup>2</sup>, MAE, RMSE, and MAPE values of 0.9621, 0.6542 ppm, 0.9925 ppm, and 0.1602%, respectively. However, the model demonstrated poor performance in independent site validation, with R<sup>2</sup>, MAE, RMSE, and MAPE of 0.8101, 1.4736 ppm, 1.9322 ppm, and 0.3585%, respectively. Compared with the model trained on datasets with CAMS, there is only a slight loss of accuracy in CV, while estimation accuracy decreased in independent site validation, with RMSE increasing from 1.55 ppm to 1.93 ppm. In addition, if data from 2020 onwards is added for training model, it may improve estimation accuracy to an extent. Therefore, it is feasible to generate later XCO<sub>2</sub> datasets by DSC-DF-LGB model trained on datasets without CAMS, but the estimation accuracy will inevitably decrease.



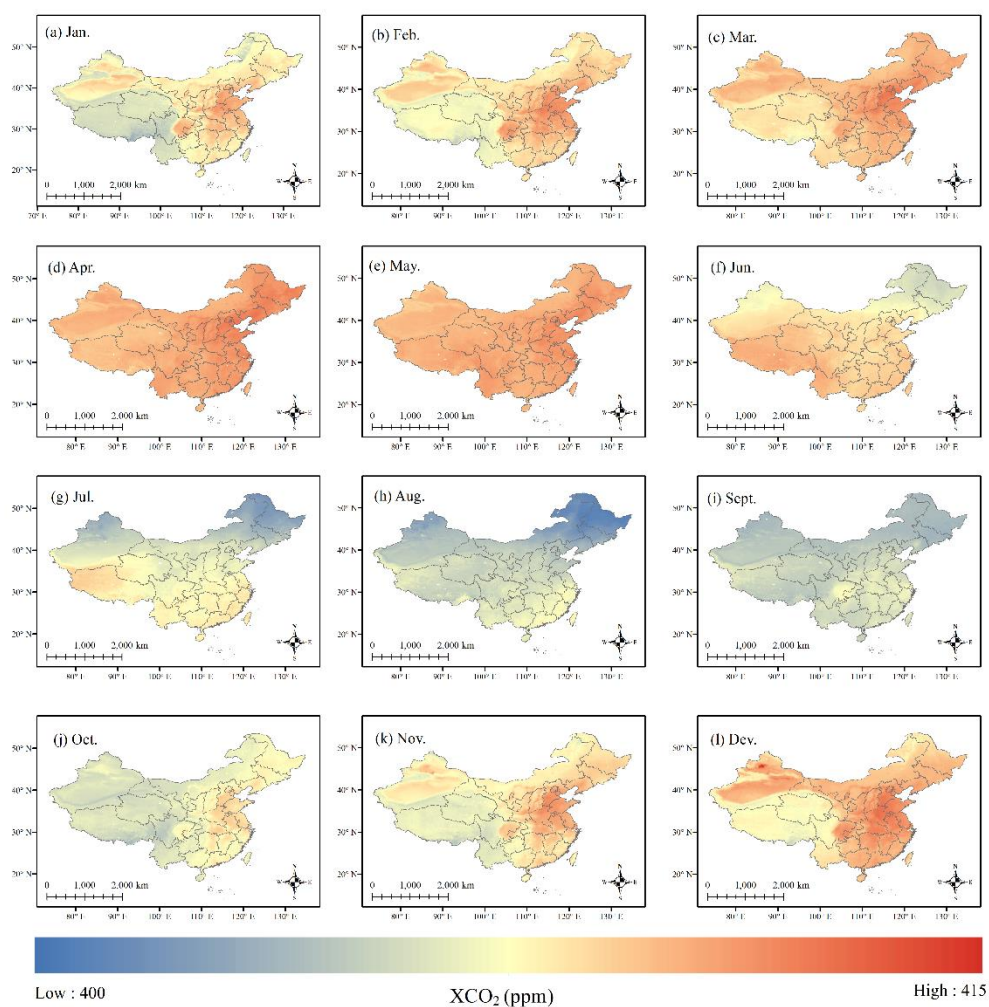
**Fig. 6.** Performance evaluation of DSC-DF-LGB models trained on datasets without CAMS. (a) shows the CV validation result of the model, (b) represents the TCCON independent site validation result, and (c) demonstrates the comparison results with the model trained on datasets with CAMS.

### 3.3 The spatiotemporal distribution of XCO<sub>2</sub> in China

Fig.7 shows the spatial distribution of monthly average XCO<sub>2</sub> in 2018. The seasonal variation of atmospheric CO<sub>2</sub>



concentration in China is significant. The atmospheric CO<sub>2</sub> concentration is higher in spring (from March to May), with the  
260 highest CO<sub>2</sub> concentration occurring in April. Subsequently, the atmospheric CO<sub>2</sub> concentration began to decrease and  
reached its lowest point in August. And from August to April of the following year, the atmospheric CO<sub>2</sub> concentration  
continued to rise again. The seasonal variation of atmospheric CO<sub>2</sub> is mainly caused by the growth and death of vegetation.  
Vegetation undergoes vigorous photosynthesis in summer, absorbing a large amount of CO<sub>2</sub> from the atmosphere. In the  
autumn and winter seasons, when vegetation dies and decomposes, CO<sub>2</sub> is released into the air (Tiwari et al., 2013). In  
265 addition, the atmospheric CO<sub>2</sub> concentration in Northeast China was lower in July and August, which is related to the strong  
carbon sequestration ability of black soil (Liu et al., 2019).

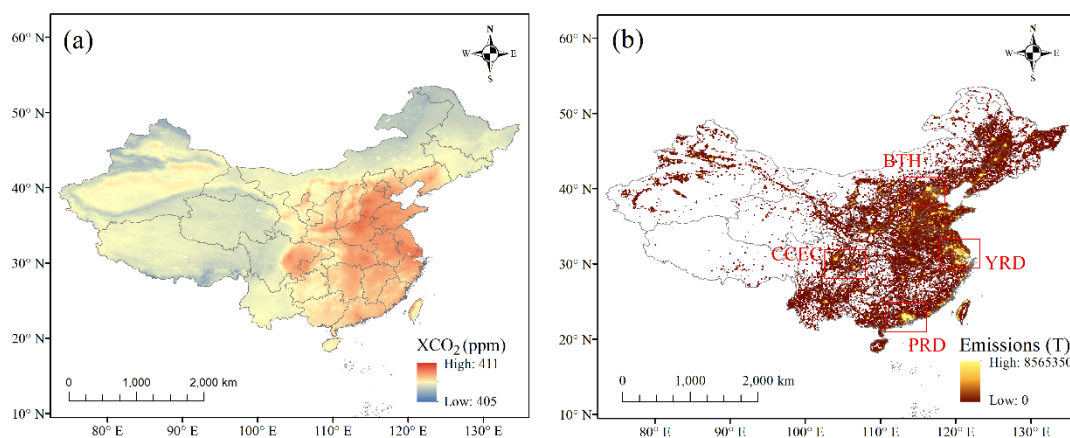


**Fig. 7.** Monthly average XCO<sub>2</sub> in China in 2018. (a)-(l) show the spatial distribution of XCO<sub>2</sub> from January to December.

Fig. 8 shows the spatial distribution of annual average XCO<sub>2</sub> in 2018, which is compared to carbon emissions. The  
270 atmospheric CO<sub>2</sub> concentration exhibits significant spatial heterogeneity. The CO<sub>2</sub> concentration in the eastern coastal areas  
is significantly higher than that in the western regions. This distribution pattern is basically consistent with that of carbon



emissions, indicating an inseparable relationship between excessive carbon emissions and the increase in atmospheric CO<sub>2</sub> concentration. Excessive carbon emissions have led to higher atmospheric CO<sub>2</sub> concentrations, especially in the Beijing Tianjin Hebei (BTH), Yangtze River Delta (YRD), and Pearl River Delta (PRD) regions where industry is developed. Besides, the significant carbon emissions from the Chengdu Chongqing Economic Circle (CCEC) have also led to higher atmospheric CO<sub>2</sub> concentrations in the region compared to surrounding cities. This indicates that the concentration of atmospheric CO<sub>2</sub> is significantly influenced by human activities.



**Fig. 8.** Comparison of Annual Average XCO<sub>2</sub> and Total Carbon Emissions in 2018. (a) represents the spatial distribution of average XCO<sub>2</sub> in 2018, (b) represents the spatial distribution of carbon emissions in 2018.

Subsequently, the annual average XCO<sub>2</sub> in China from 2015 to 2020 was calculated. As shown in Fig. 9, the annual average XCO<sub>2</sub> in China has increased from 400.11 ppm in 2015 to 413.04 ppm in 2020. The annual average growth is 2.59 ppm/yr, manifesting an overall downward trend. Except for the annual average XCO<sub>2</sub> growth of 3.25 ppm in 2016, the growth in all other years is below 3 ppm. This indicates the tremendous efforts made by the Chinese government to limit global climate change after signing the Paris Agreement.

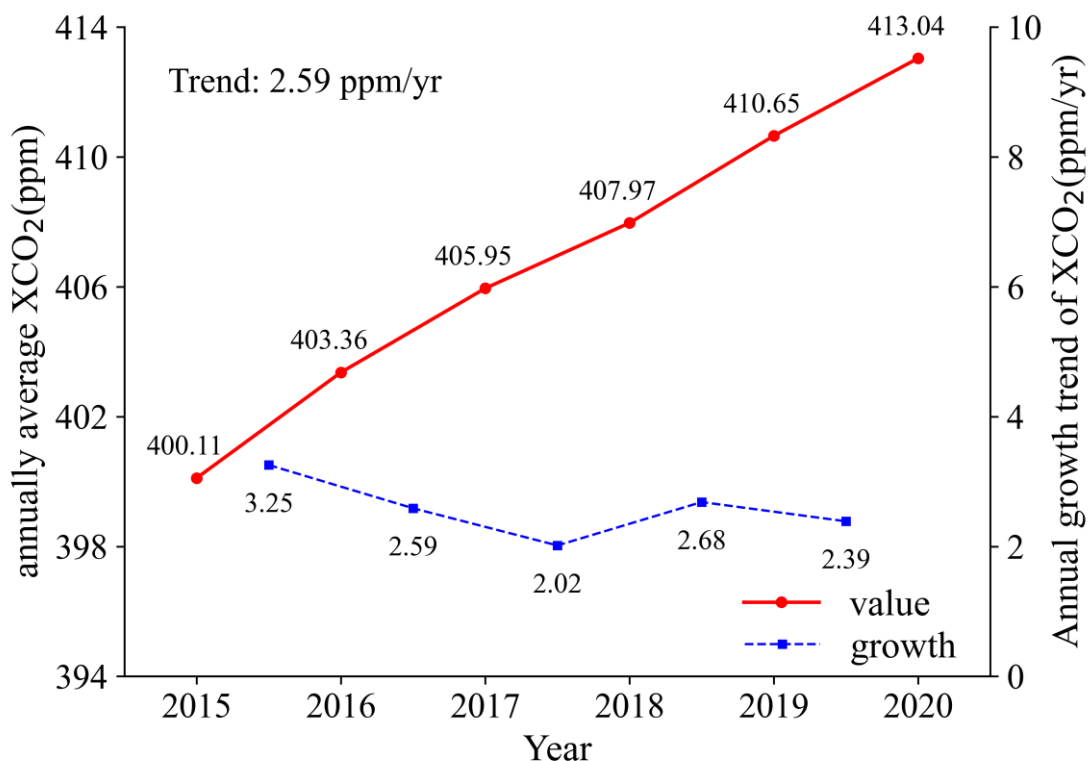


Fig. 9. Annual average XCO<sub>2</sub> and annual growth in China from 2015 to 2020.

#### 4 Code and Data availability

The full-coverage 0.1° daily XCO<sub>2</sub> dataset and the code are available at <https://zenodo.org/doi/10.5281/zenodo.12696674> (Huang, 2024).

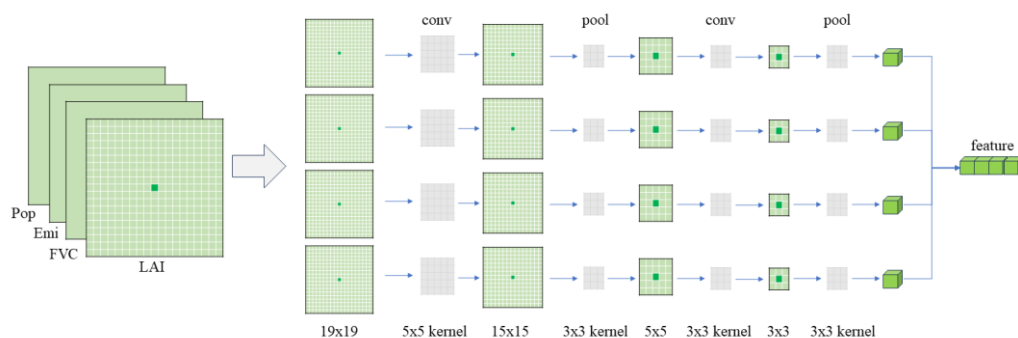
#### 5 Conclusion

This study generated a daily full-coverage XCO<sub>2</sub> dataset based on DSC-DF-LGB. By calculating, monthly and annual average XCO<sub>2</sub> datasets can be also generated. Compared to CAMS reanalysis, the generated XCO<sub>2</sub> dataset has higher spatial resolution and data accuracy. However, although the model has strong spatial generalization, its temporal generalization is poor, making it unable to generate earlier or later XCO<sub>2</sub> datasets. Subsequently, an in-depth analysis was conducted on the spatiotemporal distribution of XCO<sub>2</sub> in China. The results show that the XCO<sub>2</sub> concentration is highest in April and lowest in August, demonstrating a clear seasonal cycle, mainly due to the growth and death of vegetation; The spatial distribution of XCO<sub>2</sub> is consistent with that of carbon emissions, with higher CO<sub>2</sub> concentrations in the BTH, YRD, PRD and CCEC in China, which indicates that the spatial distribution of XCO<sub>2</sub> is significantly influenced by human activities; The XCO<sub>2</sub> is



300 increasing year by year, but its growth is gradually slowing down. This dataset generated in this study can be further used for  
 related research on carbon sources and sinks.

## Appendix A



305 **Fig. A1.** The structure of DSC. The window size is 19x19. And features are extracted through two convolutional layers and average pooling layer.

## Appendix B

**Table B1** TCCON site information

ID	Name	Longitude	Latitude	Data range
1	Hefei	117.17	31.90	2015.11~2022.12
2	Xianghe	116.96	39.80	2018.06~2023.02

### Author contributions

310 Conceptualization: HY and XH; methodology: XH and HF; validation: XH, QL and LC; Investigation: YQ, YY and XH;  
 writing – original draft preparation: XH; writing – review and editing: HY, GF and XH; funding acquisition: HY.

### Competing interests

The authors declare that they have no conflict of interest.

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The OCO-2 XCO<sub>2</sub> retrievals used in this study were produced by the OCO-2 project at the Jet Propulsion Laboratory, California Institute of Technology, and obtained from the OCO-2 data archive maintained at the NASA Goddard Earth Science Data and Information Services Center.

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