Supplementary Materials

Text S1. Details of Air-Transformer

In each validation round, we evaluated model performance by comparing original OCO-2 retrievals against model estimates using three key indicators: the coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE) (Equations (S1)–(S3)). These metrics quantify the deviation between predictions and observations, thereby offering a robust benchmark for the model's accuracy.

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{\sum_{i=1}^{n} (\hat{y}_i - \bar{\hat{y}}_i)^2} \tag{S1}$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2} \tag{S2}$$

$$MAE = \frac{1}{n} \sum_{i=1}^{n} | \hat{y}_i - y_i | \tag{S3}$$

where $\hat{y}_i$ and y_i are the observed and predicted values for the i-th sample respectively, $\bar{\hat{y}}$ is observed mean values, and n is the total number of samples.

Table S1. Comparison of Air-Transformer models with mainstream machine learning and neural network models

Validation mode	Model	R^2 ↑	RMSE ↓
Sample 10-fold	Air-Transformer	**0.9831**	**0.6843**
	Resnet	0.9720	0.8581
	Random Forest	0.9516	1.1453
	LightGBM	0.9409	1.1277
Temporal 10-fold	Air-Transformer	**0.9452**	**1.2197**
	Resnet	0.9293	1.3244
	Random Forest	0.9105	1.6975
	LightGBM	0.9078	1.8324
Spatial 10-fold	Air-Transformer	**0.9493**	**1.1496**
	Resnet	0.9428	1.2229
	Random Forest	0.9367	1.2837
	LightGBM	0.9230	1.3646

Table S2. Results of STL decomposition.

Regions	Trend strength	Seasonal strength	Residual strength
China	0.892	0.205	0.001
NE	0.730	0.340	0.003
SC	0.901	0.211	0.003
EC	0.870	0.243	0.002
NC	0.799	0.287	0.002
NW	0.916	0.173	0.002
SW	0.935	0.164	0.002

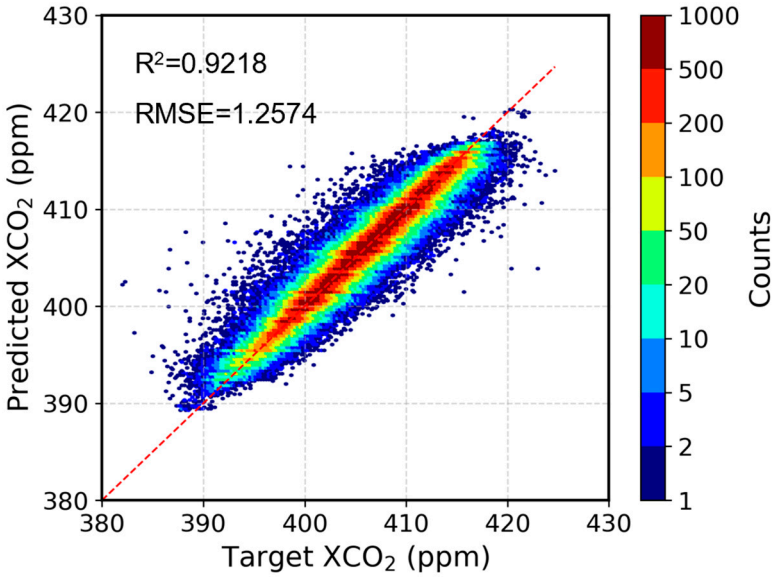


Figure S1. Fitting effect of the LightGBM surrogate model

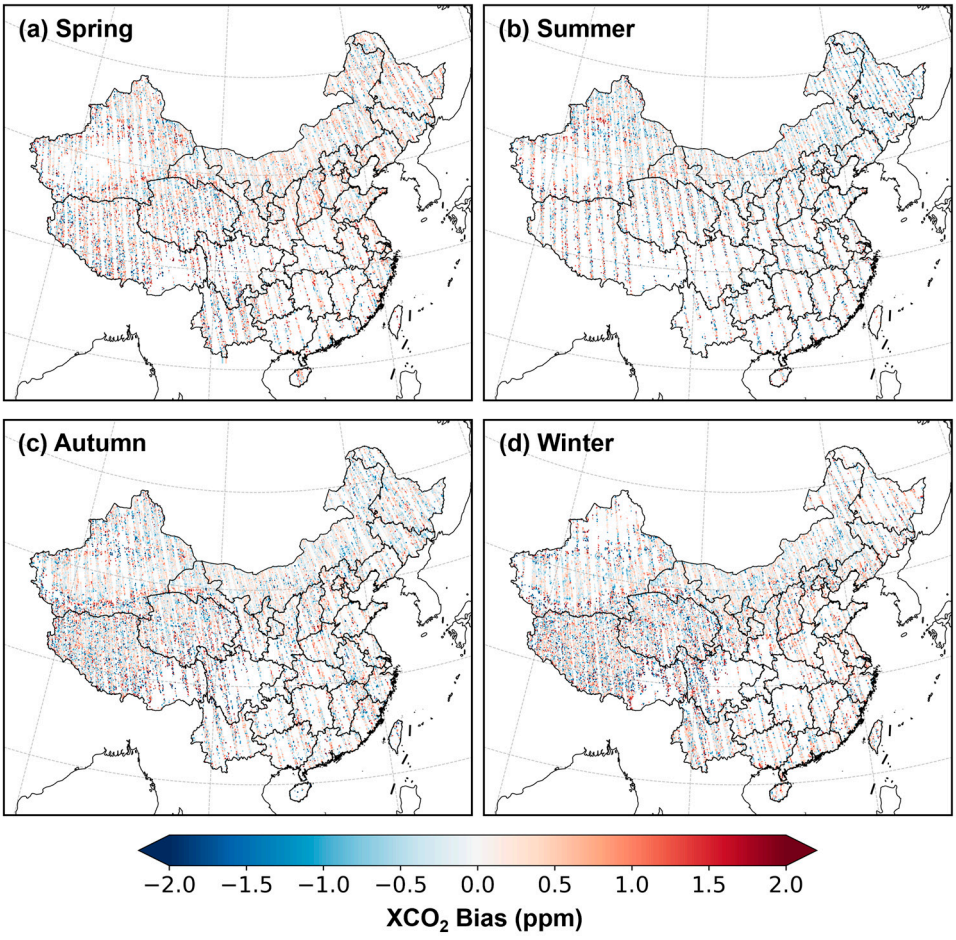


Figure S2. Spatial bias between model output and satellite data in four seasons

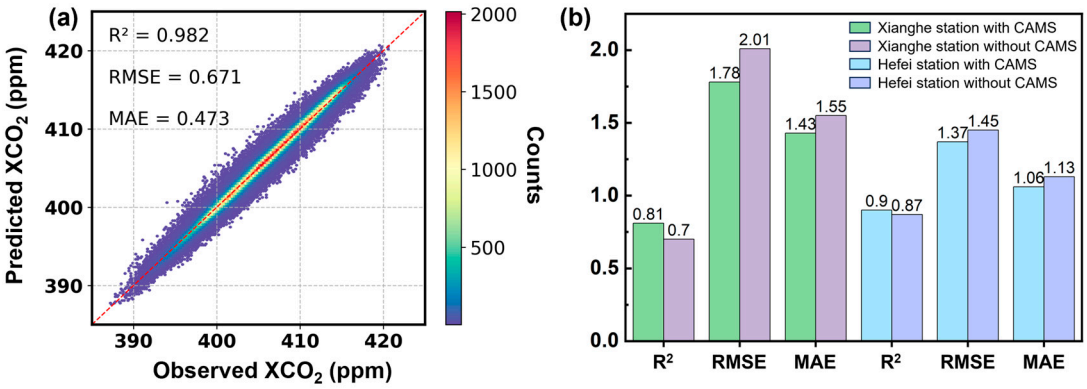


Figure S3. Model performance validation and sensitivity analysis regarding CAMS input. (a) Comparison between daily OCO-2 observations and model predictions without CAMS. (b) TCCON-based performance evaluation at Xianghe and Hefei stations. Units: RMSE (ppm), MAE (ppm).

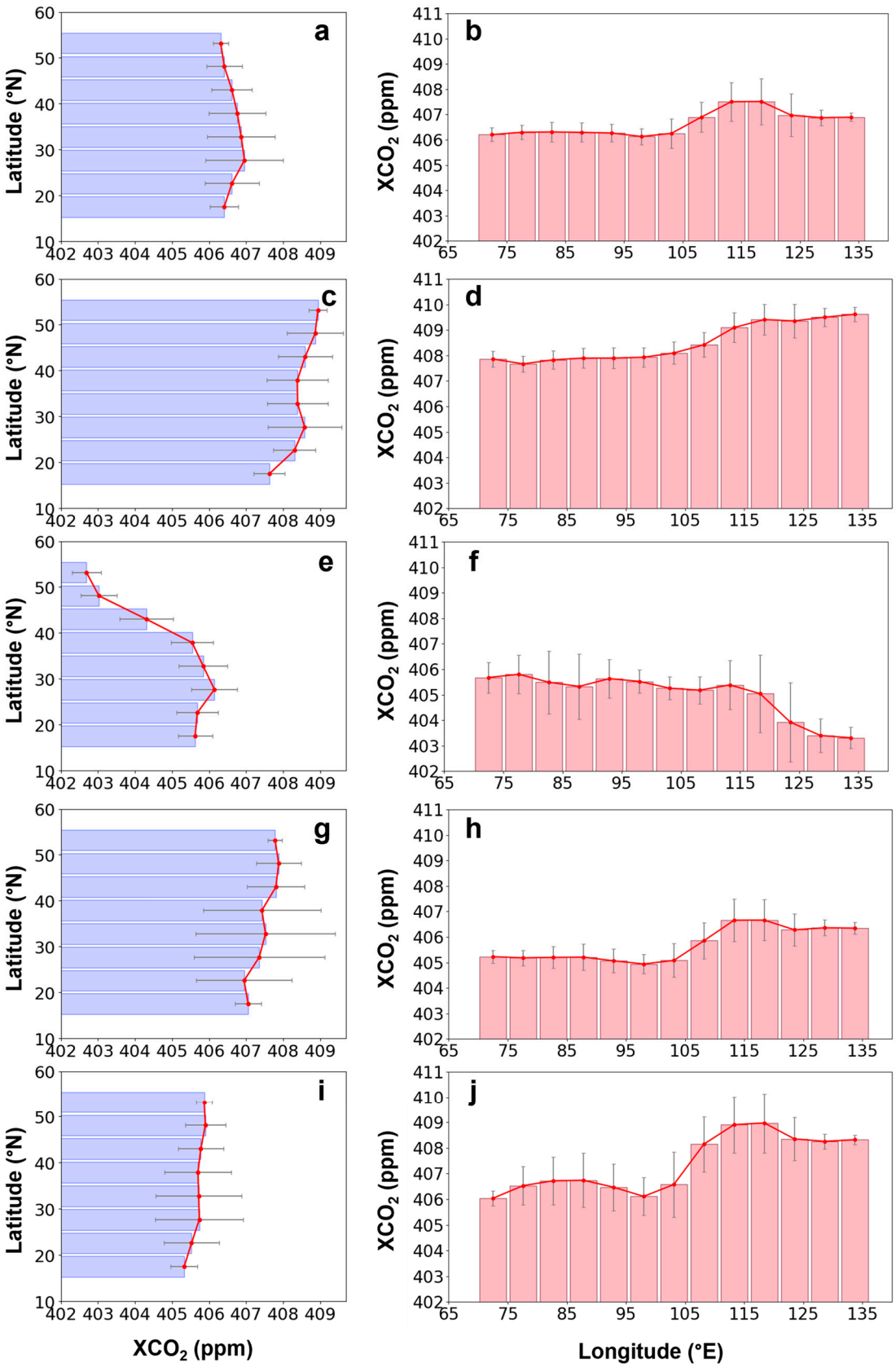


Figure S4. Latitude and longitude variations in XCO_2 concentrations: (a–b) 6-years mean concentrations; (c–d) spring; (e–f) summer; (g–h) autumn; (i–j) winter.

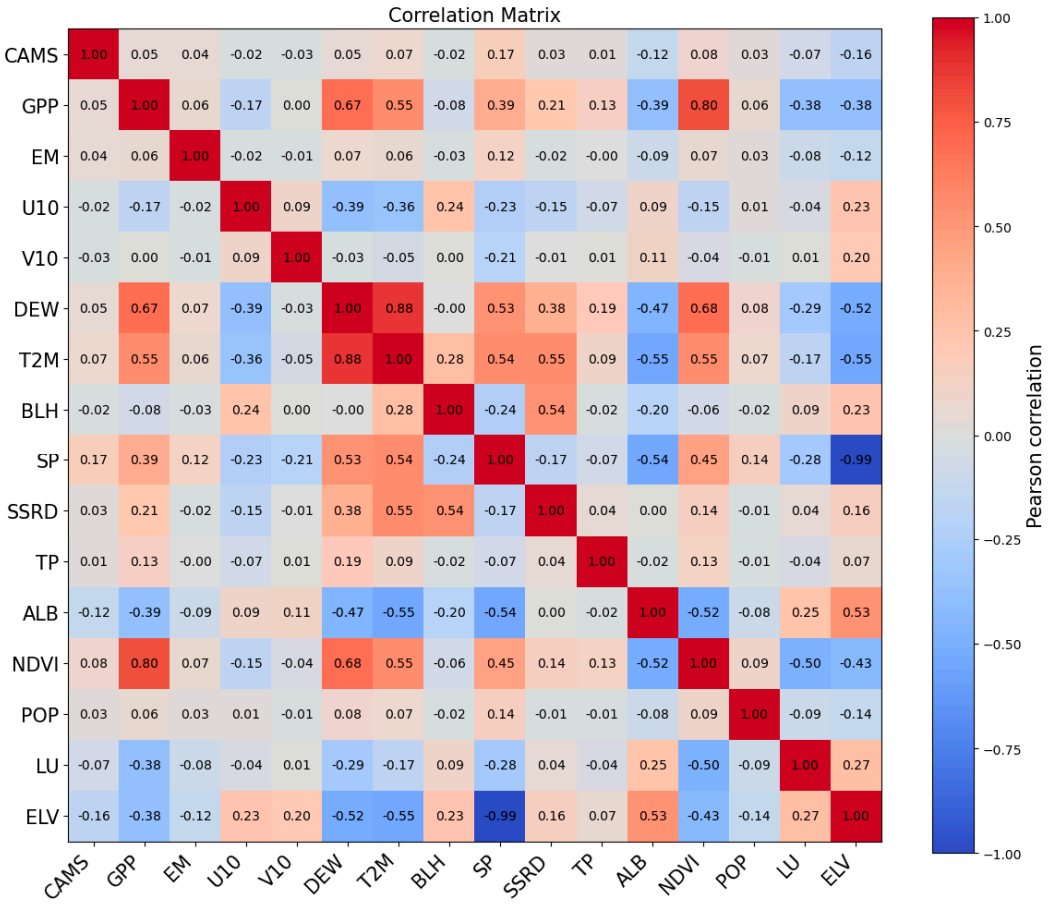


Figure S5. Correlation Matrix of Model Input Variables

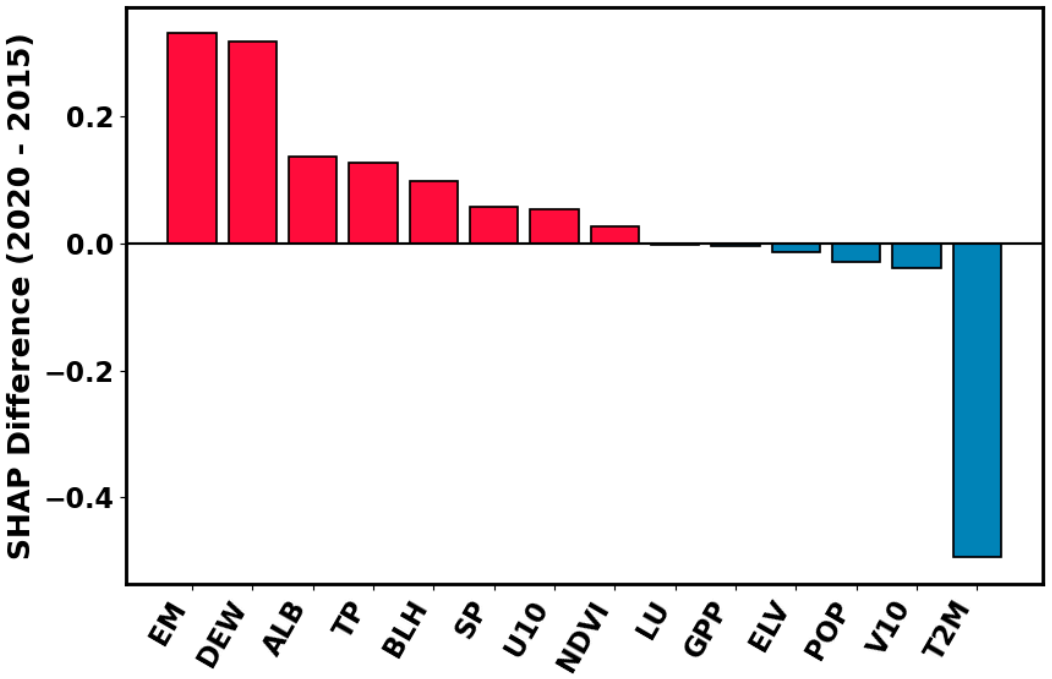


Figure S6. Changes in SHAP values for different features in 2020 relative to 2015