

Figure S1. Snapshots of the PM_{2.5} observations at 1074 air quality stations. Panels a-c are in parallel with the RFSML predictions shown in Fig.8 panels a-c.

$$\text{NMB} = \frac{1}{n} \sum_{i=1}^n \frac{\hat{y}_t - y_t}{y_t} \cdot 100\% \quad (1)$$

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (\hat{y}_t - y_t)^2} \quad (2)$$

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |\hat{y}_t - y_t| \quad (3)$$

$$\text{R} = \frac{E[(\hat{y}_t - E(\hat{y}_t))(y_t - E(y_t))]}{\sqrt{E[\hat{y}_t - E(\hat{y}_t)]^2} \cdot \sqrt{E[y_t - E(y_t)]^2}} \quad (4)$$

5 where n is the size of the test dataset; \hat{y}_t and y_t are the predicting values and ground observations of PM_{2.5} concentration at time t .

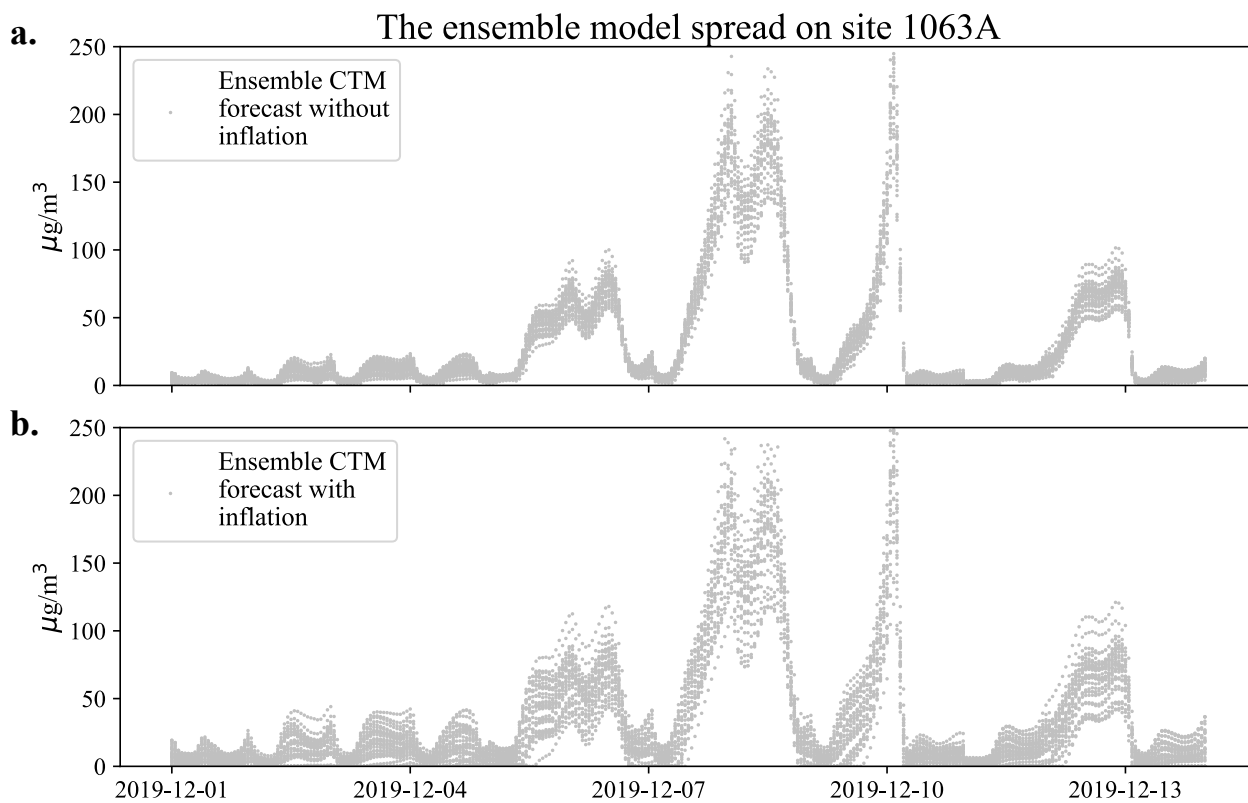


Figure S2. Panels a and b are the ensemble CTM model spread before and after inflation on an environmental monitoring station (Latitude:40.98°N, Longitude:117.95°E) in Chengde, Hebei Province.

CTM forecast vs Observation

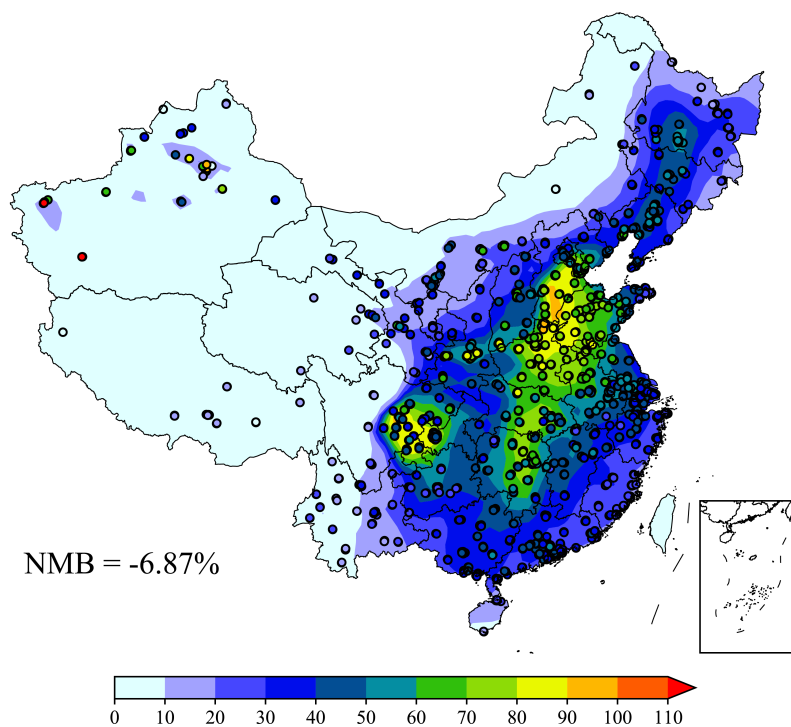


Figure S3. The average time results of CTM forecast versus Observations over the entire test period. Normalized mean bias (NMB) between the CTM forecast and observation is -6.87%.

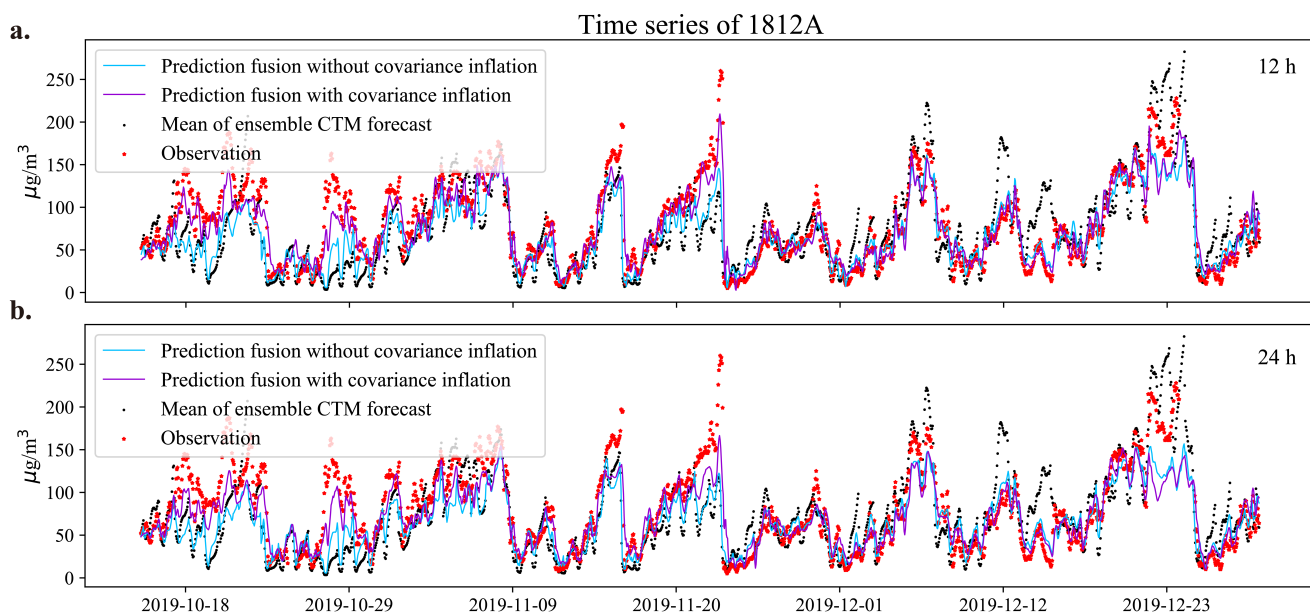


Figure S4. Time series of an environmental monitoring station (Latitude:34.65°N, Longitude:112.39°E) in Luoyang, Henan Province, which is one of the validation set. Markers of deep sky blue solid line, dark violet solid line, red star, and black dot represent prediction fusion without covariance inflation, prediction fusion with covariance inflation, ground observation, and mean of ensemble CTM predictions respectively. Subplots a and b represent forecasts 12 and 24 h ahead, respectively.