Response to reviewers

We thank the two reviewers for their thorough and constructive reviews of this manuscript. We have incorporated most of the suggestions and believe the revised paper is substantially improved. Please find below the author's responses point-by-point. The original comments by the reviewer are in *blue italics*, our responses are in black. The revised manuscript with tracked changes is also appended.

Reviewer #1:

Major Comments

This study by Zhang et al. entitled "Unleashing the Potential of Geostationary Satellite Observations in Air Quality Forecasting Through Artificial Intelligence Techniques" presents a new machine-learning framework – GeoNet – that synthesizes geostationary observations of columnar NO2 from the Geostationary Environment Monitoring Spectrometer (GEMS) with meteorological parameters to forecast surface-level NO2 in East China. Overall, this study represents a significant advancement in surface-level pollution forecasting given its use of the unprecedented hourly data provided by GEMS. I believe that this manuscript is well-written and consistent; however, I have a few comments below.

We appreciate the reviewer for the positive comments. We have addressed the following concerns point-by-point below:

1. *First, if possible, it would be useful to validate the GEMS observations using ground-based spectrometers (e.g., PGN) specifically for the study region and time period.*

We thank the reviewer for this suggestion! In our previous work (e.g., (Li et al., 2023)), we validated the GEMS NO_2 retrievals with the six ground-based MAX-DOAS distributed over the Jing-Jin-Ji region, Yangtze River Delta, Pearl River Delta, and Sichuan-Chongqing Basin in China. Generally, the correlation coefficient between GEMS and MAX-DOAS NO_2 retrieval ranges between 0.69-0.92 for different sites (see Fig. R1), indicating high consistency between both datasets. We have now discussed these results in L125-127, section 2.1:

> *Our previous validation results indicated that GEMS NO_2 retrievals generally agreed well with ground-based MAX-DOAS measurements from 6 sites in China, with correlation coefficients ranging between 0.69-0.92 (Li et al., 2023).*

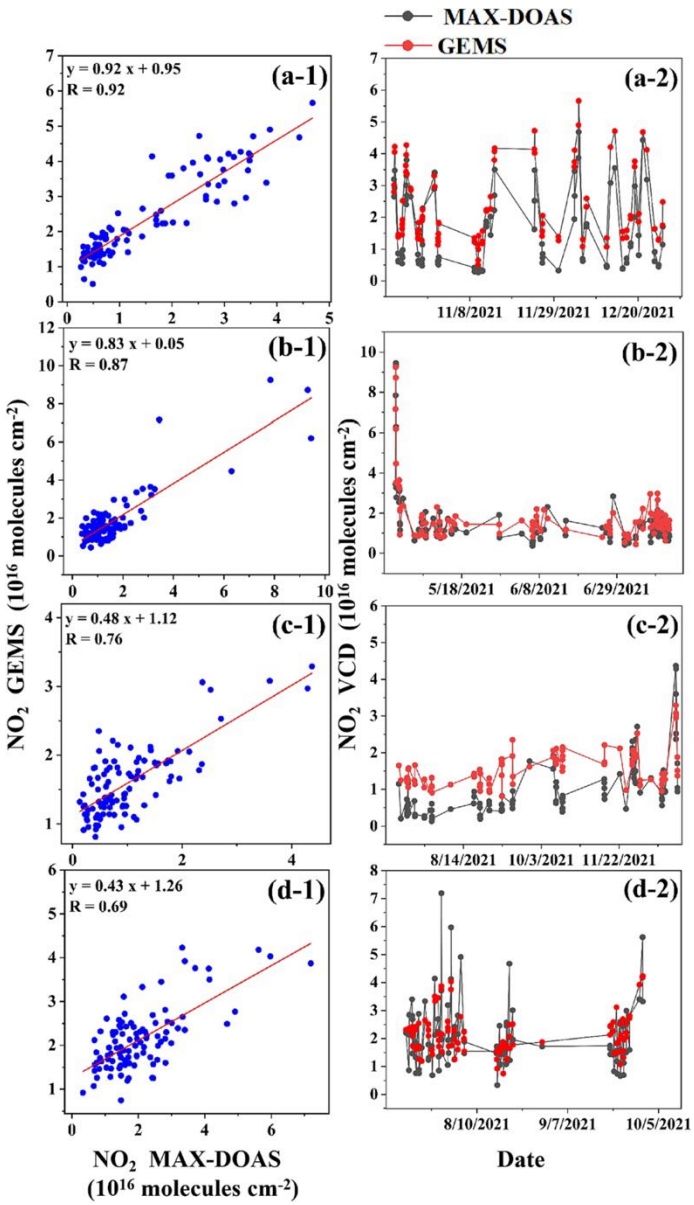

Fig. R1 (from Li et al., 2023). The comparison between GEMS and the MAX-DOAS NO_2 VCDs data from different stations. Panels (a-1), (b-1), (c-1), and (d-1) represent the comparisons with CAMS, GIG, HNU, and CQ stations, respectively. Panel (a-2), (b-2), (c-2), and (d-2) represent time series plots with CAMS, GIG, HNU, and CQ stations, respectively.

2. *Additionally, unless I missed it, I don't believe the time periods for model training and validation were ever stated; if this is the case they should be added to the main text.*

We thank the reviewer for this helpful reminder! We now add the following descriptions in L185-187, section 2.3:

> *We train the GeoNet model with input features during the whole year of 2021. The training datasets were randomly selected from 75% of the whole samples, while the remaining 25% were used as validation sets.*

3. *Second, when investigating feature importance, it would be useful to also identify variability in the feature importance to uncover whether some components are more stable than others in GeoNet and to identify if the significance of geostationary observations is consistent across different days and seasons.*

We now investigated the temporal variations of these features' importance across different seasons. Fig. R2 is similar to Fig. 3a in the main text, but for the feature importance in Spring, Summer, Autumn, and Winter. We added the following discussions in L321-322:

> *The significance of the different input variables remained generally consistent across seasons, with minor variations (as shown in Fig. S12).*

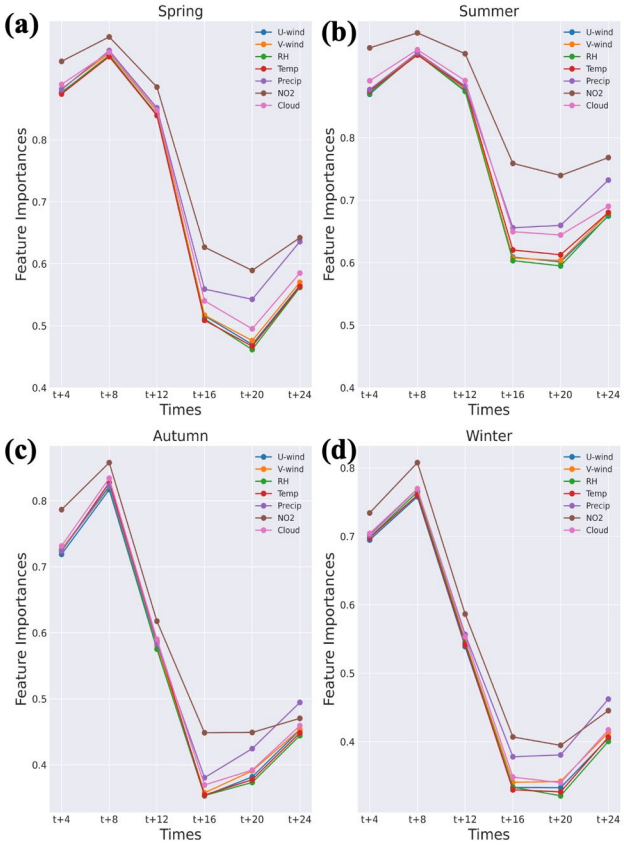

Fig. R2 (also moved into the Supplementary Information, Fig. S12). Similar to Fig 3a, but for different seasons, including Spring (a), Summer (b), Autumn (c), and Winter (d).

4. *Lastly, I suggest that the authors update their analysis in Figure 4 to include the GeoNet predictions regridded to the CAMS grid to identify how much of the improvement in predictions is attributable specifically to enhancements in spatial resolution.*

Thanks for this suggestion! We now re-grid the GeoNet predictions to the CAMS grid in Fig. R3 (and also replaced it with Fig. 5). It can be seen that GeoNet prediction results between the original (0.1°) and CAMS resolution (0.4°) are similar in spatial patterns overall.

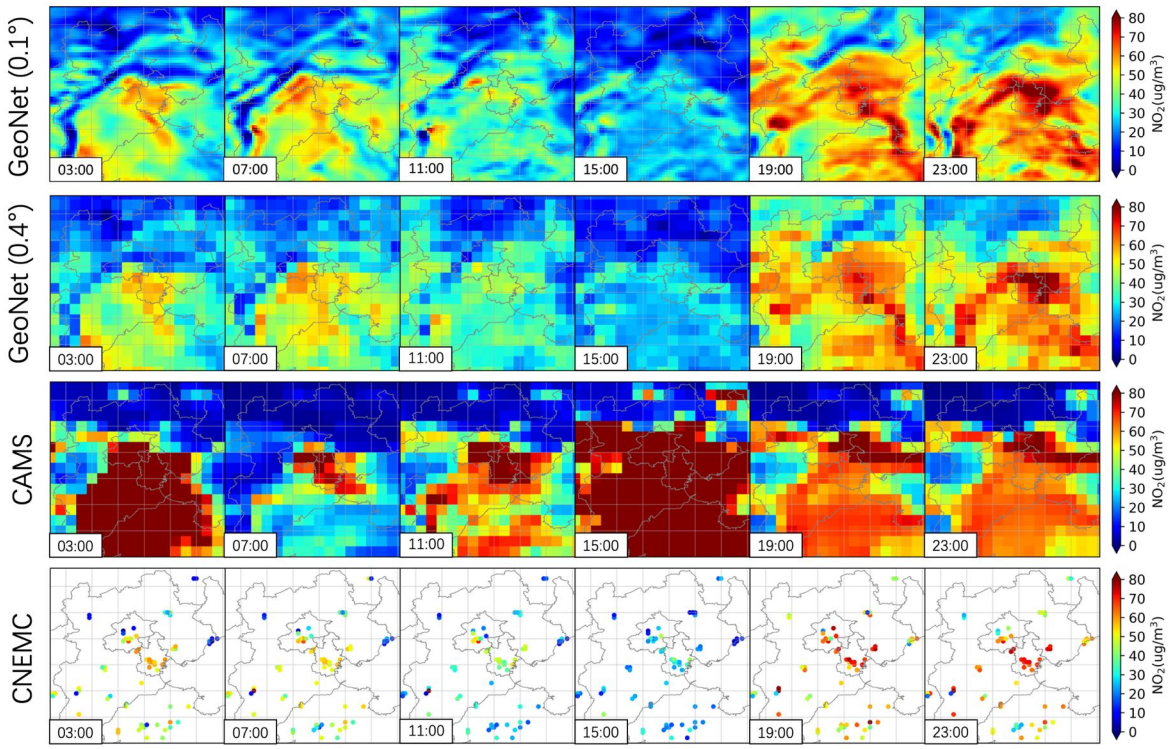

Fig. R3 (Fig. 5 in the revised manuscript). The spatial distribution comparisons of surface NO_2 concentration between (a) GeoNet prediction at the original resolution of 0.1°, (b) GeoNet prediction resampled to the CAMS resolution of 0.4°, (c) CAMS prediction, and (d) ground-based CNEMC site measurements. Note that the results are presented for different continuing local hours (labeled text in the subplot) on 23 November 2021.

I have included line-specific comments below:
Minor Comments

1. *L53-54: While I agree with this statement, it should be mentioned that for air pollution forecasting to facilitate health benefits, infrastructure needs to be created that communicate risks and appropriate responses to risks to the public.*

We added the following lines to mention the necessity of implementing infrastructure to communicate air quality risks and public recommendations, in L50-52 of the revised manuscript:

> Meanwhile, air quality health risk (AQHI) forecasts and corresponding public response recommendations need to be communicated to the public promptly through public facilities (Fino et al., 2021; Tang et al., 2024).

2. *L55: I think you can drop the second limited in this line.*

Removed.

3. *L75: Maybe it would be useful to give an example or two here (i.e., TROPOMI + OMI).*

Added “such as the Ozone Monitoring Instrument (OMI) and the TROPospheric Monitoring Instrument (TROPOMI)”.

4. *L78-81: Another limitation of the polar orbiting satellites that is worth mentioning is that typically (at least in the case of TROPOMI) the satellite observes at roughly the same time of day (early afternoon) which makes it difficult to predict concentrations at other times of the day with different meteorological (boundary layer height) and photochemical conditions.*

Thanks for your suggestion. We added the following sentences in L84-86:

However, these observations at a fixed daily overpass time could hardly support the prediction of atmospheric trace gas concentrations at other times of the day under different meteorological conditions.

5. *L92: It would be better to describe GEMS as having "unprecedented temporal and spatial resolution and coverage" as ground-level monitors can observe hourly NO2 but are limited in time and aircraft remote-sensing can observe NO2 at sub hourly resolution but over a limited temporal coverage (usually a few days or weeks). The resolution alone isn't necessarily unique but rather than combined spatial + temporal resolution with extended spatial and temporal coverage.*

Corrected.

6. *L117-120: Were you able to validate these data for the study time period / domain? If possible, it may be useful to compare GEMS to ground-based spectrometers in the study domain to get an idea of performance.*

Please refer to the response to major comment #1.

7. *L207-208: I don't think you need this sentence as it is already mentioned in the methods section.*

Removed.

8. *Figure 3: It would be interesting to present the variance of these different components as well in a). Are these importance values pretty consistent regardless of season and day, or do they vary substantially day to day?*

Please refer to the response to major comment #3.

9. *Figure 4: Have you assessed how much of the reductions in performance are attributable to resolution? If not, I suggest regridding the GeoNet prediction to the resolution of CAMS and comparing this "GeoNET_coarse" product to the observations to characterize how much of the improved performance is attributable to enhanced spatial resolution.*

Please refer to the response to major comment #4.

10. *Figure 5: The colorbar in a is not labeled, and throughout the font is small (especially in the yaxis of c and d), I suggest updating to improve readability.*

Thanks for your helpful suggestion! We added the figure label and increased the font as follows.

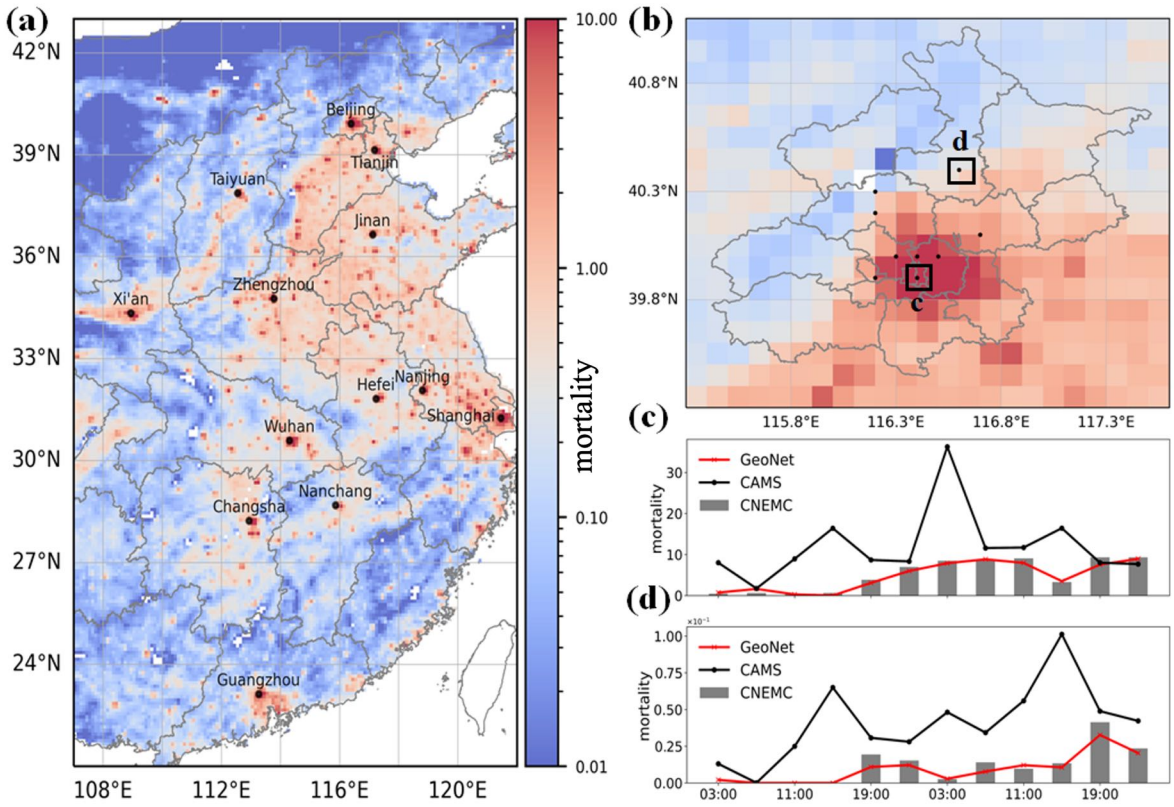

Fig R4 (Fig. 6 in the manuscript). Mortality risk of short-term NO_2 exposure based on the GeoNet prediction on November 23, 2021. (**a**) mean mortality due to the predicted NO_2 exposure in East China; (**b**) a zoom-in map over Beijing and its neighboring area; (**c**) and (**d**) are comparisons of mortality estimation over the Beijing urban and rural regions (the rectangle areas presented in **b**), respectively, based on different NO_2 exposure prediction among GeoNet, CAMS, and CNEMC.

11. L338-339: I don't believe the timeframe of this study was mentioned at all in the main text. What months / years was this prediction trained on and for what period was it validated?

Please refer to the response to major comment #2.

Reviewer #2:

The authors attempted to improve the short-term prediction of surface NO2 at a high spatial and temporal resolution by taking advantage of the GEMS NO2 prodcuts and a neural network model. They successfully forecasted full-coverage surface NO2 for the next 24 hours and identifed the critical role of GEMS NO2. Their results demonstrate the potential application of the GEMS products in air quality prediction.
Overall, this is an important study and the results presented here will be useful for future applications of GEMS products as well as the geostationary satellite observations. I am happy to see its publication in due course. However, before that, I still have a few concerns or suggestions for the authors.

We appreciate the reviewer for the positive comments. We have addressed the following concerns point-by-point below:

1. *I would sugget to move the model configuration and optimization into the main text. This will be very helpful for readers to understand the model.*

Thanks for your suggestion. We now moved the model configuration and optimization details to the L188-219 (Section 2.4) of the main text. Please refer to the details in the revised manuscript.

2. *In the handling of missing data, the authors tried to set them to a fill value of zero. Is it reasonable? It looks reasonable to fill values of diurnal NO2 climatology (e.g., the seasonal mean diurnal NO2). In addition, as shown in Fig.2, it looks the three methods of handling missing data perform similarly in term of R2 and RMSE. So I don't think it is necessary to highlight the "weakest" or "strongest" configuration.*

We greatly appreciate the reviewer's concerns regarding our method of handling missing data.

The reason we chose to use a direct fill value of zero is that during the experiments, we observed that this approach, combined with the model's feature extraction capability, could effectively mitigate the negative impact of missing data on prediction performance. Meanwhile, by incorporating cloud cover (mainly effectors of the missing satellite measurements), this method allows the model to fully leverage its potential, overcoming the issues caused by missing data. We acknowledge the reasonableness of using diurnal NO_2 climatology, as the reviewer suggested. However, the data discontinuities between satellite NO_2 measurements and gap-filled NO_2 climatology could lead to systematical biases in model predictions. Moreover, as indicated by the results, R^2 and RMSE metrics did not show significant differences across the various methods of missing data handling. Therefore, we believe our current approach is valid, with minimum effect on data discontinuities.
In general, we now provide a more detailed discussion of the different missing data handling techniques, clarifying the rationale for our choice and highlighting the positive role that cloud-cover data plays in enhancing the model's performance. Please refer to the detailed revisions in L256-263 of the manuscript:

> *The comparison results to the validation datasets indicate that the scenario using CAMS meteorology datasets and replacing missing satellite NO_2 data with fill-values (Fig. 2c), corresponds to a modest NO_2 prediction performance with R^2=0.68 and RMSE=12.26 $\mu g/m^3$. In contrast, the configuration scenario using ERA-5 reanalysis meteorology and imputing with WRF-Chem simulations (Fig. 2a), corresponds to the best prediction*

performance of R^2=0.69 and RMSE=11.88 μg/m^3. This may indicate that the importance of satellite missing data imputation may be diminished by cloud mask inputs, especially since the model can extract informative features from spatial and temporal neighboring inputs.

3. *I would also suggest to move Fig.S12 in the main text which shows the advantage of GEMS measurements.*

Done. We moved Fig. S12 into the main text (Fig. 4).

4. *The authors also show that the performance of GeoNet model degrades notably after t+16h. Is there any possible solution to overcome this short predicability?*

We appreciate the valuable feedback regarding the performance degradation of our short-term air quality forecasting model beyond t+16h. We acknowledge that this is a common phenomenon in many air quality prediction models, particularly due to the inherent uncertainties in meteorology, emissions, and chemical reactions that significantly affect longer-term forecasts. Although the accuracy of predictions after t+16h declines, the results still provide meaningful insights. In future work, we aim to improve long-term forecasting performance by adopting more sophisticated model architectures and incorporating enhanced observational data or physical constraints.

In response to this comment, we also revised the manuscript in the following aspects:

(1) Explicitly discuss the reasons for the model's performance degradation beyond t+16h in the manuscript.

(2) Outline future research directions, including the exploration of model frameworks with better temporal generalization and the integration of stronger observational and physical constraints to improve long-term predictions.

Please refer to L387-392 in the revised manuscript:

The variation of the model forecasting performance also shows that accurate prediction for longer time windows and heavy pollution events is still a major difficulty. This may be due to the high level of uncertainty in emissions and meteorology. In the future, a combination of higher resolution and more accurate multi-source data constraints, as well as machine learning models coupled with atmospheric physical mechanisms, may be needed to improve the existing forecasts.

5. *As mentioned in my last comment, the authors also highlight the possible applications to other air pollutants. However, the chemistry and lifetime of other air pollutants might be very different from NO2. For example, if the GEMS tropospheric ozone measurement is useful for the prediction of surface ozone? Some more detailed discussions on the possible application to other pollutants would be very insightful.*

Thanks for your comment. We elaborated it in the L398-402 in the revised manuscript:

This work also has important implications for the prediction of near-surface O3 and particulate matter. For example, the integration of using vertical O3 profiles from the GEMS satellite, in particular near-surface layer concentrations, and their joint observations of important O3 precursors including NO2 and HCHO, is expected to significantly improve the uncertainty of existing estimates of near-surface air pollution.

6. *BTW, I am not sure whether it is necessary to include NO2 in the Title of this manuscript since the authors didn't talk too much about major air pollutants (i.e., PM2.5 and ozone)*

Thanks for your comment. Considering the broad implications of this research for forecasting other pollutants using Geostationary satellite measurement (also discussed in response to comment #5), we think it would be better to retain the current title.

References:

(1) Fino, A., Vichi, F., Leonardi, C., & Mukhopadhyay, K. (2021). An overview of experiences made and tools used to inform the public on ambient air quality. *Atmosphere, 12*(11), 1524.

(2) Li, Y., Xing, C., Peng, H., Song, Y., Zhang, C., Xue, J., et al. (2023). Long-term observations of NO2 using GEMS in China: Validations and regional transport. *Science of The Total Environment, 904*, 166762.

(3) Tang, K. T. J., Lin, C., Wang, Z., Pang, S. W., Wong, T.-W., Yu, I. T. S., et al. (2024). Update of Air Quality Health Index (AQHI) and harmonization of health protection and climate mitigation. *Atmospheric Environment, 326*, 120473.

Unleashing the Potential of Geostationary Satellite Observations in Air Quality Forecasting Through Artificial Intelligence Techniques

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Abstract.

Air quality forecasting plays a critical role in mitigating air pollution. However, current physics-based air pollution predictions encounter challenges in accuracy and spatiotemporal resolution due to limitations in the understanding of atmospheric physical mechanisms, observational constraints, and computational capacity. The world's first geostationary satellite UV-Vis spectrometer, i.e., the Geostationary Environment Monitoring Spectrometer (GEMS), offers hourly measurements of atmospheric trace gas pollutants at high spatial resolution over East Asia. In this study, we successfully incorporate Geostationary satellite observations into a neural network model (GeoNet) to forecast full-coverage surface nitrogen dioxide (NO_2) concentrations over eastern China at 4-hour intervals for the next 24 hours. GeoNet leverages spatiotemporal series of satellite NO_2 observations to capture the intricate relationships among air quality, meteorology, and emissions in both temporal and spatial domains. Evaluation against ground-based measurements demonstrates that GeoNet accurately predicts diurnal variations and spatial distribution details of next-day NO_2 pollution, yielding the coefficient of determination of 0.68 and root mean square of error of 12.31 $\mu g/m^3$, significantly surpassing traditional air quality model forecasts. The model's interpretability reveals that geostationary satellite observations notably improve NO_2 forecast capability more than other input features, especially over polluted regions. Our findings demonstrate the significant potential of geostationary satellite observations in artificial intelligence-based air quality forecasting, with implications for early warning of air pollution events and human health exposure.

Keywords: air quality forecast; deep learning; health impact; satellite remote sensing; nitrogen dioxide;

1 Introduction

Since the industrial revolution, numerous countries worldwide have encountered severe air pollution issues such as photochemical ozone smog and haze pollution (Hong et al., 2019), which significantly affect human health, crop yields, and the global environment (Guarin et al., 2024; Manisalidis et al., 2020; Sathe et al., 2021). Recent studies have shown that both long-term and short-term exposure to air pollutants such as nitrogen dioxide (NO_2) can significantly affect human health, especially the respiratory system (Meng et al., 2021). Accurate and high spatial resolution predictions of air pollutant concentrations can provide critical information for sensitive persons to mitigate health risks. Meanwhile, air quality health risk (AQHI) forecasts and corresponding public response recommendations need to be communicated to the public promptly through public facilities (Fino et al., 2021; Tang et al., 2024). In recent decades, the advancement of atmospheric monitoring and modeling has enabled significant progress in air quality forecasting based on our understanding of atmospheric physics and chemistry (Peuch et al., 2022). Air pollution forecasting not only facilitates responses to environmental health risks but also improves the accuracy of climate and weather simulations (Makar et al., 2015). However, due to our still limited understanding of atmospheric mechanisms and observational and emission constraints, existing air quality forecasts based on physical or statistical models still face challenges in terms of temporal, spatial, and accuracy aspects (Campbell et al., 2022; Zhong et al., 2021).

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Artificial Intelligence (AI) technology has made breakthroughs in the field of Earth science (Boukabara et al., 2020; Zhong et al., 2021), particularly excelling in addressing complex problems that are challenging for traditional physical paradigms to simulate (Irrgang et al., 2021), such as weather and climate forecasting (Andersson et al., 2021). Concerning meteorological data, some large-scale deep learning models have surpassed the predictive capabilities of existing numerical weather models to some extent, examples include Climax

(Nguyen et al., 2023), Pangu-Weather (Bi et al., 2023), and GraphCast (Lam et al., 2023). Despite significant progress and impressive performance achieved in meteorological variables forecasting with AI methods, there are still limitations in predicting atmospheric pollutant compositions. Compared to meteorological parameters, the prediction of air pollutant concentrations is affected by synoptic meteorology, chemistry, and anthropogenic emission activities, usually with more complex driven mechanisms and associated uncertainties. Current AI-based air quality forecasts often involve time series predictions at a limited number of observation stations, rather than full-coverage predictions over the entire spatial domain (Du et al., 2021). This is primarily due to the lack of effective air quality observations with high temporal and spatial resolution simultaneously.

While past polar-orbiting satellite observations such as the Ozone Monitoring Instrument (OMI) and the TROPospheric Monitoring Instrument (TROPOMI), have provided extensive coverage of atmospheric pollutant distributions such as nitrogen dioxide (NO_2), sulfate dioxide (SO_2), ozone (O_3), and aerosols, they are limited to once-daily overpasses and usually affected by clouds (Chan et al., 2023; Van Geffen et al., 2022). This frequency usually exceeds the chemical lifetimes of many reactive gas pollutants like NO_2, making it challenging to offer effective observational constraints for machine learning short-term air quality forecasting (Shah et al., 2020). However, these observations at a fixed daily overpass time could hardly support the prediction of atmospheric trace gas concentrations at other times of the day under different meteorological conditions. In February 2020, the world's first geostationary satellite payload for air pollution monitoring, the Geostationary Environment Monitoring Spectrometer (GEMS), began to provide high-coverage and high-precision air quality observations at an hourly rate for the East Asian region (J. Kim et al., 2020). The dynamic processes of air pollutants including emission, transformation, and transport can be observed by the geostationary satellite during the daytime. This monitoring capability may advance data-driven

air quality forecasting such as machine learning techniques by offering unprecedented observational constraints with high spatial and temporal coverage. Recent observing system simulation experiments (OSSE) indicate that assimilating trace gas observations by geostationary satellites into chemical models can effectively improve surface ozone simulations (Shu et al., 2023), nitrogen oxides (NO_x), and emission estimates (Hsu et al., 2024).

Here, based on the unprecedented temporal and spatial resolution and coverage of the GEMS satellite (J. Kim et al., 2020), we incorporated Geostationary satellite remote sensing of tropospheric NO_2 column densities (refer to section 4 for details) into a neural Network model (GeoNet), to forecast full-coverage surface NO_2 concentration over the next day from the current time *t* (i.e., t+24h). Compared with previous air quality forecasting based on the simulation of atmospheric physics and chemistry possibly combined with data assimilation approaches, GeoNet relies solely on geostationary satellite measurements and ancillary meteorology data. GeoNet effectively addresses the complex nonlinear relationships between future short-term air quality and current satellite observations, as well as temporally adjacent meteorological variables (C. Zhang et al., 2022). The method employs satellite and meteorological variables within the spatial vicinity of individual air quality monitoring sites as input features, with site observations serving as labels for model training. The resulting model achieves accurate and comprehensive air quality predictions across the entire domain over East China, which is a significant achievement given that past machine learning technologies have relied on only a few stations or polar-orbiting satellite observations.

2 Materials and Methods

2.1 Geostationary satellite observations of atmospheric NO_2

GEMS is the first UV-Vis spectrometer at a geostationary satellite orbit, measuring atmospheric pollutants such as NO_2, SO_2, O_3, and HCHO over East Asia, at a spatial resolution of 3.5 km × 7.5 km at nadir and a temporal resolution of 1 hour during the daytime (J. Kim et

al., 2020). Based on the unique spectral absorption of trace gases, the atmospheric NO_2 column can be retrieved in visible wavelengths from the spectra of back-scattered sunlight. The details of the GEMS NO_2 retrieval can be found in the Algorithm Theoretical Basis Document (available at https://nesc.nier.go.kr/ko/html/satellite/doc/doc.do, last access: June 1, 2023). In this study, we used the tropospheric NO_2 column from the GEMS NO_2 version 2.0 product, as well as the cloud fraction for each satellite ground pixel. Overall, GEMS NO_2 measurements have a good correlation with ground-based remote sensing instruments, with correlation coefficients (R) between 0.69-0.81, and root mean square of errors (RMSE) between 3.2-4.9×10^{15} *molecules/cm*^{2} (S. Kim et al., 2023). Our previous validation results indicated that GEMS NO_2 retrievals generally agreed well with ground-based MAX-DOAS measurements from 6 sites in China, with correlation coefficients ranging between 0.69-0.92 (Li et al., 2023).

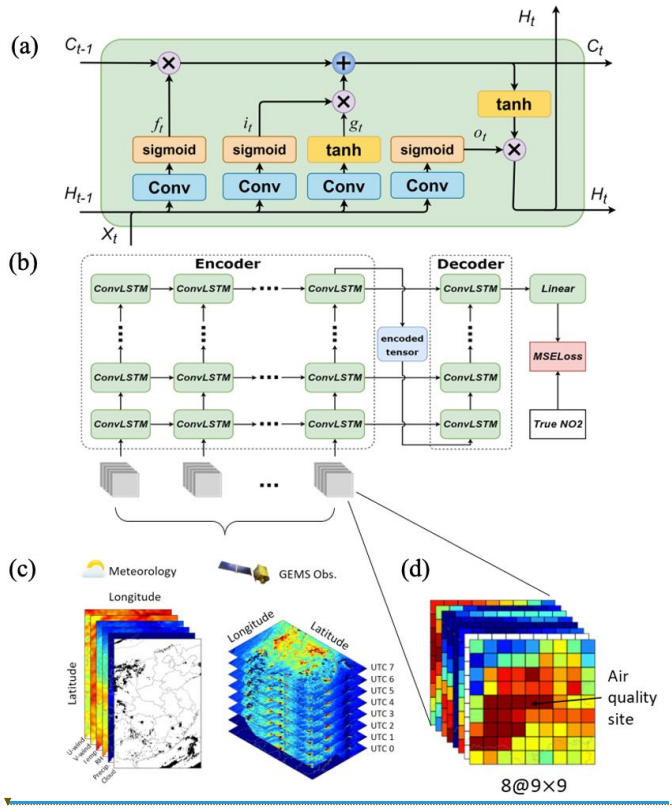
2.2 Ancillary datasets

Other input information including meteorological datasets is necessary to better constrain the prediction of future NO_2 pollution. Here, both the ERA5 meteorology reanalysis (Hersbach et al., 2020) and the CAMS forecast (Peuch et al., 2022) were used to provide meteorological parameters such as zonal and meridional wind (U-wind and V-wind), temperature (Temp), relative humidity (RH), and precipitation (Precip). In addition, the fraction of cloud cover available from the satellite NO_2 datasets was also considered. To fill the missing gaps in the satellite NO_2 measurements, we use both the NO_2 concentrations from the WRF-Chem model (C. Zhang et al., 2022) and the CAMS forecast of atmospheric composition. Note that the reanalysis datasets were typically updated with a week delay from real-time, while the forecast datasets can provide future 7-day meteorology from the current time. Therefore, the latency of input datasets would affect the operational prediction of the GeoNet model. Surface NO_2 measurements were used as the ground-truth label in the model training phase, available from

over 1000 national air quality sites by the China National Environmental Monitoring Centre (CNEMC) (Kong et al., 2021).

The preprocessing steps of model input datasets, including outlier detection, missing value handling, resampling, and normalization, are described in Supplementary Text S1.

2.3 The GeoNet model



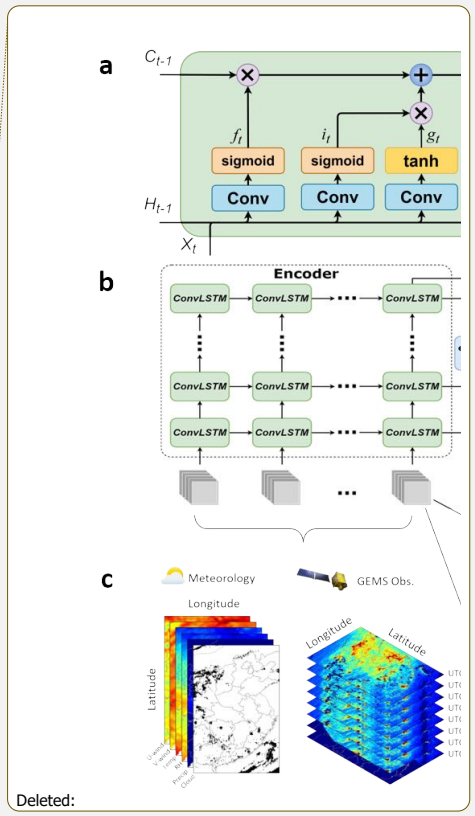


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Figure 1. The framework of predicting surface NO_2 map based on Geostationary satellite measurements and a ConvLSTM neural network model (GeoNet). (a) the structure of the ConvLSTM block; (b) a diagram of GeoNet model structure with inputs and output; (c) an illustration of the model input parameters including meteorological variables and hourly NO_2 measurements by the Geostationary satellite; (d) the input data cube of different features for single training batch, which is centered at an air quality site.

Fig. 1 illustrates the structure and methodology of the artificial intelligence air quality forecasting model established in this study. Given the distinctive nature of spatiotemporal

sequence data for air quality, predictions must consider not only temporal relationships but also spatial correlations. The deep learning model employed in this research utilizes convolutional long short-term memory (ConvLSTM) as its kernel, a variant of the LSTM model designed for the time series forecasting (Lin et al., 2020). It incorporates a convolutional network structure to capture spatial features of three-dimensional inputs. Both input-to-state and state-to-state transitions involve convolutional structures. ConvLSTM determines the future state of a unit within a grid based on inputs from its local neighbors and past states, allowing it to effectively model the spatiotemporal dynamics of air quality. The ConvLSTM kernel structure employed in training is illustrated in Fig. 5a. Here, X_t represents the input at time t, H_t and H_{t-1} denote the outputs at times t and t-1, and C_t and C_{t-1} represent the states at times t and t-1. The computational process is as follows:

$$i_t = \sigma(X_t * w_{xi} + H_{t-1} * w_{hi} + b_i) \quad (1)$$

$$f_t = \sigma\left(X_t * w_{xf} + H_{t-1} * w_{hf} + b_f\right) \quad (2)$$

$$o_t = \sigma(X_t * w_{xo} + H_{t-1} * w_{ho} + b_o) \quad (3)$$

$$g_t = tanh\left(X_t * w_{xg} + H_{t-1} * w_{hg} + b_g\right) \quad (4)$$

$$C_t = f_t \times C_{t-1} + i_t \times g_t \quad (5)$$

$$H_t = o_t \times tanh(C_t) \quad (6)$$

Where the asterisk ($*$) represents the convolution operator, w is the convolution kernel, b is the offset, $tanh$ is the hyperbolic tangent function, and σ is the activation function of Sigmoid.

The model primarily consists of three components: an encoder, a decoder, and fully connected layers. Tropospheric NO_2 observations from the GEMS satellite for different consecutive hours within a day, along with corresponding meteorological forecast field data, serve as input features for model training. The encoder processes the spatiotemporal sequences of input features for the preceding 8 hours (t-7h, t-6h, …, t), which are then decoded by the decoder. The final output, representing NO_2 concentrations at 4-hour intervals for the next 24

hours (t+4h, t+8h, t+12h,…, t+24h), is produced through fully connected layers. The loss function of mean squared error (MSE) is calculated by comparing the model output with the actual values from station observations, and the model undergoes iterative training. In the training task for a single station sample, the model utilizes continuous and distinct hourly dynamic images of all variables within the spatiotemporal vicinity of the station as input (see Fig. 1c-d). This effectively considers the intricate correlations in time and space between air quality, satellite observations, and meteorological input features. We train the GeoNet model with input features during the whole year of 2021. The training datasets were randomly selected from 75% of the whole samples, while the remaining 25% were used as validation sets.

2.4 The model configuration and optimization

The model configurations and hyperparameters such as the optimizer, loss function, L1 or L2 regularization, dropout, training steps, and epochs can make a difference to the model performance including the prediction accuracy and generalizability. The performance metrics such as the coefficient of determination (R^2), root mean square of error (RMSE), mean absolute error (MAE), and mean absolute percentage error (MAPE), were used to diagnose the model (see definition in Supplementary Text S2). Thus, several scenarios of model hyperparameters have been tested during the model training phase. The model accuracy on validation datasets and the learning rate curve were used to diagnose the model hyperparameters. The model parameters mainly include the number of layers and the dimensions of the hidden layers, both control the model's capacity. If the model capacity is relatively small, underfitting may occur; overfitting may exist if it is too large. Therefore, selecting an appropriate model capacity is crucial for improving model performance. During the pre-training process, the model is trained by combining different numbers of layers and dimensions of the hidden layers. The Mean Squared Error (MSE) Loss is recorded for each training iteration, and a heatmap is generated as shown in Fig. S2. From the heatmap, it can be observed that when the number of layers is 2

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and the dimension of the hidden layer is 256, the model achieves the minimum MSE Loss. Fig. S3 shows the sensitivity test results of model loss varying with different batch size settings, indicating that a batch size of 64 is optimal. Based on the model's MSE loss under different hyperparameter configurations, the best-fitting model can be selected.

The Adam optimization algorithm controls the learning rate, which can design independent adaptive learning rates for different parameters. The three initialization parameters ϵ, $\rho 1$, and $\rho 2$ of the Adam algorithm are set to be 0.0001, 0.9, and 0.99, respectively. For the epoch, its size is controlled by the early stop method. The early stop method monitors the change of the model's loss function on the validation set during the training process and stops the model training immediately when the validation loss of the model starts to become larger. Due to the fluctuation of the loss function, a threshold p is set for the early stopping method in practice, and when the validation loss of the model becomes large for p consecutive epochs, the model is rolled back to the lowest validation loss and the training is stopped, and the threshold p is set to 10 in this paper. Fig. S4 shows a typical learning curve of the MSE loss in training and validation data sets for different learning steps in training an optimal model. Such diagnostics can be used to avoid the model overfitting.

2.5 The importance of the model input feature

Permutation feature importance is a technique used to assess the significance of each input feature in a machine-learning model (Altmann et al., 2010). The core idea is to evaluate the impact of each feature on model performance by randomly shuffling its values and observing the resulting change in the model's accuracy. In this study, for each input feature of the GeoNet, we iteratively shuffle its value independently while keeping other features unchanged, and then observe the model prediction on the modified input. The difference in the model prediction performance between using the original and shuffling input quantifies the feature's importance. Here, we measure the relative importance of each input feature using the metric of $1\text{-}R^2$, due

to its good standardized and indicative ability (C. Zhang et al., 2022). Generally, a larger performance drop indicates greater importance, as the model heavily relies on that feature for predictions. Conversely, smaller drops or increases suggest the feature may be less crucial or redundant. By permuting the input feature array based on the different spatial and temporal domains, we can gain a deeper understanding of how feature importance varies spatially and temporally. For example, the relative importance of one meteorology variable may vary with different diurnal, weekly, and monthly cycles, revealing the variability of its impact on the predicted NO_2 levels.

3 Results and Discussion

3.1 Model performance

Based on the GeoNet model and necessary input data (refer to section 2), we have achieved preliminary predictions of near-surface NO_2 concentration with full spatial coverage and a spatial resolution of 0.1 degrees over eastern China, at four-hour intervals over the next 24 hours. In this study, we first tested the impact of using reanalysis and forecast meteorology datasets and filling in missing values in satellite observation data on the model predictions. The reanalysis datasets usually have higher precision than the forecast. Previous studies revealed that the accuracy of the information on meteorology and chemical composition significantly affects the performance of machine learning models in estimating air pollutant concentrations (Wang et al., 2024; Zuo et al., 2023). Due to the shielding effect of clouds, a considerable proportion of missing values may even exist in satellite NO_2 observations. Recent air quality big-data research usually requires the gap-filling of missing satellite data before inputting it into the machine learning model, either by spatial interpolation or regression techniques (M. Kim et al., 2021). We tested three methods for handling missing data, such as setting them to a fill value of zero, or replacing them by real-time CAMS simulated NO_2, or WRF-Chem simulated NO_2 results (not real-time, but with higher precision).

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The comparison results to the validation datasets indicate that the scenario using CAMS meteorology datasets and replacing missing satellite NO_2 data with fill-values (Fig. 2c), corresponds to a modest NO_2 prediction performance with R^2=0.68 and RMSE=12.26 μg/m^3. In contrast, the configuration scenario using ERA-5 reanalysis meteorology and imputing with WRF-Chem simulations (Fig. 2a), corresponds to the best prediction performance of R^2=0.69 and RMSE=11.88 μg/m^3. This may indicate that the importance of satellite missing data imputation may be diminished by cloud mask inputs, especially since the model can extract informative features from spatial and temporal neighboring inputs. To compromise between the performance of real-time and accuracy, we selected the configuration scenario of using CAMS meteorology and imputing with CAMS NO_2 (Fig. 2d) for subsequent discussion and operational forecasting, with an R^2=0.68 and RMSE=12.31 μg/m^3. In summary, the use of higher-precision meteorology and filling missing NO_2 data enhances the model's prediction accuracy on the validation dataset, but to a rather limited extent. This suggests that, unlike previous machine learning techniques, GeoNet can effectively adapt to three-dimensional inputs of varying accuracy and type, fully explore the spatiotemporal correlation of data features, and demonstrate strong model generalization capabilities.

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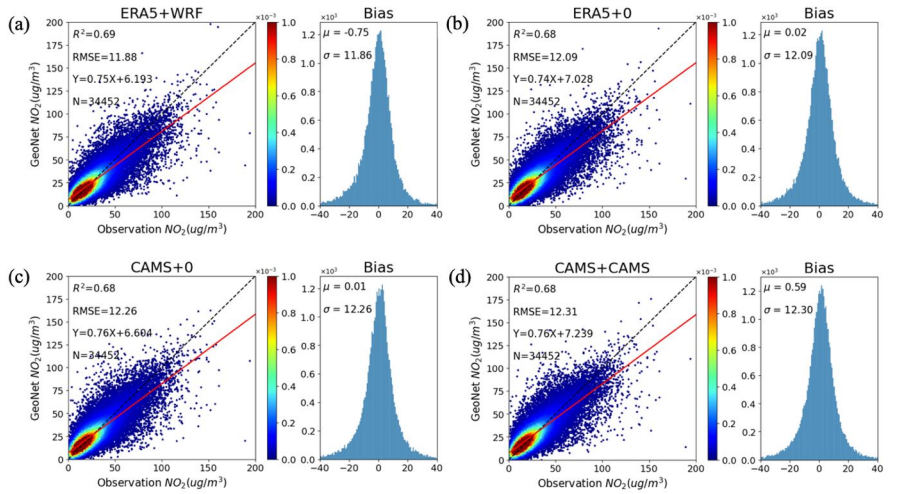

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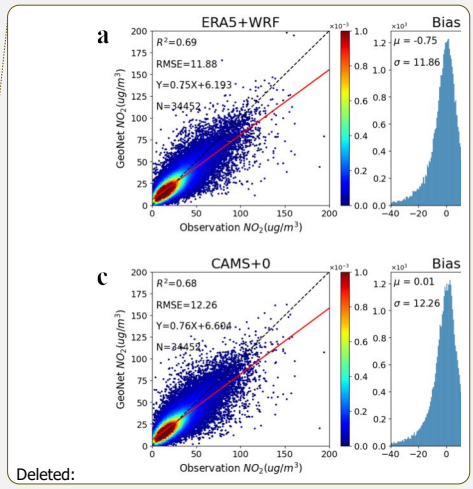


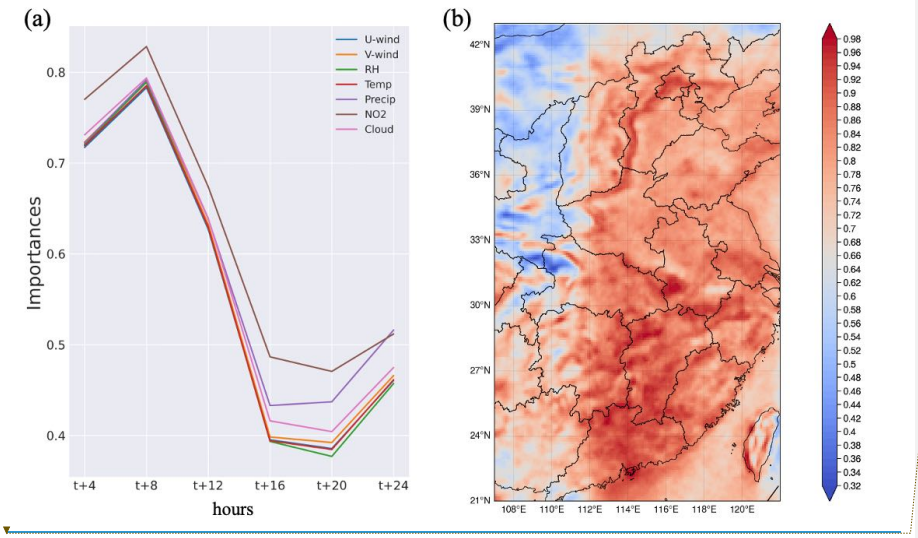
Figure 2. The GeoNet prediction performance of the surface NO_2 concentration compared to the validation samples, based on different input datasets of meteorology and atmospheric composition: (**a**) use ERA5 meteorology and fill satellite measurement gaps with WRF-Chem simulated NO_2; (**b**) use ERA5 meteorology and NO_2 fill-value of zero for over gaps; (**c**) use CAMS meteorology and NO_2 fill-value of zero for gaps; (**d**) use CAMS meteorology and CAMS NO_2. The left plot shows the scatter comparisons between GeoNet predictions and site observations, while the right plot shows the bias distribution between the two.

Figs. S5-S8 provide an overview of the major metrics (e.g., R^2, RMSE, MAE, and MPE) of GeoNet prediction performance varying with prediction hours from t+4h to t+24h in different months. The results indicate that the model exhibits a higher correlation in NO_2 forecast during the spring and winter seasons compared to the summer, while the RMSE errors show the opposite trend. This could be attributed to much higher NO_2 pollution levels in winter months. Additionally, GeoNet's NO_2 prediction errors gradually increase during the next 24 hours, particularly after t+20h. This is primarily due to the short lifetime of atmospheric NO_2, leading to a diminishing constraint from historical observational data on future NO_2 predictions. Similar phenomena are also observed in machine learning or model-assisted weather forecasts (Andersson et al., 2021).

To assess the GeoNet model's performance for short-term pollution events, we compared it with near-surface NO_2 from CAMS forecasts, and in situ observations from CNEMC ground stations. Fig. S9 illustrates the daily time series of t+4h NO_2 from GeoNet, CAMS, and CNEMC for three typical sites in Beijing, Shanghai, and Guangzhou in 2021. As shown from the plot, NO_2 predictions by both GeoNet and CAMS generally agreed with the variation trends of CNEMC measurement. However, CAMS forecasts systematically overestimate the surface NO_2 concentration by 100%, possibly resulting from the biases in the NO_x emission inventory (Douros et al., 2023). Compared to CAMS, the GeoNet prediction closely aligns with the ground-truth observations at CNEMC sites over eastern China, with an overall $R^2 > 0.5$ and mean bias < 5 μg/m^3 for polluted regions (see Fig. S10 and S11, respectively).

3.2 Main factors in NO_2 forecast and their implications

Previous physics-based numeric models of air quality prediction, e.g., the CAMS global forecast model and the regional WRF-CMAQ model (Kuhn et al., 2024; Kumar et al., 2021; Liu et al., 2023), can simulate the atmospheric physical and chemical processes (such as advection, diffusion, deposition, and chemical reactions) by solving the atmospheric equations. Recent data assimilation techniques further take real-time monitoring data from satellite and ground-based platforms as model constraints to better predict air quality variables (Antje Inness et al., 2022). Compared with physics-based models, "black-box" models such as the deep learning technique usually lack interpretability and explainability (Q.-s. Zhang & Zhu, 2018). This hinders the understanding and implications for predicting air quality variables such as NO_2. Here, we measure the relative importance of each input feature on the NO_2 forecast accuracy, by iteratively permuting the input array and observing its influences on the model prediction.



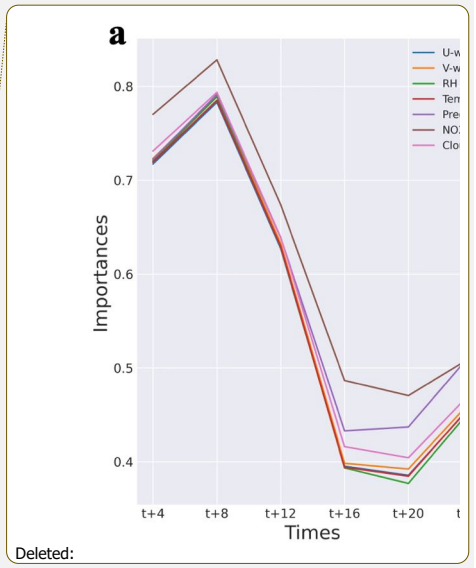


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Figure 3. (a) The overall relative importance of different input features such as wind, surface pressure, satellite NO_2, and cloud mask, in GeoNet NO_2 forecast, varying with different hour steps from t+4h to t+24h. (b) The spatial distribution of the relative importance of satellite NO_2 measurements in the GeoNet NO_2 forecast in 2021.

Fig. 3a presents the relative importance ($1\text{-}R^2$) of different input features varying with prediction hour steps from t+4h to t+24h. The geostationary satellite NO_2 measurements play the highest role in predicting surface NO_2 levels of the next day, although it degrades after t+8h. Other meteorological input features also show a major impact on NO_2 prediction performance. The significance of the different input variables remained generally consistent across seasons, with minor variations (as shown in Fig. S12). By permutating the input array for each ground pixel, Fig. 3b derived the spatial distribution of the relative importance of geostationary satellite NO_2 in the predicting performance. Overall, satellite NO_2 has a higher impact in densely populated areas experiencing severe air pollution, such as the Pearl River Delta, Yangtze River Delta, and Jianghuai Plain, than in western China. Such results highlight the underappreciated role of satellite NO_2 measurements with high spatial and temporal coverage in air pollution forecasts.

3.3 NO_2 pollution episodes and health exposure forecast

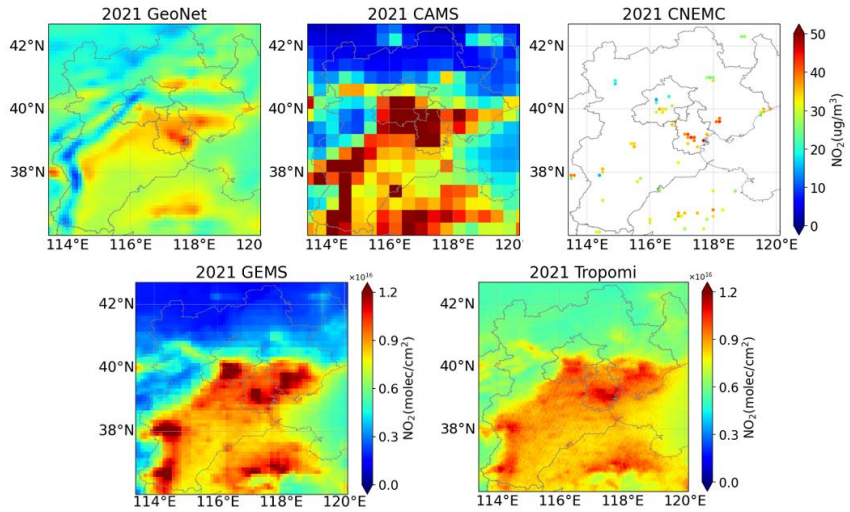

Figure 4. The comparisons of annual surface NO_2 concentrations from GeoNet, CAMS, and CNEMC, respectively, (in the top panel), as well as the tropospheric NO_2 column observations from GEMS and TROPOMI over East China in 2021 (in the bottom panel).

Beyond its prediction accuracy, GeoNet exhibits a pronounced advantage in spatial coverage and resolution, allowing for capturing finer-scale details in the pollutant distribution. Illustrated in Fig. 4, GeoNet demonstrates remarkable performance in predicting spatial nuances of NO_2 pollution, particularly when contrasted with ground-based and satellite observations. During a typical winter NO_2 pollution event (as shown in Fig. 5), GeoNet accurately simulates a significant decrease in concentrations at 11:00 and 15:00, probably led by intense photochemical activity in the daytime, coincident with ground-based observations. It also outperforms CAMS in predicting NO_2 variations throughout the day. The GeoNet model also retains the distributional differences in NO_2 concentrations between urban and rural areas, consistent with emission source characteristics and satellite observations. The suboptimal performance of CAMS predictions can be attributed to insufficient observational constraints and the use of outdated emission inventories (Douros et al., 2023). In the European region, the assimilation of TROPOMI observations into CAMS forecasts significantly improves the

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simulation accuracy of near-surface NO_2 concentrations and tropospheric column densities (A. Inness et al., 2019). Neural network methods, similar to GeoNet, could be used to correct and downscale forecast results by existing models (Baghanam et al., 2024). This approach holds promise for achieving operational air quality forecasts that balance efficiency and accuracy.

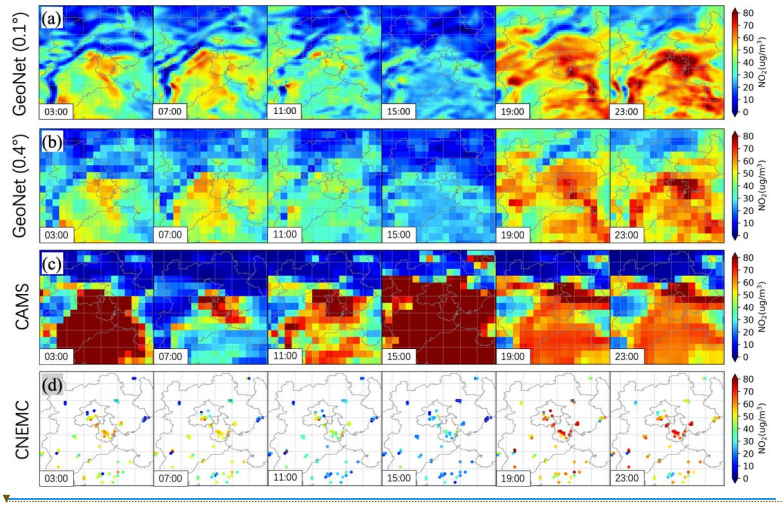
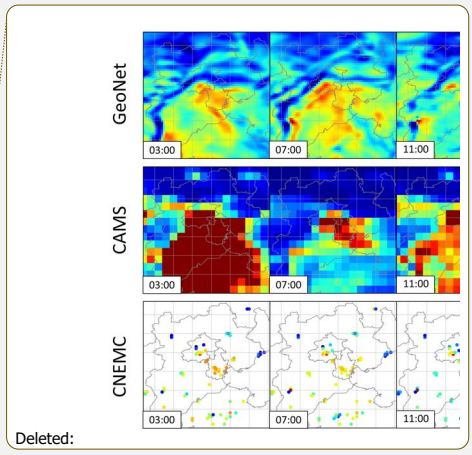


Figure 5. The spatial distribution comparisons of surface NO_2 concentration between (a) GeoNet prediction at the original resolution of 0.1°, (b) GeoNet prediction resampled to the CAMS resolution of 0.4°, (c) CAMS prediction, and (d) ground-based CNEMC site measurements. Note that the results are presented for different continuing local hours (labeled text in the subplot) on 23 November 2021.

In this study, we used a simplified linearized risk model for the short-term NO_2 exposure (Meng et al., 2021; C. Zhang et al., 2022) to calculate the distribution of all-cause mortality risks based on GeoNet NO_2 predictions (see Fig. 6). Short-term NO_2 exposure leads to remarkable regional differences in all-cause mortality, which are mainly concentrated in highly polluted and densely populated urban areas. For both urban and suburban locations in Beijing (see Fig. 6c-d), GeoNet-based NO_2 pollution exposure predictions are more consistent with actual in situ observations than the CAMS forecasts. Current air quality health indices forecasting based on limited station data has significant gaps, making it difficult to meet the refined needs for different populations in urban, suburban, and rural areas. Integrating GeoNet



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forecasts based on hourly geostationary satellite observations can support spatially comprehensive and fine-scale air quality health risk prediction. This, in turn, guides managing the risks of air pollution exposure-related diseases in sensitive populations and communities.

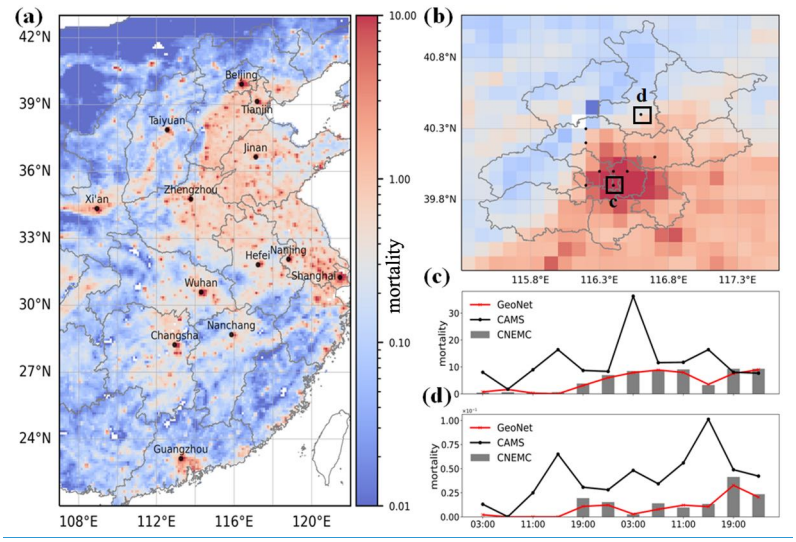

Figure 6. Mortality risk of short-term NO_2 exposure based on the GeoNet prediction on November 23, 2021. (**a**) mean mortality due to the predicted NO_2 exposure in East China; (**b**) a zoom-in map over Beijing and its neighboring area; (**c**) and (**d**) are comparisons of mortality estimation over the Beijing urban and rural regions (the rectangle areas presented in **b**), respectively, based on different NO_2 exposure prediction among GeoNet, CAMS, and CNEMC.

4 Conclusion

The GeoNet model utilizes the unprecedented hourly air quality observations from geostationary satellites and resolves nonlinear associations in spatiotemporal proximity across multiple data sources. It achieves seamless short-term regional air quality predictions, exhibiting significant performance advantages over existing machine-learning air quality prediction models. To strike a balance between real-time and accuracy requirements, we evaluated the impact of using reanalysis- and forecast-based meteorology datasets, as well as imputing the missing values of satellite NO_2. The findings reveal that the GeoNet model demonstrates robust generalization across diverse datasets, with minimal fluctuations in

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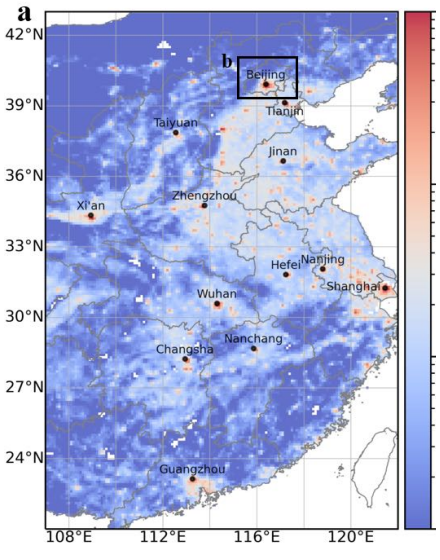

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prediction performance. Overall, the model achieves an RMSE of 12.31 μg/m^3 and an R^2 of 0.68 in predicting NO_2 concentrations every 4 hours for the next 24 hours. However, validation accuracy notably diminishes after t+16h within the next 24 hours, with stronger predictive correlations observed in seasons characterized by severe pollution, such as spring and winter, compared to summer. The variation of the model forecasting performance also shows that accurate prediction for longer time windows and heavy pollution events is still a major difficulty. This may be due to the high level of uncertainty in emissions and meteorology. In the future, a combination of higher resolution and more accurate multi-source data constraints, as well as machine learning models coupled with atmospheric physical mechanisms, may be needed to improve the existing forecasts.

Compared to traditional chemical model forecasts and data assimilation predictions, the GeoNet model handles various data sources, including meteorological simulations and air quality observations, and more accurately captures spatial intricacies of air pollution evolution. The GeoNet framework elucidated in this study forecasts short-term near-surface NO_2 concentrations and demonstrates transferable learning potentials for predicting other pollutants. This work also has important implications for the prediction of near-surface O_3 and particulate matter. For example, the integration of using vertical O_3 profiles from the GEMS satellite, in particular near-surface layer concentrations, and their joint observations of important O_3 precursors including NO_2 and HCHO, is expected to significantly improve the uncertainty of existing estimates of near-surface air pollution. This study underscores the pivotal role of next-generation stationary satellite observations of air pollution constituents in air quality forecasting, with the potential to advance operational air quality forecasting and mitigate associated health risks by integrating machine learning technologies.

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Data and code availability. The GEMS NO_2 v2.0 data is available from the National Institute of Environmental Research (NIER) of South Korea (https://nesc.nier.go.kr/en/html/index.do, last access: December 10, 2023). We downloaded the NO_2 measurements from the CNEMC real-time air quality platform (https://air.cnemc.cn:18007/, last access: Jun 8, 2023). ERA-5 reanalysis meteorological data is obtained from the European Center for Medium-Range Weather Forecasts (https://climate.copernicus.eu/climate-reanalysis, last access: December 8, 2023). CAMS forecast of meteorological and atmospheric NO_2 datasets are retrieved from the CAMS Atmosphere Data Store (https://ads.atmosphere.copernicus.eu/, last access: December 8, 2023). The source codes of the GeoNet model, surface NO_2 prediction, and necessary input data can be obtained from Chengxin Zhang (zcx2011@ustc.edu.cn) upon reasonable request.

Contributions: C.Z. implemented the GeoNet model and analyzed the data. C.L. supervised the study. C.Z. wrote the manuscript with input from all co-authors.

Competing interests: The contact author has declared that none of the authors has any competing interests.

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