Dear Editor and Reviewer,

We are grateful for the helpful comments. We have made the modifications in response to comments. Attached is a point-by-point response to the comments. We hope that you and the referees will find the changes satisfactory, and we look forward to hearing from you soon.

I) Comments from the editor

I am pleased to inform you that your manuscript is accepted for publication in ACP after considering the technical corrections given by the referee (see referee report) and the notification to the authors from review file validation (see box above) plus the ones from me listed in the following:

Comment: L213-214: "The XGBoost model was implemented in this study to convert columnar measurements into ground-level NO2 concentrations." and L215-216: "In this study, a nested machine learning model was developed to incorporate the NMH to convert columnar 215 measurements into ground-level NO2 concentrations."

Doubling? Please check and rephrase.

Response: Thank you for the comment. We have removed the doubling.

Comment: Is the XGBoost the machine learning model that you are using? If yes, you should clearly state this and decide if you then write in the following "XGBoost" or "machine learning model". Or are these two different models? Is XGBoost the model that you later (L234-235) denote as model 1 and the nested machine learning model the one you later denote as model 2?

Response: Thank you for the comment. Yes, the XGBoost model is the machine learning model that we used in this study. We have trained two models in our study. Model I is a basic XGBoost machine learning model trained without considering NMH. Model II is a nested XGBoost machine learning model, which includes an inner model designed to consider NMH as input parameters. Specifically, within this nested XGBoost machine learning model (Model II), the inner model predicts the NMH, which is then input into the main XGBoost model to predict ground-level NO₂ concentrations. We clarify the nested XGBoost machine learning model throughout the manuscript, such as (lines 236-238):

"To reveal the impacts of the NMH, we compared the performance of the basic XGBoost machine learning model without considering the NMH (Model I) and the nested XGBoost machine learning model after considering the NMH (Model II)."

Comment: L349: in further analyses -> in the further analyses

Response: Thank you for the comment. We have revised it accordingly (line 356).

Comment: L383: Abbreviation AQG has not been introduced? I found it in the introduction, but it would

be good to repeat it here.

Response: Thank you for the comment. We have revised and added it in lines 390-393.

"All provinces depicted population exposure levels of NO_2 exceeding the Air Quality Guidelines (AQG) levels of 10 µg/m³. Hainan Province had the lowest population-weighted mean NO_2 concentrations of 10.57 µg/m³, which closely approached the levels set by the AQG."

Comment: Figure 10 caption: "one standard deviation"? Do you mean one sigma standard deviation?

Response: Thank you for the comment. It is one sigma standard deviation and we added in the caption (line 410-411).

Comment: Figure 11 caption: same here

Response: Thank you for the comment. It is one sigma standard deviation and we added in the caption (line 434-435).

Comment: L428: average -> averaged

Response: Thank you for the comment. We have revised it accordingly (line 437).

II) Comments from referee:

The authors have revised the manuscript throughly. I believe it is ready for publication as long as several technical corrections are made.

Minor comments:

Comment: Line 23: This nested model was designed to ... and explore its impact on performance. Was this nested model really designed to explore its impact on performance? This statement sounds awkward.

Response: Thank you for the comment. We have revised the statement (line 26-27).

"This nested model was designed to directly incorporate NMH into the methodological framework to estimate satellite derived ground-level NO₂ concentrations."

Comment: Line 27: estimating ground-level NO2 concentration -> ground-level NO2 concentration estimates.

Response: Thank you for the comment. We have revised it accordingly (line 30).

Comment: Line 27: reducing bias and improving the R2 values to 0.93 ... -> reducing the bias by <a value> and improving the R2 values from <a value> to 0.93 ...

Response: Thank you for the comment. We have revised as per suggestion in lines 29-31.

"The inclusion of NMH significantly enhanced the accuracy of ground-level NO₂ concentration estimates, i.e., the R^2 values were improved from 0.73 to 0.93 in 10-fold cross-validation and

from 0.88 to 0.99 in the fully trained model."

Comment: Line 136: According to Kim et al. (2020), the nominal spatial resolution of GEMS baseline products is ~7 km x 8 km. However, the GEMS NO2 product has a spatial resolution of ~7 km x 8 km x 2 px (due to spatial bining, i.e., ~ 14 km x 8 km). Please double check if your statement is correct here.

Response: Thank you for the comment. We have checked the statement and described it in lines 139-140.

"The nominal spatial resolution of the GEMS NO₂ product was 7 km × 7.7 km, by binning two pixels of 3.5 km × 7.7 km each (Ahmad et., 2024)."

Comment: Line 261: Suggest replacing semicolons (;) with commas (,) in this sentence.

Response: Thank you for the comment. We have replaced the semicolons with commas in the sentence as per suggestion.

Comment: Line 263: Is 365 the maximum value or the maximum possible value?

Response: Thank you for the comment. 365 is the maximum possible value here. We have revised accordingly in line 267.

Comment: Line 280: Looks like you are interpreting m differently here and in Line 263. Try to avoid this as it may confuse the readers. One possible solution is to use one letter for 24 hours of a day, and another letter for 365 days of a year (366 if a leap year).

Response: Thank you for the comment. To avoid possible confusion for the readers, we have added a new equation to obtain the annual correction factor and its corresponding description in lines 282-288.

"Similarly, to obtain the annual correction factor, we estimated the ratio between the annual average of all available ground-measured NO_2 concentrations for 24 hours and the annual average of ground-measured NO_2 when the satellite data was available (Eq. 3).

$$F = \frac{\frac{1}{j} \sum_{i=1}^{j} C_g(i)}{\frac{1}{p} \sum_{i=1}^{p} C_g(i)}$$
(3)

Here, *F* represents the annual correction factor, C_g represents ground-measured NO₂ concentrations, *j* shows all ground measurements of NO₂, and *p* corresponds to ground measurements of NO₂ only when the satellite data was available. For the annual correction factor, the maximum possible value of *j* index in Eq. 3 is 8760 for one year."

Comment: Figure 3: Is 'Tree-n' supposed to be the same as 'Tree-1'? Also, the placement of 'Ground Measured NO2', 'Output', and 'Input' (the bottom one) looks confusing. I suggest placing all inputs at top and te output (ground-level NO2 predictions) at bottom, and reorganizing your arrow/flows accordingly.

Response: Thank you for the comment. The trees from Tree-1 to Tree-n could be different. We have

modified the subplot for Tree-n. Further, Fig. 3 has been revised as per suggestion. All the inputs are placed on top and output at bottom.

Comment: Figure 13: Vertical bars are overlapping.

Response: Thank you for the comment. We have replotted the figure to solve the overlapping issue.

III) Comments from Notification to the authors:

Comment 1:

The system indicates that at least one of the (co-)authors is a member of the editorial board of ACP (Fangqun Yu). Please add this information into the *.pdf manuscript under the headline "Competing interests" with the next revision. See more: https://www.atmospheric-chemistry-and-physics.net/submission.html#manuscriptcomposition > 16. Competing interests > 3.

Response: Thank you for the comment. We have added the information accordingly (line 673-674).

Comment 2:

Please ensure that the colour schemes used in your maps and charts allow readers with colour vision deficiencies to correctly interpret your findings (see e.g. F09). Please check your figures using the Coblis Color Blindness Simulator (https://www.color-blindness.com/coblis-color-blindness-simulator/) and revise the colour schemes accordingly.

Response: Thank you for the comment. We have revised the colour schemes of F09, F10, F11 as per suggestions.