A LASSO-based reduced-form CMAQ model for predicting ozone and $PM_{2.5}$ responses to emission changes in South Korea

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Abstract

Reduced-form models of the Community Multiscale Air Quality Modeling System (CMAQ) enable efficient prediction of air quality responses to emission changes. In this study, we developed a reduced-form CMAQ model based on the least absolute shrinkage and selection operator (LASSO) to approximate CMAQ outputs in high-dimensional settings where the number of emission variables exceeds the number of training samples. CMAQ simulations were generated using 118 emission scenarios covering seven emission sectors across 17 provincial-level administrative regions in South Korea. To account for the bounded nature of pollutant concentrations and to better represent nonlinear responses, an adaptive logit transformation was applied within the LASSO framework. The model was trained on 100 simulations and evaluated on 18 test scenarios, achieving mean root mean square errors of 0.1 ppb for ozone and 0.1 μg/m^3 for $PM_{2.5}$. The model also identifies a small subset of influential sector–region emission variables, enabling interpretable analysis of emission impacts and supporting the design of targeted emission scenarios. A web-based interface was developed to demonstrate the applicability of the approach, allowing interactive exploration of pollutant responses to emission changes. The reduced-form model enables rapid prediction of air quality responses with substantially lower computational cost than CMAQ simulations.

Introduction

Air pollution poses significant risks to human health. Major pollutants, such as ozone and $PM_{2.5}$, are associated with premature mortality, particularly from cardiovascular and respiratory diseases [1-5]. Controlling their ambient concentrations is therefore important and requires the regulation of precursor emissions. However, predicting the effects of emission controls is challenging because of diverse meteorological conditions and complex chemical reactions. Chemical transport models [6] are extensively used for this purpose. Among them, the Community Multiscale Air Quality Modeling System (CMAQ) is one of the most widely applied models [7].

CMAQ integrates meteorological and emissions data to simulate hourly pollutant concentrations but requires substantial computational resources. For example, a single control-policy simulation over several months can take multiple days on a typical computing server. As a result, comparing a large number of emission control scenarios using CMAQ alone is impractical.

To address this issue, reduced-form models have been developed to approximate CMAQ responses to emission changes. Among them, response surface models based on multidimensional kriging have been proposed as fast surrogates for CMAQ [8, 9], and later improved by integrating principal components analysis with statistical kriging for ozone prediction [10]. Polynomial-based response surface models have also been developed [11]. Subsequent studies extended this framework using deep learning and regression-based input selection methods [12, 13]. More recently, various deep learning approaches have been explored for efficient emulation of CMAQ [14-17]. These approaches aim to efficiently approximate CMAQ responses to emission changes using statistical or machine learning models.

However, air quality policy analysis often requires evaluating emission controls across multiple sectors and regions, which can lead to a large number of emission variables. Because CMAQ simulations are computationally expensive, the number of available training scenarios is typically limited. As a result, the number of input variables may exceed the number of training samples, leading to a high-dimensional regression setting that poses challenges for reliable model estimation. Many existing reduced-form

approaches have been developed for problems with relatively small numbers of emission variables. Deep learning approaches have also been explored for CMAQ emulation, but they usually require large training datasets and may be less suitable when the number of variables is large relative to the number of training samples.

To address this challenge, we develop a reduced-form CMAQ model for efficiently evaluating emission scenarios for ozone and $PM_{2.5}$. The emission inventory considered in this study includes 119 sector–region emission variables, representing seven emission sectors across 17 provincial-level administrative regions in South Korea. The proposed model is based on the least absolute shrinkage and selection operator (LASSO) [18], a linear regression method that is well suited for problems with many predictors and limited training data [19]. In addition to improving model generalization, LASSO performs variable selection, allowing the identification of sector–region emission variables that most strongly influence ozone and $PM_{2.5}$ concentrations. Because ozone and $PM_{2.5}$ concentrations often exhibit nonlinear relationships with precursor emissions [20-23], we introduce a nonlinear transformation of the response variable within the LASSO framework. The resulting model enables rapid prediction of hourly pollutant concentrations while maintaining the ability to approximate CMAQ outputs. Consequently, the proposed reduced-form model facilitates efficient evaluation of air quality responses to emission changes.

Materials and methods

CMAQ simulations

The CMAQ simulation domain covered South Korea with 67 × 82 grid cells at a spatial resolution of 9 km × 9 km. Baseline emissions were based on the 2015 national emission inventory provided by the National Institute of Environmental Research, Korea, through an official data request in July 2018. The original emission source categories were aggregated into seven sectors: Power, Industry, Residential,

Solvent, Mobile, Agriculture, and Others (S1 Table). Emissions were reported for the 17 provincial-level administrative regions in South Korea (hereafter regions; Fig 1).

Fig 1. CMAQ simulation domain. The 17 provincial-level administrative regions are shown in different colors, with their names indicated.

Emission control scenarios were generated by randomly scaling each of the 119 sector-region emission variables (7 sectors × 17 regions) between 0.5 (50% reduction) and 1.5 (50% increase). Using Latin hypercube sampling [24], 118 scenarios were generated to evenly cover this range. Emissions for these scenarios were converted to hourly values for all grid cells using the SMOKE-Asia model [25] and used as inputs to CMAQ.

Meteorological inputs were generated from the Weather Research and Forecasting model version 3.9.1 [26] with 2017 as the reference year. CMAQ version 4.7.1 [27] was run for four representative months—January, April, July, and October—representing winter, spring, summer, and fall. These simulations produced hourly ozone and $PM_{2.5}$ concentrations for all grid cells over 123 days (31 days for January, July, and October; 30 days for April). Hourly concentrations were extracted for each grid cell and used to train and evaluate the reduced-form models.

Machine learning-based reduced-form CMAQ models

A reduced-form CMAQ model was developed to learn the relationship between emission control scenarios and pollutant concentrations using the CMAQ simulations described above. Each scenario was represented by 119 input variables corresponding to emission scaling factors for seven sectors across 17 regions.

Among the 118 CMAQ simulations, 100 were used for training and 18 for evaluation. Each example consisted of an emission control scenario and the corresponding CMAQ-simulated ozone or $PM_{2.5}$

concentrations. The number of predictors (119) exceeds the number of training samples (100), resulting in a high-dimensional regression setting.

The model predicts hourly pollutant concentrations for each grid cell and time step. Separate models were built for ozone and $PM_{2.5}$, and independent models were trained for each grid cell and hour. In total, 16,218,288 models (24 hours × 123 days × 5,494 grid cells) were trained for each pollutant, each mapping the 119 emission variables to a single concentration value at a specific grid cell and hour.

The reduced-form model is based on LASSO, which performs coefficient shrinkage and variable selection. The regularization parameter λ was selected using five-fold cross-validation on the training data. In some cases, the training responses showed little variation across emission scenarios. When the number of unique response values in the training data was five or fewer, LASSO training was skipped and the mean response value was used instead.

Because ozone and $PM_{2.5}$ concentrations are nonnegative and exhibit nonlinear relationships with precursor emissions, we applied an adaptive logit transformation to the response variable:

$$\log\left(\frac{Y}{y_{upper}-Y}\right), \quad (1)$$

where Y is the pollutant concentration and y_{upper} is defined as the maximum concentration in the training data plus its standard deviation. This transformation constrains predictions within the range $(0, y_{upper})$ and improves the ability of the linear model to represent nonlinear concentration responses.

Model performance was evaluated using the root mean square error (RMSE) between predicted and CMAQ-simulated concentrations. To ensure robust evaluation, the 118 scenarios were randomly divided into training and test sets (100 and 18 scenarios), and this procedure was repeated ten times with different random splits. RMSE values were averaged across the repetitions.

Results

Prediction accuracy of the reduced-form model

This subsection evaluates the prediction accuracy of the proposed reduced-form CMAQ model. Using 100 CMAQ simulations for training, the reduced-form model reproduced CMAQ outputs with high accuracy. In the CMAQ simulations, the average ozone concentration was 41.5 ppb. The reduced-form model achieved a mean RMSE of approximately 0.1 ppb across all grid cells and hourly predictions, indicating that the prediction error is small relative to the magnitude of the simulated concentrations. Similarly, the average $PM_{2.5}$ concentration in the CMAQ simulations was 12.1 $\mu g/m^3$. The reduced-form model produced a mean RMSE of approximately 0.1 $\mu g/m^3$, again indicating high predictive accuracy.

Figure 2 compares the CMAQ-simulated concentrations to the reduced-form model predictions for the test scenarios. The predictions closely follow the one-to-one line for both ozone ($R^2 = 0.9998$) and $PM_{2.5}$ ($R^2 = 0.9997$), indicating that the reduced-form model accurately reproduces CMAQ variability across grid cells and time steps.

Fig 2. Scatterplots comparing CMAQ-simulated and model-predicted pollutant concentrations. Each point represents a grid cell-hour pair from the test scenarios for (A) ozone and (B) $PM_{2.5}$. Due to the large number of comparisons (18 test scenarios × 10 trials × 16,218,288 grid cell-hour pairs), 25% of the total data points are shown, while the reported R^2 and RMSE values are computed using the full dataset.

In some grid cells, particularly outside the 17 regions (e.g., ocean cells), the training data showed little variation across emission scenarios, so LASSO models were not fitted for those cells. As described in Materials and methods, the mean response value was used in such cases. Although this occurred in about 10% of all grid cells for ozone, it was uncommon within the 17 regions that are the focus of the analysis (S2 Table).

Spatial distribution of prediction errors

To examine spatial variations in model accuracy, RMSE values were calculated separately for each grid cell by aggregating prediction errors across all test scenarios and hourly predictions. Figure 3 shows the spatial distribution of RMSE for ozone and $PM_{2.5}$ concentrations. Overall, prediction errors remained small across most regions of South Korea. For ozone, RMSE values were typically around 0.1 ppb, with somewhat higher errors (up to about 0.5 ppb) observed in several localized areas. For $PM_{2.5}$, RMSE values were also generally close to 0.1 $\mu g/m^3$. Slightly higher errors (around 0.5 $\mu g/m^3$) were observed in a small number of localized areas (roughly two), and a single localized area showed higher errors reaching approximately 0.8 $\mu g/m^3$.

Fig 3. Spatial distribution of prediction errors. RMSE values for each grid cell for (A) ozone and (B) $PM_{2.5}$.

S1 Fig shows the spatial distribution of the standard deviation of CMAQ-simulated pollutant concentrations, which is similar to the pattern in Fig 3. This suggests that errors were higher in areas with greater concentration variability.

Interpretation of LASSO coefficients

A key advantage of LASSO is its interpretability. Each coefficient in an individual LASSO model represents the influence of emissions from a specific sector in a specific region on ozone or $PM_{2.5}$ concentrations at a particular location (grid cell) and time (hour). Across these models, an average of 23.5 variables for ozone and 22.0 for $PM_{2.5}$ had nonzero coefficients, meaning that only about 20% of the 119 emission variables were used to predict concentrations. This sparsity indicates that the model effectively selected the most influential emission variables.

Sectoral influence across regions

To examine the overall influence of emission sectors, coefficients from LASSO models for grid cell-hour pairs within the 17 regions were aggregated. For each sector, the absolute values of coefficients associated with its sector–region emission variables were summed across all models. The influence ratio for each sector was then calculated by dividing this sector-specific sum by the total sum across all sectors. The direction of influence of a sector was determined from the signed sum of the coefficients for that sector. These influence ratios and directions represent the overall effects of each sector across the 17 regions, averaged over grid cells and time steps.

Figure 4A shows the sectoral influences on ozone responses. The Mobile sector dominated the ozone response, accounting for 57.0% of the total influence. Most sectoral influences were negative, indicating that increased emissions from many sectors were associated with lower ozone concentrations. In contrast, emissions from the Solvent and Others sectors were generally associated with increased ozone concentrations.

Fig 4. Sectoral influences across the 17 regions. Sectoral influence ratios for (A) ozone and (B) $PM_{2.5}$ are shown. The colors of the ratio values indicate the direction of influence (positive in green, negative in red).

Figure 4B shows the sectoral influences on $PM_{2.5}$ responses aggregated across the 17 regions. The Agriculture sector had the largest influence (36.5%), followed by Industry (19.9%) and Mobile (18.5%). Unlike ozone, all sectoral influences were positive, indicating that increased emissions from these sectors were associated with higher $PM_{2.5}$ concentrations.

Sector-region influence for individual regions

To identify the most influential emission variables for each region, sector–region emission variables were analyzed separately by region. For each region, the absolute values of coefficients associated with each sector–region variable were summed across all models for grid cell-hour pairs within that region. The influence ratio for each variable was then calculated by dividing this sum by the total sum across all sector–region variables. The direction of influence of each sector-region variable was determined from the signed sum of its coefficients. The five variables with the largest influence ratios were identified as the most influential variables for each region (S2 and S3 Figs).

Across regions, the combined influence ratios of the top five variables ranged from 50.2% to 78.0% for ozone and 34.0% to 69.8% for $PM_{2.5}$, indicating that pollutant responses in each region were substantially influenced by a limited number of emission variables.

For ozone, the Mobile sector was consistently among the most influential variables across all regions. In many regions, ozone concentrations were influenced not only by local emissions but also by emissions from nearby regions, reflecting regional transport.

For $PM_{2.5}$, influential variables varied more across regions. The most influential variables were mainly from the Agriculture, Industry, Others, and Mobile sectors, although their relative importance differed by region. As with ozone, emissions from nearby regions often appeared among the most influential variables, indicating the importance of cross-regional effects.

Emission scenario design and evaluation

To demonstrate how the coefficient analysis can inform emission scenario design, we evaluated example scenarios based on the sector–region variables identified in the previous subsection. Seoul was selected for ozone and Jeju for $PM_{2.5}$, as the five most influential variables accounted for the largest shares of total influence in these regions (78.0% and 69.8%, respectively; see S2C and S3Q Figs). Emission scenarios were constructed by modifying these five variables for each selected region.

Starting from the baseline emissions, two scenarios were considered: a 10% reduction and a 10% increase in emissions for the selected variables, while all other emissions were held constant. The trained LASSO models were then used to predict the resulting changes in pollutant concentrations across the simulation domain.

For ozone in Seoul, a 10% reduction in the five most influential variables increased the annual mean concentration by 10.0% (12.0 to 13.2 ppb), whereas a 10% increase reduced it by 5.8% (12.0 to 11.3 ppb). For $PM_{2.5}$ in Jeju, a 10% reduction decreased the annual mean concentration by 1.1% (9.3 to 9.2 $\mu g/m^3$), while a 10% increase raised it by 1.1% (9.3 to 9.4 $\mu g/m^3$).

These results demonstrate that the proposed approach can identify a small subset of influential emission variables from a large candidate set and use them to construct targeted emission scenarios. In this study, the LASSO models reduced the 119 sector–region variables to a small subset, enabling efficient evaluation of emission control strategies focused on the most relevant sources.

Web server for rapid emission scenario evaluation

To facilitate practical use of the proposed model, we developed a web server that enables users to evaluate emission scenarios interactively (http://220.70.0.234:8080/). Users can specify emission changes for the sector–region emission variables, and the server then runs the LASSO-based reduced-form CMAQ model to predict air quality responses.

The server displays the resulting annual mean ozone and $PM_{2.5}$ concentrations on a map, showing grid cell-level values along with the overall mean and range across all grid cells. When a user hovers over a grid cell, the region containing the cell and the predicted annual mean concentration for that cell are shown. When a cell is clicked, the server provides the five most influential sector–region variables for that region along with their influence ratios. These variables provide guidance for designing targeted emission scenarios for the selected region.

In addition to map-based visualization, the server allows users to download hourly concentration files for the four simulated months (see Materials and methods). This enables more detailed analysis beyond the annual mean summaries shown on the map.

The publicly available web server is deployed on a system equipped with an Intel(R) Core(TM) i7-7700 CPU at 4.20 GHz with 44 GB RAM, on which execution of the reduced-form models for both ozone and $PM_{2.5}$ requires less than 30 seconds. This demonstrates that the web server can provide rapid evaluation of emission scenarios while retaining the spatial and temporal detail of CMAQ predictions.

Discussion

This study developed a LASSO-based reduced-form CMAQ model to efficiently evaluate air quality responses to emission changes across multiple emission sectors and regions. The model achieved high predictive accuracy for both ozone and $PM_{2.5}$, with very small RMSE values relative to the magnitude of the concentrations and near-perfect agreement with CMAQ outputs. These results demonstrate that the proposed approach can successfully approximate CMAQ responses despite the high-dimensional input space and limited number of training scenarios. The adaptive logit transformation further improved the model's ability to represent nonlinear concentration responses, which are commonly observed for both ozone and $PM_{2.5}$.

A key advantage of the proposed approach is its ability to identify a small subset of influential emission variables from a large set of sector-region combinations. Across all models, only about 20% of the 119 emission variables were selected, indicating substantial sparsity in the relationships between emissions and pollutant concentrations. This sparsity enables meaningful interpretation of model coefficients and facilitates the identification of key emission sources. The sectoral analysis showed that mobile emissions dominated ozone responses, whereas agricultural emissions played the largest role in $PM_{2.5}$ formation. These findings are consistent with the known roles of NO_x emissions in ozone chemistry and

ammonia emissions in secondary $PM_{2.5}$ formation, supporting the physical plausibility of the model results.

The results also highlight the importance of regional interactions in air quality responses. For both ozone and $PM_{2.5}$, influential variables often included emissions from nearby regions, indicating that pollutant concentrations are affected not only by local emissions but also by regional transport. This suggests that effective air quality management requires coordinated emission control strategies across administrative boundaries rather than region-specific policies alone.

The scenario analysis further demonstrates the utility of the proposed framework for emission scenario evaluation. By focusing on a small number of influential variables, the model enables the design of targeted emission scenarios that can produce meaningful changes in pollutant concentrations. For example, in regions where the most influential variables explain a large fraction of the total influence, such as Seoul for ozone and Jeju for $PM_{2.5}$, modifying these variables led to notable changes in concentrations. Specifically, reducing emissions from the most influential variables in Seoul increased ozone concentrations, whereas similar changes resulted in decreases in $PM_{2.5}$ concentrations in Jeju. These contrasting responses between pollutants highlight the pollutant-specific nature of emission impacts. Overall, the results illustrate how the model can provide insights into pollutant- and region-specific responses and support the development of more effective and region-specific emission scenarios.

Compared with existing reduced-form approaches, the proposed method is particularly well suited for high-dimensional settings where the number of emission variables is large relative to the number of training simulations. While deep learning models have been increasingly applied for CMAQ emulation, they typically require large training datasets and may be less interpretable. In contrast, the LASSO-based approach used here provides both computational efficiency and interpretability, making it suitable for applications with limited training data and a need for transparent analysis of emission scenarios.

The developed web server was used to demonstrate the practical applicability of the proposed approach by enabling rapid, interactive evaluation of emission scenarios. Through this interface, users can explore

air quality responses at the grid-cell level and identify key emission drivers for specific regions, illustrating how the model can support intuitive and efficient scenario design. The ability to generate predictions in under a minute highlights the computational efficiency of the reduced-form model compared with traditional CMAQ simulations, which require substantially longer run times.

Despite the advantages of the proposed approach, several limitations should be noted. First, the model was developed under fixed meteorological conditions based on a single reference year and does not account for meteorological variability. However, because this study focuses on relative changes in pollutant concentrations in response to emission perturbations, the use of a consistent reference year provides a stable basis for comparison. Second, the model does not explicitly represent temporal dynamics, as independent models were trained for each grid cell and time step. Third, emission scenarios were constructed by independently scaling sector–region variables, whereas real-world emission changes may involve dependencies across sectors and regions. Finally, the analysis is based solely on CMAQ simulations and was not evaluated against observational data.

Future work could address these limitations by incorporating meteorological variability and temporal dynamics into the modeling framework, enabling application beyond a single reference year. The framework could also be extended to additional pollutants beyond ozone and $PM_{2.5}$.

Conclusion

This study developed a LASSO-based reduced-form CMAQ model to efficiently evaluate air quality responses to emission changes across multiple sectors and regions. The model achieved high predictive accuracy while substantially reducing computational cost compared with full CMAQ simulations. By identifying a small subset of influential sector–region variables, the proposed approach enables efficient interpretation of emission impacts and the design of targeted emission scenarios. Overall, the results demonstrate that the proposed framework provides a practical and computationally efficient tool for emission scenario evaluation with high-dimensional inputs.

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Supporting information

S1 Fig. Spatial distribution of pollutant concentration variability. Standard deviation of CMAQ-simulated pollutant concentrations for each grid cell, for (A) ozone and (B) $PM_{2.5}$.

S2 Fig. Influence ratios of the top five sector-region emission variables for ozone in individual regions. Regions: (A) Incheon, (B) Gyeonggi, (C) Seoul, (D) Gangwon, (E) Chungbuk, (F) Sejong, (G) Daejeon, (H) Chungnam, (I) Gyeongbuk, (J) Daegu, (K) Ulsan, (L) Busan, (M) Gyeongnam, (N) Jeonbuk, (O) Gwangju, (P) Jeonnam, and (Q) Jeju. The colors of the ratio values indicate the direction of influence (positive in green, negative in red). The value in the lower right corner of each plot indicates the sum of the top five influence ratios.

S3 Fig. Influence ratios of the top five sector-region emission variables for $PM_{2.5}$ in individual regions. Regions: (A) Incheon, (B) Gyeonggi, (C) Seoul, (D) Gangwon, (E) Chungbuk, (F) Sejong, (G) Daejeon, (H) Chungnam, (I) Gyeongbuk, (J) Daegu, (K) Ulsan, (L) Busan, (M) Gyeongnam, (N) Jeonbuk, (O) Gwangju, (P) Jeonnam, and (Q) Jeju. The colors of the ratio values indicate the direction of influence (positive in green, negative in red). The value in the lower right corner of each plot indicates the sum of the top five influence ratios.

S1 Table. Grouping of the emission source categories into seven sectors.

S2 Table. Cases with insufficient variation for model training. A total of 162,182,880 cases were considered (5,494 cells × 123 days × 24 hours × 10 trials), of which 46,936,800 correspond to the 17 regions (1,590 cells × 123 days × 24 hours × 10 trials).

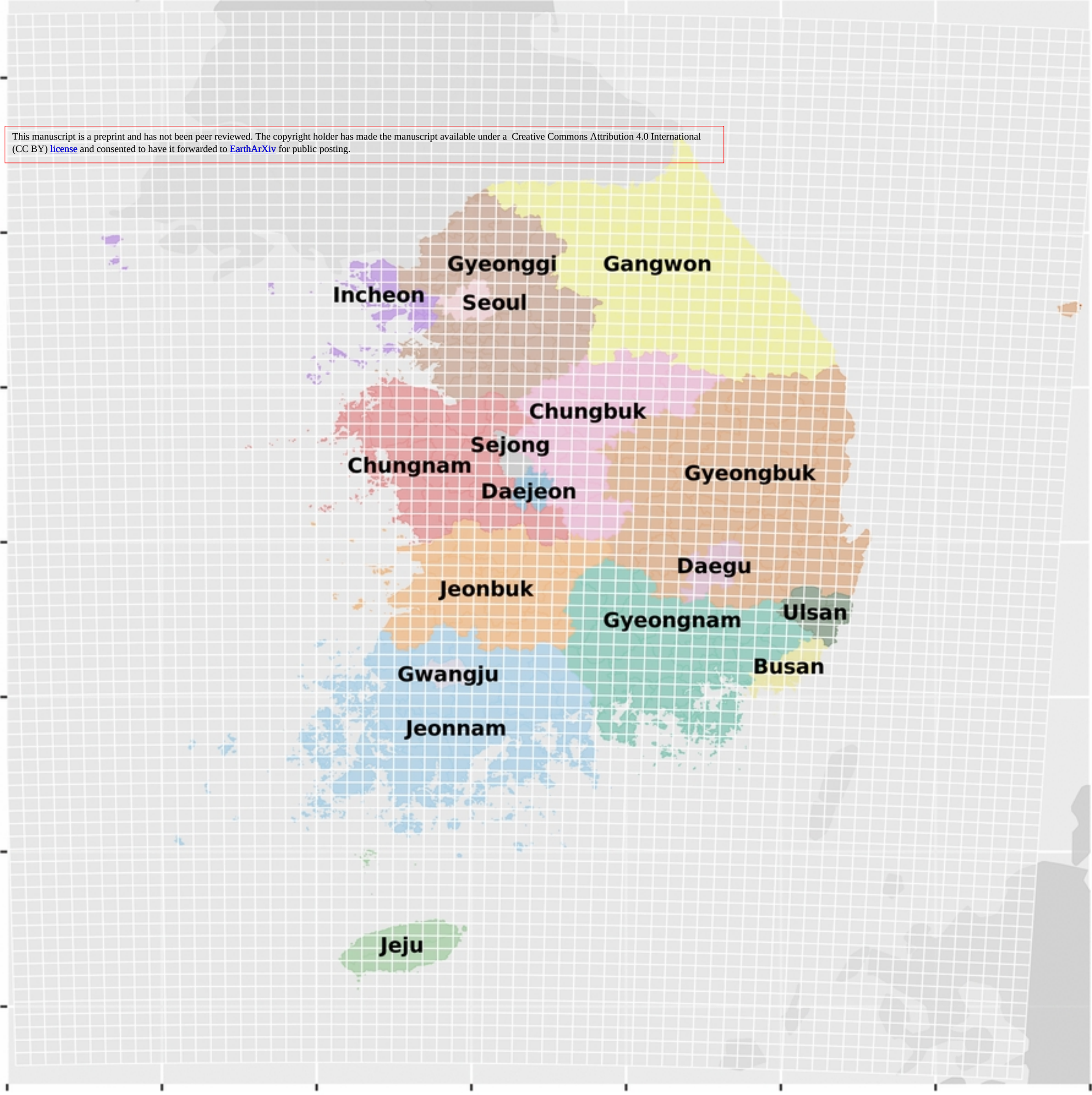


Fig 1

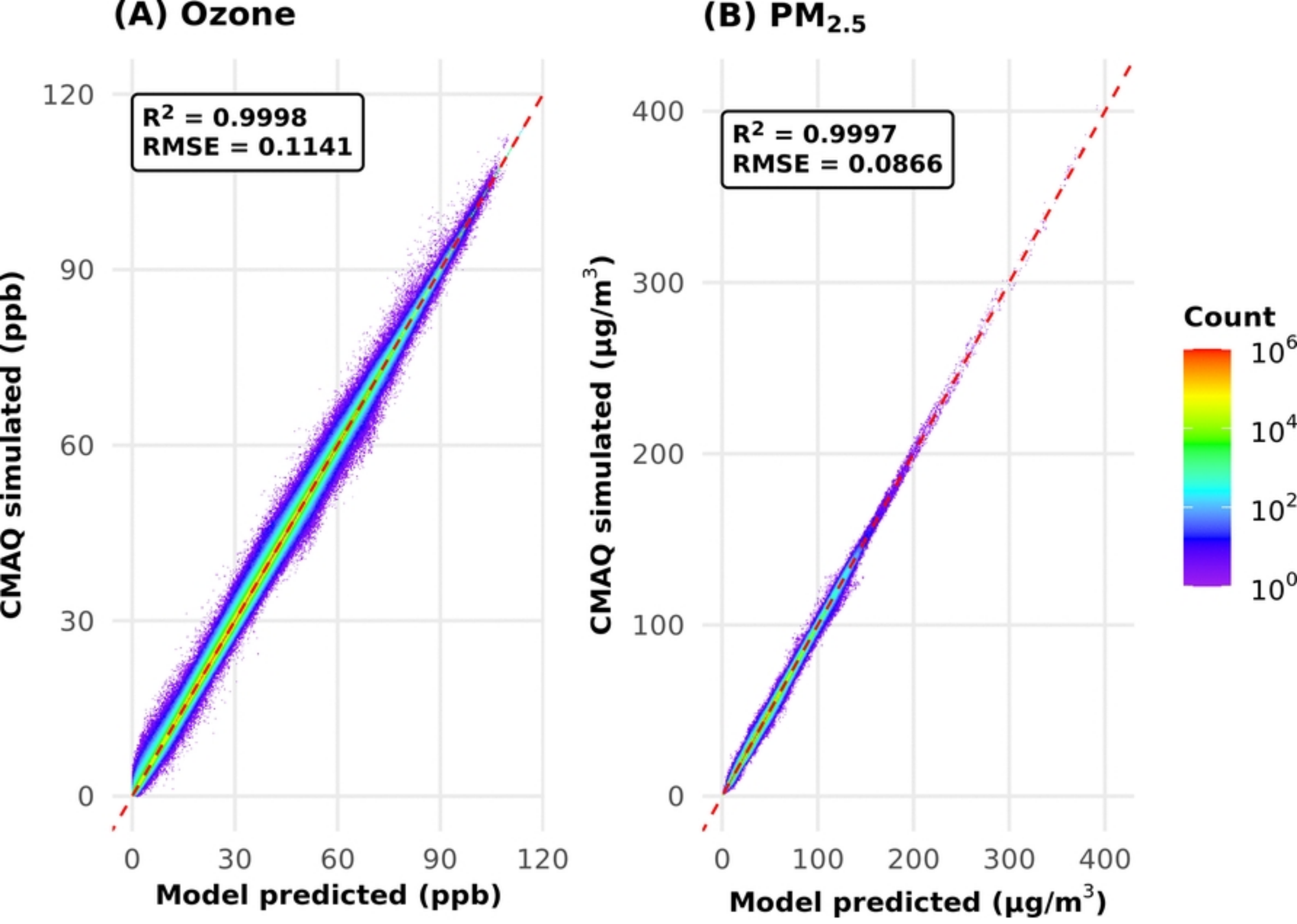
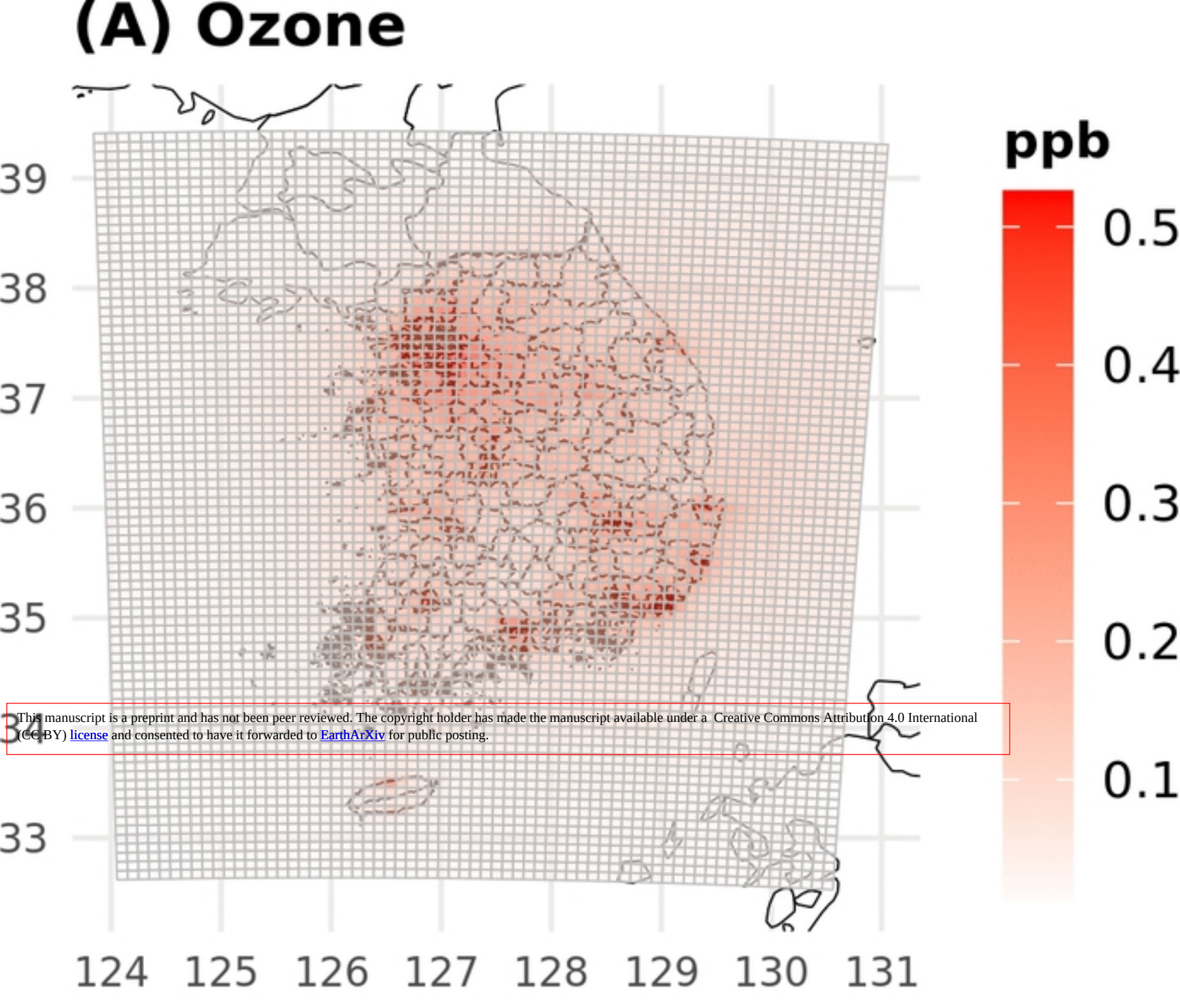

(A) Ozone
R² = 0.9998
RMSE = 0.1141
CMAQ simulated (ppb)
Model predicted (ppb)
0
30
60
90
120
(B) PM2.5
R² = 0.9997
RMSE = 0.0866
CMAQ simulated (µg/m3)
Model predicted (µg/m3)
0
100
200
300
400
Count
10^6
10^4
10^2
10^0

Fig 2



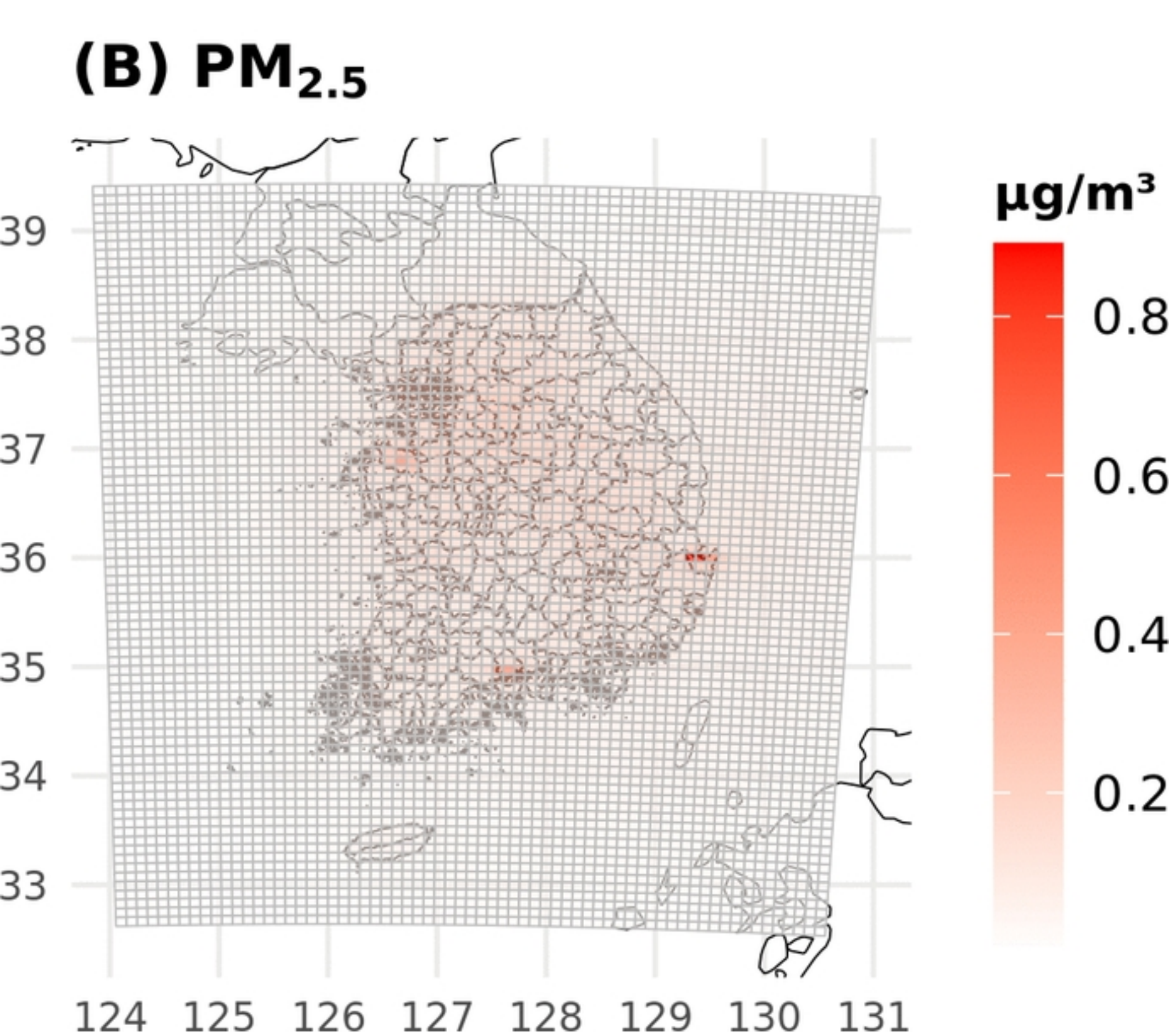


Fig 3

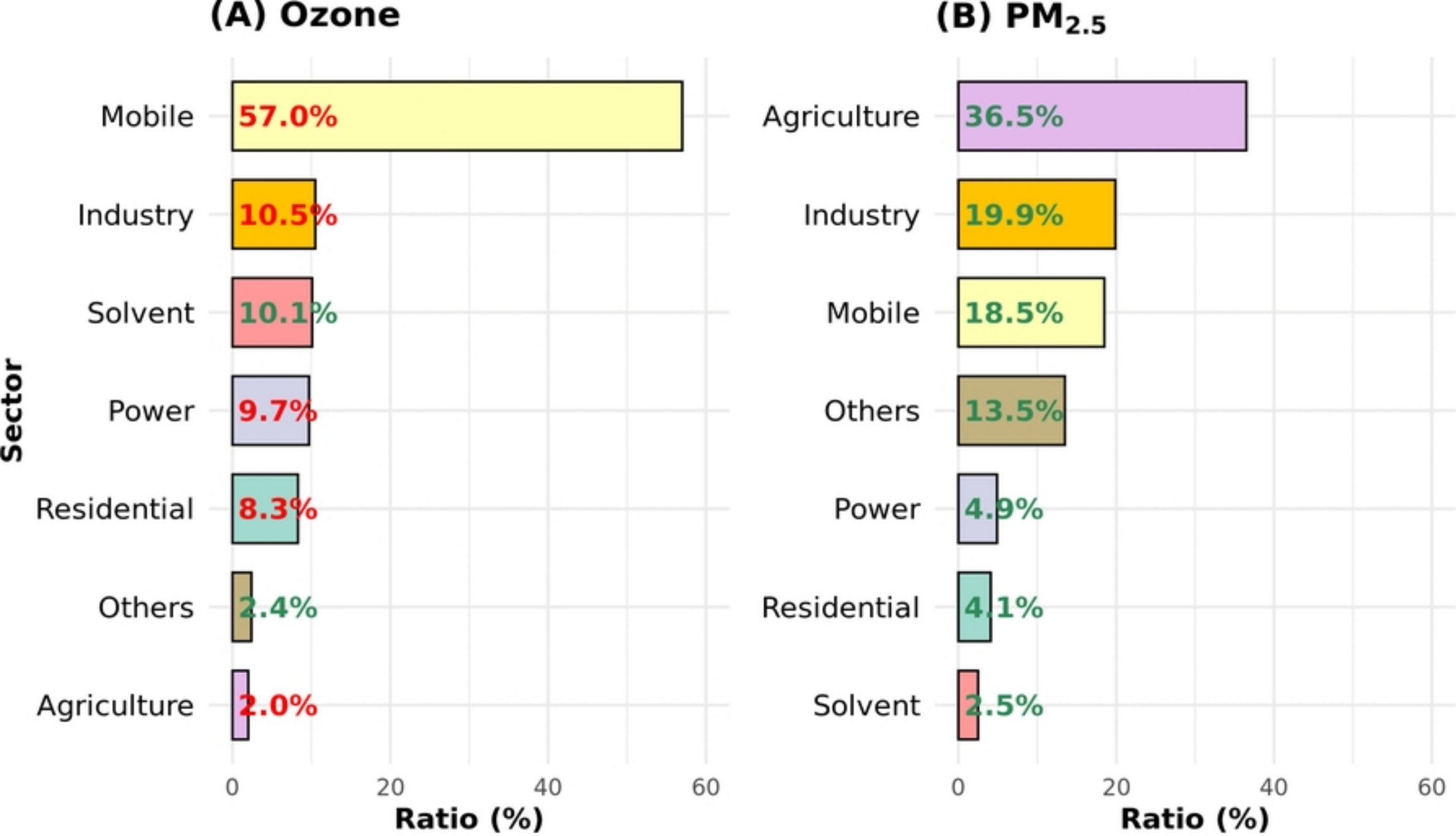

(A) Ozone
Mobile
57.0%
Industry
10.5%
Solvent
10.1%
Power
9.7%
Residential
8.3%
Others
2.4%
Agriculture
2.0%
Sector
0
20
40
60
Ratio (%)
(B) PM2.5
Agriculture
36.5%
Industry
19.9%
Mobile
18.5%
Others
13.5%
Power
4.9%
Residential
4.1%
Solvent
2.5%
0
20
40
60
Ratio (%)

Fig 4