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RESEARCH

Improvement of Speciated Anthropogenic VOC Emissions in Support of KORea-United States Air Quality (KORUS-AQ) Field Campaign

Jinseok Kim[1,2] · **Hyejung Hu**[2] · **Younha Kim**[3] · **Jung-Hun Woo**[2,4]

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Abstract

This study aims to improve the accuracy of anthropogenic volatile organic compound (VOC) speciation in Korea by developing region-specific chemical speciation profiles based on available Korean data supplemented with datasets from Northeast Asia. Current air quality modeling in Korea often relies on VOC emission profiles that inadequately represent domestic emission characteristics, leading to discrepancies between modeled and observed pollutant concentrations. In 2015, solvent use accounted for approximately 61% of national VOC emissions, while transportation was a major contributor in urbanized regions, together with residential combustion and industrial processes. Due to the limited availability of detailed, source-resolved VOC speciation measurements in Korea, this study combined domestic emission information with chemically resolved VOC composition data from Northeast Asia to address data gaps. These external datasets were not directly adopted but were systematically integrated and adjusted to reflect Korean emission sectors, activity patterns, and regulatory classifications. New source-specific profiles were developed with particular emphasis on solvent use and transportation, the two dominant VOC emission sources in Korea. Compared with the widely used KORea–United States emission inventory (KORUSv1) and the U.S. Environmental Protection Agency's SPECIATE profiles, the revised profiles increased aromatic allocations by 20–120% and olefin allocations by 24–40%, while reducing non-reactive VOC fractions by up to 95%. When implemented in the Community Multiscale Air Quality (CMAQ) model, these profiles significantly improved model performance. Nationwide correlation coefficients increased from 0.59 to 0.61 for ozone and from 0.40 to 0.60 for $PM_{2.5}$, while the mean $PM_{2.5}$ bias was reduced from -15.4 to $+3.0$ $\mu g\ m^{-3}$. In the Seoul Metropolitan Area, ozone correlation increased from 0.54 to 0.68 and $PM_{2.5}$ from 0.47 to 0.63. These results demonstrate that integrating Korean emission data with Northeast Asian chemical composition information effectively reduces uncertainties in secondary pollutant simulations and provides a stronger scientific basis for air quality management in Korea.

✉ Jung-Hun Woo
woojh21@snu.ac.kr

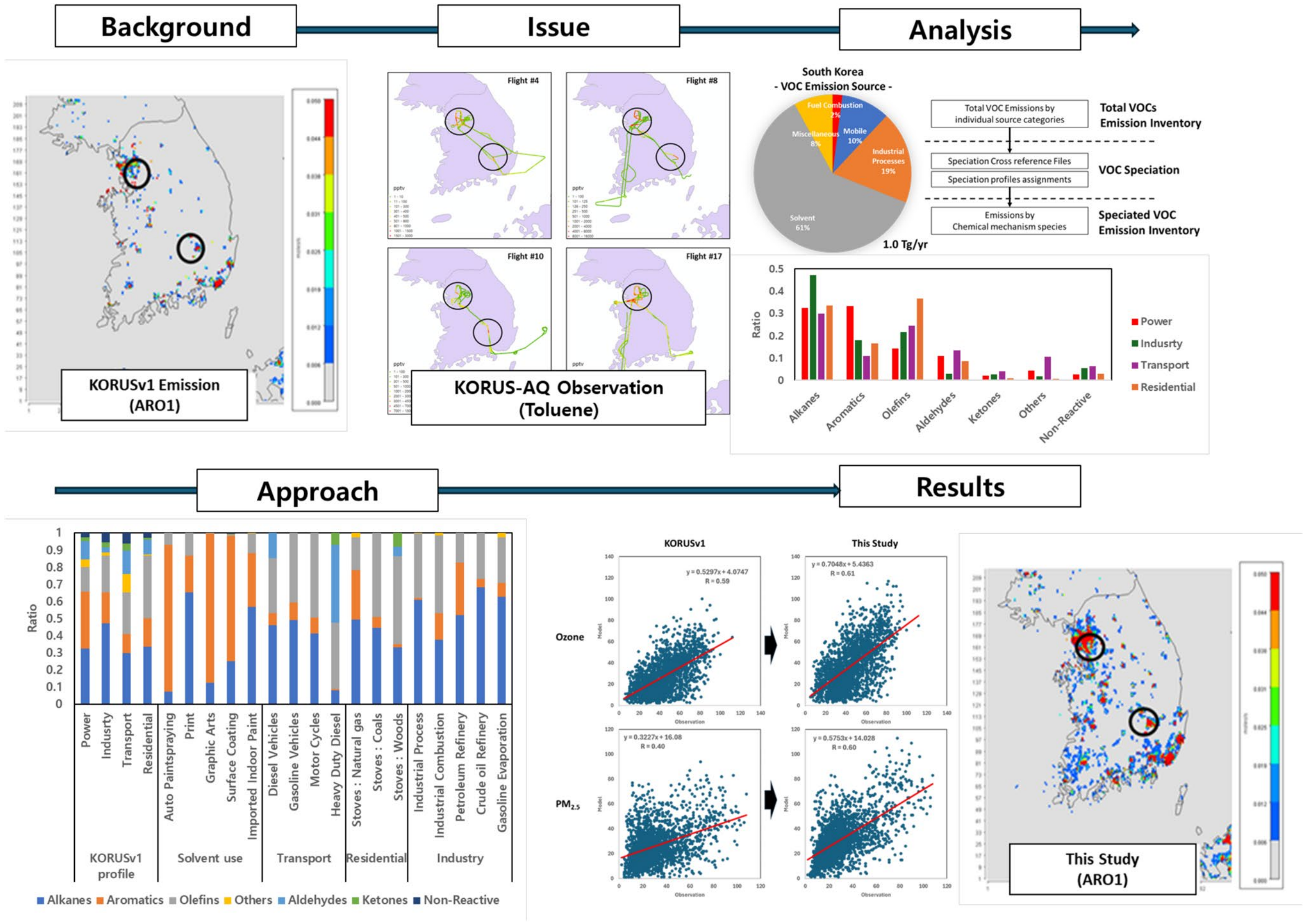
[1] Department of Advanced Technology Fusion, Konkuk University, 120 Neungdong-Ro, Gwangjin-Gu, Seoul, South Korea

[2] Environmental Planning Institute, Seoul National University, 08826 Seoul, South Korea

[3] International Institute for Applied Systems Analysis, 2361 Laxenburg, Austria

[4] Graduate School of Environmental Studies, Seoul National University, 08826 Seoul, South Korea

Graphical Abstract



Keywords KORUS-AQ · Speciated anthropogenic VOCs · Chemical speciation · Secondary pollutant · Emission processing

1 Introduction

Rapid industrialization and urbanization in East Asia have substantially increased anthropogenic emissions of air pollutants, including volatile organic compounds (VOCs). In Korea, VOCs play a particularly critical role in urban air quality because they are key precursors for the formation of tropospheric ozone and secondary organic aerosols (SOA). These pollutants not only degrade visibility and contribute to smog formation but also have profound impacts on public health and climate. Hence, accurate representation of VOC emissions in air-quality models is essential for both scientific understanding and policy formulation.

VOCs encompass hundreds of species with widely varying chemical reactivities and lifetimes. Their oxidation in the atmosphere drives the formation of photochemical oxidants and fine particles, thereby influencing the oxidative capacity of the troposphere. Because the reactivity and product yield of each compound differ markedly, total VOC emissions alone are insufficient for chemical transport modeling (CTM). Instead, VOC emissions must be chemically speciated—that is, decomposed into representative species or groups according to their molecular structure and reactivity within the mechanism used by the CTM. The accuracy of this speciation process directly determines the model's ability to reproduce observed concentrations of ozone and SOA. However, due to the difficulty of building emission inventories with detailed speciation, most inventories report only total VOC emissions without distinguishing between species. Therefore, chemical speciation profiles are commonly used to estimate the distribution of individual VOC species based on total VOC emissions for CTM modeling.

Furthermore, VOCs are not only precursors to secondary pollutants such as ozone and $PM_{2.5}$, but also often include several toxic chemical species such as benzene and toluene, which have high potential to cause cancer (Pan et al. 2015). Recent studies highlighting their impacts on various diseases and disorders have drawn increasing attention to the health effects of long-term exposure. In particular, aromatic and halogenated hydrocarbons are recognized as substances requiring special management because of their various adverse effects (Zhou et al. 2023; Li et al. 2023).

A chemical speciation profile provides the relative proportions of individual species in total VOC emissions and should ideally reflect the emission characteristics of the target region. Previous $PM_{2.5}$ and ozone modeling studies in Northeast Asia have utilized the U.S. Environmental Protection Agency (US EPA)'s SPECIATE database (https://www.epa.gov/air-emissions-modeling/speciate-4), including composite profiles tailored to national emission characteristics (Li et al. 2014, 2019). Korea lacks region-specific speciation profiles, leading researchers to rely on SPECIATE (Moon 2015; Kim and Kim 2000; Choi et al. 2017). Since this database does not fully capture the characteristics of Korean VOC emissions, it may lead to under- or overestimation of specific species.

These limitations were highlighted by the KORea–United States Air Quality (KORUS-AQ) campaign (Crawford et al. 2021), a collaborative air quality field study conducted by Korea's National Institute of Environmental Research (NIER) and National Aeronautics and Space Administration (NASA) from April to June 2016. During this study, CTM predictions were compared with airborne measurements. High concentrations of aromatic VOCs (e.g., toluene) were frequently observed over major urban areas such as the Seoul Metropolitan Area and Daegu (Simpson et al. 2020), but these were not reflected in the model results. This discrepancy arose because the VOC speciation profiles used in the models, based on the SPECIATE database, did not adequately reflect emission characteristics in Korean cities, resulting in underestimated emissions of aromatic VOCs.

Previous studies have similarly reported that the use of non-region-specific VOC profiles can lead to biased predictions of ozone and secondary organic aerosol. For example, Li et al. (2018) showed that chemical transport models using default SPECIATE profiles underestimated the contribution of aromatic compounds in East Asian megacities, resulting in a systematic low bias in peak ozone. Souri et al. (2020) also demonstrated that inaccurate VOC emissions were a primary driver of discrepancies between satellite-derived formaldehyde columns and model simulations across East Asia. More recently, Kim et al. (2022) found that missing reactivity from underrepresented VOC species led to underestimates of OH reactivity and ozone production during the KORUS-AQ campaign. In addition, Park et al. (2021) reported that revisions from the initial KORUSv1 inventory to updated speciation profiles substantially improved the performance of air quality simulations, particularly by reducing biases in ozone concentrations over the Seoul Metropolitan Area. Collectively, these studies underscore that the representativeness of VOC speciation profiles is a critical factor in reproducing observed levels of ozone and $PM_{2.5}$, emphasizing the necessity of developing localized profiles tailored to regional emission characteristics.

The characteristics of VOC emissions in the previously used chemical speciation profile, the KORUSv1 profile, are shown in Fig. S1. This profile was employed in the KORUS-AQ air quality campaign and is primarily based on emissions data from China, the largest VOC emitter in Northeast Asia (Model Inter-Comparison Study for Asia; MICS-Asia; Li et al. 2017).

Figure 1 shows the regional characteristics of VOC emissions in 2015, based on inventories from Korea (Clean Air Support System; CAPSS) (Lee et al. 2015), the United States (National Emission Inventory; NEI), Europe (European Monitoring and Evaluation Programme/European Environment Agency; EMEP/EEA) (EEA 2023), and China (KORUSv1). The comparison highlights differences in source contributions and regional characteristics. The primary sources of VOC emissions vary significantly across countries due to differences in industrial structure, energy use, and regulatory frameworks. A sector-by-sector comparison shows that solvent use is the largest source of VOC emissions in Korea (61%), while mobile sources dominate in the United States, industrial processes and product use are the main contributors in Europe, and household fuel combustion is the primary source in China.

While the relative contributions of emission sectors differ among countries, observational studies suggest that urban VOC composition in East Asian megacities shares common features. In particular, aromatic VOCs such as toluene, ethylbenzene, and xylenes are consistently reported as major components in major East Asian megacities, including Seoul, Beijing, and Shanghai. In addition, similar source characteristics have been identified, with traffic emissions and solvent use recognized as dominant contributors in these urban environments. To support this, we compiled and compared VOC composition and dominant species reported in previous studies (Cai et al. 2010; Cui et al. 2022; Han et al. 2023; Kang et al. 2022; Lee et al. 2023) for Seoul, Beijing, and Shanghai (Table S1). The comparison indicates that VOC mixtures in these East Asian megacities exhibit comparable compositional patterns, particularly with respect to aromatic compounds and their associated emission sources. This study aims to improve the accuracy of secondary pollutant simulations in Korea by developing chemical speciation profiles appropriate for the region. By applying VOC emissions that reflect Korea-specific characteristics, the simulation of $PM_{2.5}$ and tropospheric ozone—key indicators of air quality and climate change—can be enhanced.

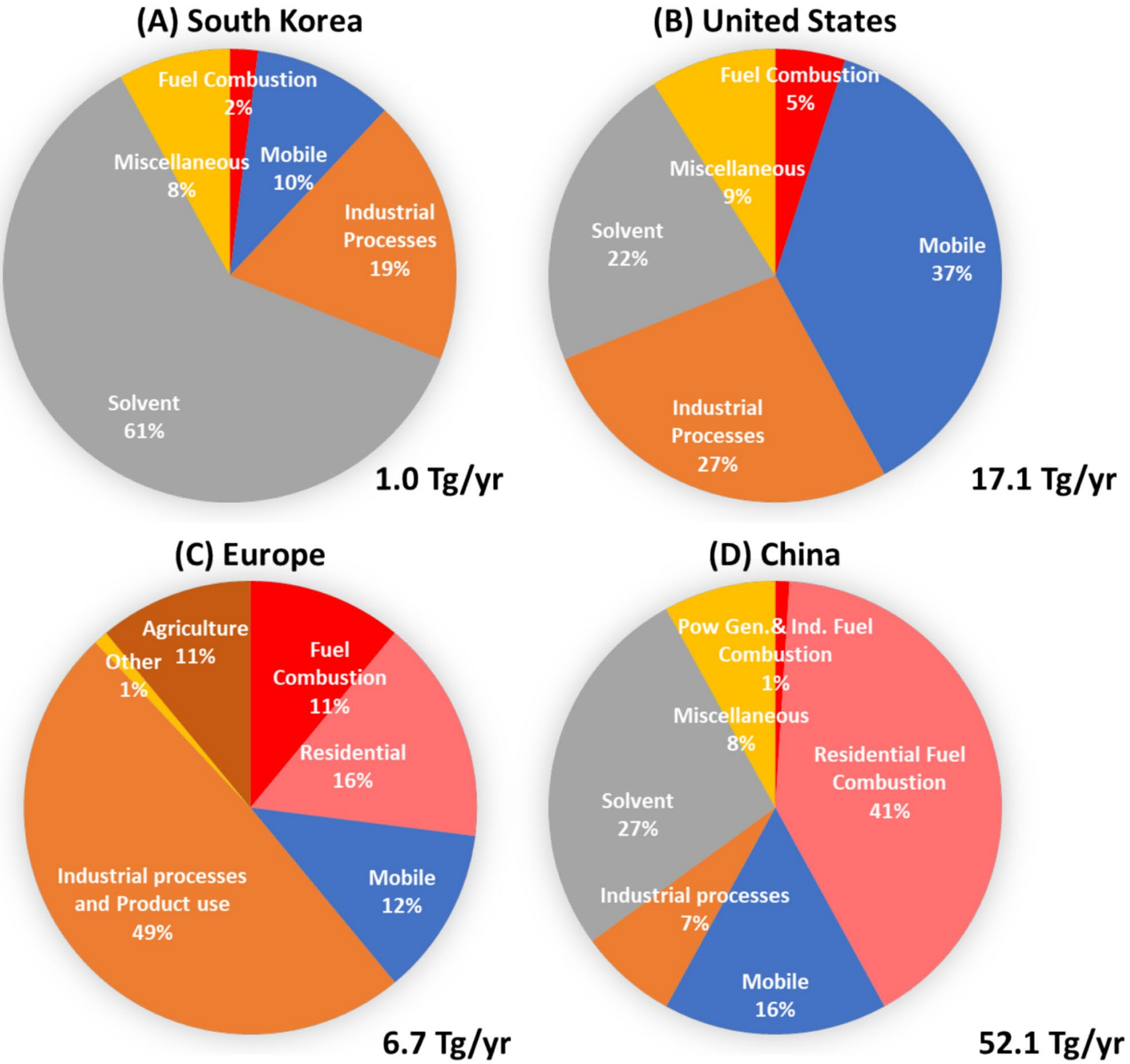


Fig. 1 Sectoral composition of anthropogenic VOC emissions by country. (Data sources: **A** South Korea (CAPSS), **B** United States (NEI), **C** Europe (EMEP/EEA), **D** China (KORUSv1))

An updated speciation profile was developed based on recent literature, and the anthropogenic VOC input used in air quality modeling was revised accordingly. Model performance was evaluated by comparing simulated results with observations to assess whether the updated profiles improved accuracy.

2 Methods

2.1 Emission Inventory and Source Characteristics

It should be noted that the inter-country comparison shown in Fig. 1 is based on 2015 inventories to maintain temporal consistency with the KORUS-AQ modeling period. Although more recent emission inventories such as MEIC (Multi-resolution Emission Inventory model for Climate and air pollution research; http://meicmodel.org.cn) have been developed for China, the comparison here aims to highlight the structural differences in dominant VOC emission sectors among countries, rather than to represent current absolute emission magnitudes. The discussion of China's residential fuel combustion as a major source thus reflects the situation in 2015 and not the present-day conditions.

Figure 2 shows the distribution of VOC emission sources across Korea's 17 metropolitan and provincial local governments. At the national level (as shown in

Fig. 2 Sectoral composition of anthropogenic VOC emissions by region

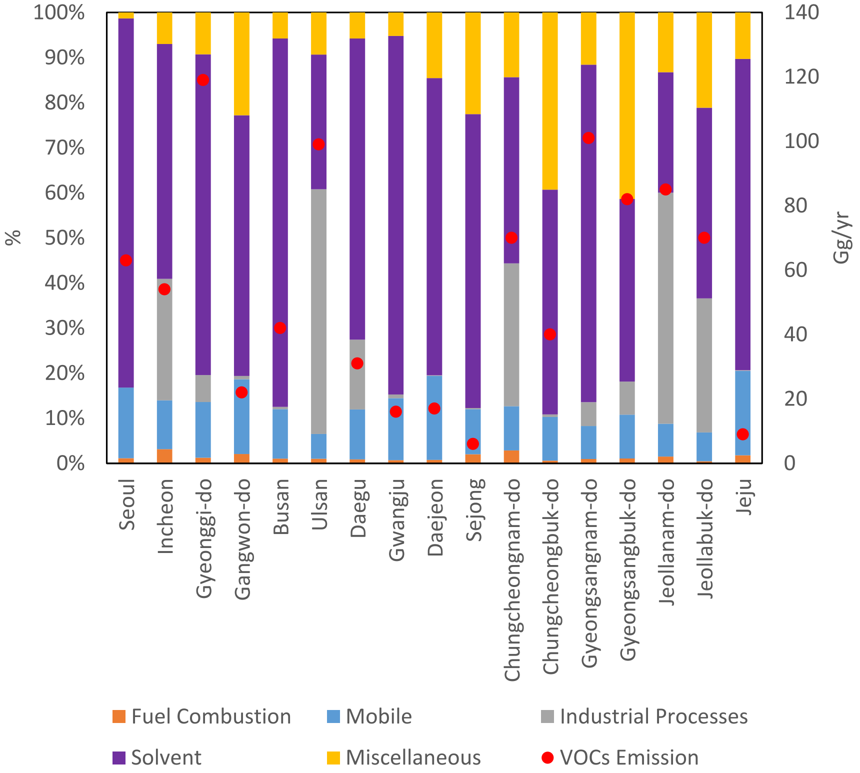


Fig. 1A), VOC emissions are primarily dominated by the solvent use, industrial process, and mobile sectors. However, the relative contributions of these sectors differ by region. Solvent use remains the dominant source in most regions, except for Ulsan and Jeollanam-do, where industrial processes contribute the highest proportion. This trend is likely attributable to the presence of large-scale industrial complexes in these areas. In particular, Ulsan and Jeollanam-do exhibit the highest proportions of industrial process-related VOC emissions in the country.

The mobile sector contributes significantly to VOC emissions in highly urbanized and densely populated areas such as Seoul, Gwangju, and Daejeon, where traffic volumes are high. Conversely, regions like Gangwon and Jeju show comparatively low total VOC emissions. The miscellaneous sector, which includes emissions from waste incineration and the burning of agricultural residues, has a relatively higher proportion in rural areas.

These regional differences in industrial activity and population density result in varying dominant sources of VOC emissions. Such characteristics should be carefully incorporated into air quality modeling studies for Korea. In particular, it is crucial to develop detailed chemical speciation profiles for the solvent use, industrial process, and mobile sectors—the three largest contributors to VOC emissions in Korea—to improve the accuracy of chemical transport model simulations.

2.2 Development of VOC Chemical Speciation Profiles

In this study, total VOC emissions from the emission inventory were chemically speciated during SMOKE-Asia emission processing to generate mechanism-resolved species for CMAQ simulations. To construct region-specific speciation profiles for Korea, the following procedure was implemented.

The chemical speciation process can be summarized as follows (refer Fig. S2). In this process, emission sources from the inventory are first categorized, and a corresponding chemical speciation profile is assigned to each category. Source-specific VOC emissions are then matched to a speciation cross-reference file, which assigns a profile number to each source group based on similar emission characteristics. Each profile number corresponds to a predefined VOC composition ratio. These ratios are used to disaggregate total VOC emissions into individual chemical species. At the end of the chemical speciation process, emissions are represented in terms of classified VOC chemical species that can be used in CTM simulations.

For the chemical speciation process, this study utilized the Spares Matrix Operator Kernel Emissions (SMOKE)—Asia emission processing system (Woo et al. 2012), which was developed for the Asian region based on the U.S. EPA's SMOKE framework. In this study, the improved

VOC chemical speciation profile was specifically applied during the chemical speciation stage.

The SAPRC-99 (Statewide Air Pollution Research Center 1999) chemical mechanism (Carter 2000) was adopted to map VOC emissions to lumped surrogate species during the SMOKE-Asia chemical speciation process for CMAQ simulations. SAPRC-99 represents VOCs using lumped surrogate species that are grouped according to their chemical reactivity and structure (Table S2). It includes an extensive set of reactions for alkanes, alkenes, aromatics, and oxygenated VOCs, allowing for a more detailed and realistic simulation of ozone and secondary organic aerosol (SOA) formation.

In KORUSv1 chemical speciation profile, alkanes, aromatics, and olefins constitute the largest portions of VOC emissions across all sectors. Notably, aromatic VOCs dominate the emissions in the power generation sector, while alkanes are the most prevalent in the industrial, transportation, and residential sectors. These results indicate that the composition of VOC chemical species varies significantly by emission source.

However, the KORUSv1 profile has a key limitation: it applies a simplified chemical speciation scheme that categorizes VOC emissions into only four broad sectors—power, industry, transportation, and residential. This coarse sectoral resolution may lead to inaccuracies in representing the detailed VOC composition needed for high-resolution air quality modeling, particularly when applied to regions such as South Korea with more diverse and sector-specific emission characteristics.

In this study, detailed chemical speciation profiles were developed for the four major VOC emission sources in South Korea: solvent use, mobile sources, residential combustion, and industrial processes. To construct these profiles, a range of peer-reviewed studies and technical reports on VOC measurements from emission sources in both South Korea and China were consulted to develop regionally applicable profiles for East Asia (Lee et al. 2015, 2021; Yuan et al. 2010; Wu and Xie 2018; Liang et al. 2017; Zhou et al. 2020).

The process consisted of several steps. First, a comprehensive literature review (Species average fractions) was conducted to compile representative VOC composition data for major Korean emission sources. Priority was given to studies conducted in South Korea; however, when sufficient source-specific measurements were unavailable, studies from regions with comparable economic development levels and similar emission source characteristics were also considered to supplement the dataset. Second, the data were organized by sector (Tier 1 and Tier 2) and classified into model-ready chemical species following mechanisms such as SAPRC. Third, the profiles were reformatted for compatibility with the SMOKE emissions processing system. Finally, the new profiles were compared with existing ones (KORUSv1 and SPECIATE), analyzed, and applied in air quality modeling to assess their performance.

To clarify the chemical speciation workflow, the following step-by-step procedure was implemented.

(1) A two-level source taxonomy was established, defining Tier 1 (solvent use, transport, residential combustion, and industry) and corresponding Tier 2 subcategories (e.g., auto-painting, printing, diesel/gasoline vehicles, natural gas stoves, petroleum refining).
(2) A literature screening was performed for studies from 2015–2016 representative of East Asian sources, ensuring consistency in analytical methods (GC–MS/FID, PTR–MS, 2D–GC) and completeness for SAPRC mapping.
(3) From each selected study, species-level mass fractions were standardized so that total VOC fractions summed to one, then mapped to SAPRC-99 lumped groups.

The finalized profiles and cross-references were implemented in SMOKE-Asia during the chemical speciation stage and coupled with CMAQ v4.7.1 using the SAPRC-99 mechanism. The details of the improved VOC speciation profiles and their evaluation are described in Sect. 3. All species-level data used for profile construction and their corresponding references are provided in the Supplementary Material (Tables S4 and S6).

2.3 Modeling Configuration and Observations

2.3.1 Modeling Configuration

Air quality modelings were conducted to evaluate the impacts of the updated VOC speciation profiles on modeled ozone and $PM_{2.5}$ concentrations. The modeling framework is summarized in Table S3.

The CTM employed was CMAQ version 4.7.1, developed and distributed by the U.S. EPA (Foley et al. 2010). The chemical mechanism applied was SAPRC-99. Emission processing was conducted using SMOKE-Asia, and meteorological inputs were generated using the Weather Research and Forecasting (WRF) model developed by the National Center for Atmospheric Research (NCAR, Skamarock et al. 2008).

The simulation period was set from April to June 2016, coinciding with the KORUS-AQ field campaign. This period was selected because it provides both airborne (KORUS-AQ aircraft) and surface observation data, enabling a comprehensive comparison between model outputs and real-world measurements.

The modeling domain consisted of two nested grids. The outer domain had a horizontal resolution of 27 km to capture long-range transport of pollutants, particularly from China.

The inner domain, resolved at 9 km, was used to allow for more accurate simulation of secondary pollutant concentrations over South Korea.

To compare the model results with observations, grid cells from the inner domain (9 km × 9 km resolution) were selected based on spatial correspondence with air quality monitoring sites. Quantitative analysis was then performed by comparing modeled and observed concentrations within these selected grid cells.

2.3.2 Observation Data and Model Evaluation Methods

Model validation was conducted for the Seoul Metropolitan Area (SMA) and Daegu. During the KORUS-AQ campaign, model performance in these regions was lower than in other areas, with aromatic VOCs notably underestimated (Kwon et al. 2021; Fried et al. 2020). To assess the effectiveness of the improved profiles, observations and model results were compared at these locations (Fig. S3).

Hourly concentration data from monitoring stations located within each region were compiled, and the sites falling within the corresponding model grid cells were identified. The observed values from these stations were then averaged to produce representative concentrations, which were compared with the model outputs for the same grid cells. This approach ensured spatial representativeness and allowed for a consistent comparison between model simulations and observations.

Ground observations were obtained from the AirKorea urban monitoring network (https://www.airkorea.or.kr/eng, last accessed: 1 June 2025) operated by the National Institute of Environmental Research (NIER). In 2016, the network consisted of 264 monitoring stations across South Korea (Fig. S4). The purpose of the urban air measurement network is to determine the average air quality concentration in urban areas to determine whether environmental standards are met (NIER 2017).

The urban atmospheric measurement network provides hourly measurements of SO_2, CO, NO_2, PM_{10}, $PM_{2.5}$, and ozone. Among these, this study uses $PM_{2.5}$ and ozone observations. $PM_{2.5}$ is measured using the gravimetric concentration method or an equivalent automatic measurement method, and ozone is measured using the ultraviolet (UV) photometric method. In this study, data from the urban air measurement network observed during the 2016 KORUS-AQ air campaign (April–June) were collected and compared with the model results. In addition, ground observation data were extracted and compared separately for the SMA and Daegu region, which were areas of VOC underestimated during KORUS-AQ (Souri et al. 2020; Simpson et al. 2020; Travis et al. 2024).

To quantitatively evaluate the performance of the CTM simulations, several statistical metrics were used to compare modeled and observed concentrations of ozone and $PM_{2.5}$. Model performance was evaluated using mean bias (MB), normalized mean bias (NMB), root mean square error (RMSE), and the correlation coefficient (R). These metrics together offer a comprehensive evaluation of model accuracy and reliability.

3 Results and Discussion

3.1 Developed VOC Chemical Speciation Profiles

Chemical speciation profiles were developed based on results from studies conducted in major cities across Northeast Asia megacities (Liu et al. 2016; Mo et al. 2016; Shao et al. 2016; Wang et al. 2014; Wei et al. 2014a; Wei et al. 2014b; see Table S4). The table summarizes the types and sources of chemical speciation profiles for representative emission categories. Four Tier 1 emission sources—solvent use, transportation, residential, and industry—were profiled, as these represent the primary VOC emission sources in South Korea. Additionally, to enable more detailed classification, a secondary level (Tier 2) was established for these Tier 1 sources. Detailed speciation profiles for each category are provided in Supplementary materials (Figs. S5–S8, Tables S5, S6). The data were synthesized and reformatted to be compatible with air quality modeling applications.

The composition ratios of chemical species are presented for each detailed emission source within the four Tier 1 level categories: solvent use, mobile, residential, and industrial sources (see Fig. 3). Compared to the previous version, these profiles enable a more detailed reflection of the emission characteristics of major VOC sources in Korea. As shown in Fig. 3, each profile exhibits distinct proportions of VOC chemical species depending on the source characteristics.

Within the solvent use sector, aromatic VOCs are the dominant chemical components. For the transportation sector, alkanes VOCs are the major contributors; however, for heavy-duty diesel vehicles, olefins and aldehydes VOCs constitute a significant share of emissions. In the residential sector, the emitted chemical species vary according to the fuel type used. When combustion involves solid fuels such as coal and wood, emissions are characterized by higher proportions of alkanes (about 37%) and olefins (about 50%) VOCs. Conversely, natural gas combustion leads to elevated emissions of aromatic VOCs. Given that most households in Korea utilize natural gas, emissions of aromatic VOCs are expected to be comparatively high. Lastly, the industrial sector is primarily dominated by alkanes VOCs.

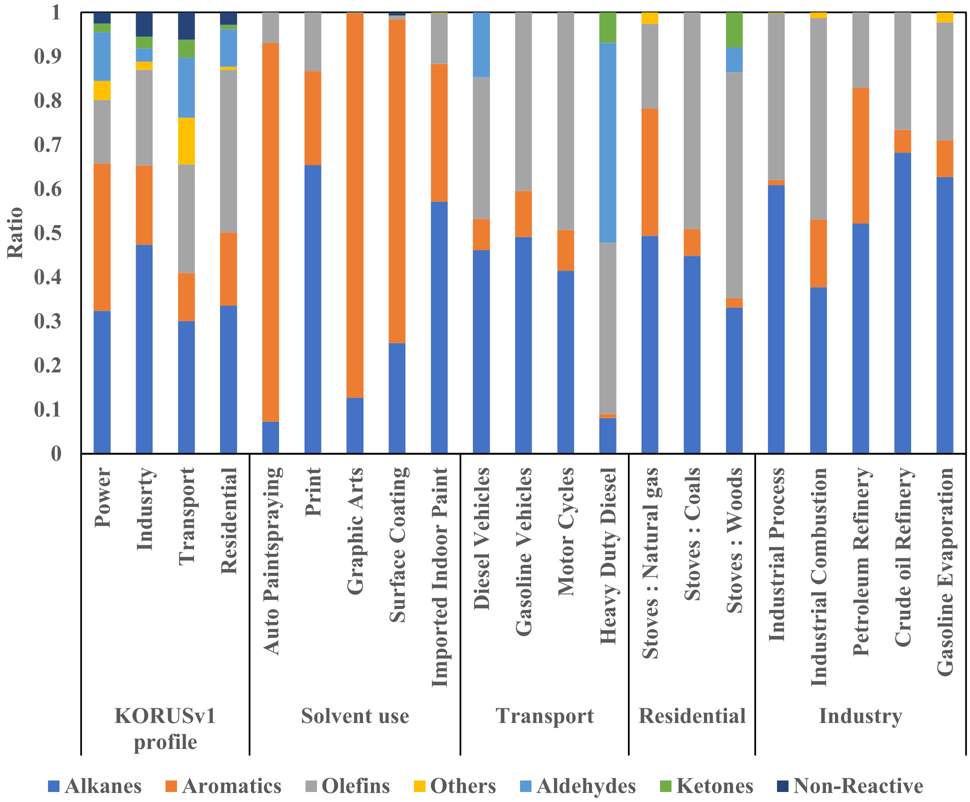


Fig. 3 Chemical speciation profiles of solvent, mobile, residential, and industry sectors

3.2 Comparison with Existing Speciation Profiles

The improved chemical speciation profiles were compared with the previously used SPECIATE and KORUSv1 profiles (Fig. S9). Compared with the earlier profiles, the revised profiles show higher proportions of reactive species such as alkanes (about 1.2 times), olefins (about 1.8 times), and aromatics (about 2.3 times), along with a marked reduction in non-reactive organic gases (NROG). Because olefins and aromatics play a key role in secondary pollutant formation, these adjustments are expected to enhance the simulated concentrations of secondary pollutants in chemical transport models.

Table 1. compares the VOC species allocation values among the improved profile, the SPECIATE profile, and the KORUSv1 profile. For instance, the emission rate of aromatics assigned by the improved profile is 1.09 times higher than that of the SPECIATE profile. Compared to the KORUSv1 profile, this rate is increased by a factor of 1.21. Relative to the previously used profiles, the improved profile developed in this study is expected to allocate fewer emissions to NROG and more to aromatics, alkanes, and olefins.

The updated VOC profiles show stronger agreement with observation-based source apportionment studies than earlier profiles. Reactive olefins (0.31) and aromatics (0.19) account for substantially larger fractions than in both SPECIATE and KORUSv1. These adjustments are consistent with

Table 1 Inter-comparison of chemical speciation ratio (Bold: rate of change for major VOC lumped species). Bold: rate of change for major VOC lumped species

Species(Ratio)	SPECIATE	KORUSv1	This Study	This Study /SPECIATE	This Study /KORUSv1
Alkanes	0.38	0.39	0.44	**1.16**	**1.15**
Aromatics	0.17	0.15	0.19	**1.09**	**1.21**
Olefins	0.22	0.25	0.31	**1.4**	**1.24**
Others	0.01	0.05	0.01	0.69	0.20
Aldehydes	0.06	0.08	0.03	0.48	0.39
Ketones	0.01	0.03	0.01	1.13	0.28
Non-Reactive	0.14	0.05	0.01	0.05	0.13
Sum (Total VOC)	1.00	1.00	1.00	–	–

KORUS-AQ findings: positive matrix factorization (PMF) of aerosol mass spectrometer (AMS) measurements over Seoul indicated that locally produced SOA was dominant, with short-lived aromatics such as toluene and xylenes contributing nearly one-third of SOA precursors (Nault et al. 2018). Likewise, PMF of VOCs and satellite HCHO inversions showed that inventories underestimated reactive VOCs—particularly aromatics and olefins—that drive OH reactivity and ozone formation (Souri et al. 2020). Airborne observations also revealed elevated aromatic VOCs over Seoul and Daegu, which were not captured by models using default SPECIATE profiles (Simpson et al. 2020). Collectively, these results indicate that the updated profiles align well with factorization-based attribution studies and more accurately represent urban emission characteristics in Korea.

Furthermore, although Table 1 presents national-average VOC allocation ratios, region-specific patterns were identified. In the Seoul Metropolitan Area (SMA), where solvent use is a dominant source, the fraction of aromatic VOCs increased substantially, whereas Daegu showed higher ratios of ARO2 and olefin groups associated with industrial complex emissions. These region-specific increases enhance secondary pollutant formation through well-known photochemical mechanisms. Reactive aromatics (e.g., toluene, xylene) rapidly react with OH radicals to produce RO_2/HO_2 radicals, accelerating $NO \rightarrow NO_2$ conversion and ozone formation under NO_x-rich urban conditions. Their multigenerational oxidation also generates semi-volatile organic compounds that partition into the particle phase, driving secondary organic aerosol (SOA) formation and thus $PM_{2.5}$ mass. The increased allocation to olefins (fast kOH reaction rates) further amplifies radical production and O_3 generation. These mechanistic pathways explain the observed improvements in model performance (Sect. 3.4.2), where ozone and $PM_{2.5}$ biases decreased significantly after applying the updated speciation profiles.

3.3 Impact on Spatial Distribution of VOC Emissions

To generate modeling emissions data using the chemical speciation profiles, emissions were processed and compared by region. Fig. S10 shows the results of the comparison by summing grid emissions by region, while Fig. S11 shows the differences between the grid emissions of KORUSv1 and those obtained in this study. As described in Sect. 1, the KORUS field campaign identified an underestimation of aromatic VOCs such as toluene. Therefore, this study examined how the improved emissions of aromatic and olefin VOCs affect the eastern and southern regions of China (Northeast China, Central East China, Southeast China) and South Korea, which have a significant impact on Korea.

ARO1 emissions in eastern China and South Korea increased approximately fourfold, while ARO2 emissions increased by about 1.2 times. Additionally, OLE1 emissions increased by about 1.6 times and OLE2 by about 1.8 times. Here, ARO1 represents aromatics with kOH less than 2×10^4 ppm^{-1} min^{-1}, exemplified by toluene, whereas ARO2 represents aromatics with kOH greater than 2×10^4 ppm^{-1} min^{-1}, exemplified by xylene. OLE1 refers to alkenes (excluding ethene) with kOH less than 7×10^4 ppm^{-1} min^{-1}, and OLE2 refers to alkenes with kOH greater than 7×10^4 ppm^{-1} min^{-1}. These increases in aromatic and olefin VOC emissions indicate a higher potential for secondary pollutant transport into Korea through long-range atmospheric transport.

Gridded emission comparisons indicate that ARO1 emissions increase across eastern and southern China. In China, ARO2 emissions generally decrease or show limited change, except in some parts of eastern China. In South Korea, increases in ARO2 emissions are primarily observed in regions with large industrial complexes and power plants. In contrast, decreases in ARO2 emissions occur in residential areas such as North Korea and in the northeastern and southeastern parts of China located near the domain boundaries. These residential regions likely exhibit lower aromatic VOC emissions due to reduced solvent use and a higher reliance on coal- and wood-based residential combustion.

For olefin compounds, emissions increased in areas containing large industrial complexes, showing patterns similar to ARO2. This is attributable to increased allocation of OLE1 and OLE2 in emission sources such as industrial processes, industrial combustion, and petroleum refineries, as defined in the industry sector profiles developed in this study. In contrast, in non-industrial regions, the allocation ratio of OLE1 decreased in the solvent use, transport, and residential sectors, whereas OLE2 remained similar to or increased relative to the previous profile. Overall, these changes resulted in an increasing nationwide trend in reactive VOC emissions.

3.4 Air Quality Model Performance Evaluation

Model simulations and observations for ozone and $PM_{2.5}$ concentrations during April, May, and June 2016 were compared. Finalized hourly air pollutant data from the national monitoring network (AirKorea), which had undergone official quality assurance and quality control (QA/QC) procedures by the NIER, were used for evaluation. Figures 4, 5, 6 show these comparisons. The top two graphs on the left present model results using the KORUSv1 profile compared with observations, while the top two graphs on the right show model results using the improved profile compared with observations. Table 2 summarizes descriptive statistics for these data, including RMSE, R, Normalized RMSE (NRMSE), MBE, NMB, and Index of Agreement (IOA).

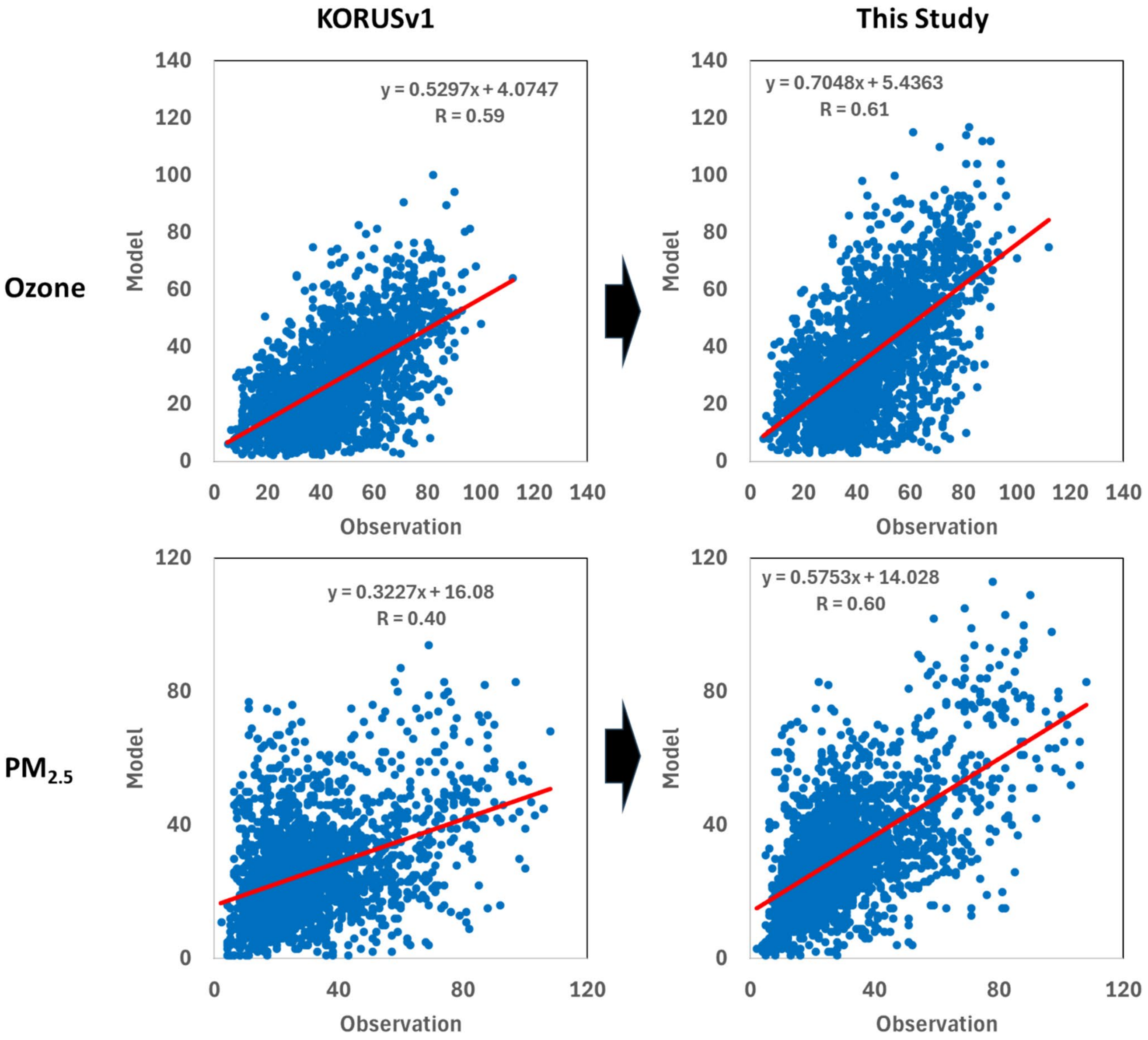


Fig. 4 Model vs. Observed comparison of ozone and $PM_{2.5}$ across South Korea (Ozone: ppb, $PM_{2.5}$: µg/m^3)

3.4.1 Validation of Meteorological Data

Before evaluating the modeling results, the meteorological input data were first assessed, as these are a major source of uncertainty in chemical transport modeling and a prerequisite for reliable air quality applications. According to the U.S. EPA and previous studies (Emery and Tai 2001; U.S. EPA 2007, 2017), reasonable performance is assumed when near-surface meteorological variables fall within the following ranges: mean temperature bias within ± 2 K, wind speed bias within ± 2 m s^{-1}, wind direction error within ± 20°, and relative humidity bias within ± 10%. Correlation coefficients above 0.5–0.7 are also generally considered acceptable, although thresholds may vary depending on domain size, resolution, and modeling objectives. These benchmarks provide a practical basis for determining whether meteorological fields are of sufficient quality to support air quality modeling.

Overall, the model generally met these criteria for key meteorological variables (Figs. S12, S13). Observed patterns of wind speed, wind direction, relative humidity, and temperature were reasonably well reproduced in both the Seoul Metropolitan Area and Daegu, although wind speeds in Daegu tended to be overestimated, potentially introducing uncertainties into the simulation of pollutant dispersion and concentrations.

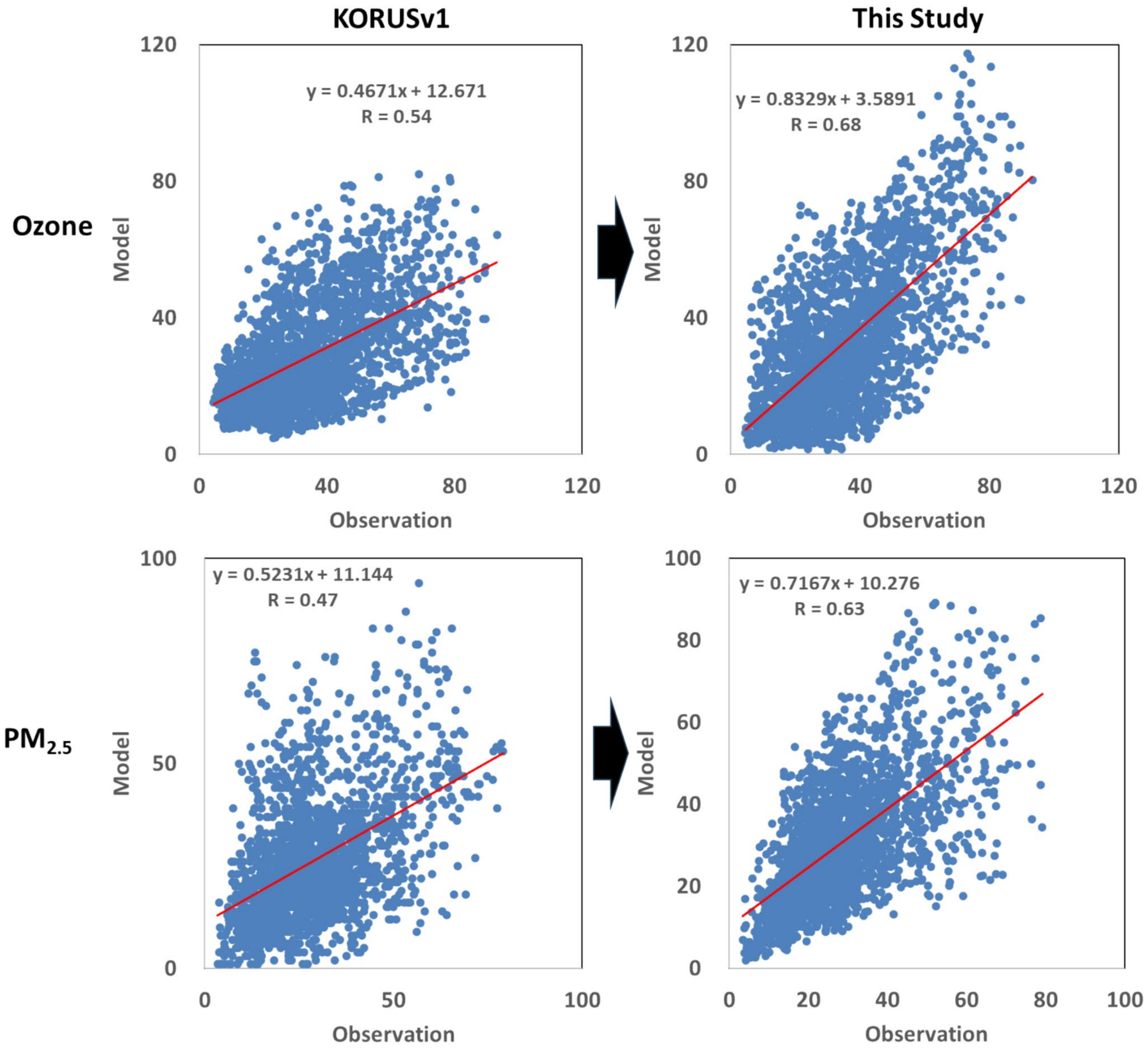


Fig. 5 Model vs. Observed ozone and $PM_{2.5}$ in the SMA (Ozone: ppb, $PM_{2.5}$: μg/m^3)

3.4.2 Effects of Updated VOC Speciation on Simulated $PM_{2.5}$ and Ozone

3.4.2.1 South Korea In Fig. 4, which compares results for the entire South Korea, the correlation coefficient for simulated ozone concentrations increased from 0.59 (using the KORUSv1 profile) to 0.61 with the improved profile. Additionally, the slope of the trend line rose from 0.5297 to 0.7048, moving closer to the ideal value of 1. This improvement is attributed to the adjusted allocation of VOC chemical species, with a greater proportion assigned to highly reactive aromatic VOCs such as toluene (about 2.1 times) and xylene (about 1.4 times), which enhances ozone formation through chemical reactions. Similarly, $PM_{2.5}$ simulation performance improved, with the correlation coefficient increasing from 0.40 to 0.60 and the slope of the trend line from 0.3227 to 0.5753.

As shown in Table 2, both ozone and $PM_{2.5}$ simulations in this study outperformed those using the KORUSv1 profile. Among the two pollutants, $PM_{2.5}$ showed a relatively greater improvement. Specifically, the R increased from 0.40 to 0.60, the MB improved significantly from − 15.38 to 3.04, and the IOA increased from 0.63 to 0.77.

3.4.2.2 South Korea—SMA In Fig. 5, the R for ozone concentrations simulated using the improved profile increased

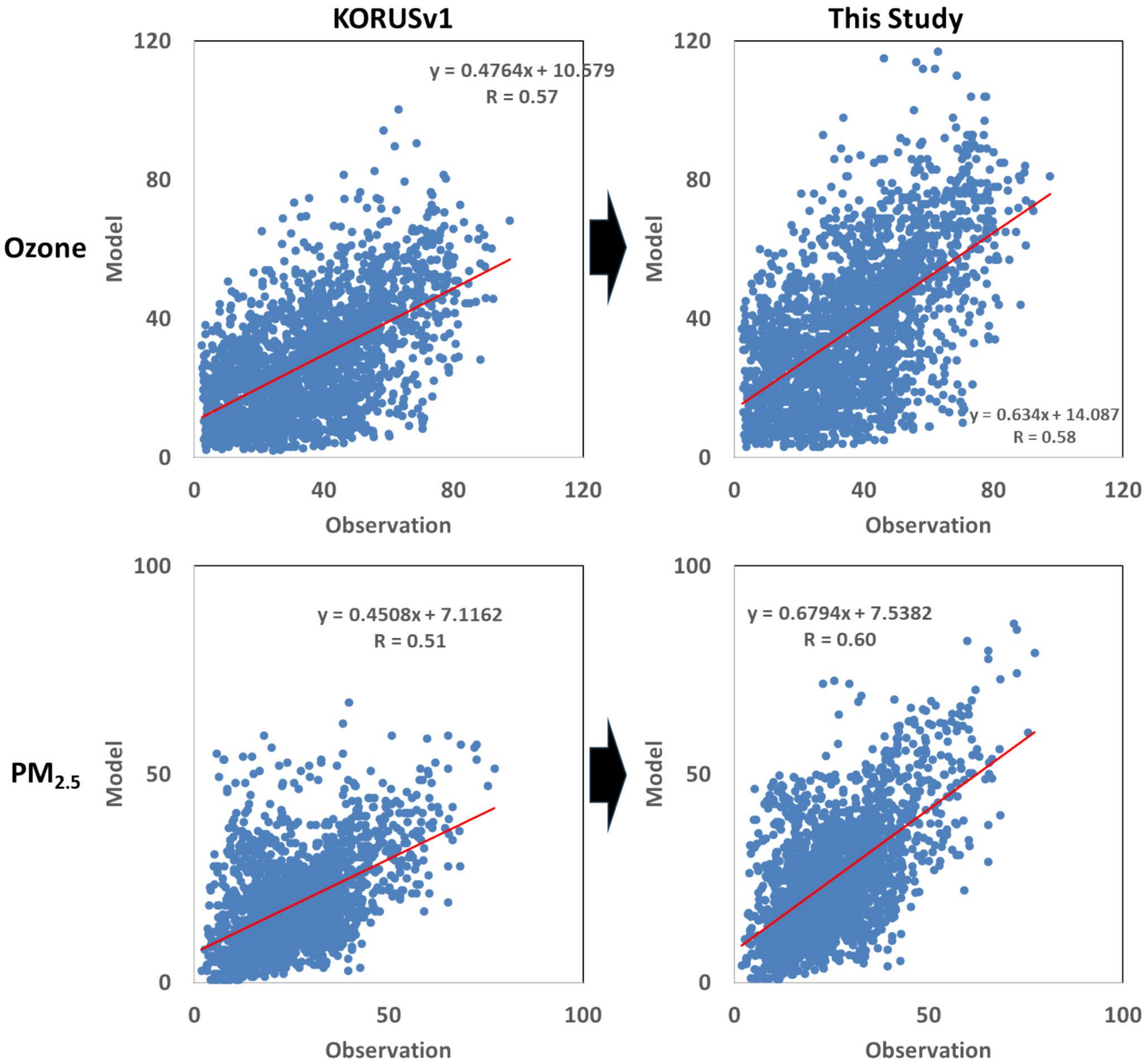


Fig. 6 Model vs. Observed ozone and $PM_{2.5}$ in Daegu (Ozone: ppb, $PM_{2.5}$: µg /m^3)

from 0.54 to 0.68 compared to the KORUSv1 profile, and the slope of the trend line rose from 0.4671 to 0.8329, approaching 1. This improvement is attributed to the different allocation ratios of VOC chemical species at the regional level, leading to enhanced ozone formation due to a higher proportion of highly reactive aromatic VOCs such as toluene and xylene. Notably, the Seoul metropolitan area (about 2.1 times), with its higher proportion of solvent use, shows a larger increase in aromatic VOC emissions than the national average (about 1.2 times). For $PM_{2.5}$, the R increased from 0.47 to 0.63, and the slope of the trend line improved from 0.5231 to 0.7167.

As shown in Table 2, the performance for both ozone and $PM_{2.5}$ in the metropolitan area improved in this study compared to the KORUSv1 profile, with a more pronounced increase observed for $PM_{2.5}$. Specifically, for $PM_{2.5}$, the MB shifted from − 2.52 to 2.16, and the IOA increased from 0.69 to 0.79.

3.4.2.3 South Korea—Daegu In Fig. 6, the ozone concentration simulated for Daegu in this study shows a slight increase in the R from 0.57 to 0.58 compared to the existing KORUSv1 profile, while the slope of the trend line improved from 0.4764 to 0.634, moving closer to 1. Similarly, the R

Table 2 Model performance statistics

Unit (Ozone: ppb, $PM_{2.5}$: μg/m^3)	Ozone		$PM_{2.5}$	
	KORUSv1	This study	KORUSv1	This study
South Korea				
RMSE (unit)	23.52	19.97	19.56	16.50
R	0.59	0.61	0.40	0.60
NRMSE (%)	0.52	0.44	0.62	0.53
MB (Unit) = MBE	−16.66	−7.33	−4.76	0.94
NMB (%)	−37.16	−16.35	−15.38	3.04
IOA	0.64	0.73	0.63	0.77
SMA				
RMSE (unit)	17.15	16.50	15.01	12.73
R	0.54	0.68	0.47	0.63
NRMSE (%)	0.48	0.46	0.52	0.44
MB (Unit) = MBE	−6.35	−2.37	−2.52	2.16
NMB (%)	−17.78	−6.65	−8.80	7.53
IOA	0.71	0.81	0.69	0.79
Daegu				
RMSE (unit)	18.95	18.67	13.38	11.69
R	0.57	0.58	0.51	0.60
NRMSE (%)	0.51	0.51	0.52	0.46
MB (Unit) = MBE	−8.72	0.60	−6.95	−0.67
NMB (%)	−23.66	1.61	−27.14	−2.63
IOA	0.71	0.76	0.67	0.78

for $PM_{2.5}$ increased from 0.51 to 0.60, with the slope of the trend line rising from 0.4508 to 0.6794.

Table 2 shows the performance improvements in Daegu. For both ozone and $PM_{2.5}$, the results from this study demonstrate better performance compared to the KORUSv1 profile. $PM_{2.5}$, in particular, exhibited a relatively large improvement. Specifically, the MB improved from −6.95 to −0.67, and the NMB increased from −27.14 to −2.63, indicating a significant reduction in the previous underestimation. Additionally, the IOA improved from 0.67 to 0.78. Time series of observed and simulated $PM_{2.5}$ and Ozone concentrations are presented in Figs. S15 and S16 to provide detailed temporal comparisons between observations and model results.

Application of the chemical speciation profiles developed in this study improved the simulation performance of both ozone and $PM_{2.5}$, although the extent of improvement varied by region depending on emission source characteristics. In SMA, where solvent use and mobile sources dominate, a substantial increase in aromatic VOCs was observed. This resulted in higher correlation coefficients for ozone (from 0.54 to 0.68) and $PM_{2.5}$ (from 0.47 to 0.63), while the mean bias (MB) of $PM_{2.5}$ decreased from −2.52 to +2.16 μg/m^3.

In Daegu, the combined influence of solvent use and emissions from industrial complexes led to an increase in reactive VOCs, contributing to significant gains in model performance. The ozone MB declined markedly (from −8.72 to −0.60 μg/m^3), and the $PM_{2.5}$ MB was also greatly reduced (from −6.95 to −0.67 μg/m^3). Grid-level emission comparisons revealed that ARO2 and olefin groups increased more prominently in industrial areas, reflecting the characteristics of Daegu, whereas the higher share of solvent use in the SMA resulted in a more pronounced increase in aromatic VOCs. These differences account for the region-specific improvements in model performance.

Despite these improvements, uncertainties associated with the developed VOC speciation profiles should be noted. These include variability in source-profile measurements, limited availability of source-specific data in South Korea for certain emission categories, and uncertainties introduced by mapping individual VOC species to lumped surrogate species in the SAPRC mechanism. These factors may influence the quantitative interpretation of model results.

Beyond model evaluation, the findings also suggest implications for emission control strategies. In the SMA, regulatory measures targeting solvent products (e.g., paints, coatings, and printing inks) and mobile sources may be particularly effective, whereas in Daegu, additional management strategies for petrochemical and refinery facilities—especially for aromatic (ARO2) and olefin compounds—are likely to be necessary.

3.4.3 Impact of VOC Speciation Update on SOA Concentration

The results of the SOA simulations using the existing KORUSv1 profile and the profiles developed in this study are presented in Fig. 7 and S14. As shown in Fig. 7, the SOA concentration simulated with the new profiles (mean: 12.75 μg/m^3) was higher than that obtained using the KORUSv1 profile (mean: 8.50 μg/m^3). This increase can be attributed to the higher allocation ratios of aromatics and olefins—species with high SOA production reactivity—in the VOC speciation profiles developed in this study.

Fig. S14 presents the daily average time series for April, May, and June. Consistent with Fig. 7, the time series graph also shows that the SOA concentrations simulated using the new profile were approximately 1.5 times higher than those simulated with the KORUSv1 profile. In addition, during the modeling period, the monthly average $PM_{2.5}$ concentrations (April: 35.0 μg/m^3, May: 30.1 μg/m^3, June: 30.0 μg/m^3) indicated that the SOA contribution was higher when the new profile was used (April: 37%, May: 43%, June: 41%) than when the KORUSv1 profile was used (April: 26%, May: 28%, June: 26%). This increase is attributed to the higher allocation ratios of aromatic compounds and olefins with high SOA formation reactivity in the VOC speciation profiles developed in this study.

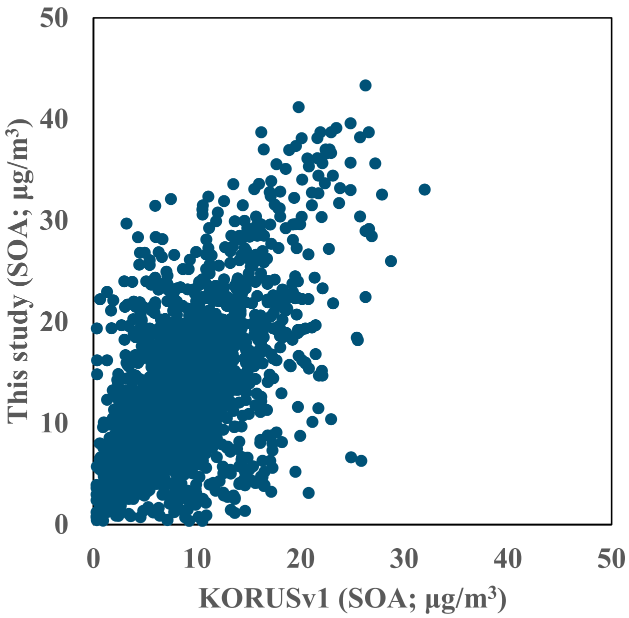


Fig. 7 Comparison of simulated SOA concentrations: KORUSv1 Profile vs. This Study profile

4 Conclusions

This study developed region-specific VOC chemical speciation profiles to improve the representation of anthropogenic VOC emissions in Korea. Previous studies during the KORUS-AQ campaign identified significant underestimation of aromatic VOC emissions (e.g., toluene and xylene) in existing emission inventories. To address this limitation, refined chemical speciation profiles were constructed for 19 emission sectors using recent source-profile measurements relevant to Korean emission characteristics. The improved profiles show a marked decrease in the fraction of NROG and a corresponding increase in reactive species such as aromatics and olefins. Specifically, emissions classified as ARO1 increased by approximately 3 to 7 times, ARO2 by 1.2 times, and olefin compounds by 1.6 times compared to previous profiles (OLE1 by 1.6 times, OLE2 by 1.8 times). Regional analysis further revealed that ARO1 emissions in the East China region increased roughly fourfold, with ARO2 emissions increasing by 1.2 times. Also, OLE1 emissions are increasing by 1.7 times, and OLE2 emissions are increasing by 1.8 times.

These changes in VOC composition led to significant improvements in air quality model performance. Ozone simulations showed increased correlation coefficients, rising from 0.59 to 0.61 at the national scale and from 0.54 to 0.68 in the Seoul Metropolitan Area. $PM_{2.5}$ simulations exhibited even greater improvement, with the correlation coefficient increasing from 0.40 to 0.60 at the national level. In addition, the mean bias (MB) for $PM_{2.5}$ improved substantially, shifting from -15.38 to 3.04 μg/m^3, while the index of agreement (IOA) increased from 0.63 to 0.77. These results indicate that the updated speciation profiles effectively reduced the underestimation of secondary pollutants and improved the model's ability to capture both the magnitude and temporal variability of observed concentrations.

It should also be noted that the updated VOC speciation profiles developed in this study have been used to construct the KORUS v2 and v5 emission inventories. Previous studies (Oak et al. 2019; Kim et al. 2024) evaluated these emission datasets against observational measurements, including VOCs and their precursors, and reported improved agreement in terms of VOC composition and atmospheric reactivity. This provides additional support that the improved model performance in this study is closely linked to the enhanced representation of VOC chemical speciation.

The revised VOC profiles incorporate feedback from the KORUS-AQ aircraft observations, which revealed underestimation of reactive species such as aromatics and olefins in the baseline simulation. This update improved the model's ability to reproduce ozone and $PM_{2.5}$ concentrations across key regions, demonstrating the effectiveness of the refined Tier 2 sectoral framework.

These findings highlight the importance of accurately representing VOC chemical composition in emission inventories. The refined Tier-2 sectoral framework developed in this study provides a more realistic representation of emission sources and their chemical characteristics, offering a practical approach for improving VOC emissions used in regional air quality modeling.

In summary, the application of a VOC chemical speciation profile specifically developed for Korean conditions led to marked improvements in the simulation of secondary pollutants. This approach effectively addresses the underestimation issues caused by reliance on foreign-centric emission profiles that inadequately reflect the Korean industrial landscape and residential energy use. The results underscore the critical importance of incorporating realistic, region-specific emission data in air quality modeling to enhance prediction reliability.

Despite these improvements, several sources of uncertainty remain in the developed speciation profiles. First, the profiles were constructed using species composition data compiled from previous source-profile studies. Such measurements can vary depending on sampling conditions, analytical methods, fuel composition, and operating characteristics of emission sources. As a result, the derived profiles represent averaged source characteristics rather than fully capturing the variability of individual emission sources. Second, the availability of source-profile measurements in South Korea remains limited for certain emission sectors. In these cases, measurements from regions with comparable emission characteristics were incorporated to supplement the dataset, which may introduce additional uncertainties. Finally, uncertainties may also arise from the mapping of individual VOC species to lumped surrogate species in the SAPRC chemical mechanism, which simplifies the representation of VOC reactivity and secondary aerosol formation potential. Despite these limitations, previous studies of the KORUS-AQ campaign have shown that inaccuracies in VOC species classification can lead to significant bias in ozone and secondary organic aerosol simulations (Simpson et al. 2020; Crawford et al. 2021; Kim et al. 2022). For example, the underrepresentation of aromatic VOCs was identified as a major factor in the underestimation of ozone in urban areas. These results highlight the importance of improving VOC species classification profiles, even with the existence of inherent uncertainties.

Future work should extend the application of the developed chemical speciation profiles to various seasons and geographic regions to comprehensively evaluate their robustness and predictive capability. Additionally, expanding the scope and precision of observational datasets will facilitate the construction of even more reliable speciation profiles. This study demonstrates the improved representation of VOC speciation and its impacts on SOA formation and air quality during the KORUS-AQ period. However, analyzing other seasons and periods remains an important task for future research, and this work will be extended using the methodology established in the present study. Such efforts will contribute to adaptive policy-making that reflects dynamic emission environments and changing climate conditions, thereby supporting the advancement of efficient and effective air quality management strategies.

The findings highlight the necessity for emission treatment strategies that are customized to local emission characteristics, particularly in densely populated metropolitan and industrial regions with diverse emission sources. These tailored approaches provide an essential foundation for developing effective, science-based air quality management policies. For example, solvent-related emissions dominate in the Seoul Metropolitan Area, while industrial emissions play a larger role in regions such as Daegu. Sector and Region-specific emission control strategies based on local source structures may therefore be more effective for reducing ozone and secondary particulate matter formation. Moreover, the methodological framework developed in this study can be extended to other East Asian metropolitan or industrial regions with similar emission characteristics, supporting transboundary air-quality management and policy coordination.

Despite these limitations, the results demonstrate that improving VOC chemical speciation alone can significantly enhance model performance within a controlled emission framework.

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Author contributions J.K. contributed to conceptualization, data curation, formal analysis, investigation, methodology, software, validation, visualization, and writing—original draft preparation. H.H. contributed to methodology, project administration, validation, and writing—review and editing. Y.K. contributed to data curation, formal analysis, methodology, and validation. J.H.W. contributed to conceptualization, funding acquisition, project administration, resources, supervision, and writing—review and editing. All authors reviewed and approved the final manuscript.

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Data Availability The data used in this study include observational data, published chemical speciation profiles, and newly processed emission and model simulation data generated for air quality modeling. Observational data are available from the AirKorea database (https://www.airkorea.or.kr/web/). Chemical speciation information was obtained from previously published literature, as cited in the reference list. The processed emission data and model outputs supporting the findings of this study are available from the corresponding author upon reasonable request.

Declarations

Conflict of Interest The authors declare that they have no conflict of interest.

Consent to Participate Not applicable.

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