

Evaluating the EPICC-Model for Regional Air Quality Simulation: A Comparative Study with CAMx and CMAQ

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Abstract

This study presents a systematic evaluation of the EPICC-Model developed in China for regional PM_{2.5} and MDA8 O₃ simulations against established international models, using WRF meteorological fields and a multi-source integrated emission inventory. Results highlight the strengths of the EPICC-Model in several aspects: it achieves relatively high spatial consistency with measurements for PM_{2.5}, with an annual index of agreement (IOA) of 0.80, and accurately captures pollution patterns in heavily polluted North China. It also demonstrates improved performance in simulating summer O₃ peaks, reducing maximum bias by more than 20 $\mu\text{g m}^{-3}$; this performance may be partly associated with its inclusion of heterogeneous HONO formation and particulate nitrate photolysis. The model exhibits the highest hit rate (45.6%) for MDA8 O₃ pollution events exceeding 160 $\mu\text{g m}^{-3}$ and successfully reproduces persistent pollution episodes. However, all models share common limitations, including insufficient capability in reproducing heavy pollution episodes, systematic underestimation of SO₄²⁻, and uncertainties in SOA-related OC simulations. Future improvements should focus on refining secondary aerosol chemistry and emission inventories and further evaluating the representation of vertical turbulent mixing under stable boundary-layer conditions. This study benchmarks the performance of the EPICC-Model against established established chemical transport models (CTMs) and identifies priorities for its further development and regional application.

1 Introduction

With rapid urbanization and industrialization, China faces increasingly severe multi-pollutant air quality challenges. Among them, fine particulate matter (PM_{2.5}) and ozone (O₃) are key threats to public health and ecosystems, and their coordinated control has become a priority. Specifically, PM_{2.5} comprises both directly emitted particles and secondary components formed from SO₂, NO_x, NH₃, and volatile organic compounds (VOCs), with its levels also affected by regional transport and meteorology (Zhang et al., 2012; Jing et al., 2020; Zhai et al., 2021; Bao et al., 2023). Emission control policies have reduced population-weighted PM_{2.5} exposure by ~48% from 2013 to 2020 (Xiao et al., 2022), yet severe winter haze episodes persist in regions like Beijing-Tianjin-Hebei. In contrast, O₃ is formed through photochemical reactions involving NO_x and VOCs, and its production exhibits nonlinear responses to precursor levels, characterized by NO_x-sensitive and VOC-sensitive regimes (Haagen-Smit and Fox, 1956; Sillman, 1999). Ambient O₃ levels are also strongly influenced by meteorological factors, including solar radiation, temperature, humidity, and boundary-layer dynamics (Li et al., 2019b; Gao et al., 2022). In many Chinese urban clusters, PM_{2.5} concentrations have decreased, whereas warm-season maximum daily 8 h average (MDA8) O₃ concentrations increased at a rate of 1.2 ± 1.3 ppb yr⁻¹ during 2013-2022 (Wang et al., 2024). The combined pollution of PM_{2.5} and O₃ exhibits complex spatiotemporal evolution patterns and formation mechanisms (Lyu et al., 2025; Zhu et al., 2023), posing significant challenges for sustained air quality improvement in China.

To better understand the formation of complex air pollution and assess control strategies, Chemical Transport Models (CTMs) are widely used for regional air quality analysis and policy evaluation (Li et al., 2021; Gao and Zhou, 2024). Representative CTMs include the Community Multiscale Air Quality Modeling System (CMAQ) developed by the U.S. Environmental Protection Agency (EPA) (Byun and Schere, 2006; Foley et al., 2010; Appel et al., 2017, 2021), the Comprehensive Air Quality Model with Extensions (CAMx) developed by Ramboll (Ramboll, 2020; Emery et al., 2024), WRF-Chem for regional-scale simulations (Grell et al., 2005), and GEOS-Chem, which is widely applied for global-scale studies (Eastham et al., 2018; The International GEOS-Chem User Community, 2025). However, current CTMs still exhibit significant uncertainties in simulating PM_{2.5} and O₃ under specific pollution scenarios in China, primarily manifested as systematic biases in peak concentrations, spatiotemporal distribution errors, and inaccuracies in capturing seasonal variability (Bessagnet et al., 2016; Chen et al., 2019). Against this backdrop, China has developed the Emission and atmospheric Processes Integrated and Coupled Community Model (EPICC-Model) to enhance capabilities in simulating complex pollution processes. Supported by the National Natural Science Foundation of China (Major Program) and the Earth System Numerical Simulation Facility (EarthLab), the model was officially released on November 8, 2024 (EPICC-Model Working Group, 2026) (for detailed description, see Section 2.1).

As a newly released CTM, the EPICC-Model has undergone preliminary single-model performance evaluations (EPICC-Model Working Group, 2026; Wang et al., 2025), but systematic multi-model comparisons under nationwide, multi-season conditions remain lacking. Multi-model intercomparison not only helps reveal differences among models in pollutant transport, chemical reactions, and meteorological feedbacks, but also serves as a key approach to quantifying simulation uncertainties and improving model robustness and reliability (Carmichael et al., 2008). Although substantial efforts have been made in evaluating CTMs over China and East

Asia, such as the MICS-Asia phase studies on PM_{2.5} and O₃ (Chen et al., 2019; Gong and Liao, 2019; Itahashi et al., 2020; Li et al., 2019a), regional comparisons in the Pearl River Delta (Wu et al., 2012), and recent multi-model analyses over eastern China (Gao et al., 2024), most focus on earlier-generation or established models. Likewise, large-scale assessments within CMIP5/6 have consistently revealed systematic biases in simulating PM_{2.5} and components across China (Li et al., 2020; Ren et al., 2024). Given the structural innovations and representations in the EPICC-Model, it is both timely and necessary to conduct a systematic comparison with established CTMs over China, in order to comprehensively assess its strengths and weaknesses and provide a scientific basis for subsequent model improvement and application.

Therefore, this study implements a consistent model intercomparison framework to systematically compare the simulation performance of three models (EPICC-Model, CMAQ, and CAMx) for PM_{2.5} and O₃ concentrations over China in 2021, based on a unified meteorological driving field and a multi-source integrated emission inventory. The objectives are to comprehensively assess the capabilities of the EPICC-Model, identify common issues and their potential causes across multiple models, and propose targeted improvements. The paper is structured as follows: Section 2 introduces the configuration schemes of the three models, emission data sources, the WRF-based meteorological forcing, and the evaluation of meteorological simulations. Section 3 presents the research results, including comparative analyses of the spatiotemporal distribution simulations of PM_{2.5} and O₃, PM_{2.5} chemical composition analysis, assessments of the Air Quality Index (AQI) and pollution forecast accuracy, as well as comparisons of model performance in simulating persistent pollution events. Section 4 summarizes the key findings and discusses future directions for model improvements and prospects.

2 Data and methods

2.1 Overview of simulation domain, period, and CTM configurations

This study employed a two-level nested grid configuration with the model domain centered at (35°N, 105°E). The outer domain covers East Asia with a 45 km horizontal resolution (228 × 165 grid cells), while the inner domain focuses on China at a 15 km resolution (465 × 300 grid cells), starting from grid point (36, 39) within the outer domain. All analyses and results are derived from the inner domain simulations. The simulation period extends from 12:00 UTC on 14 December 2020 to 18:00 UTC on 31 December 2021, with the initial 17.25 days (until 18:00 UTC on 31 December 2020) dedicated to model spin-up.

To systematically evaluate the operational model configurations, this study employed consistent meteorological driving fields generated by the Weather Research and Forecasting (WRF) model and a harmonized multi-source emission inventory to drive year-long simulations using the EPICC-Model, CAMx, and CMAQ. The EPICC-Model is a three-dimensional tropospheric CTM developed in China with an independent modular framework (EPICC-Model Working Group, 2026). Several major process-level routines and numerical algorithms were inherited or adapted from CAMx and CMAQ, whose foundational contributions are explicitly acknowledged. Building on these foundations, the EPICC development team designed a modular and plug-in architecture and independently integrated several specialized chemistry treatments,

including sulfate formation, heterogeneous HONO production, and N₂O₅ hydrolysis. Although the EPICC-Model supports multiple interchangeable scientific options within its plug-in architecture, the present study evaluates a single operational configuration (Table 1) rather than performing intra-model comparisons of alternate process representations or numerical schemes. Such option-to-option assessments have been reported elsewhere (Wang et al., 2025; EPICC-Model Working Group, 2026). Featuring highly modular architecture and parallel computing capabilities, it simulates key physical and chemical processes including emissions, transport, gas-phase and heterogeneous reactions, aerosol thermodynamics, and dry/wet deposition. CAMx (Ramboll, 2020) is a versatile photochemical grid model widely used for air quality scientific assessments and policy support. It follows the “one atmosphere” approach, accommodating pollution simulations from urban to regional scales (Emery et al., 2024). CMAQ (EPA, 2021) is a continuously evolving open-source modeling platform featuring an open architecture and multi-processor parallel computing capabilities. It efficiently simulates air pollution processes including O₃, particulate matter, toxic pollutants, and acid deposition (EPA, 2021).

Table 1. Key configuration schemes of the EPICC-Model, CMAQ, and CAMx.

	EPICC-Model	CAMx	CMAQ
Model version	v1.0	v7.00	v5.3.3
Vertical layers	20 terrain-following σ_z layers (surface to 20 km)	14 time-varying height-interface layers	14 non-hybrid eta layers (MCIP v4.5)
Horizontal advection	Walcek (Walcek and Aleksic, 1998)	PPM (Colella and Woodward, 1984)	PPM
Vertical advection	Walcek	Fully implicit backward Euler (Ramboll, 2020)	PPM
Horizontal diffusion	Multi-scale	Multi-scale	Multi-scale
Vertical diffusion	First-order K-theory (YSU-based diffusivity)	First-order K-theory (WRF/YSU-derived diffusivity; Ramboll, 2020)	ACM2 (Pleim, 2007)
Gas-phase mechanisms	CB6r5 (Yarwood et al., 2020)	CB05 (Yarwood et al., 2005)	CB6r3 (Emery et al., 2015)
Aqueous-phase chemistry	RADM (Walcek and Taylor, 1986)	RADM	AQCHEM
Aerosol processes	ISORROPIA v2.2 (Fountoukis and Nenes, 2007)	CF/ISORROPIA v1.7 (Nenes et al., 1998)	AE7/ISORROPIA v2.2
Secondary organic aerosol	Two-product model (Pandis et al., 1992; Odum et al., 1997)	SOAP2.2 (Ramboll, 2020)	AE7/VBS
Dry deposition	ZHANG03 (Zhang et al., 2001, 2003)	ZHANG03	M3DRY
Wet deposition	Henry's law (William, 1803)	Henry's law	AQCHEM
Photolysis	Full-science TUV (preprocessor) + streamlined TUV (in-model adjustment)	Full-science TUV (preprocessor) + streamlined TUV (in-model adjustment)	Binkowski et al., 2007
Boundary conditions	MOZART	Default	Default

The key configuration parameters of the EPICC-Model, CAMx, and CMAQ are summarized in Table 1. In the operational configurations adopted in this study, the EPICC-Model employed 20 terrain-following normalized-height (σ_z) layers extending from the terrain surface to a fixed model top of 20 km, whereas CAMx and CMAQ were configured with 14 vertical layers. For CMAQ, MCIP v4.5 selected and collapsed layers from the original non-hybrid WRF-ARW terrain-following eta coordinate. For CAMx, WRFCAMx aggregated selected WRF layers and converted their full-level geopotential heights into time-varying physical layer-interface heights. The 14-layer configurations of CAMx and CMAQ used here reflect operational forecasting setups

adopted for the study period, rather than a model-required or intrinsically coarser vertical capability; both models can be configured with finer vertical structures. For future controlled intercomparisons aimed at isolating process-level differences, harmonizing vertical and horizontal grid resolutions across models would be desirable. For three-dimensional transport, the EPICC-Model employed the Walcek scheme for both horizontal and vertical advection, and a first-order K-theory approach for vertical diffusion with diffusivities based on the YSU boundary-layer parameterization. CMAQ used the Piecewise Parabolic Method (PPM) for both horizontal and vertical advection and the Asymmetric Convective Model version 2 (ACM2) for vertical diffusion. WRF meteorological fields generated with the ACM2 scheme are commonly used in CMAQ applications to maintain consistency in boundary-layer treatment. CAMx used PPM for horizontal advection and a fully implicit backward Euler solver for vertical advection. Its vertical diffusion followed a first-order K-theory approach, with vertical diffusivities diagnosed from WRF meteorological fields based on the YSU parameterization. Thus, CAMx does not directly employ the complete online YSU scheme. In terms of chemical mechanisms, the EPICC-Model employed the CB6r5 gas-phase mechanism coupled with RADM aqueous-phase chemistry, allowing the representation of gas-aqueous reactions contributing to secondary organic aerosol (SOA) formation, particularly under high-humidity conditions where aqueous-phase reactions can influence SOA production (Yarwood et al., 2020). The CMAQ v5.3.3 configuration used in this study employed the CB6r3 mechanism in combination with the AE7/VBS module to represent SOA formation, and from version 5.2 onward, incorporated additional parameterizations such as Potential Combustion SOA (PCSOA) to compensate for combustion-related semivolatile organic compound (SVOC) and intermediate-volatility organic compound (IVOC) emissions not captured in current inventories (Murphy et al., 2017). Newer CMAQ versions include CB6r5 and its variants. CAMx used the CB05 gas-phase chemical mechanism coupled with the Secondary Organic Aerosol Partitioning (SOAP) module to parameterize SOA formation, simulating the oxidation of both anthropogenic and biogenic VOCs and their partitioning into the aerosol phase. The CB05 chemical mechanism adopted in CAMx has been widely applied in regional air quality simulations, providing a reasonable balance between chemical representation and computational efficiency. Although CAMx v7.00 also supports the more recent CB6r4 mechanism, CB05 was retained because this study aims to objectively evaluate the models using their actual operational forecasting configurations during the study period, rather than to compare or optimize chemical mechanisms. The operational use of CB05 also reflects the computational-efficiency and forecast-timeliness requirements of routine forecasting, and its applicability to regional CAMx simulations over China has been demonstrated in previous studies (Wen et al., 2021). For photolysis calculations, both the EPICC-Model and CAMx used the full Tropospheric Ultraviolet and Visible (TUV) radiative-transfer model as a preprocessor to generate photolysis-rate input files. A streamlined TUV module was then applied internally to adjust these rates for cloud and aerosol effects. Regarding boundary conditions, the EPICC-Model incorporated MOZART outputs as the initial and lateral background fields. Although CMAQ and CAMx also support the use of

global model outputs, such as MOZART, to provide initial and lateral boundary conditions, simpler profile-based approaches were adopted for these two models to retain their operational configurations during the study period. Specifically, CMAQ boundary conditions were generated based on the CB6r3 profile file, and CAMx initial and boundary conditions were prepared using the icbcprep procedure with the corresponding profile configuration, which can be found in the Zenodo repository (<https://doi.org/10.5281/zenodo.17055755>). These initial and lateral boundary conditions were not harmonized across the three models, and their individual influence was not isolated through sensitivity simulations. Consequently, differences among the model results may reflect the combined effects of internal model formulations and initial and lateral boundary conditions, particularly for regional background concentrations and areas influenced by boundary inflow. Free-tropospheric LBCs may also influence surface O₃ and PM_{2.5} away from the domain edges through rapid transport aloft and subsequent downward mixing (Mathur et al., 2017; Hogrefe et al., 2018; Zhang and Arunachalam, 2018). A comparison of O₃ and PM_{2.5} near ~2 km along the dominant inflow boundary was not performed, which limits diagnosis of LBC contributions in this surface-oriented evaluation. These differences in physical parameterizations, chemical mechanisms, and initial and lateral boundary conditions provide important context for interpreting the differences in PM_{2.5} and MDA8 O₃ simulations among the three models.

2.2 WRF model configuration and meteorological simulation evaluation

Key configuration parameters of the WRF model used in this study are summarized in Table 2. The simulations were conducted using WRF v3.9.1, with initial and boundary conditions derived from the National Centers for Environmental Prediction (NCEP) Final 1° × 1° reanalysis data (FNL, ds083.2), featuring a temporal resolution of 6 hours. To enhance the accuracy of the WRF simulations, four-dimensional data assimilation (FDDA) grid nudging was applied during the simulation. The WRF v3.9.1 simulation used the original non-hybrid terrain-following dry-hydrostatic-pressure eta coordinate and without the hybrid vertical coordinate option.

Table 2. Key configuration parameters of the WRF model.

WRF v3.9.1	
Horizontal resolution	45 km-15 km (one-way nested)
Vertical coordinate	30 non-hybrid eta layers, model top at 50 hPa
Longwave Radiation	RRTMG (Iacono et al., 2008)
Shortwave Radiation	RRTMG
Microphysics	Thompson (Thompson et al., 2008)
Land-surface Model	Unified Noah Land Surface Model (Tewari et al., 2004)
Advection	Monotonic transport
Planetary boundary layer (PBL) scheme	YSU (Hong et al., 2006)
Cumulus option	Kain-Fritsch Scheme (Kain, 2004)
Nudging options	FDDA

This study systematically evaluated the performance of the WRF model in simulating surface meteorological fields over mainland China for the year 2021, based on comprehensive observational data. The evaluation utilized daily observations from representative stations in 335 cities nationwide (excluding Jiayuguan and Wujiaqu due to data unavailability), covering key meteorological variables such as 2 m air temperature, 2 m relative humidity, 10 m wind speed, 10 m wind direction, precipitation, and surface pressure. To ensure seasonal representativeness, January, April, July, and October were selected to represent winter, spring, summer, and autumn, respectively, for comparative analysis (see Fig. S1- Fig. S24 and the Supplement for details, including the evaluation metrics).

The evaluation results indicated that the WRF model accurately captured the diurnal variations of key meteorological variables across most regions. For 2 m temperature simulations, the Pearson correlation coefficient (R) exceeded 0.7 in January and October, with the Root Mean Square Error (RMSE) below 5 °C and the Mean Bias (MB) constrained within ± 2 °C in North, East, and South China. Simulations of 2 m relative humidity also performed well, with R values generally above 0.7 and RMSE below 15% in April and July; MB values in East and South China were less than $\pm 9\%$. However, relatively large humidity biases were observed in parts of Southwest and Northwest China, where MB in the southwest exceeded 15% and RMSE surpassed 17%. Previous studies suggest that simulations can be considered reliable when $R \geq 0.6-0.7$, RMSE for temperature ≤ 5 °C, and RMSE for humidity $< 15\%$ (Lou et al., 2025; Oyegbile et al., 2024). Therefore, the WRF model used in this study demonstrated adequacy in simulating temperature and humidity. Simulations of 10 m wind speed showed consistent performance, with R exceeding 0.7 and RMSE below 8 m/s in most regions. Nevertheless, systematic overestimations were observed in the Sichuan Basin, Xinjiang, and parts of Tibet. Although the wind speed RMSE exceeds typical values reported in some studies (4-6 m/s), it remains within an acceptable range given the seasonal variability at the national scale (Xu et al., 2020; Yu et al., 2022b). In contrast, the performance for 10 m wind direction was relatively poor, with R values below 0.4 in most areas, except for moderate improvement in the Beijing-Tianjin-Hebei region, East China, Central China, and South China. This finding aligns with previous research noting WRF's general limitations in reproducing wind direction (Jiménez and Dudhia, 2013). For precipitation, correlation coefficients were generally above 0.4 nationwide. However, substantial errors were observed in parts of Southwest, Northwest, and South China, especially in regions with complex terrain, consistent with previous findings (Yu et al., 2022a). Surface pressure simulations exhibited high consistency, with R values exceeding 0.7 across the country. While parts of Southwest and Central China exhibited slight underestimation (MB < 20 hPa), likely associated with unresolved terrain altitude differences at the model resolution, surface pressure was slightly overestimated in Guizhou and Chongqing. Overall, the WRF model provided adequate meteorological forcing fields for CTMs.

2.3 Emission inventory and observational data sources

The anthropogenic emissions data used in this study for China were derived from

the Multi-resolution Emission Inventory for China (MEIC) developed by Tsinghua University, with a base year of 2019 (Geng et al., 2024). This inventory includes major source sectors such as transportation, industry, power generation, and residential combustion, and covers multiple pollutants including CO, SO₂, NO_x, VOCs, PM₁₀, PM_{2.5}, black carbon (BC), and organic carbon (OC). Emissions of ammonia over China were obtained from the PKU-NH₃ inventory (Huang et al., 2012a; Kang et al., 2016), while emissions from biomass burning are taken from the “China Open Biomass Burning Emissions Inventory” with a base year of 2017 (Huang et al., 2012b; Song et al., 2009). The Emissions Database for Global Atmospheric Research (EDGAR) v5.0 dataset (Crippa et al., 2020), with a base year of 2015 and a spatial resolution of 0.1° × 0.1°, was used to represent anthropogenic emissions outside China. Biogenic emissions were simulated online using the Model of Emissions of Gases and Aerosols from Nature (MEGAN) v3.2 model (Guenther et al., 2012). It should be noted that although the base years of the emission inventories do not match the simulation year of this study, the use of inventories from adjacent years remains a common practice in regional air quality modeling, especially in the absence of globally consistent, high-resolution, multi-sector emission datasets for the target year. Under the assumption of no substantial changes in regional climate and socioeconomic activities, such inventories can reasonably represent the emission patterns of the study period (Amnuaylojaroen et al., 2014; Huang et al., 2023; Wang et al., 2023). It is important to clarify that no projection or temporal adjustment of the individual emission inventory data to the 2021 simulation year was performed.

All surface observational data used in this study were obtained from the China National Environmental Monitoring Centre (CNEMC), including hourly PM_{2.5} and O₃ concentrations from 1,644 national monitoring stations across China in 2021 (station distribution shown in Fig. S25). Based on these data, daily average PM_{2.5} concentrations and MDA8 O₃ values were calculated for 337 cities. Additionally, aerosol chemical composition data were obtained from the same source for ten representative cities: Beijing (116.41°E, 40.04°N), Tianjin (117.21°E, 39.17°N), Zhengzhou (113.73°E, 34.77°N), Jinan (117.06°E, 36.66°N), Shanghai (121.53°E, 31.23°N), Nanjing (118.76°E, 32.07°N), Wuhan (114.37°E, 30.54°N), Fuzhou (119.31°E, 26.10°N), Chengdu (104.09°E, 30.64°N), and Chongqing (106.47°E, 29.62°N).

3 Results and discussion

3.1 Spatiotemporal distribution and statistical analysis of daily averages

Figure 1 presents the performance of the EPIC-Model, CAMx, and CMAQ in simulating annual PM_{2.5} concentrations, evaluated against observations from 1,644 national monitoring stations across China. Based on the time series analysis (Figure 1a), the year can be divided into three distinct phases. Phase I (January to mid-May): During this period, both the EPIC-Model and CAMx significantly underestimated PM_{2.5} concentrations and failed to capture the three major pollution episodes at the beginning of the year, as indicated by the circles in the figure (with biases ranging from 25 to 52 µg m⁻³). In contrast, CMAQ showed improved performance in capturing both the timing

and intensity of pollution peaks. This was primarily attributed to its substantially higher simulated OC levels relative to the other models and observations, which produced a compensatory effect on total $\text{PM}_{2.5}$ (Figure 6). In addition, CMAQ exhibited intermittent overestimations during several periods, which may partly reflect the sensitivity of near-surface $\text{PM}_{2.5}$ concentrations to the treatment of minimum vertical eddy diffusivity (Kz_min) in ACM2, as indicated by previous CMAQ sensitivity experiments over China (Kim et al., 2024). The contrasting pattern within the rectangular box was attributed to a dust event. Phase II (mid-May to mid-October): During this period, $\text{PM}_{2.5}$ concentrations were generally low and exhibited limited variability. This was primarily attributed to elevated planetary boundary layer heights, enhanced turbulent mixing, and frequent precipitation events during the summer, which collectively facilitated the dilution and wet deposition of near-surface particulate matter. CAMx performed best in this phase. In contrast, both the EPIC-Model and CMAQ tended to overpredict pollutant levels, with CMAQ exhibiting a notably stronger positive bias. Phase III (mid-October to December): During the heating season, observed $\text{PM}_{2.5}$ levels increased significantly, accompanied by greater spatiotemporal variability. CAMx maintained relatively good agreement with the observations, whereas the positive bias of CMAQ became more pronounced. The component evaluation in Figure 6 indicates that the substantially elevated OC concentration simulated by CMAQ was the most likely dominant contributor to this $\text{PM}_{2.5}$ overestimation, while differences in vertical mixing may have additionally influenced near-surface pollutant accumulation. The performance of the EPIC-Model was intermediate between the two.

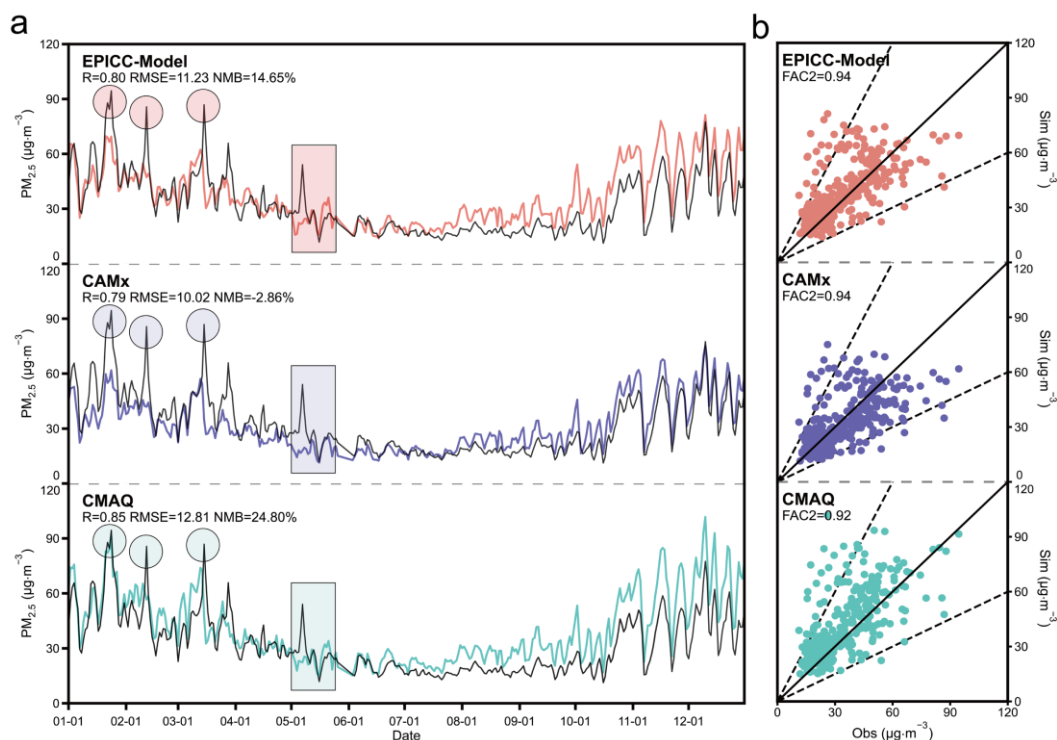


Figure 1. Comparison of simulated and observed daily $\text{PM}_{2.5}$ concentrations (i.e., daily mean $\text{PM}_{2.5}$ concentrations) across China in 2021. (a) shows the time series of daily $\text{PM}_{2.5}$, with the black line representing observations from 1,644 national air quality monitoring stations and colored lines indicating different CTMs. (b) presents scatter plots of modeled versus observed $\text{PM}_{2.5}$. All model

outputs exclude dust aerosol contributions to isolate secondary particulate formation processes.

Statistical validation analysis (Figure 1b) further corroborated the above findings. Although CMAQ exhibited the highest correlation coefficient ($R=0.85$), most of its data points lay above the 1:1 reference line, indicating a systematic overestimation. CAMx demonstrated the best overall statistical performance, with a Fraction of Predictions Within a Factor of Two (FAC2) value of 0.94 and a Normalized Mean Bias (NMB) of merely -2.86%. It is important to note that CAMx struggled to capture severe pollution episodes, markedly underestimating periods of high concentrations, which constrains its usefulness for evaluating pollution processes. In contrast, the EPICC-Model exhibited a more pronounced seasonal response. Its simulations during spring and summer are more consistent with CAMx, indicating similar performance under the generally lower ambient $PM_{2.5}$ concentrations during these seasons, particularly in summer when enhanced boundary-layer ventilation and more frequent precipitation favor pollutant dilution and wet removal. During the autumn and winter pollution seasons, its simulation trends aligned more closely with CMAQ, capturing pollution accumulation processes more effectively. At the national aggregate scale represented in Figure 1, the EPICC-Model reproduced the seasonal transition of $PM_{2.5}$ concentrations and responded to high-concentration pollution episodes while maintaining reasonably strong annual statistical performance.

Figure 2 presents the performance of the EPICC-Model, CAMx, and CMAQ in simulating MDA8 O_3 concentrations, evaluated against observations from 1,644 national monitoring stations across China. Observational data reveal a typical photochemically-driven seasonal pattern in O_3 concentrations: summer months exhibit peak levels due to enhanced VOC- NO_x chain reactions under intense solar radiation and elevated temperatures (Seinfeld and Pandis, 2016; Sillman, 1999), while O_3 concentrations remain relatively low during the colder months because weaker solar radiation suppresses photolysis and lower temperatures reduce thermochemical reaction rates, collectively weakening photochemical activity (Wang et al., 2019). The time series analysis (Figure 2a) showed that all three models reasonably reproduced the seasonal variation of O_3 concentrations, yet notable differences emerged across concentration levels. The EPICC-Model performed particularly well during high-concentration episodes, effectively capturing the peak levels of O_3 pollution. In contrast, both CAMx and CMAQ, while capable of reproducing high-concentration trends, systematically underestimated peak magnitudes with maximum negative biases reaching $-20 \mu g m^{-3}$. The improved representation of high- O_3 episodes by the EPICC-Model may be partly related to its inclusion of heterogeneous HONO formation and particulate nitrate photolysis, which can enhance radical production and O_3 formation in inland China (Bao et al., 2018; Zhang et al., 2022; Li et al., 2024). Recent EPICC-specific sensitivity and source-diagnosis studies further demonstrate that these HONO pathways, including particulate nitrate photolysis, contribute to simulated HONO and O_3 formation and improve the representation of O_3 over China (Zhang et al., 2025; EPICC-Model Working Group, 2026). At lower O_3 concentration levels, CMAQ reproduced the general temporal variation but exhibited a systematic positive bias, which may reflect the combined influence of vertical redistribution and photochemical production.

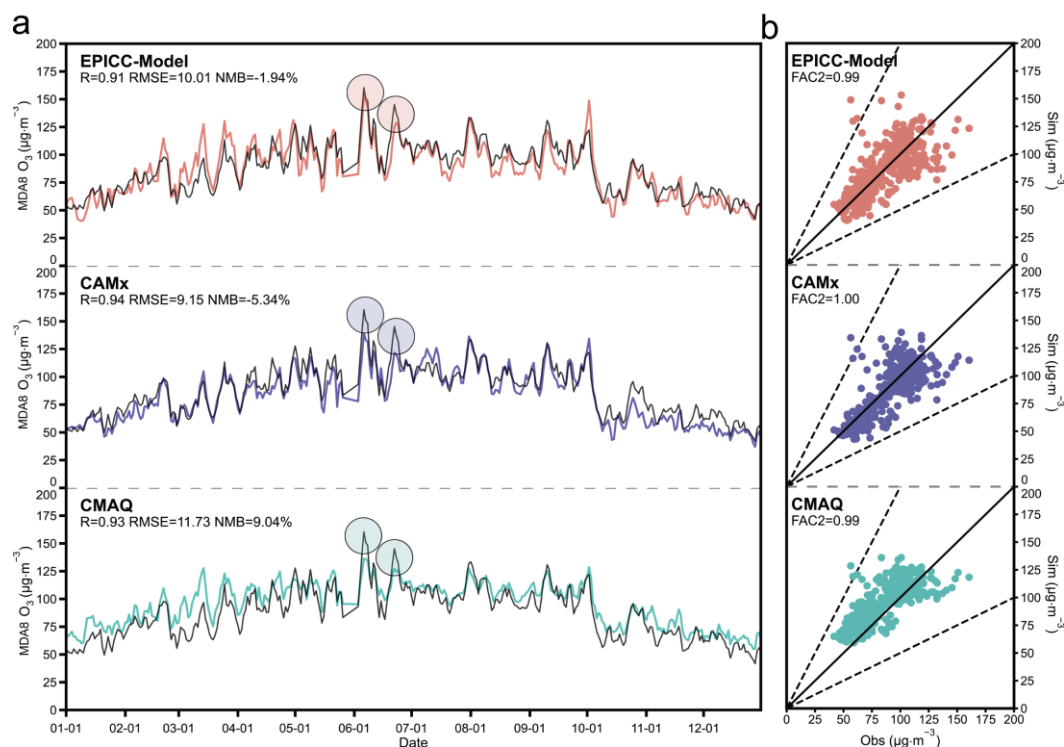


Figure 2. Comparison of simulated and observed daily MDA8 O₃ concentrations across China in 2021.

Statistical analysis indicated that CAMx achieved the highest temporal correlation ($R = 0.94$) and the lowest RMSE ($9.15 \mu\text{g m}^{-3}$), while exhibiting a modest negative mean bias ($\text{NMB} = -5.34\%$). CMAQ showed a slight overestimation throughout the year but maintained a strong temporal correlation ($R=0.93$), demonstrating good capability in capturing temporal variations. Notably, the EPIC-Model not only accurately captured peak concentrations but also achieved the lowest annual NMB, reflecting a more robust performance overall. The scatterplots in Figure 2b showed that all three models had FAC2 values close to 1, indicating comparable overall performance. The models nevertheless exhibited different statistical characteristics: CMAQ tended to overestimate MDA8 O₃, CAMx achieved the highest correlation and lowest RMSE despite a modest negative bias, and the EPIC-Model had the smallest absolute NMB.

Figure 3 compares the simulated spatial distributions of PM_{2.5} for the four seasons of 2021 produced by the EPIC-Model, CAMx, and CMAQ, revealing notable differences in regional simulation consistency and bias characteristics among the three models. As shown in Figure 3, the Index of Agreement (IOA) values vary across models and seasons, exhibiting clear seasonal patterns that quantitatively support the spatial distribution differences.

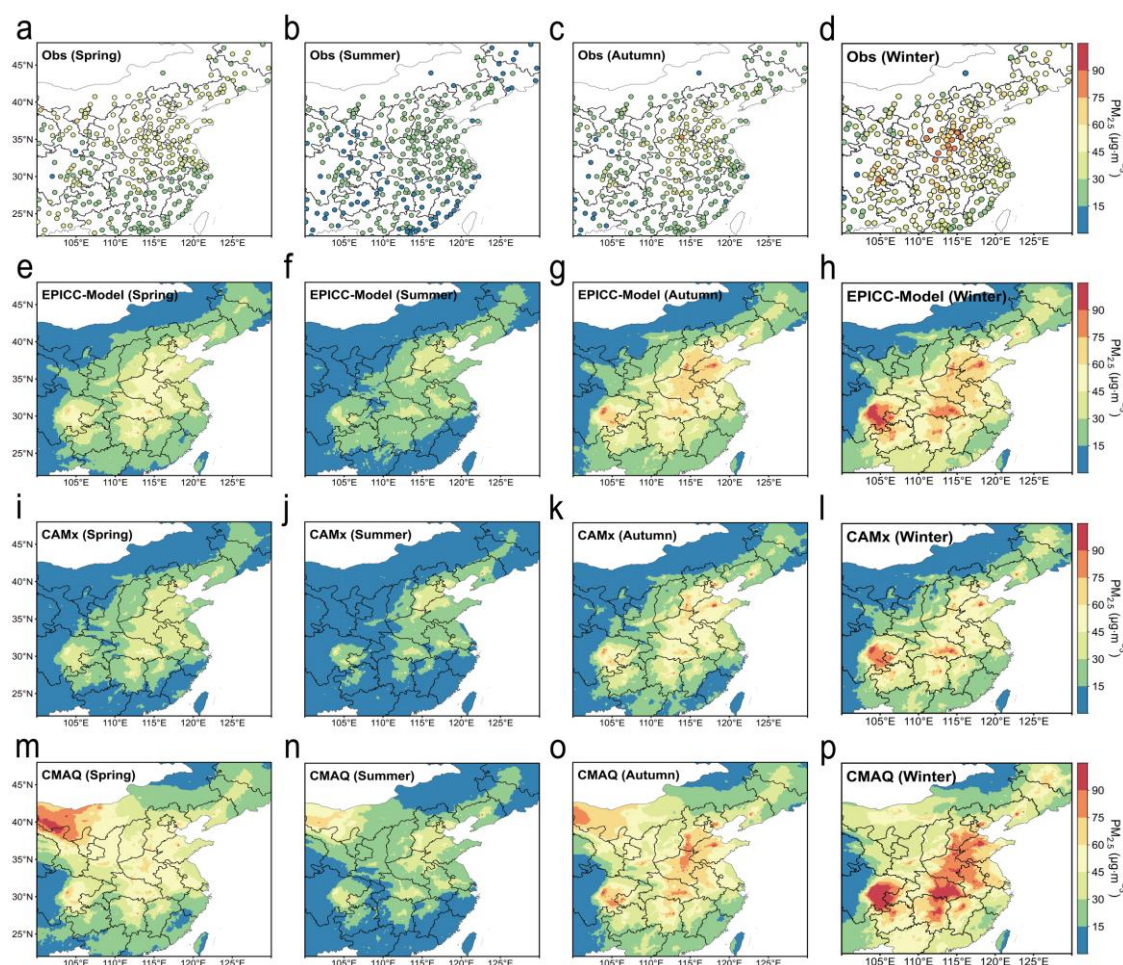


Figure 3. Seasonal spatial distributions of simulated PM_{2.5} concentrations, with spring (March-May), summer (June-August), autumn (September-November), and winter (December-February).

Table 3. IOA for the spatial distribution of PM_{2.5} simulated by different models.

	Spring	Summer	Autumn	Winter	Year
EPIC-Model	0.63	0.62	0.60	0.81	0.80
CAMx	0.60	0.64	0.68	0.76	0.78
CMAQ	0.72	0.58	0.54	0.73	0.77

In spring, elevated PM_{2.5} concentrations were observed in several geographically separated regions, including North China, the arid basins of Northwest China, and the Sichuan Basin. This spatial pattern reflects the combined influences of northwesterly dust transport, local anthropogenic emissions, and pollutant accumulation under relatively limited ventilation in basin regions. All three models effectively reproduced the pollution pattern, with IOA values exceeding 0.60, and CMAQ achieved the highest IOA of 0.72. Since dust concentrations were excluded from the particulate matter assessment in this study, all three models consistently underestimated PM_{2.5} levels in the arid Northwest and southwestern plateau regions. In summer, influenced by the southeastern monsoon and intensive precipitation, PM_{2.5} remained generally low across China with reduced regional variability. The three models exhibited similar spatial consistency nationwide, with IOA values ranging between 0.58 and 0.64. However, in the high-humidity coastal regions of South China, the EPIC-Model and CMAQ

demonstrated slight advantages over CAMx in simulation accuracy. In autumn, the nationwide PM_{2.5} concentrations rebounded due to an increase in stagnant weather conditions and a reduced boundary layer height. All three models showed varying degrees of overestimation in North China and the Sichuan Basin, likely related to ACM2/YSU schemes underestimating mixing layer height and weakening vertical diffusion at night (Jia et al., 2023). During this period, CAMx achieved the highest IOA value of 0.68, the EPIC-Model scored 0.60, while CMAQ dropped to its annual minimum of 0.54. In winter, PM_{2.5} concentrations reached their annual peak driven by low temperatures, temperature inversions, subsidence, and heating emissions. All three models successfully reproduced the pollution patterns in polluted regions like North and Central China. The EPIC-Model demonstrated exceptional performance with an IOA of 0.81, while CMAQ and CAMx maintained strong consistency at 0.73 and 0.76, respectively. However, all models unrealistically simulated higher PM_{2.5} concentrations in the Sichuan Basin compared to Henan Province. This discrepancy may have resulted from differences in emission estimates between the two regions: anthropogenic emissions in the Sichuan Basin are likely overestimated in the models, whereas frequent agricultural activities in Henan may lead to underestimation of NH₃ emissions, thereby suppressing nitrate aerosol formation. Previous studies have demonstrated that spatial errors in NH₃ emissions significantly impact nitrate-driven heavy pollution events (Kang et al., 2016; Kong et al., 2019; Liu et al., 2021).

Overall, all three models reliably simulated PM_{2.5} spatial distributions, with annual mean IOA values above 0.77. The EPIC-Model performed best (IOA=0.80), showing highest consistency in winter and heavily polluted North China. CAMx showed consistent performance (IOA=0.78) and was suitable for multi-seasonal averages but underestimated high-humidity regions and responded weakly to severe pollution. CMAQ showed slightly lower consistency (IOA=0.77), performed better in spring and winter, declined in summer and autumn, and exhibited a general positive bias, particularly in winter.

Figure 4 shows the seasonal spatial distribution of MDA8 O₃ in 2021 from the three models. Given the strong seasonal variability of O₃, model performance was quantitatively evaluated using the IOA metric, with detailed results provided in Table 4.

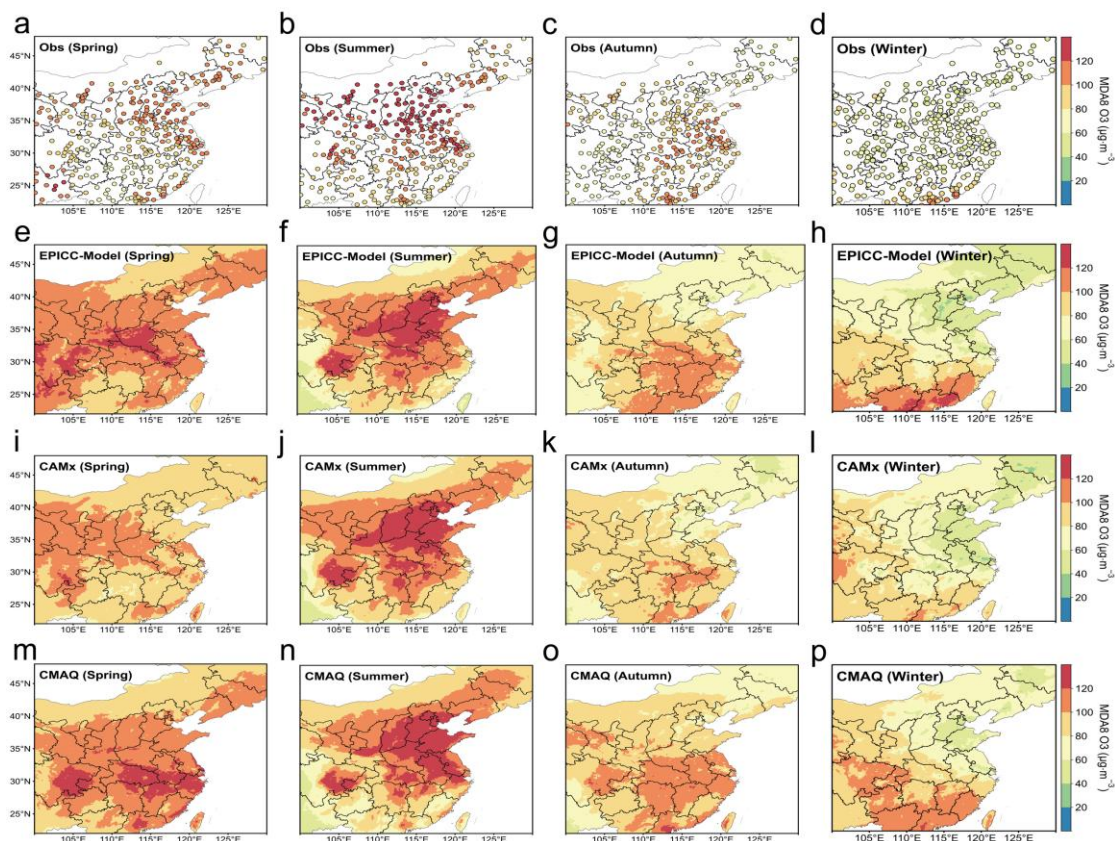


Figure 4. Seasonal spatial distributions of simulated MDA8 O₃ concentrations, with spring (March–May), summer (June–August), autumn (September–November), and winter (December–February).

Table 4. IOA for the spatial distribution of MDA8 O₃ simulated by different models.

	Spring	Summer	Autumn	Winter	Year
EPIC-Model	0.56	0.79	0.74	0.77	0.85
CAMx	0.53	0.85	0.70	0.76	0.87
CMAQ	0.33	0.85	0.78	0.75	0.84

In spring, O₃ pollution exhibited a multi-centered and scattered distribution pattern. The EPIC-Model reproduced this pattern well (IOA = 0.56) and outperformed CAMx and CMAQ, particularly in the high-concentration areas like Yunnan. CAMx generally underestimated O₃ across China, which may reflect the combined effects of its gas-phase chemistry and representation of vertical transport (Ren et al., 2022; Tang et al., 2011). CMAQ, in contrast, produced an unrealistic high-O₃ belt over the Yangtze River plain with a much lower IOA of 0.33. In summer, a high O₃ concentration belt formed over the mid-latitudes (30° N ~40° N), and all three models successfully reproduced the enhanced O₃ levels with the highest spatial consistency observed throughout the year. The summer IOA values for the EPIC-Model, CAMx, and CMAQ reached 0.79, 0.85, and 0.85, respectively. All three models were driven by meteorological inputs derived from the same WRF simulation but processed for their respective vertical structures. The simulated summer O₃ distributions therefore reflected the combined influences of regional photochemistry, meteorological transport, and lateral boundary conditions (Li et al., 2019a). In autumn, nation-wide O₃ declined as solar radiation weakens, with pollution centers shifted to eastern and southeastern coasts. All three

models performed similarly (IOA 0.70–0.78). CMAQ performed best in the Pearl River Delta, accurately reproducing localized high concentrations, as supported by previous studies (Jiang et al., 2010; Wang et al., 2010). The EPICC-Model ranked second with slight overestimation in northern Jiangxi, and CAMx continued to underestimate O₃. In winter, nationwide O₃ concentrations decreased to their annual minimum, and the relative seasonal concentration maximum shifted toward southern coastal China. This redistribution reflects weaker photochemical production and stronger NO titration over northern China, whereas comparatively stronger solar radiation sustains greater photochemical activity in the south. All models performed steadily (IOA 0.75–0.77). The EPICC-Model reproduced the relative O₃ maximum over the southern coastal region, whereas CAMx displaced it farther southwest. CMAQ reproduced O₃ reasonably well over North China but overestimated concentrations mainly over the middle and lower reaches of the Yangtze River and the Sichuan Basin. These differences reflect the models' combined representations of photochemistry, NO titration, and atmospheric transport.

The evaluation indicated that the EPICC-Model showed consistent seasonal MDA8 O₃ performance with an annual IOA of 0.85, capturing O₃ distribution across China. CAMx had slightly higher consistency (IOA 0.87) but systematically underestimated in spring, autumn, and winter and missed localized peaks. CMAQ performed well in summer and autumn, especially over the Pearl River Delta, but IOA dropped to 0.33 in spring and overestimated in winter, indicating a need to improve boundary layer and dry deposition schemes.

To comprehensively evaluate model performance, this study used Taylor diagrams to compare the EPICC-Model, CAMx, and CMAQ simulations with observations on both annual and seasonal scales. The Taylor diagram simultaneously displays the correlation coefficient (R), normalized standard deviation (STD), and centered root mean square error (RMSE). In the diagram, the radial distance represents STD, the angular coordinate indicates R, and dashed contours denote RMSE relative to observations. The “REF” point (R = 1, STD = 1) represents perfect agreement with observations. The annual results (Figure 5a) showed that all three models performed satisfactorily in simulating PM_{2.5} and MDA8 O₃, with particularly strong performance for MDA8 O₃. Correlation coefficients exceeded 0.75 for all models, while RMSE and STD remained relatively low, indicating lower variability and higher accuracy in MDA8 O₃ simulations compared to PM_{2.5}.

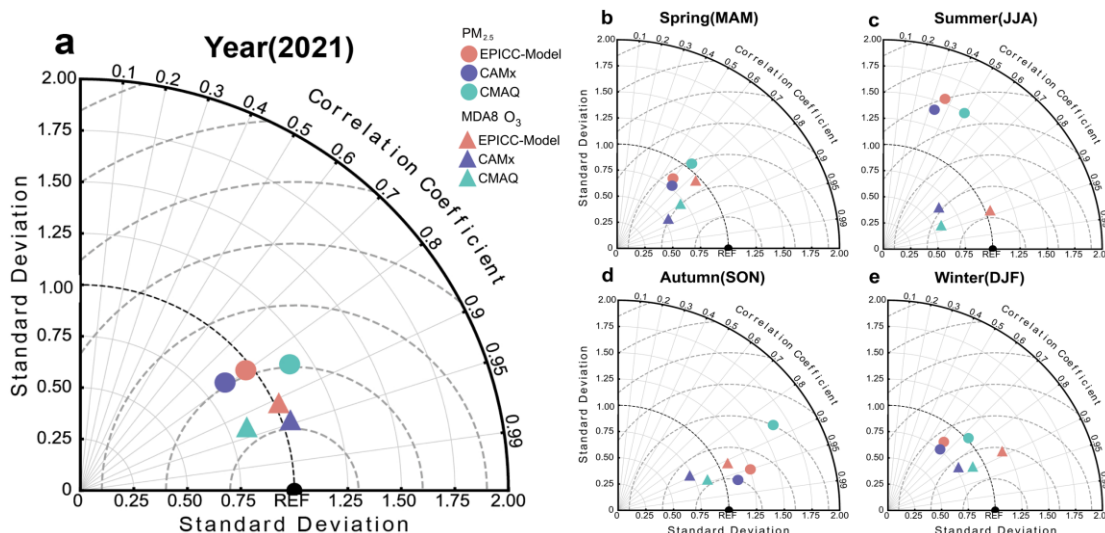


Figure 5. Taylor diagrams of PM_{2.5} and MDA8 O₃ for the three models on annual and seasonal scales.

Seasonally, PM_{2.5} simulation accuracy exhibited marked variations: during winter and spring high-concentration periods, all three models showed comparable performance, with CMAQ demonstrating greater ability to replicate pollution peaks (STD $\approx$ 1, closest to observations). Model performance declined significantly under summer's low-background conditions ($R < 0.55$, elevated RMSE/STD), indicating enhanced error during high-concentration periods. Autumn saw a recovery in performance, and CAMx achieved $R = 0.97$. In contrast, MDA8 O₃ simulations showed more robust seasonal consistency: while spring remained the weakest season ($R > 0.7$), the EPIC-Model and CMAQ maintained low errors. The EPIC-Model excelled during summer O₃ peaks ($R \approx 0.95$, lowest RMSE/STD), CMAQ led in autumn, and all models converged in winter ($R = 0.8-0.9$), effectively capturing O₃ spatiotemporal patterns.

Overall, the EPIC-Model demonstrated strong robustness in seasonal O₃ simulations, maintaining consistently low standard deviations and showing clear advantages during the summer pollution peak. In contrast, CAMx and CMAQ exhibited relative strengths in PM_{2.5} simulations: CAMx performed particularly well under the complex meteorological conditions of autumn, while CMAQ better captured pollutant accumulation processes during the stable boundary layer conditions in winter, reflecting their respective adaptability.

3.2 Evaluation of PM_{2.5} chemical composition simulations

Based on the spatiotemporal variations of PM_{2.5} total concentrations simulated by each model, the performance of the EPIC-Model, CAMx, and CMAQ in simulating major chemical components was further evaluated. Figure 6 presents the average relative contributions and absolute concentrations of key PM_{2.5} components in ten representative cities across urban clusters, including the Beijing-Tianjin-Hebei, Yangtze River Delta, Chengdu-Chongqing, and the Middle Reaches of the Yangtze River regions. Overall, all three models reasonably reproduced the observed chemical

composition structure characterized by a predominance of nitrate (NO_3^-), which is consistent with previous findings (Huang et al., 2021). Observations indicated that NO_3^- accounted for approximately 31.2% to 42.4% of $\text{PM}_{2.5}$ mass in most cities. This dominant feature was reproduced by all models, although the simulated concentrations tended to be overestimated to varying degrees.

Meanwhile, all three models consistently underestimated sulfate (SO_4^{2-}), a bias consistent with existing research findings (Shao et al., 2019), which may stem from underestimating SO_2 oxidation rates or uncertainties in intra-cloud aqueous-phase chemical mechanisms. The insufficient formation of SO_4^{2-} not only limited the production of ammonium sulphate $[(\text{NH}_4)_2\text{SO}_4]$ but also reduced the consumption potential of NH_3 (Gao et al., 2018), thereby suppressing the simulated concentration of ammonium (NH_4^+). The reduced formation of ammonium sulfate may also leave more NH_3 available to partition with HNO_3 , potentially enhancing NH_4NO_3 formation and contributing to the overestimation of particulate NO_3^- in some regions.

For OC, although certain deviations are observed in individual cities, the overall simulation performance of the three models remained within an acceptable range (Miao et al., 2020). Among them, the EPIC-Model and CAMx produced results that were closer to observations, while CMAQ tended to systematically overestimate OC concentrations. This systematic bias may stem from the introduction of Potential Combustion SOA (PCSOA) species starting from CMAQv5.2. PCSOA serves as a surrogate secondary organic aerosol species to compensate for the lack of combustion-related SVOC and IVOC emissions in current inventories. However, the model estimates PCSOA concentrations through parameterized precursor emissions and simplified processes including OH oxidation and gas-particle partitioning. The associated uncertainties may result in regional and temporal discrepancies, failing to reflect the real-world variations in PCSOA and consequently leading to simulation biases (Murphy et al., 2017; Pennington et al., 2021). Overall, all three models share substantial uncertainties in SOA-related mechanisms, representing a common limitation.

BC is the least abundant component of $\text{PM}_{2.5}$, with observed concentrations ranging from 0.7 to 2.1 $\mu\text{g m}^{-3}$. All models exhibited generally consistent performance in simulating its relative contribution, and slight overestimations were observed in Beijing, Tianjin, and Zhengzhou. In Beijing and Zhengzhou, the elevated fractions were accompanied by overestimated absolute BC concentrations, suggesting possible uncertainties in BC emission magnitude or spatial allocation, as well as in mixing, transport, and removal processes. In Tianjin, however, the absolute BC bias was small. The elevated BC mass fraction is mainly attributable to the underestimation of other measured $\text{PM}_{2.5}$ components in absolute terms (particularly OC), which reduces the simulated total of these components and thereby increases the relative contribution of BC. Differences in spatial representativeness between individual urban sites and grid-cell-averaged concentrations may introduce additional uncertainty, although their influence on the direction of the bias cannot be determined from the available data (Hong et al., 2017).

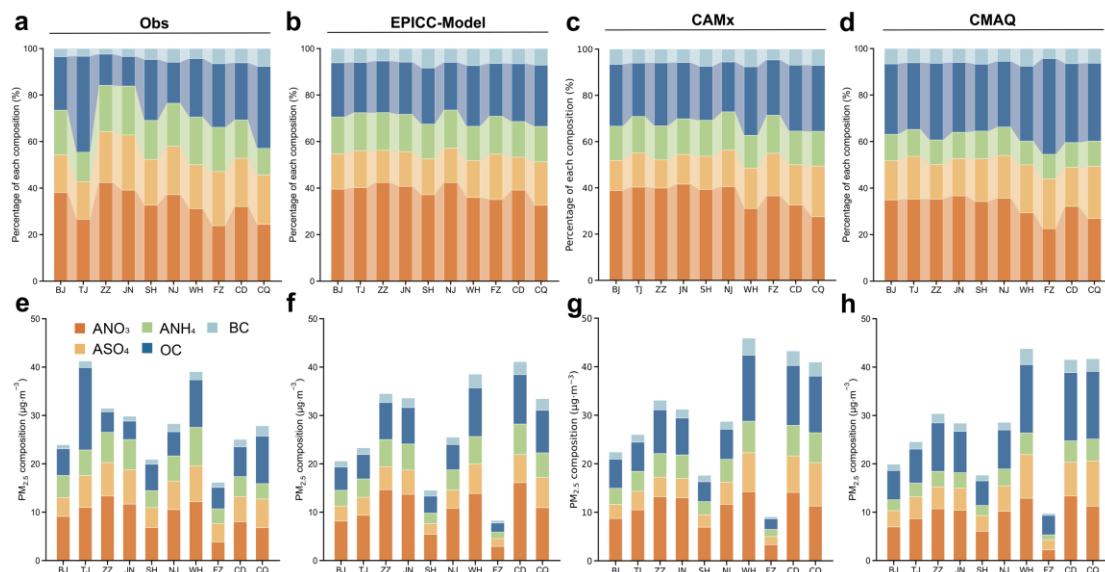


Figure 6. Comparison of simulated and observed aerosol components in representative Chinese cities. ASO₄, ANO₃, ANH₄, OC, and BC denote sulfate, nitrate, ammonium, organic carbon, and black carbon in PM_{2.5}, respectively. The locations of monitoring sites are as follows: BJ (Beijing; 116.41° E, 40.04° N), TJ (Tianjin; 117.21° E, 39.17° N), ZZ (Zhengzhou; 113.73° E, 34.77° N), JN (Jinan; 117.06° E, 36.66° N), SH (Shanghai; 121.53° E, 31.23° N), NJ (Nanjing; 118.76° E, 32.07° N), WH (Wuhan; 114.37° E, 30.54° N), FZ (Fuzhou; 119.31° E, 26.10° N), CD (Chengdu; 104.09° E, 30.64° N), and CQ (Chongqing; 106.47° E, 29.62° N).

As shown in the stacked bar charts of PM_{2.5} absolute concentrations in Figure 6e-h, Tianjin exhibits the highest levels among the selected cities, followed by Wuhan, while Fuzhou shows the lowest. This spatial pattern is closely related to regional emission intensity and meteorological conditions. The three models reasonably reproduce these concentrations in most cities, particularly in Nanjing. However, systematic biases exist in certain locations. Simulated concentrations in Tianjin are substantially lower than observations, primarily due to underestimation of OC associated with uncertainties in SOA formation mechanisms. In contrast, concentrations in Chengdu and Chongqing are consistently overestimated across all models, indicating an amplified model response to pollution episodes in central China. Overall, while the models capture the major chemical composition features, their ability to accurately reproduce absolute concentrations and regional variability remains limited, highlighting the need for refined emission inventories and improved representation of meteorological processes.

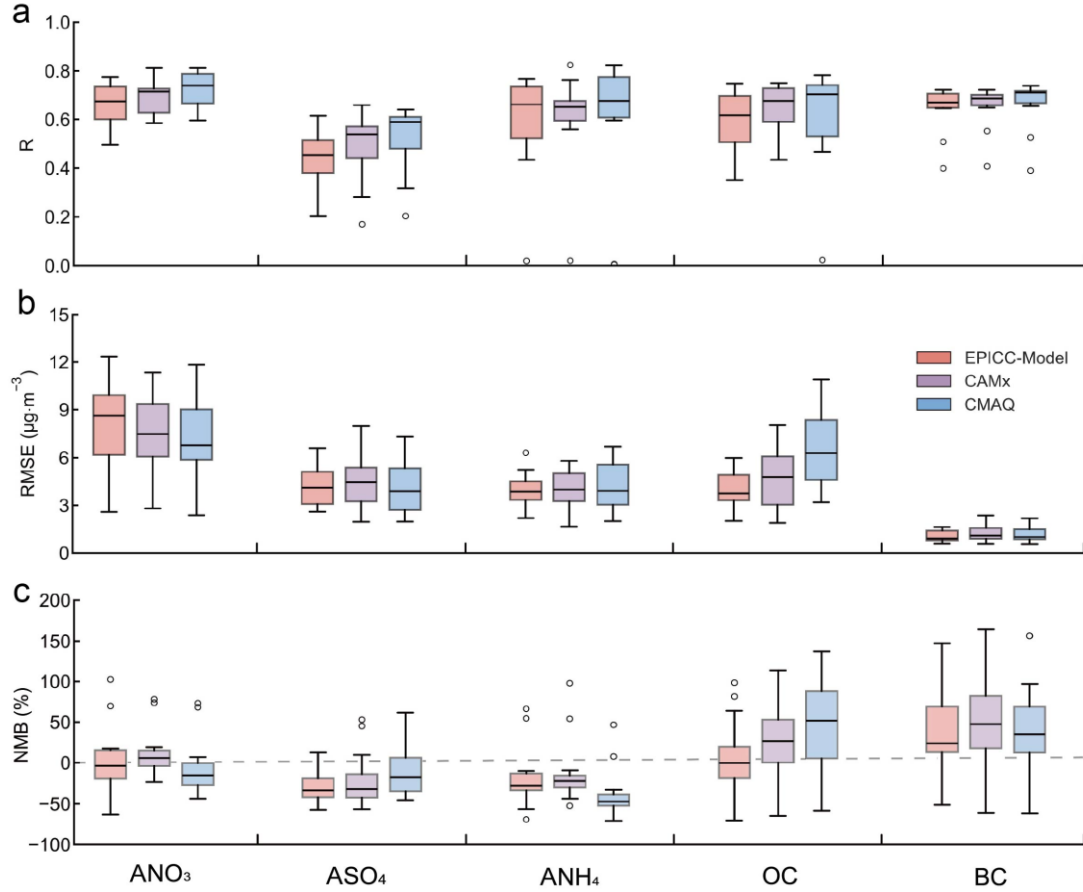


Figure 7. Performance metrics of aerosol component simulations across models in representative Chinese cities.

Figure 7 presents boxplots of statistical evaluation metrics (R, RMSE, and NMB) based on ten representative cities to quantify the simulation accuracy and systematic biases of each model. Regarding the overall distribution of R values, a clear “stepwise” difference is observed among the three models. CMAQ generally exhibits higher R values across PM_{2.5} components than the EPIC-Model and CAMx, indicating stronger capability in reproducing spatiotemporal variability. Among individual components, NO₃⁻ shows the highest correlation (median R > 0.6) with no outliers, suggesting robust representation. NH₄⁺ and OC display slightly lower R values, reflecting moderate uncertainty but acceptable overall performance. SO₄²⁻ shows dispersed correlations and some low R values, indicating substantial simulation errors, likely due to insufficient representation of regional secondary aerosol formation. BC exhibits the most compact R distribution, with low inter-city variability, reflecting robust and consistent simulation by all models. The RMSE analysis shows larger errors for NO₃⁻ and OC, with some cities reaching 12 μg m⁻³ and median values above 6 μg m⁻³, reflecting sensitivity to meteorology, secondary processes, and SOA-related uncertainties. The EPIC-Model performs well in this aspect. SO₄²⁻ and NH₄⁺ exhibit moderate RMSE, indicating relatively low variability simulations, while BC shows the lowest RMSE and most compact distribution, suggesting high accuracy. The NMB results show that the deviations of NO₃⁻, SO₄²⁻, and NH₄⁺ are relatively constrained, although overestimations or underestimations still occur in some cities. In contrast, the NMB

boxplots for OC and BC exhibit significant elongation, with deviations ranging from -50% to +150% in certain locations. The high bias of OC is mainly attributed to inaccuracies in the representation of SOA formation and precursor emissions, while the large relative deviations of BC are likely due to its low ambient concentrations, where even minor absolute errors can lead to amplified relative discrepancies.

A cross-model comparison reveals that CMAQ exhibits the highest correlation coefficients, particularly excelling in reproducing the spatial and temporal patterns of NO_3^- and NH_4^+ . However, it shows a tendency to overestimate OC concentrations. CAMx shows intermediate performance across most components. The performance of the EPIC-Model varies among chemical components and cities, with its RMSE and NMB generally falling within the ranges of the other two models.

3.3 AQI and pollution forecast accuracy

To benchmark the performance of the three CTMs across air-quality categories, we evaluated the categorical forecasts of the EPIC-Model, CAMx, and CMAQ following the *Technical guideline for numerical forecasting of ambient air quality* (HJ1130-2020) and the *Technical Regulation for the Assessment of Urban Ambient Air Quality Index (AQI) Forecasts (Trial)* (CNEMC, 2021). For the Air Quality Index (AQI) level evaluation, an AQI interval from 0.75F to 1.25F was first constructed, where F denotes the forecast AQI. This interval was converted to the corresponding air-quality-level range, and a forecast was considered correct when the observed level fell within that range. Missing observations or simulations were excluded before classification and evaluation. $\text{PM}_{2.5}$ and MDA8 O_3 were also evaluated separately using their respective individual air quality index (IAQI) categories. Because the present model configurations did not include wind-blown dust emissions, the combined heavy/severe $\text{PM}_{2.5}$ category was retained as a diagnostic evaluation of model performance under the configurations used in this study, rather than as an evaluation of dust-forecasting capability. To determine whether the statistics for this category were dominated by typical dust events, the spatial and seasonal distribution of the observed heavy/severe $\text{PM}_{2.5}$ events was additionally examined. The detailed analysis is presented in Section S4 and Table S1 of the Supplement. Overall, the categorical forecast accuracy generally decreased as the observed pollution level increased. The algorithms and definitions of AQI and IAQI are provided in the Supplement for reference.

In terms of overall forecasting accuracy, CAMx performed best for AQI, $\text{PM}_{2.5}$ IAQI, and MDA8 O_3 IAQI, with accuracies of 84%, 83%, and 90%, respectively. The EPIC-Model showed competitive performance in several light and moderate pollution categories. This performance was physically consistent with the heterogeneous pathways represented in the model, including manganese-catalyzed SO_2 oxidation at the air-liquid interface of deliquesced aerosol particles, N_2O_5 heterogeneous hydrolysis, and heterogeneous HONO formation (Wang et al., 2021; Zhang et al., 2022; Yang et al., 2024; EPIC-Model Working Group, 2026). For $\text{PM}_{2.5}$, CMAQ showed the highest accuracy in the moderate and combined heavy/severe categories, reaching 61% and 40%, respectively. Nevertheless, all three models showed substantially lower accuracy in the combined heavy/severe $\text{PM}_{2.5}$ category than in the lower pollution categories.

Table 5. Comparison of AQI level forecast accuracy for 337 Chinese cities.

Model	Excellent	Good	Light Pollution	Moderate Pollution	Heavy/Severe Pollution	Accuracy
EPICC-Model	85%	85%	62%	39%	23%	82%
CAMx	90%	87%	57%	31%	11%	84%
CMAQ	83%	88%	63%	41%	36%	82%

Table 6. Comparison of PM_{2.5} IAQI level forecast accuracy at 1,644 monitoring sites in China with observations.

Model	Excellent	Good	Light Pollution	Moderate Pollution	Heavy/Severe Pollution	Accuracy
EPICC-Model	88%	74%	66%	51%	25%	82%
CAMx	92%	69%	57%	40%	13%	83%
CMAQ	86%	75%	66%	61%	40%	82%

Table 7. Comparison of MDA8 O₃ IAQI level forecast accuracy at 1,644 monitoring sites in China with observations.

Model	Excellent	Good	Light Pollution	Moderate Pollution	Heavy/Severe Pollution	Accuracy
EPICC-Model	92%	84%	67%	47%	10%	88%
CAMx	97%	81%	66%	44%	17%	90%
CMAQ	89%	91%	72%	35%	10%	88%

Given the high sensitivity and risk posed by polluted weather and severe pollution events to public health and environmental management, this study further focused on the forecasting performance of PM_{2.5} and MDA8 O₃ pollution events. Based on metrics such as hit rate, false alarm rate, and the distance from the random operating characteristic (DROC) (definitions and calculation methods are provided in the Supplement), the forecast effectiveness for general pollution conditions (PM_{2.5} > 75 µg m⁻³ and MDA8 O₃ > 160 µg m⁻³) and severe pollution conditions (PM_{2.5} > 150 µg m⁻³) was thoroughly analyzed to elucidate the applicability and potential limitations of each model under extreme pollution scenarios.

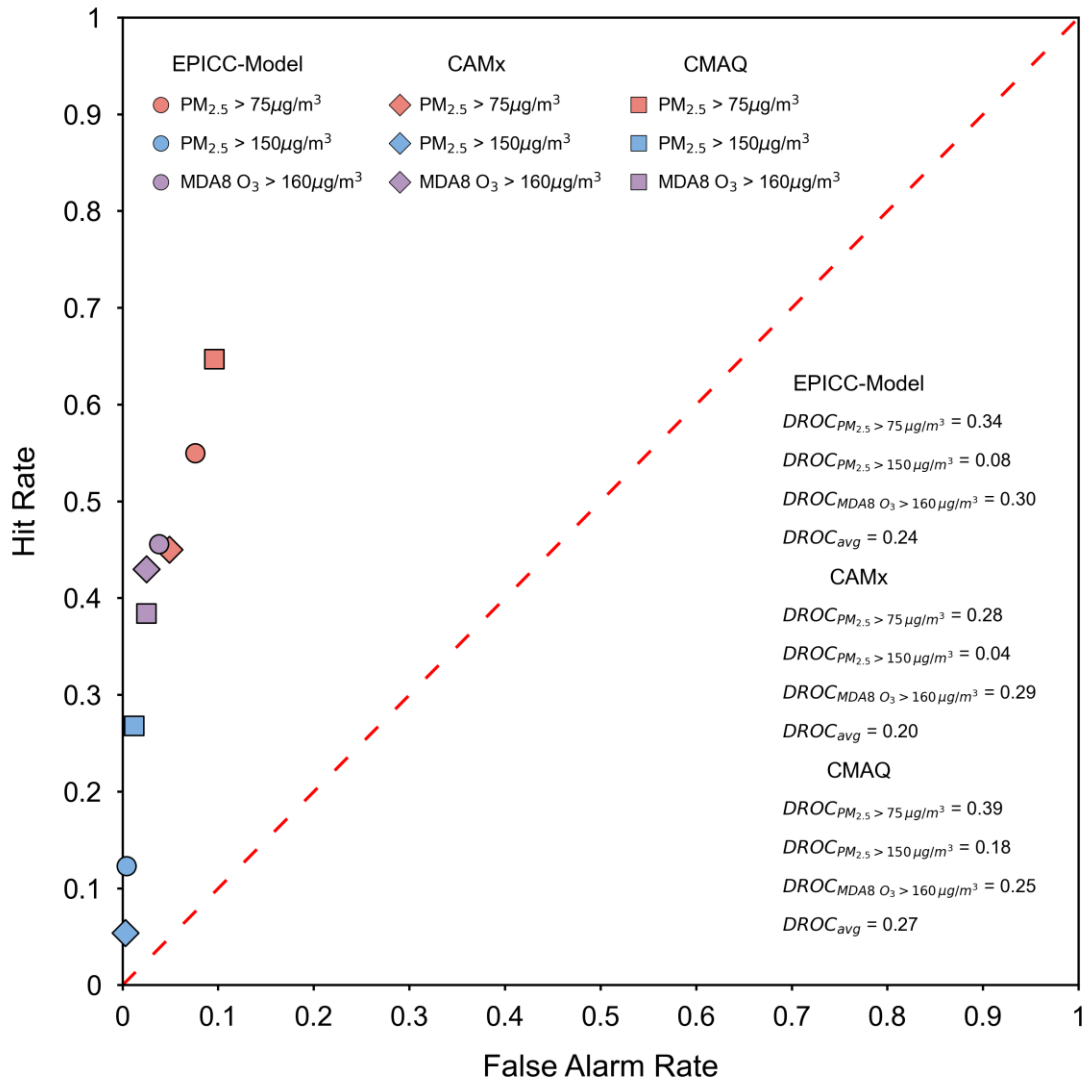


Figure 8. Comparison of CTMs performance based on hit rate and false alarm rate. Scatter points represent the performance of three models (EPICC-Model: circles, CAMx: diamonds, CMAQ: squares) under different pollution event thresholds: $PM_{2.5} > 75 \mu g m^{-3}$, $PM_{2.5} > 150 \mu g m^{-3}$, and $MDA8 O_3 > 160 \mu g m^{-3}$. The red dashed line indicates the random forecast reference line. The DROC metric, which quantifies model skill, is provided in the lower-right corner, with higher values indicating better model performance.

Figure 8 visually compared the forecast performance of three models under different pollution thresholds using scatter points in ROC space. For general pollution scenarios ($PM_{2.5} > 75 \mu g m^{-3}$), CMAQ showed the highest hit rate (64.7%) but was accompanied by a relatively high false alarm rate (9.6%), indicating a tendency toward systematic overestimation. CAMx achieved the lowest false alarm rate (4.9%), likely because it tended to underpredict $PM_{2.5}$ levels and forecast fewer high pollution events. However, its hit rate was also relatively low (45.0%), reflecting a more conservative forecasting tendency. The EPICC-Model struck a balance between hit rate (55.0%) and false alarm rate (7.6%), suggesting a trade-off between detection capability and false alarm occurrence. Under the more severe pollution condition ($PM_{2.5} > 150 \mu g m^{-3}$), the hit rates of all models decreased significantly. While CMAQ still maintained the highest

hit rate (26.8%), its miss rate reached 73.2%. The EPIC-Model and CAMx showed hit rates of only 12.3% and 5.4%, respectively, indicating limited responsiveness of current models to extreme pollution events. Nevertheless, all models maintained false alarm rates below 2%. This reflects limitations of the models in simulating extreme pollution conditions. For O₃ pollution events (MDA8 O₃ > 160 µg m⁻³), the EPIC-Model achieved the highest hit rate (45.6%), slightly higher than CAMx (43.0%) and CMAQ (38.4%), while also maintained a low false alarm rate (3.8%). The DROC values provided in the lower-right table quantitatively reflect the above observations: CMAQ had the highest DROC (0.39) for general PM_{2.5} pollution events, while the EPIC-Model performed best for O₃ events (DROC=0.30). CAMx exhibited relatively low DROC across all thresholds.

3.4 Capability in capturing regional persistent pollution events

To further evaluate the capability of the EPIC-Model, CAMx, and CMAQ in simulating trans-regional and long-duration pollution episodes, this study selected typical persistent PM_{2.5} and O₃ events in 2021, and conducted a dedicated analysis incorporating pollutant transport pathways and the spatiotemporal consistency of meteorological fields.

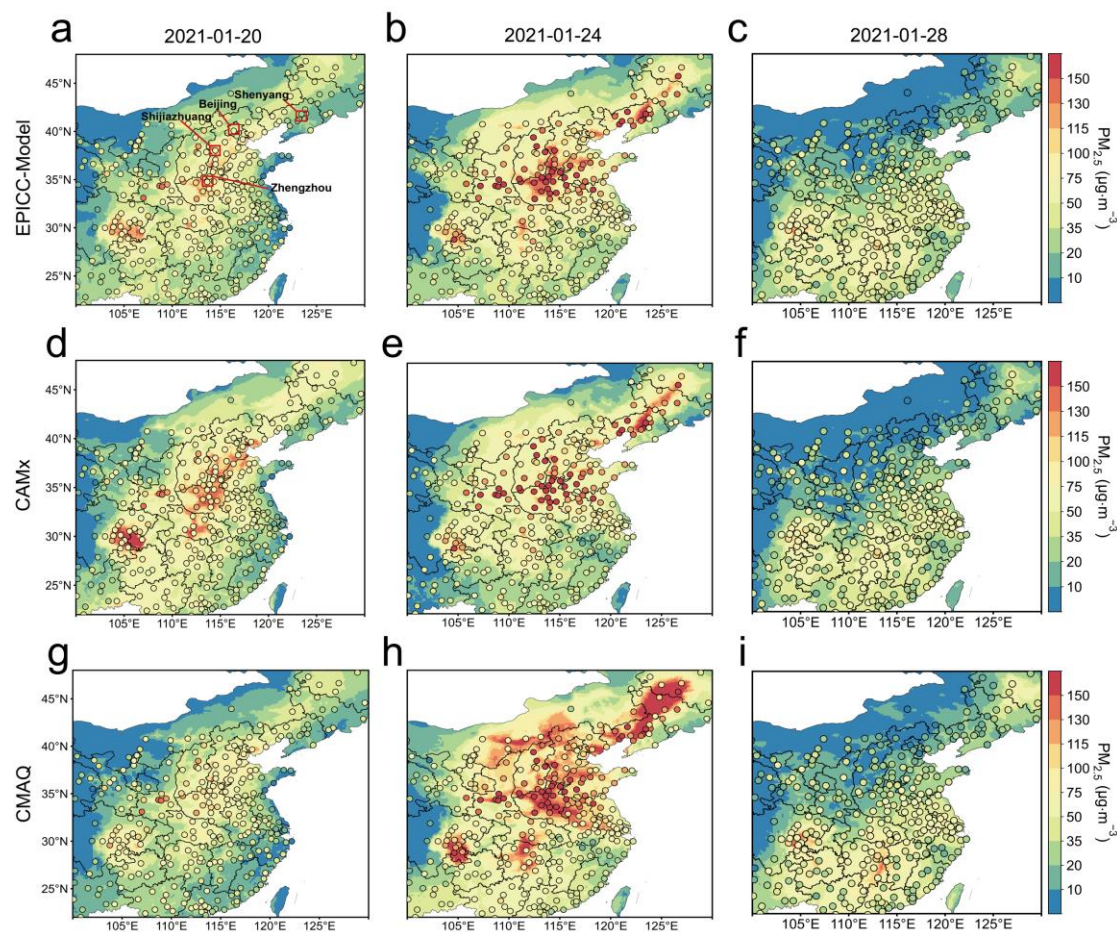


Figure 9. Spatiotemporal distribution of the persistent PM_{2.5} pollution event. Dots represent observed concentrations in 337 cities.

As shown in Figure 9, a persistent PM_{2.5} pollution event occurred in eastern and central China from January 20 to 28, 2021. Initially, pollution was concentrated between 30° N and 40° N, forming a “dual-core” pattern over the North China Plain and the Sichuan Basin. By January 24, PM_{2.5} concentrations peaked, with the pollution belt extending southeastward to the middle and lower Yangtze River regions and northeastward to the Songnen Plain. On January 28, under cold air influence, concentrations dropped below 75 μg m⁻³ in most areas, leaving only isolated hotspots. All three models captured the temporal evolution from initiation to dissipation. The EPIC-Model showed better performance in reproducing spatial gradients and temporal patterns, particularly in the center of the North China Plain and Yangtze River Middle-Reach corridor. CAMx reproduced the northeastward transport path but underestimated pollution intensity, failing to capture the strong core in Henan during the peak. CMAQ systematically overestimated concentrations.

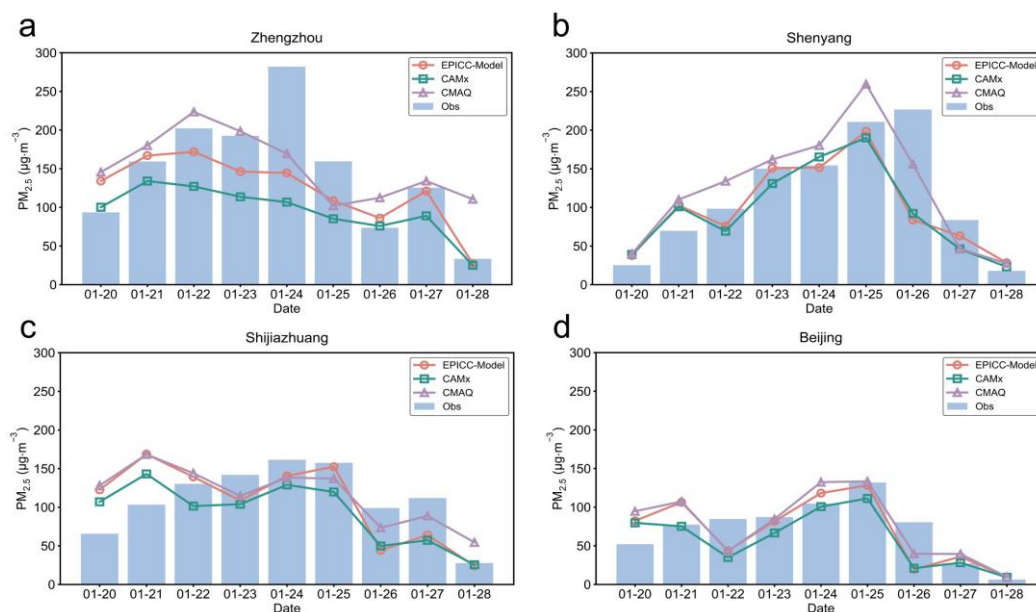


Figure 10. Time series of PM_{2.5} concentrations in key cities along the pollution belt.

As shown in Figure 10, Zhengzhou recorded the first PM_{2.5} peak (>150 μg m⁻³) on January 21, with the pollution plume spreading northeastward and causing a delayed concentration rise in Shenyang. All four cities (Zhengzhou, Shenyang, Shijiazhuang, and Beijing) reached their maxima, though peak timings varied. During the clearing phase, driven by southward cold air intrusion, concentrations declined across all cities, with faster removal in Zhengzhou and Shijiazhuang than in Shenyang and Beijing. All three models reproduced the overall process but showed systematic timing biases, with peaks in Shenyang and Zhengzhou simulated 24-48 hours earlier than observed. Such deviations may result from inaccuracies in the simulated wind field evolution within the meteorological models. In terms of magnitude, CAMx underestimated and CMAQ overestimated concentrations in Zhengzhou, while the EPIC-Model produced comparatively robust results. In the other three cities, all models tracked concentrations similarly.

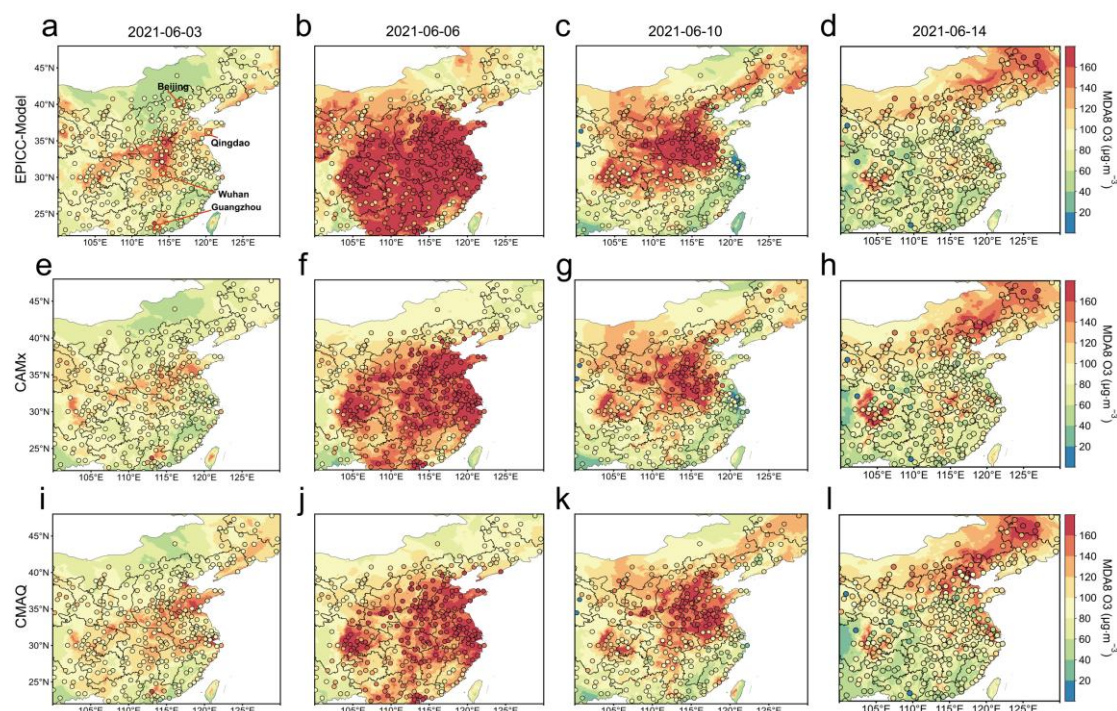


Figure 11. Spatiotemporal distribution of the persistent O₃ pollution event.

As shown in Figure 11, a persistent O₃ pollution episode occurred in China from June 3 to 14, 2021. The event began on June 3 with scattered pollution over the North China Plain and parts of Guangdong Province. By the peak stage on June 6, pollution intensity increased significantly, spreading to central, southeastern, and southern regions. By June 10, the pollution weakened and became more localized in North China and its western areas, while southern regions began clearing. By June 14, MDA8 O₃ concentrations dropped below 100 $\mu\text{g m}^{-3}$ across most areas, leaving only a few localized hotspots in Northeast China and Inner Mongolia. Elevated temperatures, strong solar radiation, and stagnant atmospheric conditions favored O₃ formation, whereas cold air intrusions promoted dispersion and removal.

During this persistent pollution event, all three models captured the full process of occurrence, development, and removal. The EPIC-Model reproduced the expansion of the elevated-O₃ area from central China toward southeastern and southern China and the subsequent clearing, although it locally overestimated O₃ over southeastern China during the peak stage on 6 June, potentially reflecting uncertainties in simulated photochemistry and regional transport. CAMx and CMAQ generally underestimated O₃ in the observed high-concentration regions, particularly on 6 and 10 June, but reproduced the local contrasts between neighboring high-O₃ and low-O₃ monitoring sites more clearly. In comparison, the EPIC-Model reproduced a broader region of elevated O₃ but produced a smoother and more spatially extensive enhancement, resulting in local overestimation in parts of central and southeastern China. Overall, the EPIC-Model showed an advantage in representing the regional extent of the elevated-O₃ area during this episode.

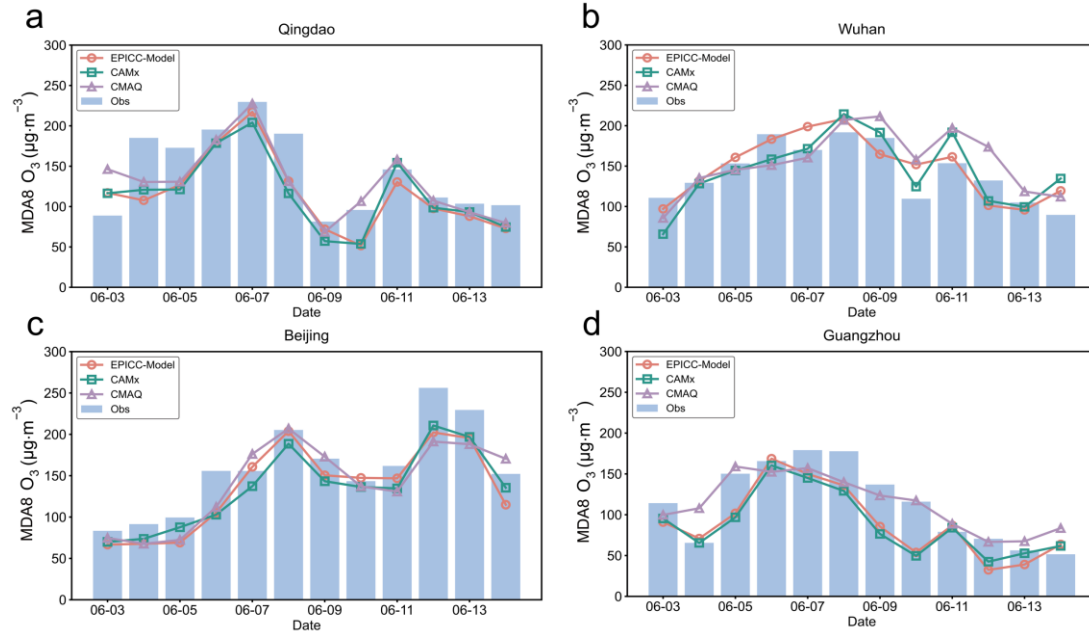


Figure 12. Time series of O₃ concentrations in key cities along the pollution belt.

The pollution event occurred over central and eastern China between 30° N and 40° N. Qingdao first entered O₃ pollution on June 4, with MDA8 O₃ exceeding 160 μg m⁻³. The pollution then maintained high concentrations and expanded northward and southward, reaching Qingdao, Wuhan, Beijing, and Guangzhou by June 6. After June 9, the first clearing phase began from south to north, with Guangzhou improving first, followed by Wuhan and Qingdao, while the pollution center shifted to the North China Plain and northeastern regions, causing a sharp rise in Beijing around June 12. By June 14, most regions had cleared, with Beijing showing the fastest decline, likely due to enhanced cold air activity and higher boundary layer. All three models captured the full progression in Beijing and Qingdao accurately. For Wuhan and Guangzhou, model predictions showed approximately one-day deviations from observations, likely due to limited responses to abrupt meteorological changes.

4 Conclusions

This study presents a systematic evaluation of three CTMs (EPIC-Model, CAMx, and CMAQ) for PM_{2.5} and MDA8 O₃ simulations over China in 2021, using meteorological fields derived from the same WRF simulation and multi-source emission inventories. The work fills a critical research gap by providing the first comprehensive comparison of the EPIC-Model against established CTMs. The results indicated that all three models could effectively reproduce the spatiotemporal evolution characteristics of PM_{2.5} and MDA8 O₃ (PM_{2.5}: R = 0.79-0.85, MDA8 O₃: R = 0.91-0.94). The PM_{2.5} bias of the EPIC-Model varied seasonally, with a tendency toward underestimation in spring and summer and overestimation in autumn and winter. Spatially, it exhibited higher consistency (annual IOA = 0.80), particularly in winter and over heavily polluted North China, effectively capturing pollution patterns and peaks. For O₃, the EPIC-Model performed well during high-concentration summer

episodes, and this performance may be partly associated with its inclusion of heterogeneous HONO formation and particulate nitrate photolysis. Furthermore, the EPICC-Model produced particularly accurate O₃ simulations over the eastern, central, and Chengdu-Chongqing regions. Notably, all three models shared common deficiencies in PM_{2.5} simulations. Systematic underestimations occurred in arid northwestern China due to unaccounted dust processes, highlighting the critical influence of natural emissions on model accuracy. Conversely, autumn-winter PM_{2.5} overestimations occurred in North China and the Sichuan Basin. Insufficient nocturnal mixing may contribute to these biases, consistent with previously reported tendencies of the ACM2/YSU boundary-layer schemes under stable conditions (Jia et al., 2023). Uncertainties in emission inventories further exacerbate regional biases, such as potential overestimation of anthropogenic emissions in the Sichuan Basin and underestimation of agricultural NH₃ emissions in Henan, which affects nitrate aerosol formation. Future improvements should incorporate dust processes, refine boundary layer parameterizations to better simulate pollutant accumulation under stable meteorological conditions, and employ higher-resolution emission inventories with improved temporal variability characterization.

In terms of PM_{2.5} component simulations, the EPICC-Model, CAMx, and CMAQ all reasonably reproduced the chemical composition characterized by NO₃⁻ dominance and associated regional variations. Compared with CAMx and CMAQ, the EPICC-Model exhibited smaller biases in SO₄²⁻ and NH₄⁺, with more robust control of absolute concentrations as reflected in RMSE and NMB, indicating a relatively consistent overall performance, although its correlation metrics are slightly lower than the other two models. Nevertheless, all three models share common limitations: SO₄²⁻ is generally underestimated, leading to insufficient formation of (NH₄)₂SO₄ and lower NH₄⁺ concentrations; SOA formation remains highly uncertain, influenced by precursor VOC emissions, oxidation pathways, and gas-particle partitioning parameterizations, resulting in spatial deviations in OC; BC simulations are highly sensitive to emission inventories, occasionally leading to slight overestimations in certain cities. Addressing these issues in future work should focus on optimizing secondary inorganic aerosol chemistry, improving SOA formation mechanisms and precursor emissions, and enhancing the resolution and accuracy of emission inventories to improve the models' capability in reproducing PM_{2.5} chemical composition.

Regarding AQI level classification ability, CAMx achieved the highest overall accuracy (84%), demonstrating particular strengths in distinguishing “excellent” and “good” air quality levels. CMAQ was relatively accurate in pollution level identification, with the highest hit rate (64.7%) in forecasting general pollution where PM_{2.5} > 75 µg m⁻³, but it had a high false alarm rate (9.6%), indicating a tendency toward over-forecasting. The EPICC-Model showed higher hit rates in forecasting PM_{2.5} light to moderate pollution levels and MDA8 O₃ general pollution, achieving 45.6% for MDA8 O₃ > 160 µg m⁻³, compared with 43.0% for CAMx and 38.4% for CMAQ. For severe PM_{2.5} pollution events exceeding 150 µg m⁻³, all three models showed low hit rates, ranging from 5.4% to 26.8%, although their false alarm rates remained below 2%. In addition, the EPICC-Model demonstrated relatively balanced

false alarm rates across all pollution types, suggesting a simulation capability comparable to other mainstream models and particular effectiveness in capturing light to moderate pollution and O₃ pollution.

In the simulation analysis of typical persistent PM_{2.5} and O₃ pollution events in 2021, the EPICC-Model demonstrated strong capabilities, particularly outperforming CAMx and CMAQ in reproducing spatial distributions and pollution evolution. The EPICC-Model successfully captured the entire process of pollution occurrence, development, and clearance, particularly in the core area of the North China Plain and the diffusion zone of the middle Yangtze River, where the simulation results were in close agreement with observational data. CAMx and CMAQ, however, performed less effectively in capturing persistent pollution events, both exhibiting significant deviations during the simulation of severe pollution phases. CAMx tended to underestimate pollution intensity during some high-concentration stages, while the models exhibited timing deviations during the development or dissipation of individual episodes.

This study establishes a multi-model evaluation framework for systematically comparing the performance of the EPICC-Model with established CTMs over China. By identifying model-specific limitations and challenges shared across the three models, the comparison highlights priorities for future model enhancements, including improved representations of natural dust, boundary-layer mixing, secondary aerosol formation, and emission inputs. The results provide benchmark information for evaluating, selecting, and further developing regional air-quality modeling systems in China. The multi-model evaluation framework and identified performance characteristics may also serve as a reference for model applications in other regions facing similar air-quality modeling challenges.

Code and data availability

All models used in this study are open source and publicly available. The EPICC-Model v1.0 source code is archived at <https://doi.org/10.5281/zenodo.20303367>. CAMx v7.00 can be downloaded from <https://www.camx.com/download/source/> (Ramboll, 2020), while CMAQ v5.3.3 is available through <https://doi.org/10.5281/zenodo.5213949>. Meteorological fields were generated using the WRF v3.9.1 (Skamarock et al., 2008), which is available from https://www2.mmm.ucar.edu/wrf/users/download/get_source.html. Initial and boundary conditions were derived from the NCEP FNL reanalysis dataset (NCEP, 2000), archived at <https://doi.org/10.5065/D6M043C6>. Anthropogenic emissions over China were obtained from the MEIC inventory developed by Tsinghua University (Geng et al., 2024), available at http://meicmodel.org.cn/?page_id=541&lang=en. Chinese NH₃ emissions were taken from the PKU-NH₃ inventory, while biomass-burning emissions were obtained from the China Open Biomass Burning Emissions Inventory (Huang et al., 2012a, 2012b; Song et al., 2009; Kang et al., 2016). Both datasets are available through the MEIC data platform at http://meicmodel.org.cn/?page_id=1772&lang=en. Emissions outside China were represented using the EDGAR v5.0 inventory (Crippa et al., 2020), available at

https://edgar.jrc.ec.europa.eu/dataset_ap50. Biogenic emissions were calculated online using MEGAN v3.2, whose source code is archived at <https://zenodo.org/records/10526206> (Guenther et al., 2012). Air quality observations were obtained from the China National Environmental Monitoring Centre (CNEMC; <https://www.cnemc.cn/>). The primary datasets generated and analyzed in this study, as well as the emission data employed (using the 15th of each month as an example), are available in Zenodo at <https://doi.org/10.5281/zenodo.20843312>. Additional supporting materials are available from the corresponding author upon reasonable request.

Author contributions

ML, QW, WengdW, and HC conceptualized and organized the study. ML performed the data analysis and drafted the manuscript. ML and XF conducted the numerical simulations, and FY optimized the simulation code. XF and WeiW provided data support. DL contributed to the meteorological model evaluation. ML, QW, WengdW, and HC validated and analyzed the simulation results. KC, JZ, and ZW reviewed the research findings and provided key feedback. All authors read and approved the final manuscript.

Competing interests

The authors declare no competing interests.

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