Reduced-complexity air quality intervention modelling over China: development of the InMAPv1.6.1-China and comparison with the CMAQv5.2 model

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Abstract. This paper presents the first development and evaluation of the reduced-complexity air quality model for China. In this study, a reduced-complexity air quality intervention model over China (InMAP-China) is developed by linking a regional air quality model, a reduced-complexity air quality model, an emission inventory database for China, and a health impact assessment model to rapidly estimate the air quality and health impacts of emission sources in China. The modelling system is applied over mainland China for 2017 under various emission scenarios. A comprehensive model evaluation is conducted by comparison against conventional CMAQ simulations and ground-based observations. We found that InMAP-China satisfactorily predicted total $PM_{2.5}$ concentrations in terms of statistical performance. Compared with the observed $PM_{2.5}$ concentrations, the mean bias (MB), normalized mean bias (NMB), and correlations of the total $PM_{2.5}$ concentrations are -8.1 μg/m^3, -18%, and 0.6, respectively. The statistical performance is considered to be satisfactory for a reduced-complexity air quality model and remains consistent with that evaluated in the United States. The underestimation of total $PM_{2.5}$ concentrations was mainly caused by its composition, primary $PM_{2.5}$. In terms of the ability to quantify source contributions of $PM_{2.5}$ concentrations, InMAP-China presents similar results in comparison with

those based on the CMAQ model, the difference is mainly caused by the different treatment of secondary inorganic aerosols in the two models. Focusing on the health impacts, the annual $PM_{2.5}$-related premature mortality estimated using InMAP-China in 2017 was 1.92 million, which was 25 ten thousand deaths lower than estimated based on CMAQ simulations as a result of underestimation of $PM_{2.5}$ concentrations. This work presents a version of the reduced-complexity air quality model over China, provides a powerful tool to rapidly assess the air quality and health impacts associated with control policy, and to quantify the source contribution attributable to many emission sources.

1 Introduction

With rapid urbanization and industrialization, fine particulate matter pollution less than 2.5 μm in diameter ($PM_{2.5}$) has become a major environmental issue in China. High $PM_{2.5}$ concentrations can be observed over eastern China from satellite observations (Xiao et al., 2020) and the $PM_{2.5}$ concentrations have been largely decreased since 2013 due to the effective control measures taken by the Chinese government (Zhao et al., 2021). $PM_{2.5}$ can affect air quality, ecosystems, and climate change and damage human health through short-term or long-term exposure. The Global Burden of Disease study reported that 1.1 million premature deaths were caused by long-term $PM_{2.5}$ exposure over China in 2015 (Cohen et al., 2017).

State-of-the-science three-dimensional air quality models (AQMs) have been widely used in China as tools to simulate regional $PM_{2.5}$ concentrations, quantify the contributions to total $PM_{2.5}$ concentrations resulting from emission sources and assess the benefits associated with control measures (Chang et al.; 2019, Li et al., 2015; Zhang et al., 2015; Zhang et al., 2019). The Weather Research and Forecasting model-Community Multiscale Air Quality Modelling System (WRF-CMAQ) (Appel et al., 2017; Chang et al., 2019), the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) (Reddington et al., 2019), the Weather Research and Forecasting model-Comprehensive Air Quality Model Extension (WRF-CAMx) (Li et al., 2015), and the Global Adjoint model of Atmospheric Chemistry (GEOS-Chem Adjoint) (Zhang et al., 2015) were frequently used in previous studies. To conduct a series of simulations for multiple scenarios or quantify the separate contributions attributable to multiple sources, large computational resources and run-time are required while utilizing conventional AQMs. To address these challenges and to improve the availability and accessibility of air quality modelling, several reduced-complexity models have been developed by the air quality research community. The three representative reduced-complexity air quality models frequently used are the Estimating Air Pollution Social Impacts Using Regression (EASIUR) model (Heo et al., 2016; Heo et al., 2017), the updated Air Pollution Emission Experiments and Policy (APEEP2) model (Muller et al., 2007; Muller et al., 2011) and the Intervention for Air Pollution model (InMAP) (Tessum et al., 2017). A recent study compares three reduced-complexity models, EASIUR, APEEP2, and InMAP, and the results indicate that these three models are consistent in their assessment of the marginal social cost at the county level (Gilmore et al., 2019). Reduced-complexity air quality models are less computationally intensive and easier to use. However, it is not available in China. Therefore, it is essential to develop a reduced-complexity air quality model over China to quickly predict $PM_{2.5}$ concentrations and the associated health impacts of emission sources.

The reduced-complexity intervention model for air pollution, InMAP, was developed by Tessum et al. (Tessum et al., 2017) to rapidly assess the air pollution, health, and economic impacts resulting from marginal changes in air pollutant emissions. Compared with conventional air quality models, InMAP has the advantage of being time-efficient, can predict annual-average $PM_{2.5}$ concentrations within a few hours but with a modest reduction in accuracy compared with CTMs. InMAP reduces the running time by simplifying the physical and chemical processes. InMAP has been used to assess marginal health damage of location-specific emission sources (Goodkind et al., 2019), to quantify the health impacts of individual coal-fired power plants in the United States (Thind et al., 2019), and to estimate the health benefits of control policies considering specific locations (Sergi et al., 2020). However, to date, a version of the reduced-complexity air quality intervention model over China is absent.

In this work, based on the source code of version 1.6.1 of InMAP model， a reduced-complexity air quality intervention model over China (InMAP-China) is developed to rapidly predict the air quality and estimate the health impacts of emission sources in China. The total consumed time for a simulation for the year 2017 using the InMAP-China established in this study is approximately an hour with a single CPU of 24 nodes. Therefore, it is convenient when conducting multiple simulations of $PM_{2.5}$ concentrations due to air pollutants emissions in 2017. The modelling system is applied over mainland China for 2017 under various emission scenarios to examine model performance. Comparisons against conventional air quality models and surface observations are performed in this study. The model applicability and limitations are also declared.

The paper is organized as follows: Section 2.1 presents the components of InMAP-China including the interface development between WRF-CMAQ and InMAP to generate parameters of the base atmospheric state, the preprocessed process of emission input data, and the exposure-response functions employed in this model. Section 2.2 introduces the evaluation protocol, including the statistical variables adopted and the simulation design in this study. Section 3 presents the evaluation of InMAP-China's predictions of $PM_{2.5}$ air quality and $PM_{2.5}$-related health impacts in several simulations. Section 4 summarizes the conclusions and limitations of this study.

2 Description of InMAP-China model

2.1 Model components and configurations

The reduced-complexity intervention model for air pollution, InMAP, was developed by Tessum et al. (Tessum et al., 2017) to rapidly assess the air pollution, health, and economic impacts resulting from marginal changes in air pollutant emissions. The model has been widely used in studies (Sergi et al., 2020; Thind et al., 2019; Goodkind et al., 2019; Dimanchevi et al., 2019) focusing on $PM_{2.5}$ pollution and health, economic impacts resulting from emission sources in the United States. In this model, the continuous equation of atmospheric pollutants is solved at an annual scale, and the run time can be reduced. The parameters used to represent physical and chemical processes for simplified simulation are calculated before using CTM output data. $PM_{2.5}$ air quality and $PM_{2.5}$-related premature mortality are predicted and output in the InMAP model.

In this work, a Chinese version of the reduced-complexity air quality intervention model InMAP-China is developed to rapidly estimate the $PM_{2.5}$ concentration and associated health impacts of emission sources. Figure 1 shows the model framework. Based on the source code of the InMAP model, three-step development work is conducted to establish InMAP-China. First, we develop a preprocessed interface to calculate physical and chemical process parameters using the WRF-CMAQ output variables to support the simplified simulation in InMAP-China. Second, air pollutant emission data are preprocessed to an appropriate format for the InMAP-China simulation. Third, the exposure-response function of the GEMM model is employed in InMAP-China and replaces the original default function to assess $PM_{2.5}$-related health impacts.

Table 1 presents the basic configurations of InMAP-China. The simulation domain is over East Asia and covers mainland China. The spatial resolution is 36 km. Fourteen vertical layers are used in InMAP-China, ranging from the surface layer to the top level of the tropospheric layer.

2.1.1 Parameter interface development for simplified simulation in InMAP-China

We develop a pre-processed interface to calculate physical and chemical process parameters using WRF-CMAQ output variables for simplified simulation in InMAP-China based on the Environmental Protection Agency's (EPA) work (Baker et al., 2020). Two NETCDF files containing the key parameters for simplified simulation are generated by using the parameter interface developed here, one is at 36km resolution across the entire mainland of China and another is at 4km resolution over the BTH region. The main step of the pre-processed interface includes meteorological and chemical variable extraction and merging, unit conversion, vertical layer mapping, physical and chemical process parameter calculation, and average processing. The hourly chemical and meteorological variable outputs from the WRF-CMAQ modelling system are converted into annual-average physical and chemical process parameters required for simplified simulation.

A NetCDF file containing the three-dimensional annually-averaged parameters to characterize atmospheric advection, dispersion, mixing, chemical reaction, and deposition is generated. Table 2 shows the relationship between the annual-average parameters for simplified simulation and the original hourly variables. In InMAP-China, the annual averaged component and the deviation of wind speed to represent advection are calculated using hourly elements. The offset of wind vectors in different directions may result in some uncertainties in this process. The parameters of eddy diffusion and convective transport are pre-calculated using hourly elements, including temperature, pressure, boundary layer height, etc. The annual wet deposition rate is determined by the rainwater mixing ratio and cloud fractions. The annual dry deposition rate of particles and gaseous pollutants at the surface level is pre-calculated using friction speed, heat flux, radiation flux, and land cover. The simplification of chemical reactions is different among pollutants. For NO_x, NH_3, and volatile organic compound (VOC) precursors, the annual averaged gas-particle partitioning is adopted and calculated before using the output concentrations of species from CMAQ. For SO_2 pollutants, the annual oxidation rate of two major conversion pathways for SO_2 is calculated using concentrations of hydroxyl radical (HO) and hydrogen peroxide (H_2O_2) in CMAQ, and the conversion is estimated in InMAP-China.

2.1.2 Prior WRF-CMAQ simulation

To generate the meteorological and chemical parameters required by InMAP-China, a one-year WRF-CMAQ simulation covering the entire mainland of China is conducted to output hourly meteorological and chemical-related variables in 2017. Besides, the nested WRF-CMAQ simulation over the BTH region is also conducted and validated using observed data. The corresponded output data is used to generate the meteorological and chemical parameters required by InMAP-China for the simulations of 4 km resolution in the BTH region. Tables S1 and S2 show the major configurations of the WRF-CMAQ modelling system. The WRF model is driven by the National Centers for Environmental Prediction Final Analysis (NCEP-FNL) (https://doi.org/10.5065/D6M043C6) reanalysis data to provide the initial and boundary conditions. The meteorological fields derived from the WRF model is used to drive the CMAQ model (Appel et al., 2016) simulations. The air pollutant emissions used here include anthropogenic emissions over China derived from the MEIC model (http://meicmodel.org/), anthropogenic emissions over the region of East Asia outside China derived from the MIX-2010 inventory (Li et al., 2015), and biogenic emissions derived from the MEGANv2.10 model. The CB05 chemical mechanism and the AERO6 aerosol module are employed in the model simulation.

Table S3 summarizes the performance statistics of meteorological variables, including surface temperature, relative humidity, and wind speed, in China in 2017, as simulated by the WRF model. The hourly observed data of major meteorological variables derived from the National Climate Data Center (NCDC) are utilized here. The results show that the meteorological variables simulated by the WRF model agree well with the surface observations, which is consistent with previous studies (Wu et al., 2019; Zheng et al., 2015; Hong et al., 2017). The model performs well on the predictions of surface temperature, with an MB of -0.7 K, an NMB of -6.1%, and an R of 0.9. The predictions of relative humidity at a height of 2 meters are relatively satisfied with an MB of 4.1% and an NMB of 6.1%. The predictions of wind speed at a height of 10 meters are slightly overestimated, with an MB of 0.3 m/s and an NMB of 12.4%, which may be caused by out-of-date USGS land use data employed in the model runs.

The SO_2, NO_2 and $PM_{2.5}$ concentrations modelled across the domain agree well with the surface observations in terms of the statistical performance and monthly variations. Table S4 summarizes the performance of the statistics of major air pollutant concentrations. The nationwide annual averaged $PM_{2.5}$ concentration simulated in 2017 in China was 42.1 $\mu g/m^3$. Compared with the observed $PM_{2.5}$ of 45.9 $\mu g/m^3$, there are slight underpredictions with an MB of 3.7 $\mu g/m^3$ and NMB of 8.1%. The CMAQ model has moderate underpredictions of the NO_2 concentrations and SO_2 concentrations, which may be related to the uncertainties of emission inputs. For modelled NO_2 concentrations, MB and NMB are -4.6 $\mu g/m^3$ and -13.9%, respectively. For modelled SO_2 concentrations, MB and NMB are -0.8 $\mu g/m^3$ and -4.5%, respectively. Figure S3 shows the monthly variation. The variation trend of the observed SO_2, NO_2, and $PM_{2.5}$ concentrations can be reproduced in the CMAQ simulations.

2.1.3 Pre-processed emission input data

We develop the pre-processed module to generate vector emission input for the InMAP-China simulation. This module can allocate air pollutant emissions vertically and horizontally to supply the missing parameters for the emission file and convert them into a shapefile vector format. The shapefile vector format's emission data of 36km resolution in the entire mainland of China and 4km resolution in the BTH region in 2017 are pre-processed by using this module.

In this module, the emission data are pre-processed by source and altitude. The anthropogenic emissions of five sectors in China in 2017 from the MEIC inventory (http://meicmodel.org/), the anthropogenic emissions over regions outside mainland China in Asia from the MIX-2010 inventory (Li et al., 2015), and the natural emissions estimated using the MEGANv2.10 model (Guenther et al., 2012) are employed in this study.

More detailed, the gridded anthropogenic emissions of 0.3 degrees for the residential, transportation, and agricultural sectors are pre-processed and input to the surface layer. The gridded air pollutant emissions of the industrial sector and non-coal power plants are pre-processed for allocation to attitudes ranging from 130 meters to 240 meters and 130 meters to 890 meters, respectively. The emissions of coal-fired power plants (CPPs) are pre-processed as point sources. The air pollutant emissions and the stack attribution of each unit are provided in the emission file. Because the stack attribution of the power unit is missed in the MEIC inventory, we supplied the information in the pre-processed module based on NEI (National Emission Inventory data) data of power units. For stack height/stack diameter, a linear relationship is first established (see Figure S1), and then, supplementation for these two parameters of Chinese power plants is conducted by using the relationships. The fixed value for the other two variables of stack attribution is set here because the $PM_{2.5}$ concentrations attributable to power plants (CPPs-$PM_{2.5}$) are less sensitive to the two variables (see Figure S2). The stack gas exit velocity and stack gas exit temperature of the power unit are 6 m/s and 313 K, respectively. The air pollutant emissions over regions outside mainland China in Asia and the natural emissions simulated by MEGANv2.10 are pre-processed and input to the surface layer.

2.1.4 Exposure-response function from GEMM

To rapidly estimate the premature mortality of $PM_{2.5}$ exposures, we employ the exposure-response function from GEMM to estimate $PM_{2.5}$-related premature mortality, which is developed by Burnett et al. (Burnett et al., 2018), and calculate the premature mortality using $PM_{2.5}$ concentration predictions of InMAP-China. Premature mortality due to non-communicable diseases (NCDs) and lower respiratory infections (LRIs) was considered in this study. Mortality is determined by the mortality incidence rate, population, and attributable fraction (AF) to certain $PM_{2.5}$ concentrations. The national mortality incidence rate and the population data were derived from the GBD2017 study (Institute for Health Metrics and Evaluation). The spatial distribution of the population in 2015 from the Gridded Population of World Version 4 (Doxsey et al., 2015) was employed to allocate the population in 2017.

2.2 Evaluation protocol

2.2.1 Evaluation method

In this study, the performances of the InMAP-China predictions are evaluated by comparison against CMAQ simulations and surface observations. Model-to-model comparison and model-to-observation comparison have both been used to evaluate the performance of reduced-complexity air quality models in previous studies (Tessum et al., 2017, Gilmore et al., 2019).

The following aspects are considered to make an evaluation. First, we examine the ability of InMAP-China to predict $PM_{2.5}$ concentrations at different emission levels, which will be introduced in Section 3.1. Second, to examine the ability to quantify source contributions to $PM_{2.5}$ concentrations, we compare the InMAP-China's predictions of the sectoral contributions attributable to power, industry, residential, transportation, and agriculture with those based on the CMAQ model, which will be presented in Section 3.2. Third, to comprehensively understand the performance at higher spatial resolution using InMAP-China, we compare the predictions of $PM_{2.5}$ concentrations at 4km spatial resolution in the BTH region both modelled by InMAP-China and conventional CMAQ with the observations, which is displayed in Section 3.3. Fourth, focusing on the health impacts, the $PM_{2.5}$-related premature mortality predicted by InMAP-China is also compared with mortality estimation based on $PM_{2.5}$ exposure derived from CMAQ, which is presented in Section 3.4.

For the observed $PM_{2.5}$ concentration data, the annual averaged observed $PM_{2.5}$ concentrations in 2017 were calculated using hourly concentration data from the China National Environmental Monitoring Center, CNEMC (http://www.cnemc.cn/). More than 1400 national monitoring sites for air pollutant concentrations are included in the simulation domain. The statistical parameters used in this study include the correlation coefficient (R), mean bias (MB), mean error (ME), normalized mean bias (NMB), normalized mean error (NME), and root mean square error (RMSE). The statistical analyses on the performance of InMAP-China are similar to our previous evaluation of conventional CTMs (Zheng et al., 2015; Wu et al., 2019).

2.2.2 Experimental design

We design twelve simulations to examine the model ability of InMAP-China in this study. Table 3 shows the sequence of simulations.

InMAP_TOT represents the baseline simulation with maximum emissions input, in which five sectoral anthropogenic emissions are derived from the MEIC inventory, natural emissions are derived from the MEGANv2.10 model, and Asian emissions outside mainland China are derived from the MIX-2010 inventory are combined as emission inputs. Five sectoral and five abatement simulations are also conducted to examine the ability of InMAP-China to predict concentration changes in response to sectoral emissions and abatement emissions. The emission inputs for these ten simulations have been declared in Table 3. The annual averaged physical and chemical process parameters are calculated based on the output variables of WRF-CMAQ model, which has already been mentioned in Section 2.1.2. Based on the above input, the particle continuity equations are solved by InMAP-China model to obtain the annual averaged $PM_{2.5}$ concentrations at the steady-state of the atmosphere. The above simulations are all conducted at 36km spatial resolution across the entire mainland of China. Besides, another simulation represented by InMAP-BTH is conducted at 4km spatial resolution over the BTH region, with the anthropogenic emission input data at 4km resolution derived from the MEIC inventory and natural emissions derived from the MEGANv2.10 model is utilized in this simulation.

To make a comparison with the InMAP-China simulations, eleven CMAQ simulations are also performed under the same emission inputs. The hourly $PM_{2.5}$ concentrations simulated by CMAQ in 2017 are averaged at obtaining the annual averaged $PM_{2.5}$ concentrations. Due to limited computational resources, each simulation is conducted for four representative months (January, April, July, and October) in 2017.

3 Results and Discussion

3.1 Model performance of $PM_{2.5}$ concentrations in China

3.1.1 Total $PM_{2.5}$ concentrations

Figure 3 shows the performance evaluation of total $PM_{2.5}$ concentrations in the InMAP_TOT simulations. Compared with the observed annual averaged $PM_{2.5}$ concentrations, the total $PM_{2.5}$ concentrations are moderately underpredicted by InMAP-China with an MB of -8.1 μg/m^3 and an NMB of -18.1%. Compared with the CMAQ predictions, the total $PM_{2.5}$ concentrations are also underpredicted, with an MB of -5.3 μg/m^3 due to the underprediction of primary $PM_{2.5}$. Consistent air pollutant emissions are employed in the CMAQ and InMAP-China simulations. Therefore, the underpredictions are caused by the different mechanisms in the two models. InMAP-China reproduces the spatial pattern of total $PM_{2.5}$ concentrations simulated by CMAQ. Notably, significant over predictions of $PM_{2.5}$ concentrations can be observed over mountain areas across Northern China, and the complex terrain and large emission intensity increase the challenge of predicting $PM_{2.5}$ concentrations using the reduced-complexity air quality model in this region.

Figure 4 shows a comparison of $PM_{2.5}$ compositions. Compared with the CMAQ results, the InMAP-China predictions of $PM_{2.5}$ compositions are satisfactory, with NMBs for SO_4^{2-}, NO_3^-, NH_4^+, and primary $PM_{2.5}$ equal to 13%, -8%, -10%, and -23%, respectively. The predictions of SO_4^{2-}, NO_3^-, and NH_4^+ perform better than those of primary $PM_{2.5}$. Figure 5 and Figure 6 compare the spatial distribution of $PM_{2.5}$ compositions, and similar over-predictions of $PM_{2.5}$ compositions can be observed in the mountain area in Northern China.

The ability of InMAP-China to predict $PM_{2.5}$ compositions is also examined at various emission levels. Figure 7 compares the concentrations of $PM_{2.5}$ compositions and the proportions of secondary inorganic aerosols (hereafter, SNA) in total $PM_{2.5}$ concentrations in different scenarios by two models. In the InMAP_TOT scenario, the proportion of SNA is 56%, which is extremely close to the 50% proportion in the WRF-CMAQ simulations. In five emission abatement simulations, the proportion was approximately equal to that in the baseline scenario because the linearly treated chemical reaction relationship of SNA was employed in InMAP-China. However, focusing on the simulations of five sectoral emission scenarios, a significant difference can be observed, which is mainly caused by the difference in chemical treatments in InMAP-China and CMAQ. In this situation, the impacts on $PM_{2.5}$ concentrations are distinct due to the nonlinear emission-concentration process.

3.1.2 Marginal change in $PM_{2.5}$ concentrations

Figure 8 compares the InMAP-China and CMAQ predictions of population-weighted $PM_{2.5}$ concentrations and $PM_{2.5}$ compositions for eleven emission scenarios. Marginal changes in air pollutant concentrations are defined as 1 $\mu g/m^3$ by normalizing the population-weighted air pollutant concentrations of each scenario using the largest value among all scenarios modelled by CMAQ. The InMAP-China reproduces CMAQ predictions on the marginal change in population-weighted $PM_{2.5}$ concentrations, with an NMB of -12% and correlations of 0.98, as shown in Figure 8(a). This performance is similar to that predicted by InMAP in the United States (Tessum et al., 2017).

Figure 8(b)-(f) compares the predictions of $PM_{2.5}$ compositions. The InMAP-China predictions of SO_4^{2-}, NO_3^-, NH_4^+ and primary $PM_{2.5}$ agree well with the CMAQ results, but the predictions of secondary organic aerosol (SOA) are the poorest. The marginal changes in NO_3^- and primary $PM_{2.5}$ concentrations are moderately underpredicted by InMAP-China, with an NMB value of -13% and -21%, respectively. Conversely, the marginal change in SO_4^{2-} concentrations are over-predicted with an NMB of 23%. The marginal change in NH_4^+ predicted by InMAP-China agrees well with the CMAQ predictions. Because few reaction pathways of SOA are included in the CB05 mechanism in the CMAQ simulations, SOAs are under-predicted in the entire modelling system.

The regional performance of the changes in $PM_{2.5}$ and its compositions for eleven emission scenarios is also examined in this study. Figures S4-S7 show the regional results. Four regions, including the Beijing-Tianjin-Hebei region (BTH), Yangtze River Delta (YRD), Pearl River Delta (PRD), and Fen Wei Plain (FWP), are analyzed here (see Figure 2). At the regional level, the CMAQ predicted marginal changes in population-weighted $PM_{2.5}$ concentrations, and its composition can be reproduced by InMAP-China, which is similar to the nationwide performance. However, the marginal change in SO_4^{2-} concentrations over the BTH is significantly over-predicted by InMAP-China, with an NMB of 135%, which is expected to be improved by optimizing the representation of the annual sulfate oxidation rate in this region.

3.2 Model performance of source contributions in China

Figure 9 shows the contribution of each sector to $PM_{2.5}$ concentrations nationwide and at the regional scale, and Table 4 displays the proportion value of sectoral contribution based on two models. The predictions of the source contributions of $PM_{2.5}$ concentrations in InMAP-China are reliable compared with those based on the CMAQ model, and the difference can be explained.

The results based on the two models indicate that the industrial and residential sectors are the first and second contributors among the five sectors. The contribution of the electricity sector is comparable when using the two models, while the contributions of transportation and agriculture are moderately different, which is mainly due to the difference in the model mechanism and the treatment of secondary inorganic aerosols in the two models. At the regional scale, the difference in the sectoral contribution caused by the mechanism in the two models is more significant than at the national scale.

3.3 Model performance of $PM_{2.5}$ predictions at higher resolution in the BTH region

We also conducted a simulation with a higher spatial resolution of 4 km in the BTH region by using InMAP-China model and make a comparison with the WRF-CMAQ nested simulation at the same area in the BTH region. Figure 10 and Figure 11 show the performance evaluation of total $PM_{2.5}$ concentration and the composition in the InMAP_BTH scenario. Compared with the observed annual averaged $PM_{2.5}$ concentrations, the total $PM_{2.5}$ concentrations are moderately overpredicted in InMAP_BTH with an NMB of 41.3% and an R of 0.5.

Further compared with the nested CMAQ predictions, the total $PM_{2.5}$ concentrations are also over-predicted by InMAP-China model. The predictions of $PM_{2.5}$ compositions in the InMAP_BTH scenario are partially satisfactory, except for SO_4^{2-}, with NMBs for SO_4^{2-}, NO_3^-, NH_4^+, and primary $PM_{2.5}$ equal to 178%, 36%, 33%, and 27%, respectively. Figure 12 further shows the comparison of the spatial distribution of $PM_{2.5}$ compositions in the BTH region. The overall spatial distribution pattern of $PM_{2.5}$ compositions is similarly modeled by two models, however, an obvious difference can be observed across the mountain area in the BTH region, for instance, the over-predictions of $PM_{2.5}$ compositions, especially, SO_4^{2-} and NO_3^- observed near the Taihang mountain area.

3.4 Model performance of $PM_{2.5}$-related premature mortality in China

To examine the performance of the predictions of $PM_{2.5}$-related premature mortality, a comparison of premature mortality using the $PM_{2.5}$ predictions from InMAP-China and CMAQ, separately, is performed here. Figure 13 shows the comparison based on two models for all provinces. The results demonstrate that, compared with the premature mortality based on CMAQ, the relative difference is ranging from -44% to 15% at the provincial level due to the difference of $PM_{2.5}$ concentrations in the two models.

At the provincial level, the $PM_{2.5}$-related premature mortality in Beijing city, Tianjin city, Hebei province, and Shanghai city is slightly over-predicted by InMAP-China, with the relative difference ranging from 4% to 15%. Conversely, for the other majority of provinces, $PM_{2.5}$-related premature mortality is under-predicted by InMAP-China, with the relative difference ranging from -3% to -44%. Overall, the $PM_{2.5}$-related premature mortality estimated using InMAP-China was 1.92 million people in 2017. Compared with the CMAQ-based estimations, 25 ten thousand deaths are under-predicted by InMAP-China because of underestimation of total $PM_{2.5}$ concentrations in the baseline simulation.

4 Conclusions

This work develops a reduced-complexity air quality intervention model over China and presents a comprehensive evaluation by comparing CMAQ simulations and surface observations. The InMAP-China aims at providing a simplified modelling tool to rapidly predict the $PM_{2.5}$ concentrations due to emission change as well as the health impact of emission sources in China. After the model is established, the total consumed time for a new simulation under the atmosphere condition in the year 2017 across the mainland of China using InMAP-China is merely an hour with a single CPU of 24 nodes. Therefore, it is time-efficient when conducting new simulations of $PM_{2.5}$ concentrations in China. Notably, the running of WRF-CMAQ simulations is merely necessary for our developing stage of InMAP-China. For the application of InMAP-China, we recommend users to select InMAP-China as a prior tool with extensive simulation demands, for instance, to quantify the $PM_{2.5}$ concentrations due to hundreds of pollution emitters or to rapidly estimate the $PM_{2.5}$ concentrations caused by dozens of control policies, separately. Besides, the variable grid can also be set in InMAP-China to allow a high spatial resolution of 1km or even higher in a certain urban area.

InMAP-China has moderately satisfactory performance in this study, however, this model has reductions in accuracy compared with conventional CTMs. Overall, InMAP-China satisfactorily predicts total $PM_{2.5}$ concentrations in the baseline simulation in terms of statistical performance. Compared with the observed $PM_{2.5}$ concentrations, the MB, NMB, and correlations of the total $PM_{2.5}$ concentrations are -8.1 $\mu g/m^3$, -18%, and 0.6, respectively. The statistical performance is satisfactory for a reduced-complexity air quality model and remains consistent with the performance evaluation in the United States. The underestimation of total $PM_{2.5}$ mainly comes from the primary $PM_{2.5}$. Moreover, the spatial pattern of total $PM_{2.5}$ concentrations can be reproduced in InMAP-China, while an overestimation over the mountain area in Northern China can be observed. The large emission intensity and complex terrain over this region increase the difficulty of modelling concentrations in this area. The predictions of source contributions to $PM_{2.5}$ concentrations by InMAP-China are comparable with those based on the CMAQ model, and the difference is mainly caused by the uncertainty of the simplification of the chemical process in the InMAP-China. The global version of the reduced-complexity air quality model (Global-InMAP) is also developed and released recently (Thakrar et al., 2021), our results of InMAP-China can provide more accurate results in the mainland of China.

This study is subject to some limitations and uncertainties. In InMAP-China, the annual-average chemical and physical processes parameters are calculated using hourly parameters from WRF-CMAQ. Complicated seasonal and daily variations affecting the formation and transportation of particulate matter are challenging to retain. The intensity of advection of the air mass is supposed to be weakened due to the offset of the wind vector in the averaging process, which was also pointed out in a previous study. Moreover, InMAP-China has difficulty predicting SOA concentrations because reaction pathways for SOA are insufficient in this modelling system. Further research work is suggested to improve the model performance. For instance, the combination of machine learning with the simplified simulation may need to research to promote the reduced-complexity air quality modeling over China.

Code and data availability

The source code for the localized version of the reduced-complexity air quality model over China (InMAP-China), which is developed based on the original InMAP model over the United States. The data related to this study as well as the user manual are available at https://doi.org/10.5281/zenodo.5111961.

Author contributions

Q. Zhang and RL. Wu designed the research and RL. Wu carried them out. RL. Wu, CW. Tessum and Y. Zhang contributed to model development. R. L. Wu and Q. Zhang interpreted the results. RL. Wu prepared the manuscript with contributions from all co-authors.

Competing interests

The authors declare no competing interests.

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Table 1. Model configurations in InMAP-China.

Category	Parameters	Configurations
Basic	Research area and period	China, 2017
	Spatial resolution	36 km × 36 km
	Vertical layers	14 layers
	Run type	Steady run
	Variable grid	Static grid
	Projection	Lambert
	Grid numbers	305816
Input	Meteorological and chemical parameters	Calculated using variables from WRFv3.8-CMAQv5.2
	Anthropogenic emissions	MEIC, MIX, MEGAN
	Population data	GPW 2015 and GBD 2017
	Baseline mortality rate	GBD 2017
Output	Air pollutants	$PM_{2.5}$ and its composition concentrations
	Mortality	$PM_{2.5}$-related premature mortality

Table 2 The relationship between parameters for simplified simulation and original variables.

WRF-CMAQ's Variables	Descriptions	InMAP-China's Parameters	Descriptions
U, V, W	Wind fields	UAvg, UDeviation VAvg, VDeviation WAvg, WDeviation	Advection and mixing coefficients
PH, PHB	Base state of geopotential and perturbation geopotential	Dz	Layer heights
PBLH	Planetary boundary layer height	M2d, M2u, Kxxyy, Kzz	Mixing coefficients
T	Potential Temperature	SO_2Oxidation, PlumeHeight	Chemical reaction rates and plume rise
P, PB	Base state pressure plus perturbation pressure		Chemical reaction rates and plume rise
QRAIN	Mixing ratio of rain	ParticleWetdep, GasWetdep	Wet deposition
QCLOUD	Cloud mixing ratio	SO_2Oxidation	Aqueous-phase chemical reaction rates
CLDFRA	Fraction of grid cell covered by clouds	ParticleWetdep, GasWetdep	Wet deposition
SWDOWN,GLW	Downward shortwave and longwave radiative flux at ground level	GasDrydep, ParticleWetdep	Dry deposition
HFX	Surface heat flux	M2d, M2u, Kxxyy, Kzz, Drydep	Mixing and dry deposition
UST	Friction velocity		Mixing and dry deposition
LU_INDEX	Land use type	M2d, M2u, Kxxyy, Kzz	Mixing
DENS	Inverse air density		Mixing and convert between mixing ratio and mass concentration
aVOC	Anthropogenic VOCs that are SOA precursors	aOrgPartitioning	VOCs/SOA partitioning
aSOA	Anthropogenic SOA		
OH, H_2O_2	Hydroxyl radical and hydrogen peroxide concentrations	SO_2Oxidation	Oxidation rates
pNO	ANO_3I, ANO_3J	NOPartitioning	

gNO	NO and NO_2		NO_x/pNO_3 partitioning
pNH	ANH_4I, ANH_4J	NHPartitioning	NH_3/pNH_4 partitioning
gNH	NH_3		

Table 3 Simulation experiments conducted using InMAP-China.

Class	Simulations	Emission input	Physical and chemical parameter input
Base	InMAP_TOT	Five sectoral anthropogenic emissions and natural emissions	
High_re	InMAP_BTH	Five sectoral anthropogenic emissions and natural emissions with 4km resolution at BTH region	
Sec1	InMAP_POW	Power plants emissions	
Sec2	InMAP_INDUS	Industrial emissions	
Sec3	InMAP_TRANS	Transportation emissions	
Sec4	InMAP_RESI	Residential emissions	
Sec5	InMAP_AGRI	Agricultural emissions	
Aba1	InMAP_RE10	Reduce the air pollutants emissions by 10% based on InMAP _TOT emissions	
Aba2	InMAP_RE30	Reduce the air pollutants emissions by 30% based on InMAP _TOT emissions	Converted using WRF-CMAQv5.2 simulation data in the year of 2017; Remain the same in all simulations.
Aba3	InMAP_RE50	Reduce the air pollutants emissions by 50% based on InMAP _TOT emissions	
Aba4	InMAP_RE70	Reduce the air pollutants emissions by 70% based on InMAP _TOT emissions	
Aba5	InMAP_RE90	Reduce the air pollutants emissions by 90% based on InMAP _TOT emissions	

Table 4 Comparison of the proportions of sectoral contributions to $PM_{2.5}$ concentrations using InMAP-China and CMAQ.

Sector	National		BTH		YRD		PRD		FWPY	
	CMAQ	InMAP-China	CMAQ	InMAP-China	CMAQ	InMAP-China	CMAQ	InMAP-China	CMAQ	InMAP-China
Power	6.9%	8.1%	6.2%	9.4%	7.4%	8.6%	10.4%	8.2%	7.0%	10.0%
Industry	30.8%	35.0%	30.2%	38.2%	33.3%	39.1%	37.5%	35.4%	27.7%	31.9%
Residential	25.9%	28.1%	24.7%	28.2%	17.9%	20.8%	19.5%	28.4%	30.0%	33.8%
Transportation	14.0%	17.3%	13.4%	15.6%	15.7%	21.2%	17.1%	17.5%	13.2%	15.0%
Agriculture	22.5%	11.5%	25.5%	10.4%	25.7%	12.4%	15.4%	11.6%	22.0%	9.4%

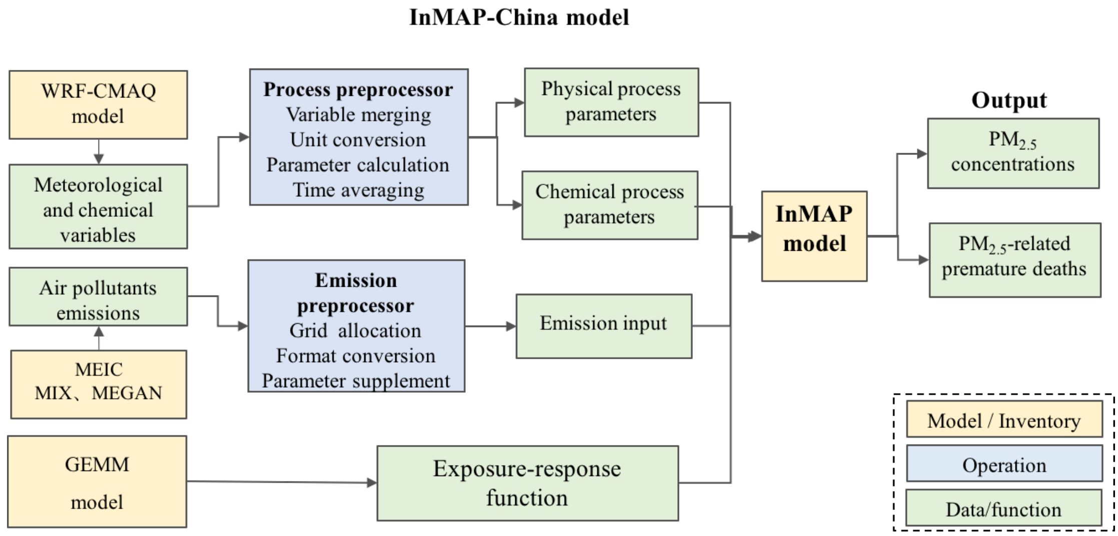

Figure 1 Model framework of InMAP-China.

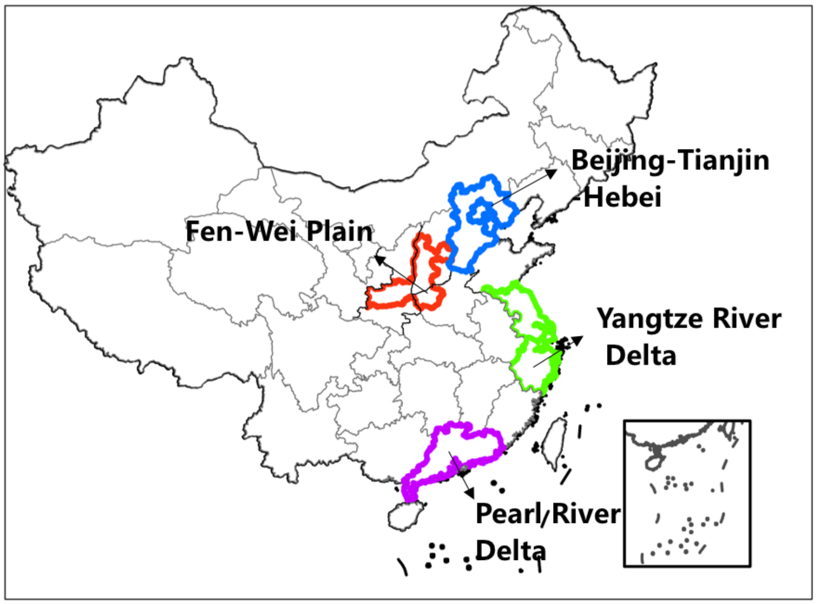

Figure 2 Four key regions are defined in this study, including the Beijing-Tianjin-Hebei region, Yangtze River Delta region, Pearl River Delta region, and Fen Wei Plain region.

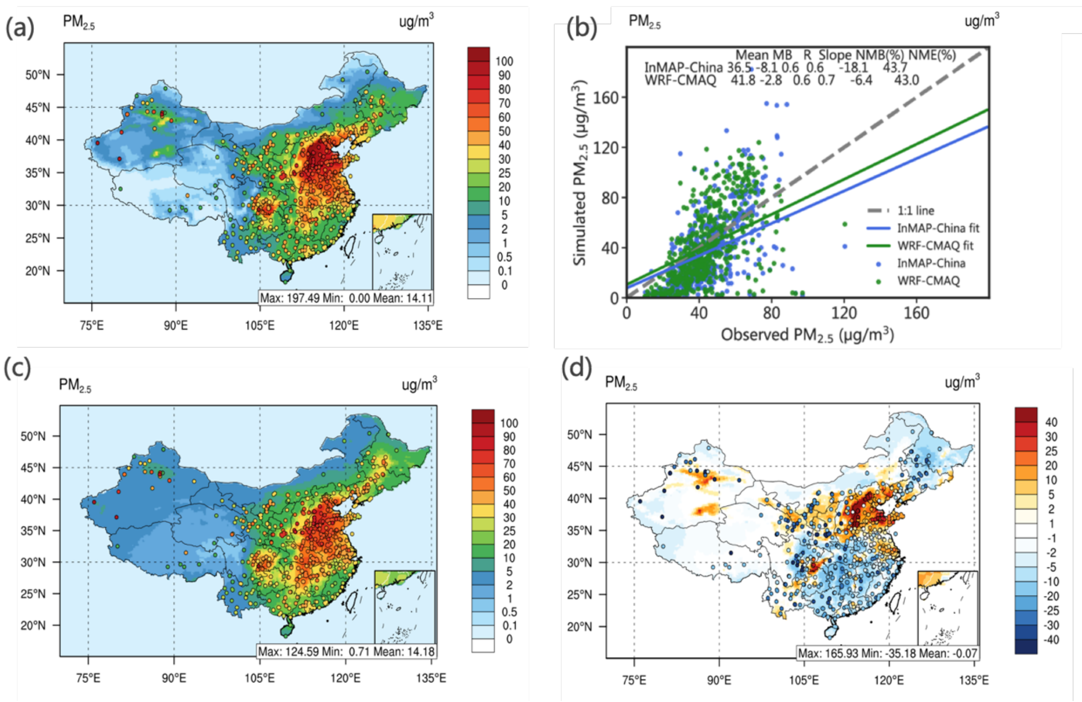

Figure 3 The spatial pattern and statistical metrics of total $PM_{2.5}$ concentrations predicted by InMAP-China and WRF-CMAQ. Panels (a) and (c) display the spatial patterns of total $PM_{2.5}$ concentrations predicted by InMAP-China and WRF-CMAQ, respectively. Panel (d) presents the difference in the spatial distribution of the total $PM_{2.5}$ concentrations predicted by the two models. Panel (b) shows the statistical metrics between the simulated and observed $PM_{2.5}$. The observed total $PM_{2.5}$ concentrations are marked as circles in panel (a) and panel (c). In panel (d), the circle shows the difference between the $PM_{2.5}$ simulated by InMAP-China and the observed $PM_{2.5}$. The same color bar is utilized in the contour and the marked circle.

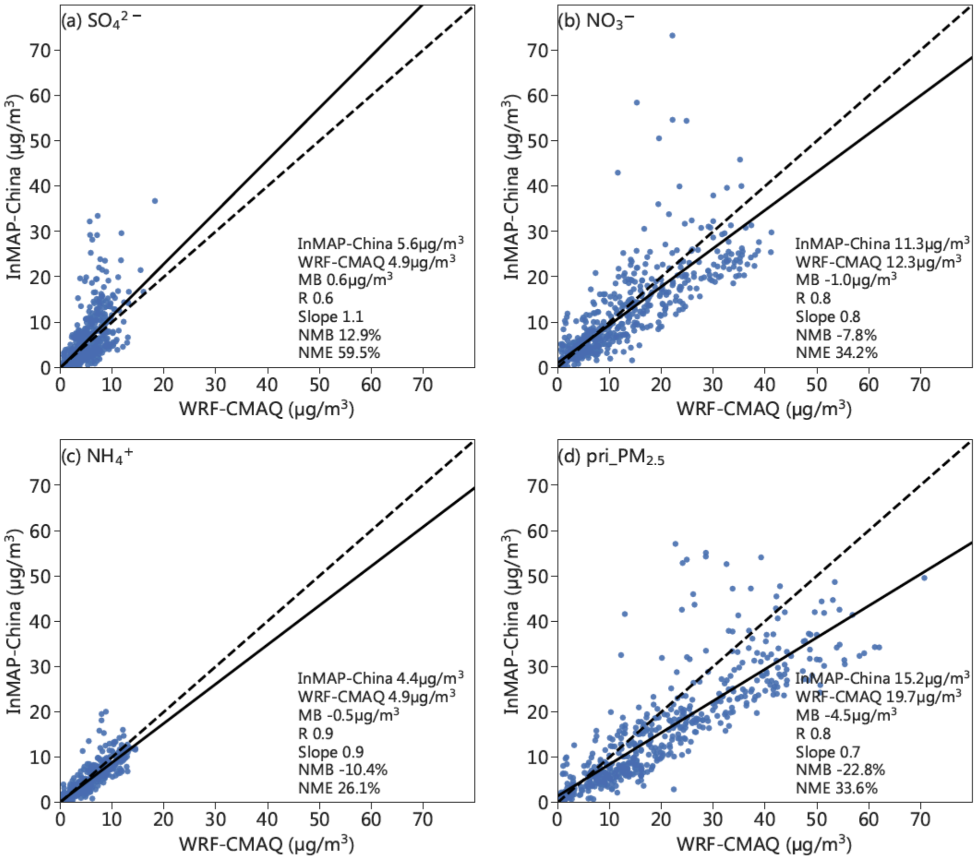

Figure 4 Scatter plot comparing the $PM_{2.5}$ composition concentration modelled by the InMAP-China and WRF-CMAQ models. Panels (a), (b), (c), and (d) display sulfate, nitrate, ammonium, and primary $PM_{2.5}$, respectively. The statistical metrics are labelled in the lower right corner of each panel.

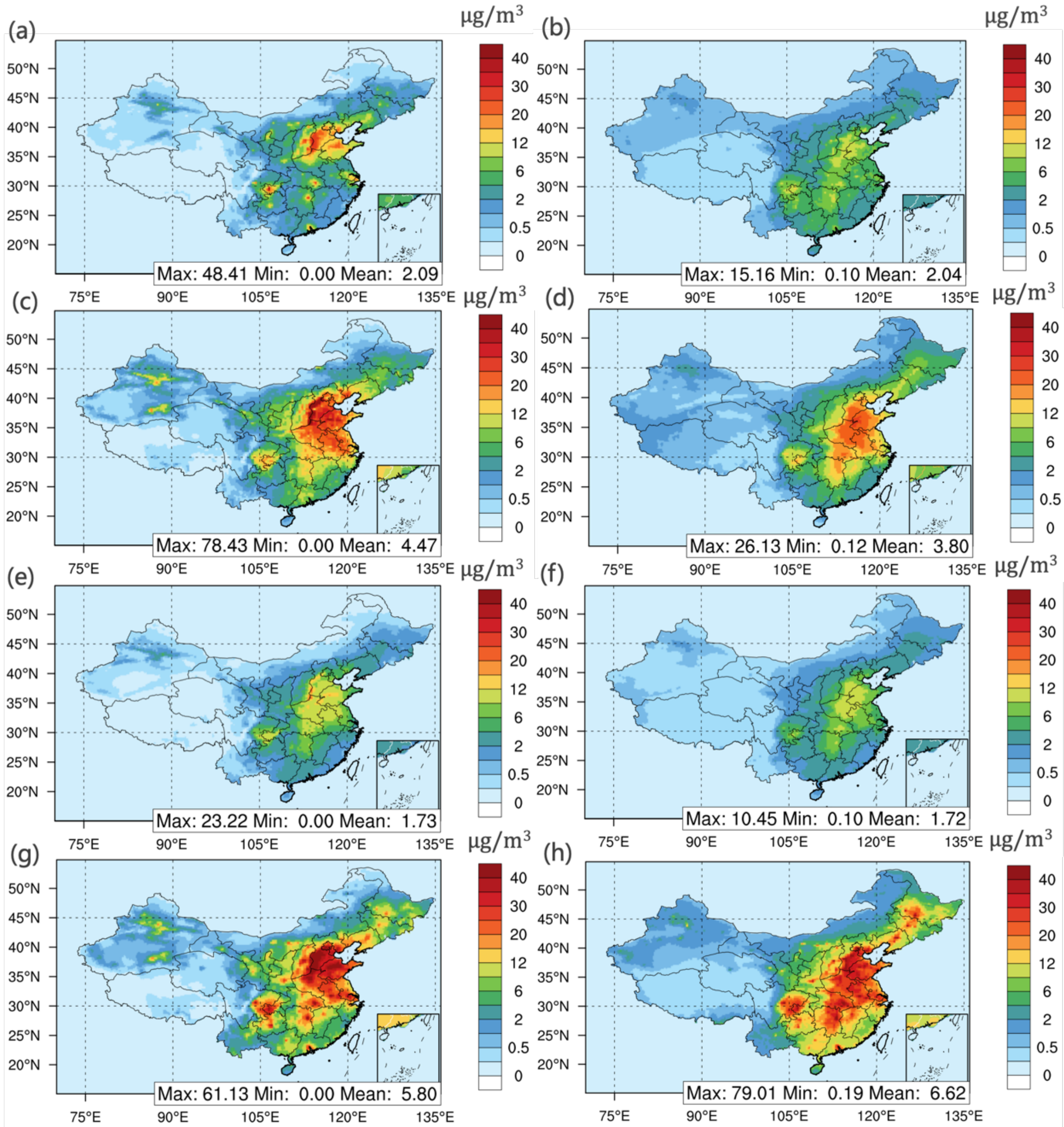

Figure 5 The spatial pattern of $PM_{2.5}$ compositions modelled by the InMAP-China and WRF-CMAQ models. Panels (a), (c), (e), and (g) present the sulfate, nitrate, ammonium, and primary $PM_{2.5}$, respectively, simulated by InMAP-China in the InMAP-TOT scenario. Panels (b), (d), (f), and (h) present the results modelled by WRF-CMAQ.

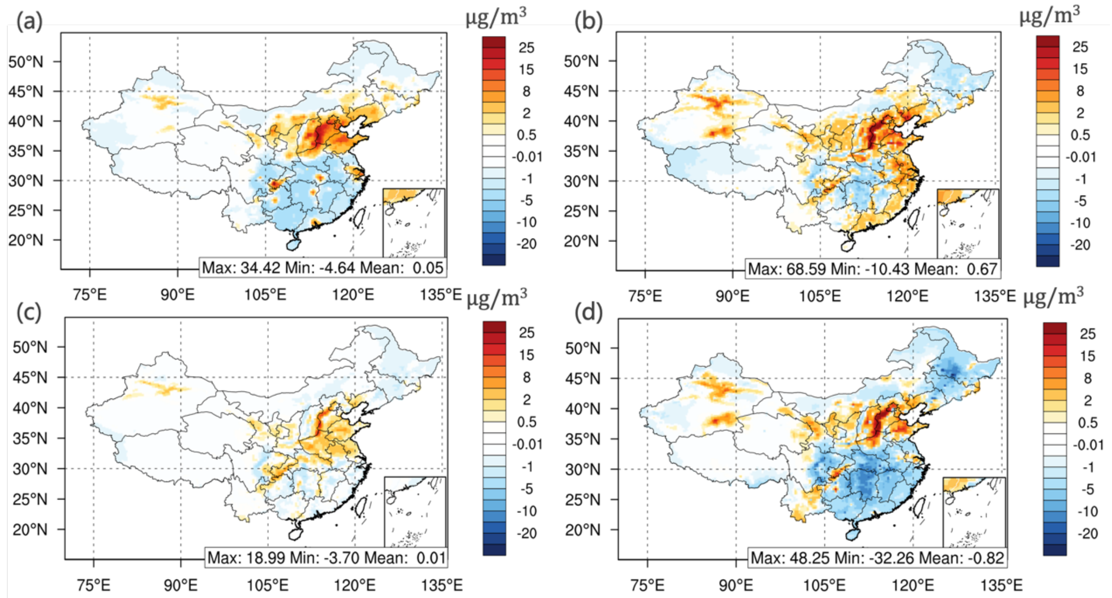

Figure 6 The difference in the spatial pattern of $PM_{2.5}$ compositions between InMAP-China and WRF-CMAQ.

Panels (a), (b), (c), and (d) display sulfate, nitrate, ammonium, and primary $PM_{2.5}$, respectively.

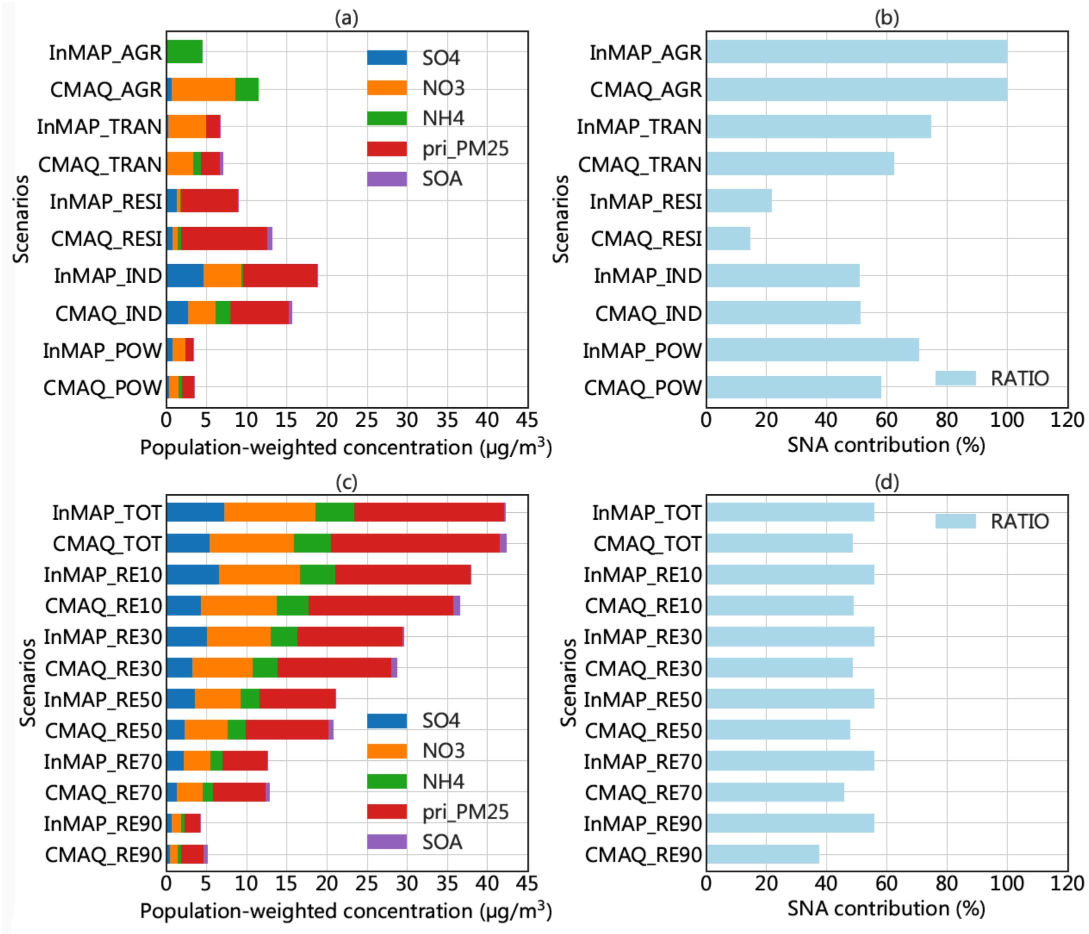

Figure 7 Comparison of $PM_{2.5}$ component concentrations and SNA contributions in these eleven simulations. (a) and (c) show the modelled $PM_{2.5}$ compositions. Panel (a) presents the results of sectoral emission scenarios, and panel (c) presents the results of the baseline and emission abatement scenarios. Panels (b) and (d) present the SNA contribution (%) for each scenario.

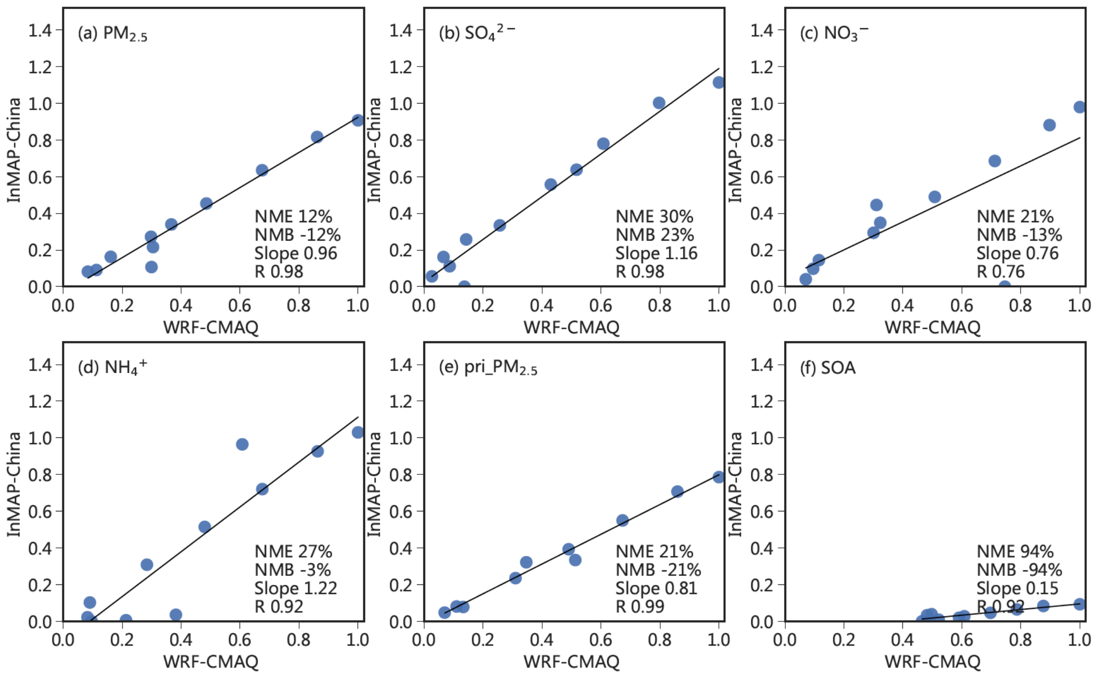

Figure 8 Marginal change in nationwide annual average population-weighted $PM_{2.5}$ concentration and its composition as modelled by InMAP-China and WRF-CMAQ for eleven emissions scenarios. The population-weighted pollutant concentration for each scenario is normalized using the largest value among all scenarios modelled by CMAQ. The eleven dots represent the eleven scenarios, and the statistical metrics are labelled in the lower right corner for each panel.

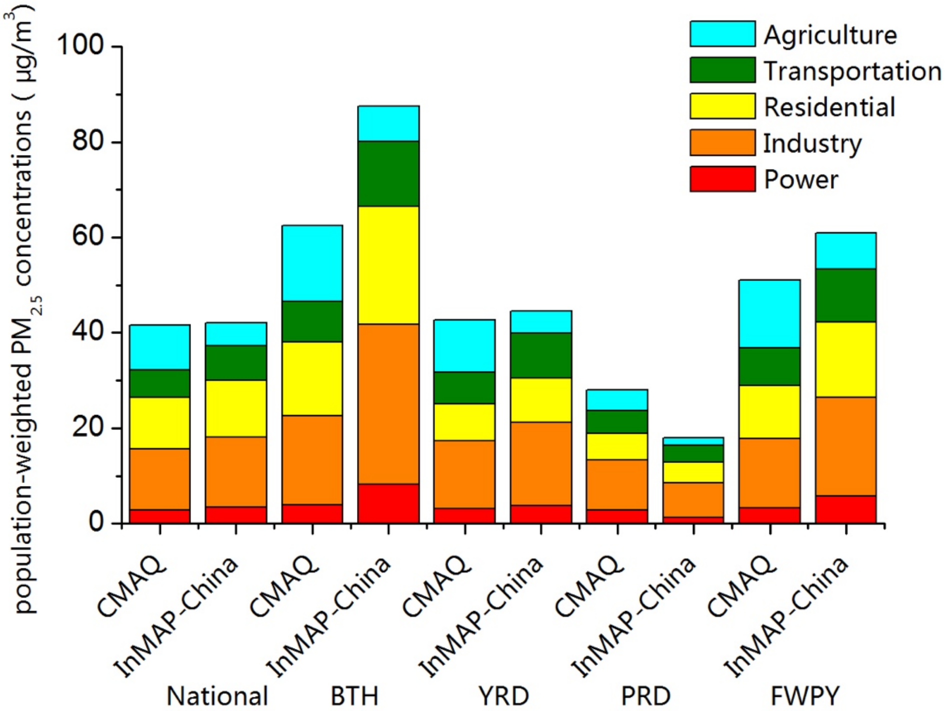

Figure 9 Comparison of source contributions to population-weighted $PM_{2.5}$ concentrations estimated by the two models.

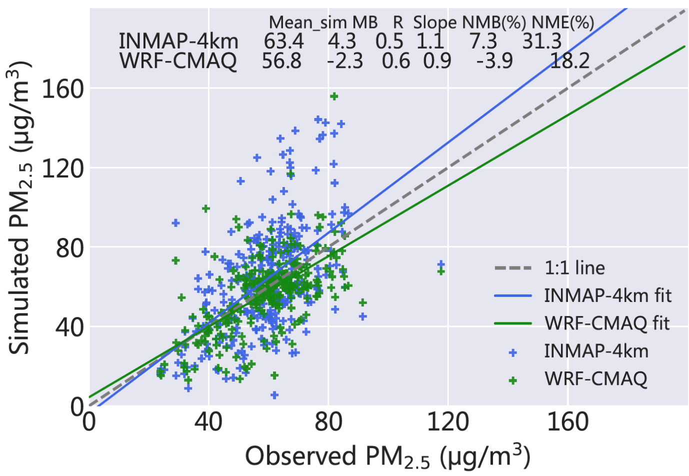

Figure 10 Scatter plot comparing the $PM_{2.5}$ concentration modeled in the BTH region with 4 km spatial resolution by the InMAP-China and WRF-CMAQ. The value of statistical metrics is labeled in the panel.

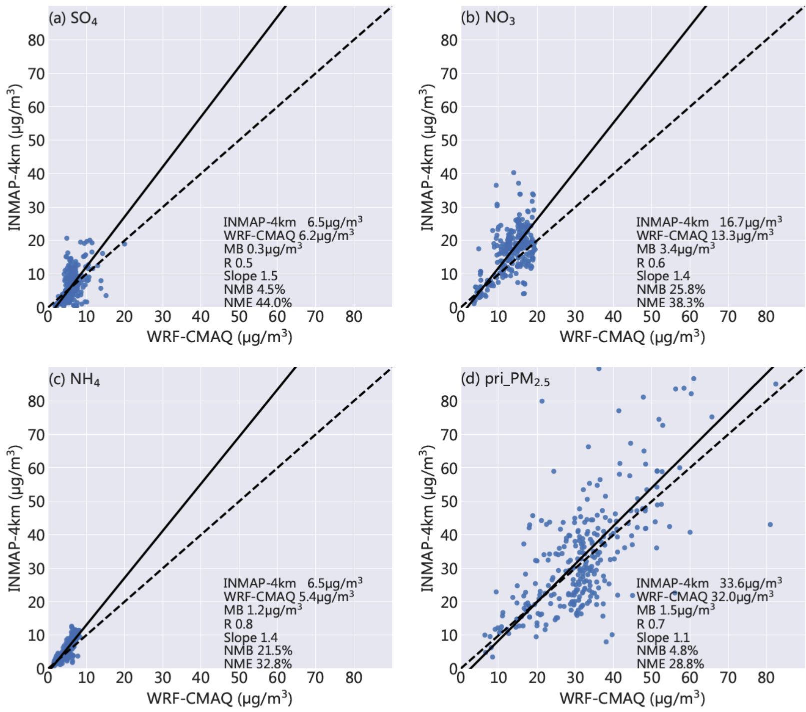

Figure 11 Scatter plot comparing the $PM_{2.5}$ composition concentration modeled at BTH region with 4km spatial resolution by the InMAP-China and WRF-CMAQ. Panels (a), (b), (c) and (d) display the sulfate, nitrate, ammonium, and primary $PM_{2.5}$, respectively. The statistical metrics are labeled in the lower right corner of each panel.

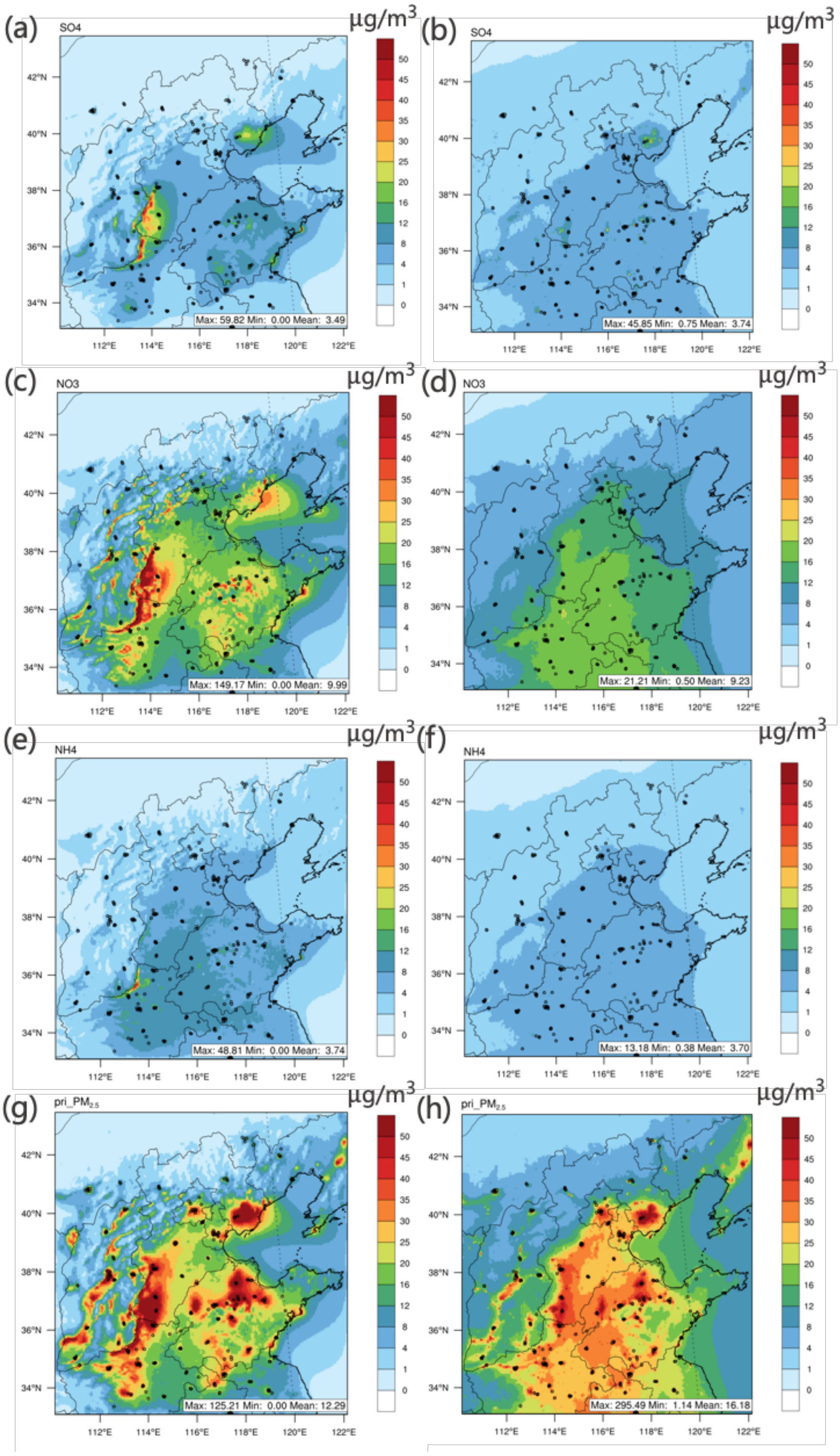

Figure 12 The spatial pattern of $PM_{2.5}$ compositions simulated in the BTH region with 4km spatial resolution by the InMAP-China and WRF-CMAQ. Panels (a), (c), (e), and (g) present the sulfate, nitrate, ammonium, and primary $PM_{2.5}$, respectively, simulated by InMAP-China. Panels (b), (d), (f), and (h) present the corresponding results simulated by WRF-CMAQ.

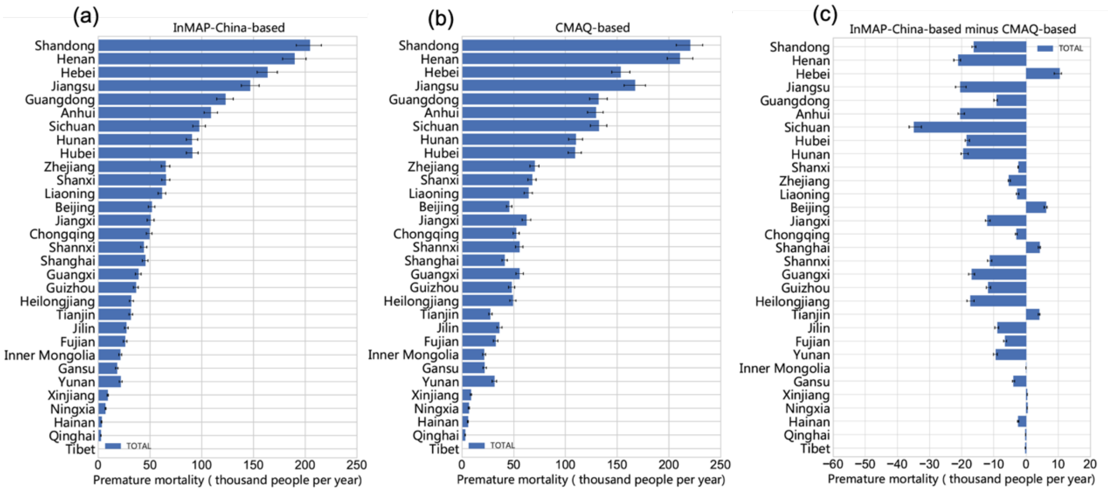

Figure 13 Comparison of $PM_{2.5}$-related premature mortality using the $PM_{2.5}$ predictions from two models.

(a) InMAP-China-based; (b) CMAQ-based; and (c) difference between the two models.