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 that 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 Chinese governments (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, a number of 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 for 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 time efficient, can predict annual-average $PM_{2.5}$ concentrations within few hours but with a modest reduction in accuracy compared with CTMs. InMAP reduces the running time by simplifying the physical and chemical process. 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 the 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 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 prior to 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 for the purpose of rapidly estimating 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 preprocessed 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). The main step of the preprocessed 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 precalculated 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 precalculated 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 is conducted to output hourly meteorological and chemical-related variables in the year 2017. 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 R of 0.9. The predictions of relative humidity at a height of 2 metres 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 metres 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 μg/m^3. Compared with the observed $PM_{2.5}$ of 45.9 μg/m^3, there are slight underpredictions with an MB of 3.7 μg/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 μg/m^3 and -13.9%, respectively. For modelled SO_2 concentrations, MB and NMB are -0.8 μg/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 basically be reproduced in the CMAQ simulations.

2.1.3 Preprocessed emission input data

Additionally, we develop the preprocessed 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 shapefile vector format. The emission data are preprocessed 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. Gridded anthropogenic emissions of 0.3 degrees for the residential, transportation, and agricultural sectors are preprocessed and input to the surface layer. The gridded air pollutant emissions of the industrial sector and noncoal power plants are preprocessed for allocation to attitudes ranging from 130 metres to 240 metres and 130 metres to 890 metres, respectively.

The emissions of coal-fired power plants (CPPs) are preprocessed 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 preprocessed 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 preprocessed and input to the surface layer.

2.1.4 Exposure-response function from GEMM

In InMAP-China, we employ the exposure-response function from GEMM to estimate $PM_{2.5}$-related premature mortality, which was developed by Burnett et al. (Burnett et al., 2018). Premature mortality due to noncommunicable 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, 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 3.3.

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).

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.

2.2.2 Experimental design

We design eleven 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 derived from the MEIC inventory, natural emissions derived from the MEGANv2.10 model, and Asian emissions outside mainland China 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 atmosphere.

In order 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 obtain 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

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. Basically, InMAP-China reproduces the spatial pattern of total $PM_{2.5}$ concentrations simulated by CMAQ. Notably, significant overpredictions 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 overpredictions 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 a 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 NMB values of -13% and -21%, respectively. Conversely, the marginal change in SO_4^{2-} concentrations is overpredicted 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 underpredicted 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 analysed 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 overpredicted 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

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 basically 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 $PM_{2.5}$-related premature mortality

Figure 10 compares the predictions of $PM_{2.5}$-related premature mortality based on two models at the provincial level. 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. At the provincial level, the $PM_{2.5}$-related premature mortality in Beijing city, Tianjin city, Hebei province and Shanghai city is slightly overpredicted 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%.

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. InMAP-China has the advantage of being time-efficient in conducting air quality predictions and health impact assessments of emission sources in China.

InMAP-China performed well for the prediction of $PM_{2.5}$ concentrations. The model 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 chemical process in the InMAP-China. Focusing on the predictions of health impacts, InMAP-China shows moderate under-predictions of 25 ten thousand people deaths compared with CMAQ-based predictions due to the underestimation of total $PM_{2.5}$ concentrations.

Although the modelling system has an acceptable performance, research work is suggested to further improve the model performance. 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.

The development of InMAP-China aims at providing an alternative to the conventional CTMs to predicting the $PM_{2.5}$ concentrations due to emission change in the mainland of China. InMAP-China has the advantage of time efficiency and a satisfactory performance in this study; however, this model has a modest reduction in accuracy compared with conventional CTMs; hence, some limitations still exist for model applications. In terms of the applicability of this modelling system, we recommend users to select InMAP-China as a prior tool with the following objectives: quantification of the contribution of multiple emission sources in baseline atmospheric conditions, for instance, the $PM_{2.5}$ air quality and health impacts contributed by dozens of categories of fine emission sources, and rapid estimation of the general air quality and health benefits attributable to a series of control policies. Instead, if the objective of simulations is to predict the actual situation and pre-estimate the reductions in $PM_{2.5}$ concentrations due to control measures, conventional CTMs are a better choice because the change in atmospheric conditions along with emission change should be taken into account.

Code and data availability

The source code for the localized version of 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

RL. Wu and Q. Zhang designed the research and RL. Wu carried them out. RL. Wu, CW. Tessum and Y. Zhang contributed to model development. 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
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	
BASE	InMAP_TOT	Five sectoral anthropogenic emissions and natural 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	
Aba3	InMAP_RE50	Reduce the air pollutants emissions by 50% based on InMAP _TOT emissions	Converted using WRF-CMAQv5.2 simulation data in the year of 2017; Remain the same in all simulations.
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%

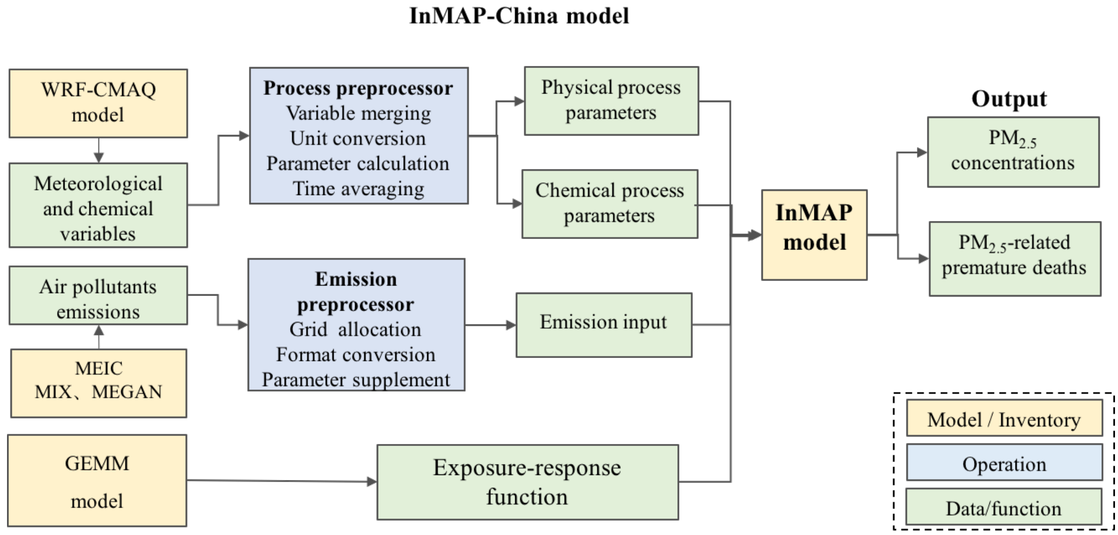

Figure 1 Model framework of InMAP-China.

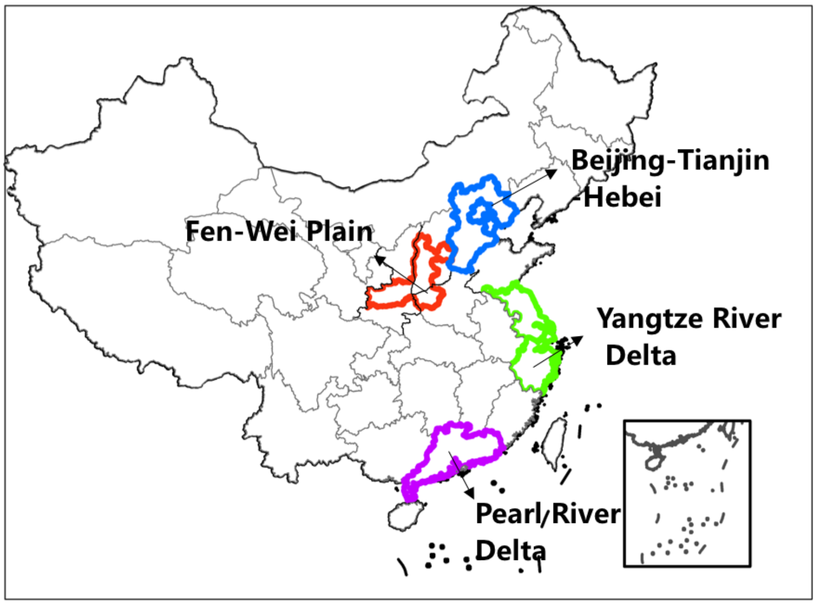

Figure 2 Four key regions defined in this study, including the Beijing-Tianjin-Hebei region, Yangtze River Delta region, Pearl River Delta region and Fen Wei Plain region.

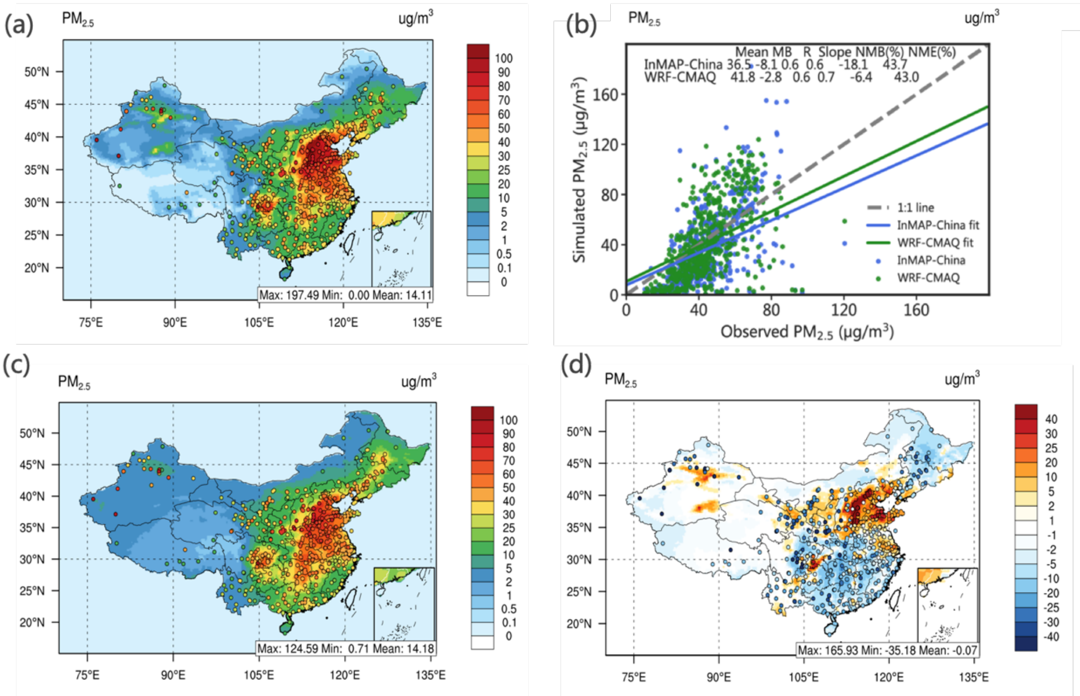

Figure 3 The spatial pattern and statistical metrics of total $PM_{2.5}$ concentrations predicted by InMAP-China and WRF-CMAQ. Panels (a) and (c) display the spatial patterns of total $PM_{2.5}$ concentrations predicted by InMAP-China and WRF-CMAQ, respectively. Panel (d) presents the difference in the 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 colorbar is utilized in the contour and the marked circle.

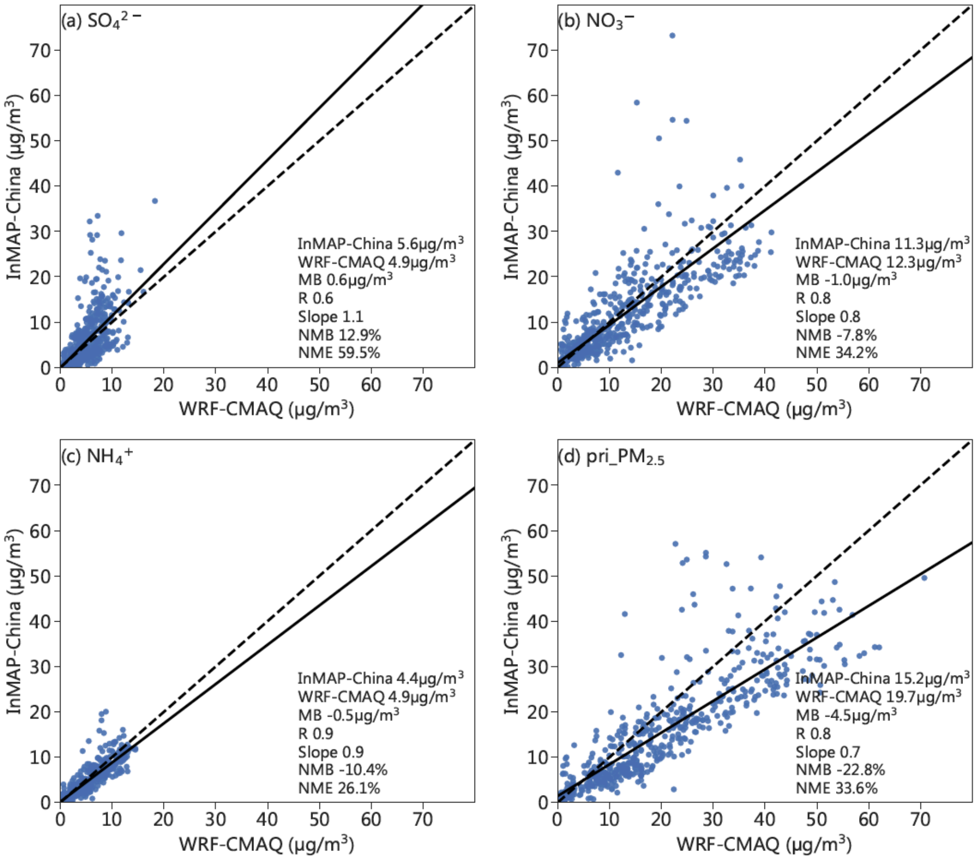

Figure 4 Scatter plot comparing the $PM_{2.5}$ composition concentration modelled by the InMAP-China and WRF-CMAQ models. Panels (a), (b), (c) and (d) display sulfate, nitrate, ammonium, and primary $PM_{2.5}$, respectively. The statistical metrics are labelled in the lower right corner in each panel.

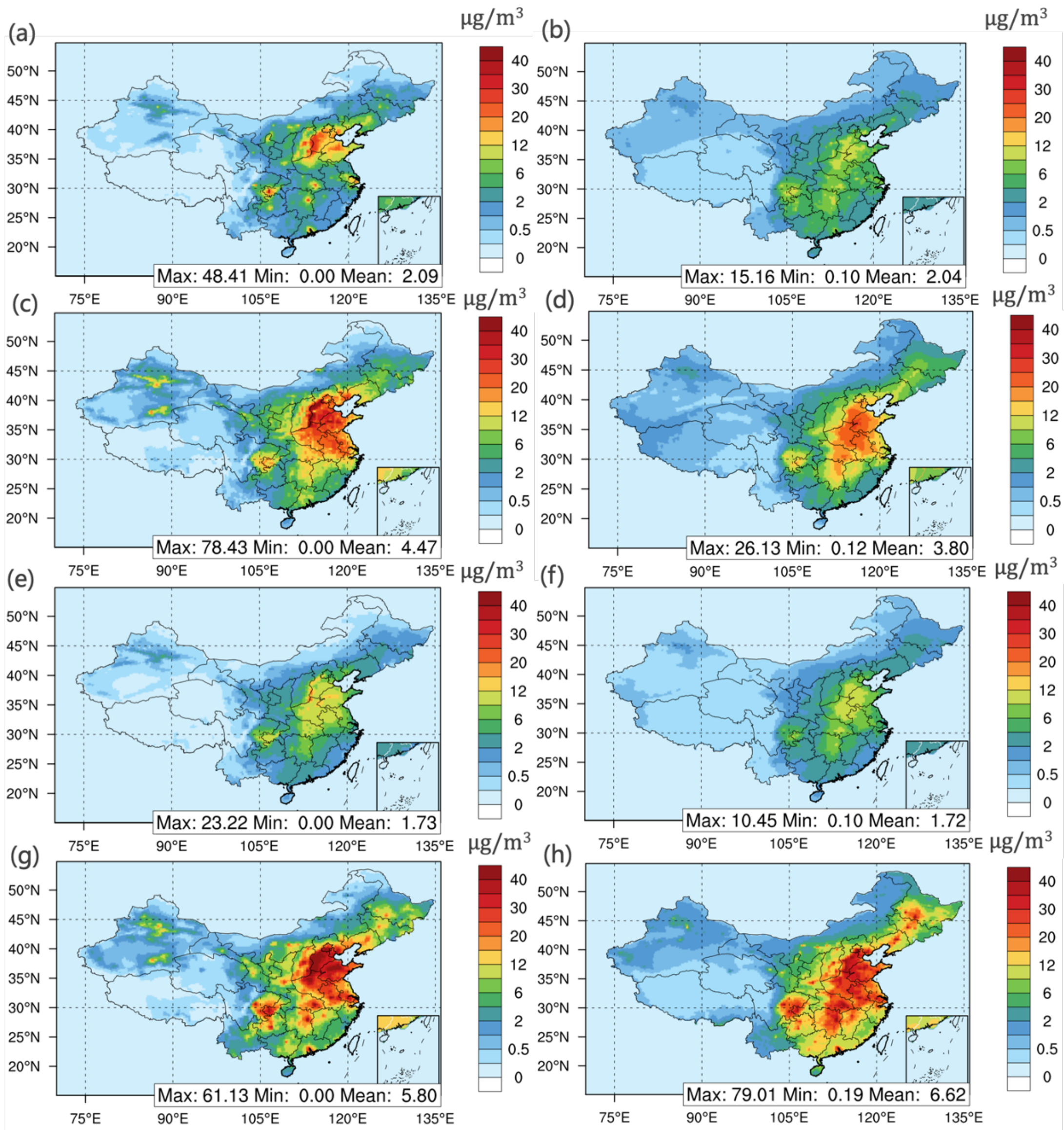

Figure 5 The spatial pattern of $PM_{2.5}$ compositions modelled by the InMAP-China and WRF-CMAQ models. Panels (a), (c), (e), and (g) present the sulfate, nitrate, ammonium, and primary $PM_{2.5}$, respectively, simulated by InMAP-China in the InMAP-TOT scenario. Panels (b), (d), (f), and (h) present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

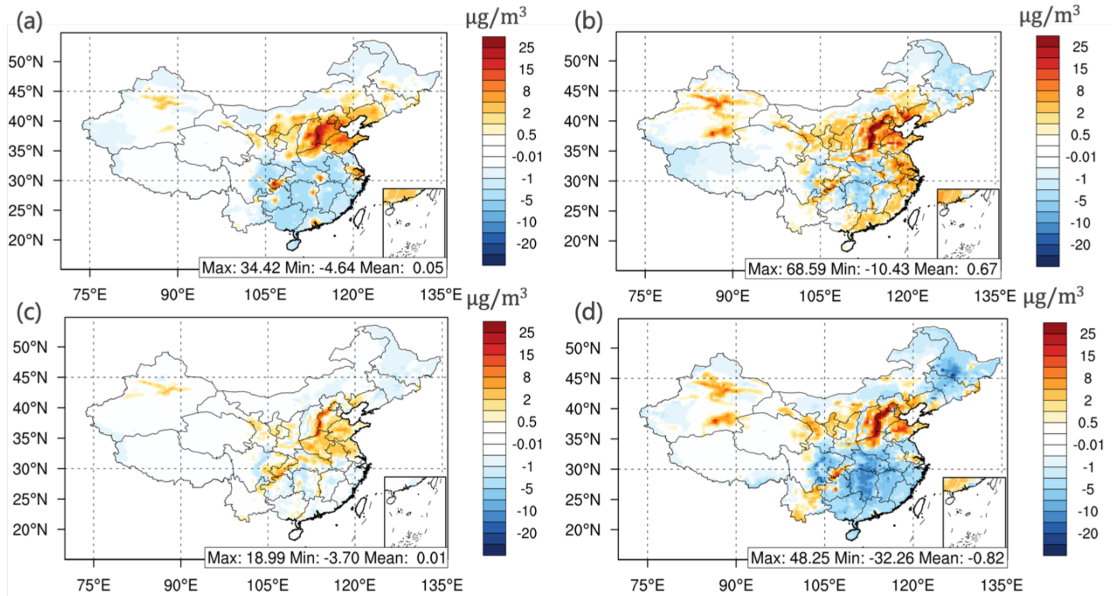

Figure 6 The difference in the spatial pattern of $PM_{2.5}$ compositions between InMAP-China and WRF-CMAQ.

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

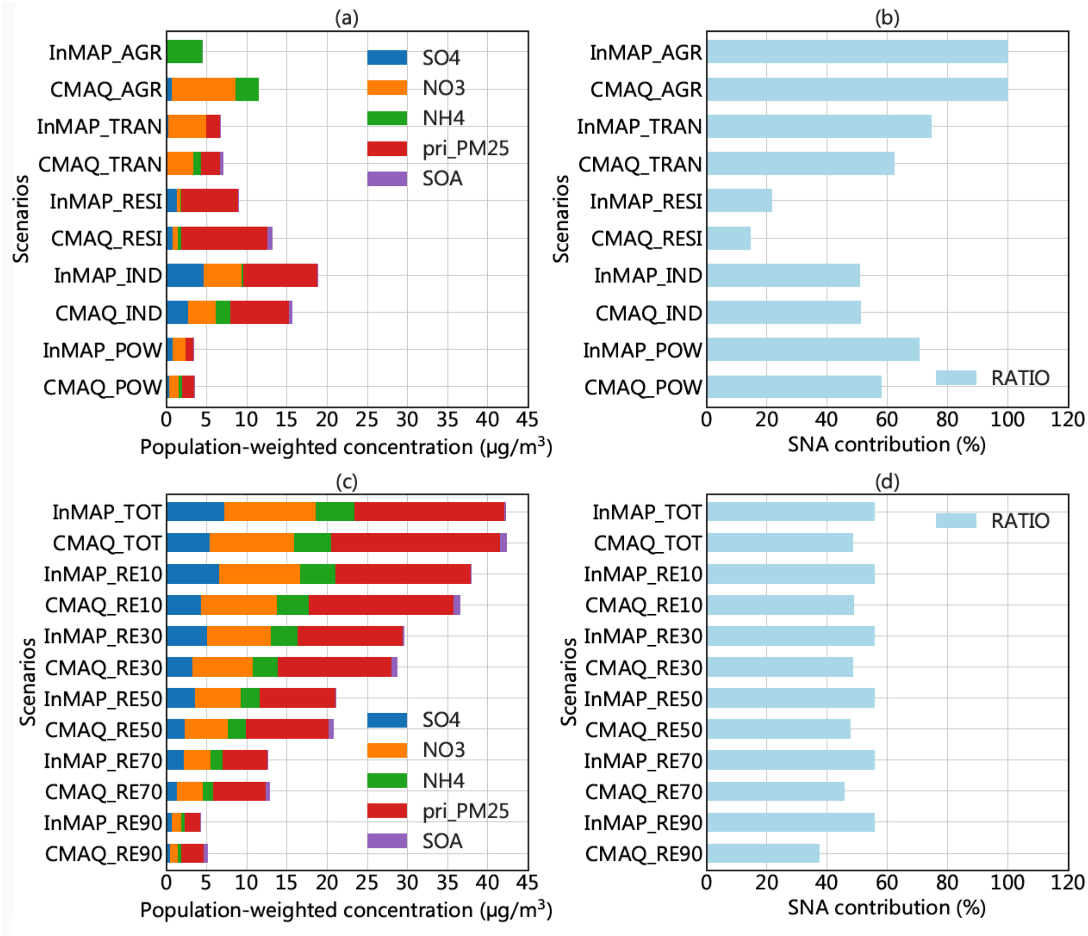

Figure 7 Comparison of $PM_{2.5}$ component concentrations and SNA contributions in these eleven simulations. (a) and (c) show the modelled $PM_{2.5}$ compositions. Panel (a) presents the results of sectoral emission scenarios, and panel (c) presents the results of the baseline and emission abatement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

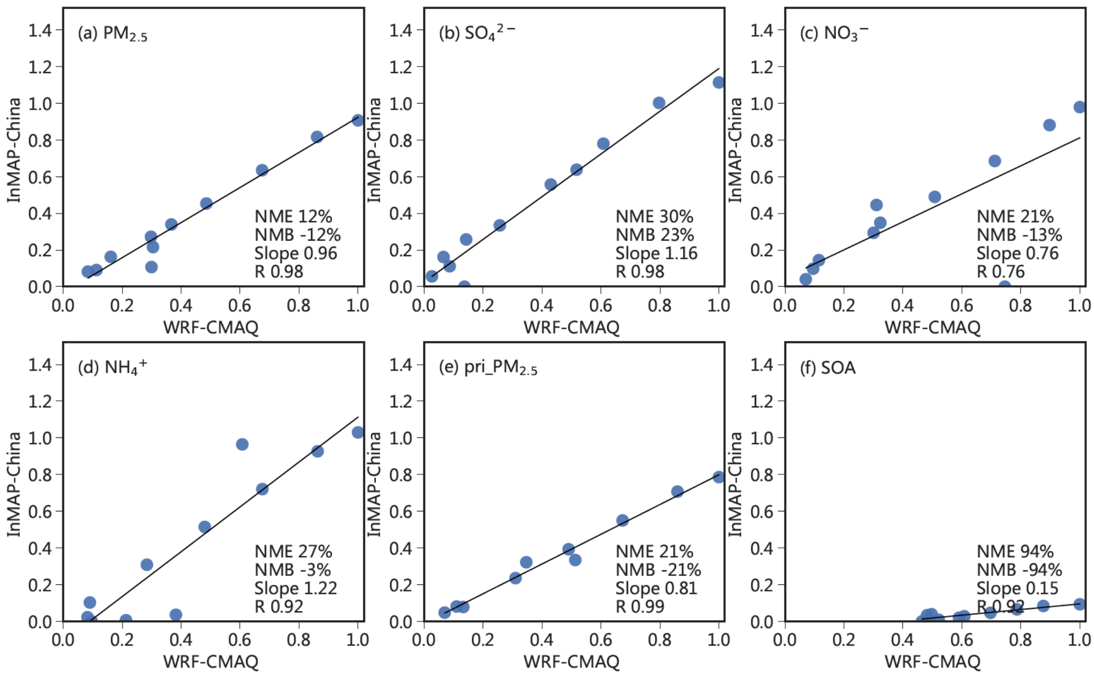

Figure 8 Marginal change in nationwide annual average population-weighted $PM_{2.5}$ concentration and its composition as modelled by InMAP-China and WRF-CMAQ for eleven emissions scenarios. The population-weighted pollutant concentration for each scenario is normalized using the largest value among 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.

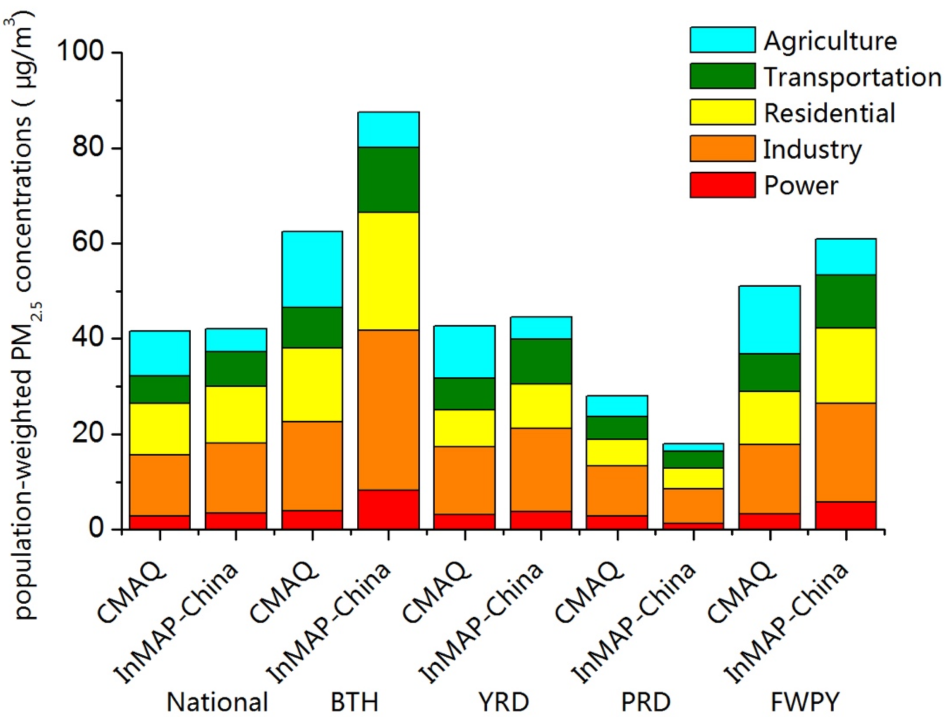

Figure 9 Comparison of source contributions to population-weighted $PM_{2.5}$ concentrations estimated by the two models.

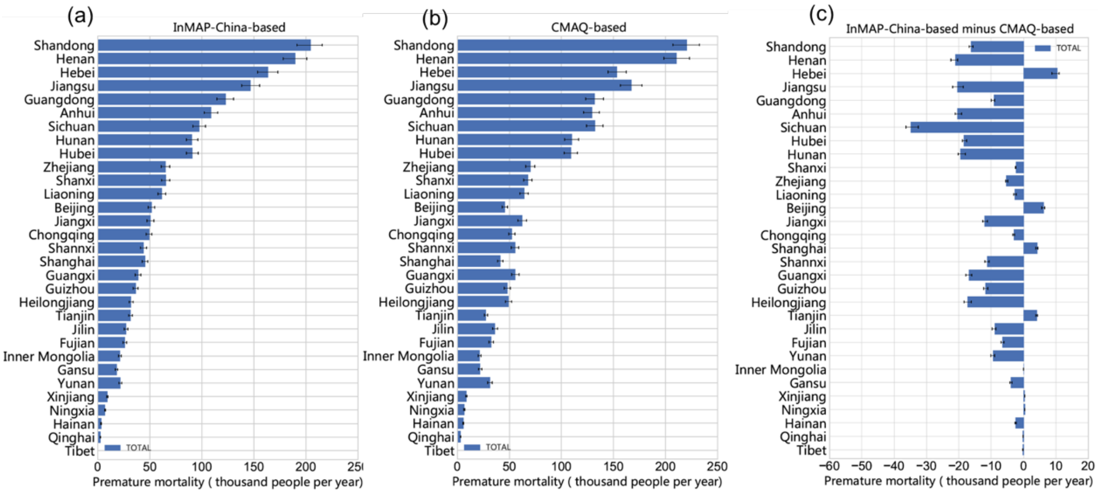

Figure 10 Comparison of $PM_{2.5}$-related premature mortality based on two models. (a) InMAP-China-based; (b) CMAQ-based; and (c) difference between the two models.