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Numerical Air Quality Forecast over Eastern China: Development, Uncertainty and Future

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Abstract

Air pollution is severely focused due to its distinct effect on climate change and adverse effect on human health, ecological system, etc. Eastern China is one of the most polluted areas in the world and many actions were taken to reduce air pollution. Numerical forecast of air quality was proved to be one of the effective ways to help to deal with air pollution. This chapter will present the development, uncertainty and thinking about the future of the numerical air quality forecast emphasized in eastern China region. Brief history of numerical air quality modeling including that of Shanghai Meteorological Service (SMS) was reviewed. The operational regional atmospheric environmental modeling system for eastern China (RAEMS) and its performance on forecasting the major air pollutants over eastern China region was introduced. Uncertainty was analyzed meanwhile challenges and actions to be done in the future were suggested to provide better service of numerical air quality forecast.

Keywords: numerical prediction, numerical forecast, air pollution, air quality, eastern China

1. Introduction

China has been suffering severe air pollution in recent years, characterized as high levels of fine particles ($PM_{2.5}$) and ozone [1–4]. As part of atmospheric composition, air pollutants play important role in climate change. For example, ozone is one of major greenhouse gases, which causes atmospheric warming [5]. Atmospheric aerosol is one of the most important and uncertain factors in both climate change and weather activities. It influences climate by

its direct radiative forcing and induced cloud adjustments and weather by the interactions of aerosol-radiation, aerosol-cloud, etc. [5]. Air pollution also leads to adverse effects on health [6, 7], including increasing of respiratory and cardiovascular diseases, excess mortality, and decreasing of life expectancy [8–11]. High particulate matter (PM) concentration under relatively high relative humidity (RH) conditions often induces haze events and causes high risk on public activities such as surface transportation, aircraft take-off and landing. Therefore, the characteristics, formation mechanisms, and influence factors of air pollution and related issues were seriously focused in recent years (e.g. in [4, 12–15]).

In policy decision aspect, the Chinese government therefore has issued series of actions to reduce air pollution in the last few years. The new Chinese national ambient air quality standards (CNAAQSQ2012) [16] was jointly released by Ministry of Environmental Protection (MEP) of the People's Republic of China and General Administration of Quality Supervision, Inspection and Quarantine of the People's Republic of China in 2012. At the first time, standards for $PM_{2.5}$ and daily maximum 8-hour averaged (DM8H) ozone (O_3 -8h) were established in China. The State Council then issued a stringent action plan to combat air pollution on September, 2013 [17]. China sponsored tens of projects and funded several billions since 2016 in a special fund named Study on Formation Mechanism of Atmospheric pollution and Control Technology. In the support of the Premier Fund, "2 + 26" cities were chosen and one scientific team was organized for each city in 2017 to deal with the air pollution in Beijing-Tianjin-Hebei and its surrounding region. Accordingly, China Meteorological Administration (CMA) established operational centers in three populated regions (Beijing-Tianjin-Hebei, Yangtze River Delta, and Pearl River Delta) to provide air quality forecasting and warning. Provincial governments took many kinds of actions to try to improve ambient air quality.

Eastern China, which covers the Yangtze River Delta, is one of the most polluted regions [1, 3]. The air quality in this region is also influenced by Beijing-Tianjin-Hebei region by the north-westerly. Study on air pollution as well as its secondarily produced haze in this region was thus widely carried out and numerical modeling played an important role. For example, Tie et al. studied ozone [18] and Zhou et al. studied particulate matter and haze [19] over Shanghai by using the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) [20]; the severe PM pollution and haze episodes over eastern China in January 2013 were modeled by using the nested air quality prediction model system (NAQPMS) [21] and revised Community Multi-scale Air Quality (CMAQ) model [22, 23], etc. In the previous studies, increase of secondary aerosols was certified to take important role in heavy PM pollution events (e.g. in [19, 23, 24]) and some new sources through heterogeneous processes were found to promote rapid increase of PM in extreme pollution episodes [14, 25]. These works proved that the usage of air quality models is one valid solution to air pollution studies.

In this chapter, the numerical forecast of air quality over eastern China is presented. This work is one of the important applications of numerical meteorological prediction and supports air quality and relevant service including temporary emission control and study of air pollution on health, etc. In the next sections, the brief history of development of numerical modeling for air pollution will be reviewed. Then the operational forecast will be emphasized, including the construction of modeling system and forecast performance. Analysis and discussion on the uncertainty and shortage in current work will be presented to help improving the forecast in the future. Brief conclusion will be given in the end.

2. Brief history of numerical air quality modeling

Air quality models are tools that describe the physical and chemical processes which influence air pollutants, including chemical reactions, transport, diffusion, scavenging, etc. in the atmosphere. They are built based on the understanding of atmospheric physics and chemistry and computation technology. The models are used in many air quality and related issues, such as analyzing the characteristics of tempo-spatial patterns and changes of air pollutants, discovering the mechanisms of formation of air pollution, and estimating the influence of the change of factors (e.g. anthropogenic emission, volcanic explosion) on air quality, etc. Usually, air quality models are more or less driven by meteorological variables and therefore are connected with meteorological models or model outputs.

Since the 1970s, three generations of air quality models have been developed sponsored by United States Environmental Protection Agency (US EPA) and other organizations. In the first-generation models, atmospheric physical processes are highly parameterized and chemical processes are ignored or just simply treated. These models introduce the dispersion profiles in different levels of discretized stability and are specialized in calculating the long-term average concentration of inert air pollutant. The second-generation models include more complicated meteorological models and nonlinear chemical reactions and the simulation domain is three-dimensionally (3-D) gridded. The chemical and physical processes are individually calculated in each grid and influence between neighbor grids is considered. This generation is used generally to treat one type of air pollution, such as photochemical smog and acid rain. In the end of the 1990s, US EPA presented the concept of “one atmosphere” and developed the third-generation air quality modeling system—Medels-3/CMAQ [26]. It is an integrated system and consists of serial modules to process emissions, meteorology inputs, chemical reaction and transport, production making, etc. The third-generation models involve relatively detailed atmospheric chemistry and physics as well as the influence and inter-conversion among air pollutants of different types or phases. In fact, the divide of different generations is not distinct and some models are still in continuous development. For example, the CALPIFF (one Lagrangian model of the first-generation) introduced much research results in the 1990s and was often implemented in the 2000s. The second version regional acid model (RADM2) increased chemical species and reactions [27] and was introduced in the very newly developed third-generation model of WRF-Chem [20].

In recent years, 3-D chemical transport models (CTMs) has been widely used in studying and forecasting air quality combined with numerical meteorological models benefited from the rapid development of models and computing technology. For example, global ozone was simulated by using the model for ozone and related chemical tracers (MOZART) and the model performance was evaluated [28, 29]. Gu et al. studied summertime ozone and nitrate aerosol in upper troposphere and lower stratosphere (UTLS) over the Tibetan Plateau and the south Asian monsoon region using the Goddard Earth Observing System chemical transport model (GEOS-Chem) [30, 31]. The CMAQ model had a great number of applications around the world, e.g. in [32, 33]. Tie et al. studied the characterizations of chemical oxidants in Mexico City using WRF-Chem [34]. Zhou et al. developed an operational mesoscale sand and dust storm forecasting system for East Asia by coupling a dust model within the CMA unified atmospheric chemistry environment (CUACE) [35]. Zhou et al. developed the CUACE

for aerosols (CUACE/Aero) to study chemical and optical properties of aerosol in China [36]. Over eastern China, there were also numerous applications of CTMs. Gao et al. studied regional haze events in the North China Plain (NCP) using WRF-Chem [37]. Zhou et al. built an operational system to forecast air quality over eastern China region and resulted good performance in forecasting the major air pollutants of $PM_{2.5}$ and ozone over this region [38]. Wu et al. analyzed the source contribution of primary and secondary sulfate, nitrate, and ammonium (S-N-A) during a representative winter period in Shanghai using online source-tagged NAQPMS [39]. Li et al. investigated ozone source by using the ozone source apportionment technology (OSAT) with tagged tracers coupled within Comprehensive Air Quality Model with Extensions (CAMx) [40].

Air quality modeling in current generation can be switched “offline” or “online” depending on the treatment of meteorology and chemistry. The offline chemical processes are treated independently from the meteorological modeling, while those in online approach are dependent. The modeling systems implemented in recent years are mostly offline, such as AIRPACT [32]. The chemical transport in this approach is driven by outputs from a separate meteorological model, typically available once per hour. This approach is computationally attractive since only one meteorological dataset can be used to produce many chemical simulations for different scientific questions. On the other hand, the “online” treatment (e.g. WRF-Chem) was newly developed to solve the loss of information in offline approach about atmospheric processes that have a time scale of less than the output time interval of meteorological models, including wind speed, wind direction, rainfall, etc. The lost information may be very important in high resolution air quality modeling. The online approach also benefits to investigate the interactions between meteorology and chemistry [21], which are out of the purpose of offline treatments. Previous studies (e.g. in [19, 21, 37, 38, 41]) on air pollution and related issues over eastern China region had proved the applicability and advantage of the online model of WRF-Chem.

Shanghai Meteorological Service (SMS), as well as the East China Meteorological Center of CMA, shares the responsibility to provide air quality forecast and air pollution warning for Shanghai and guidance for East China region. Therefore, SMS initialized numerical modeling of air quality in 2006. This work got scientific and technological supports from the World Meteorological Organization (WMO) through Shanghai WMO global atmosphere watch (GAW) urban research and meteorological environment (GURME) Pilot Project. Based on the thinking of the applicability and advantage of WRF-Chem and the extendibility on calculation of the inter-feedback between meteorological variables and air pollutants, WRF-Chem was chosen as the core model in developing our numerical air quality forecast system. An experimental forecasting system was established in 2008, in which nested domains of 16×16 -km and 4×4 -km was implemented. The outer domain covered eastern China region and the inner one covered the main YRD region. The evaluation showed that the results from two domains had comparable performance and further study in [34] showed that the 6×6 -km resolution performed best under the conditions of the model and emission data at that time. Therefore, a real time forecast system covering the YRD region with a horizontal resolution of 6-km was built in 2009 to support the air pollution (including three variables of PM_{10} , SO_2 and NO_2) forecast for Shanghai. This application showed that the forecasts from this version had acceptable performance under relatively stable conditions but poorer performance for transport cases, because there are much more air pollutants transported from areas outside the

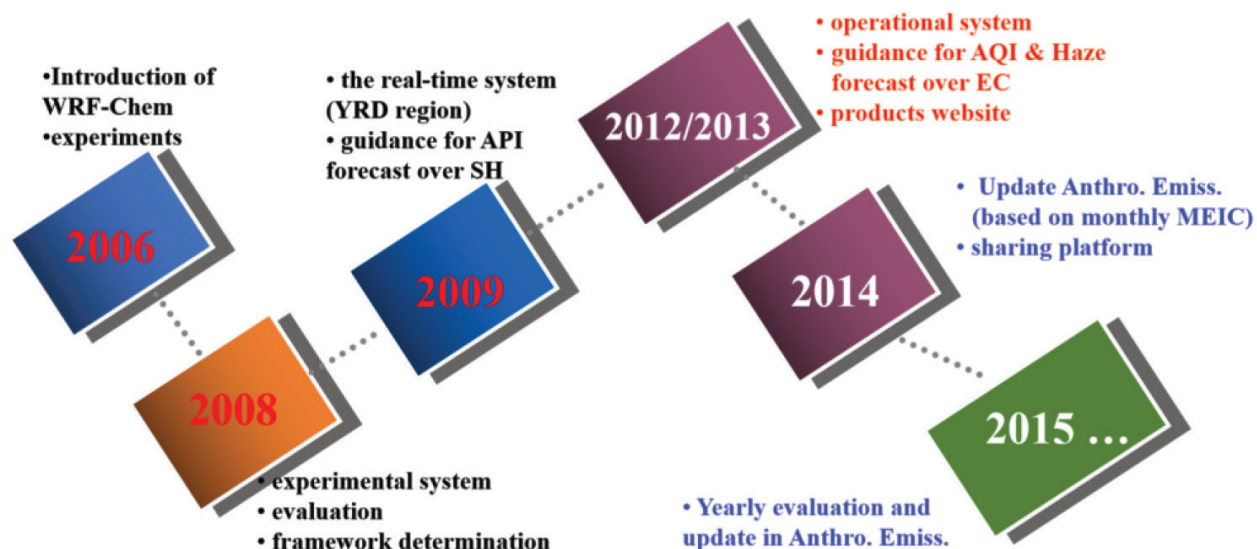


Figure 1. The brief history of development of numerical air quality forecast in SMS.

model region such as the NCP. With updates in high performance computational resource, one forecast system covering eastern China region was established in 2012, which was named as Regional Atmospheric Environmental Modeling System for eastern China (RAEMS). This system was certificated as an official operational forecast system by CMA in March, 2013. More details about the operational system will be introduced in the next section and the brief history of its development was shown in **Figure 1**.

3. The operational forecast and performance of RAEMS

3.1. Framework of the operational system

The core model in RAEMS is WRF-Chem, which was developed through the collaboration of several institutes (e.g. NOAA, NCAR, etc.). Chemistry and meteorology is fully coupled in this model, in other words, the same advection, convection, and diffusion scheme, model grids, physical schemes, and time step is used and there is no interpolation in time for meteorological fields. The modeling performance of WRF-Chem has been extensively validated [20, 42]. Several real-time prediction systems were built based on the WRF-Chem model to provide air quality forecasts around the world (e.g. China, the United States, and Brazil), as listed in [43]. In RAEMS, several improvements were made based on WRF-Chem version 3.2 by Tie et al. [44], including the introduction of aerosol effects on photolysis, adjustments of nocturnal ozone losing, and introduction of ISORROPIA II secondary inorganic aerosol scheme [45]. This modified version has been validated, showing good performance in ozone and $PM_{2.5}$ prediction for Shanghai [18, 19].

As shown in **Figure 2**, the domain encompasses the eastern China Region. Centered at (32.5°N, 118°E), it consists of 360 un-staggered grids in west-east and 400 in south-north with a 6-km grid resolution. There are 28 layers vertically, with the top pressure of 50 hPa. The time step for integration is 30-s for meteorology and 60-s for chemistry, and these for radiation, biogenic

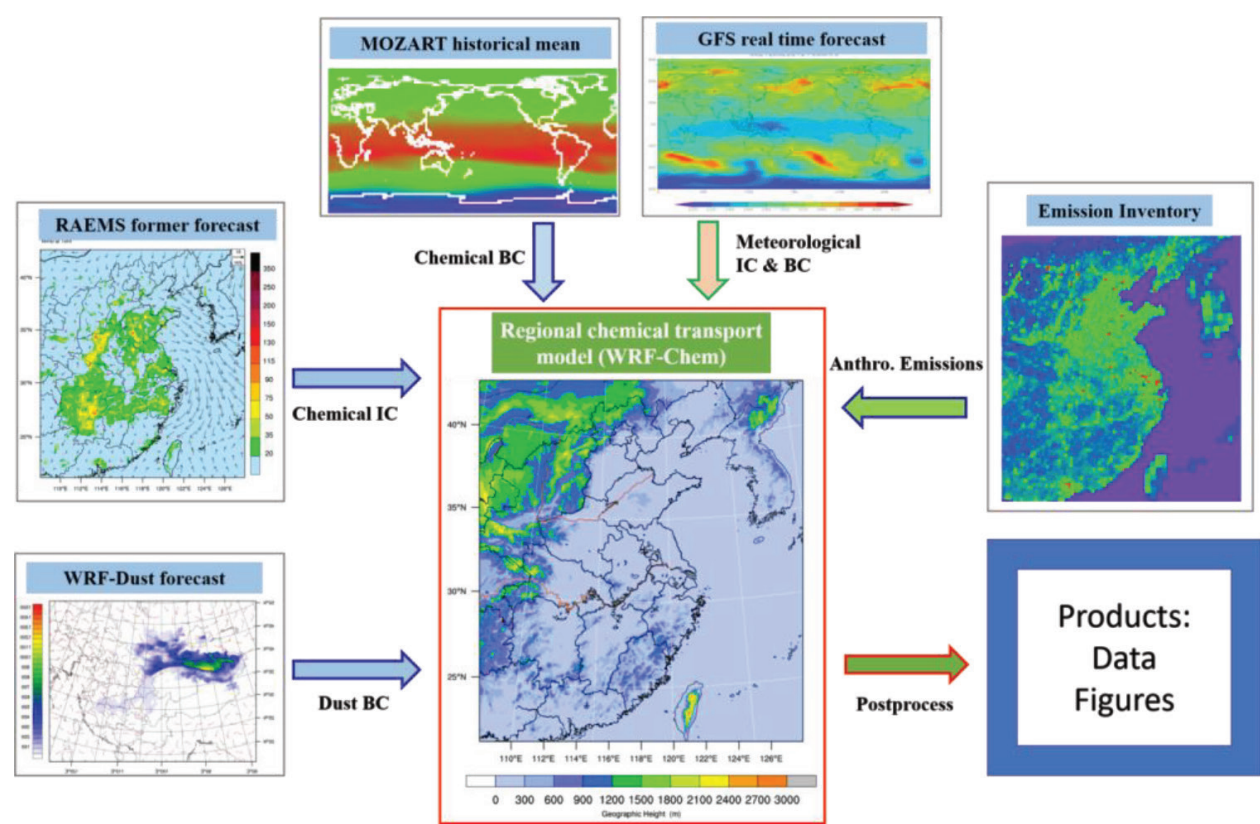


Figure 2. Components of RAEMS. Domain coverage was shown in the central component.

emission, and photolysis are 10, 30, and 15 min, respectively. Physical options are listed in **Table 1**. Specially, the Noah-modified 20-category IGBP-MODIS instead of 24-category USGS land-use was used. The RADM2 [27] was used for gas-phase chemistry. ISORROPIA II

| Parameterization scheme | Option |
|-----------------------------------|---------------|
| Micro-physics (mp_physics) | WSM 6-class |
| Cumulus parameterization (cu_phy) | Not used |
| Long-wave radiation (ra_lw) | RRTM |
| Short-wave radiation (ra_sw) | Dudhia |
| Surface layer (sf_sfclay) | Monin_Obukhov |
| Land surface (sf_surface) | Unified Noah |
| Boundary layer (bl_pbl) | YSU |
| Gas-phase chemistry | RADM2 |
| Inorganic aerosol chemistry | ISORROPIA II |
| Organic aerosol chemistry | SORGAM |

Table 1. Physical and chemical configuration in RAEMS.

secondary inorganic [45] and the Secondary ORGanic Aerosol Model (SORGAM) [46] schemes were used to treat aerosol chemistry. Madronich scheme [47, 48] was applied for photolysis.

The global forecast from the National Centers for Environmental Prediction Global Forecast System (NCEP GFS) was used for meteorological initial and boundary conditions. NCEP GFS data was used widely for weather forecast, analysis, and as the initial and lateral boundary conditions of regional modeling. 0.5-degree GFS forecast was used, and 1-degree data was also applied if higher resolution forecasts were not available. Previous forecast was used for chemical initial conditions. The gaseous chemical lateral boundary conditions were based on estimations from a global chemical transport model (MOZART-4) [28, 29]. Boundary conditions were extracted from the MOZART-4 by matching the RAEMS boundary with the MOZART cells. While maintaining diurnal variations in species concentrations, monthly averaged MOZART-4 values of the year 2009 were applied.

3.2. Biogenic and anthropogenic emissions

Biogenic emissions were calculated online using model of emissions of gases and aerosols from nature (MEGAN2, in [49, 50]). Global land cover maps including isoprene emission factor, plant functional type, and leaf area index were applied.

The multi-resolution emission inventory for China (MEIC [51, 52]) for the year 2010 was applied as the anthropogenic inventory. MEIC inventory was developed by Tsinghua University, including emissions of 10 major atmospheric pollutants and greenhouse gases (SO_2 , NO_x , CO, NMVOC, NH_3 , CO_2 , $\text{PM}_{2.5}$, PM_{10} , BC, and OC) over mainland China. MEIC supplied gridded monthly emissions from five sectors (industry, power, residential, transport, and agriculture) with a 0.25-degree resolution. Asian emission inventory for the NASA INTEX-B Mission [53] was applied for regions outside mainland China and before August, 2014. It has a resolution of 0.5-degree for the year 2008.

While being used in RAEMS system, the emissions were spatially regridded to the model grids. Emissions were also hourly allocated with the diurnal profile (in [38]) provided by Shanghai Academy of Environmental Science. NO emission took a proportion of 90% of the amount of NO_x in mole number and NO_2 took the rest 10% (as in [41]). Information of spatial distribution and total amount can be found in [38].

3.3. Operational execution and products

The RAEMS was authorized as an official operational forecasting system by CMA on Mar. 23, 2013 and has been producing forecast since then. The operational system runs once per day, initialized at 12Z UTC (20Z LST). It is started at about 2 am at local time every day and completes entire simulation and post-processing within 5 h. The predictable time length is more than 78 h and the forecast system provides forecast products for 3 local days.

Operational products are displayed on a website [54]. The link to this site is also accessible from the official NOAA WRF-Chem website [43]. The products include hourly spatial

distributions of major pollutants and air quality related meteorological conditions. Temporal variations of both meteorological elements and pollutant species at more than 500 stations as well as real-time evaluation results are also provided online.

3.4. Regular update on anthropogenic emission

The anthropogenic emission used in RAEMS was yearly updated since 2016 to fit the change of emission as well as the adaptability of the modeling system. The emission was updated monthly based on that used in the same month of previous year. These adjustments were majorly depended on the results of monthly evaluation of previous year and information of emission regulation and control implementing in that month as well as the feedback from the forecasters in operational agencies who use the products every day. In the treatment, the ratio of bias median to observational average for each city was taken as the key indicator for adjusting. At the same time, performance of NO_2 and SO_2 and primary PM emission was most focused because of the importance of S-N-A in secondary aerosol [55, 56] and that of primary aerosol. For example, the evaluation showed that NO_2 was obviously underestimated in the northern and southern parts of East China region with bias ratios of over -25% in December, 2015 (**Figure 3**). SO_2 forecasts showed more serious underestimation for most cities in these two areas. But the RAEMS overestimated NO_2 and SO_2 for many cities in the middle region, especially for the cities along the Yangtze River. Therefore, the emitting intensities of NO_2 and SO_2 in December, 2016 were increased or decreased in different amounts separately for different areas. Accordingly, other emitting species were adjusted in the similar way. The amounts were estimated experientially based on ratios and control information.

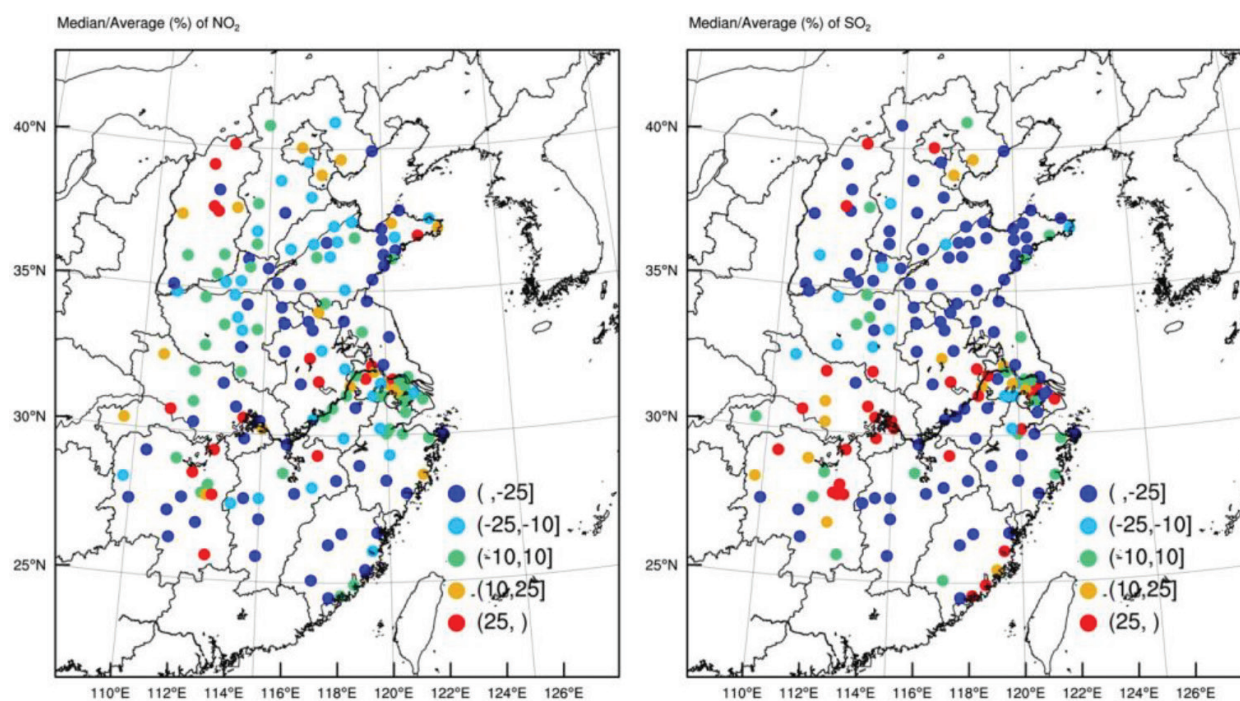


Figure 3. The distribution of the ratio of forecast bias median to the observational average in December, 2015 for NO_2 (left) and SO_2 (right).

3.5. Evaluations

A comprehensive evaluation on the performance of RAEMS was carried out in [38]. In that work, the performance in the beginning of two natural years of 2014 and 2015 was exhibited. They analyzed the series of statistical indicators for variables of $\text{PM}_{2.5}$, ozone, PM_{10} , NO_2 , SO_2 and CO. The indicators included mean bias (MB), mean error (ME), root mean square error (RMSE), correlation coefficient (R), normalized mean bias (NMB) and error (NME), factor of 2 of measurement values (FAC2, the ratio of forecast records within between half and twice of measurement values), Fractional bias (FB) and error (FE), etc. Category performance with different exceedance limits was also evaluated for the two most important pollutants of $\text{PM}_{2.5}$ and O_3 -8h. In spatial, the performance of $\text{PM}_{2.5}$ and DM8H ozone for main cities and $\text{PM}_{2.5}$ for provincial capital cities was shown. In temporal, the consistency of different forecast time length of $\text{PM}_{2.5}$ and ozone and diurnal variation and the distribution of peak time of ozone was analyzed.

In general, their results showed that the RAEMS has good performance in forecasting the temporal trend and spatial distribution of major air pollutants over eastern China region and the performance is consistent with the increasing forecast time length up to 3 days. All summarized statistical indicators of daily $\text{PM}_{2.5}$ and DM8H ozone in different forecast time lengths were comparable with each other and no distinct disagreements were shown. About half of cities have correlation coefficients greater than 0.6 for $\text{PM}_{2.5}$ and 0.7 for DM8H ozone. The forecasted $\text{PM}_{2.5}$ concentrations were generally in good agreements with observed concentrations, with most cities having NMB within $\pm 25\%$. Forecasted ozone diurnal variation was very similar to the observations and made small peak time error. The modeling system also exhibited acceptable performance for the other air pollutants. More detailed information can be found in [38].

Here more evaluation results were given for the city of Shanghai, one of the largest cities around the world, to show a glimpse on the continuity of forecast performance and how the forecast system performed after 2015. **Figure 4** shows the scattering results of observed and 48-h forecasted $\text{PM}_{2.5}$ and O_3 -8h for 4 years from 2014 to 2017. It shows that RAEMS had generally good performance in forecasting the two most important air pollutants. For $\text{PM}_{2.5}$, the four-year average observed concentration was $46.9 \mu\text{g}/\text{m}^3$ and the forecasted concentration was only $0.1 \mu\text{g}/\text{m}^3$ overestimated. The correlation coefficient between observation and prediction of $\text{PM}_{2.5}$ was 0.74. It also revealed relatively low RMSE and NMB, $22.3 \mu\text{g}/\text{m}^3$ and 8.1%, respectively and high FAC2 of 0.89. This result suggested that 89% forecasted $\text{PM}_{2.5}$ concentrations were within between half and twice of those of observed. These indicators showed excellent performance in forecasting and modeling $\text{PM}_{2.5}$. The NMB of 8.1% was much lower than the acceptable threshold value of $\pm 20\%$ recommended in the United Kingdom [57]. For example, Chen et al. reported a FAC2 of around 60% and NMB of 17 and 32% for polluted and clean periods [32]. Grell et al. reported a R^2 of 0.38 for simulating $\text{PM}_{2.5}$ over New Hampshire using WRF-Chem [20]. Foley et al. Reported a NMB of 19% [33]. Prank et al. found underestimation of 10–60% over Europe using four chemical transport models of CMAQ, EMEP, LOTOS-EUROS and SILAM [58]. Wu et al. reported FAC2 of 70–80% [39]. For O_3 -8h, the forecasts showed better performance in indicators of correlation coefficient, NMB, and FAC2, but worse in MB and RMSE comparing with corresponding indicators for $\text{PM}_{2.5}$. The performance for Shanghai has high scores among the cities over the eastern China [38].

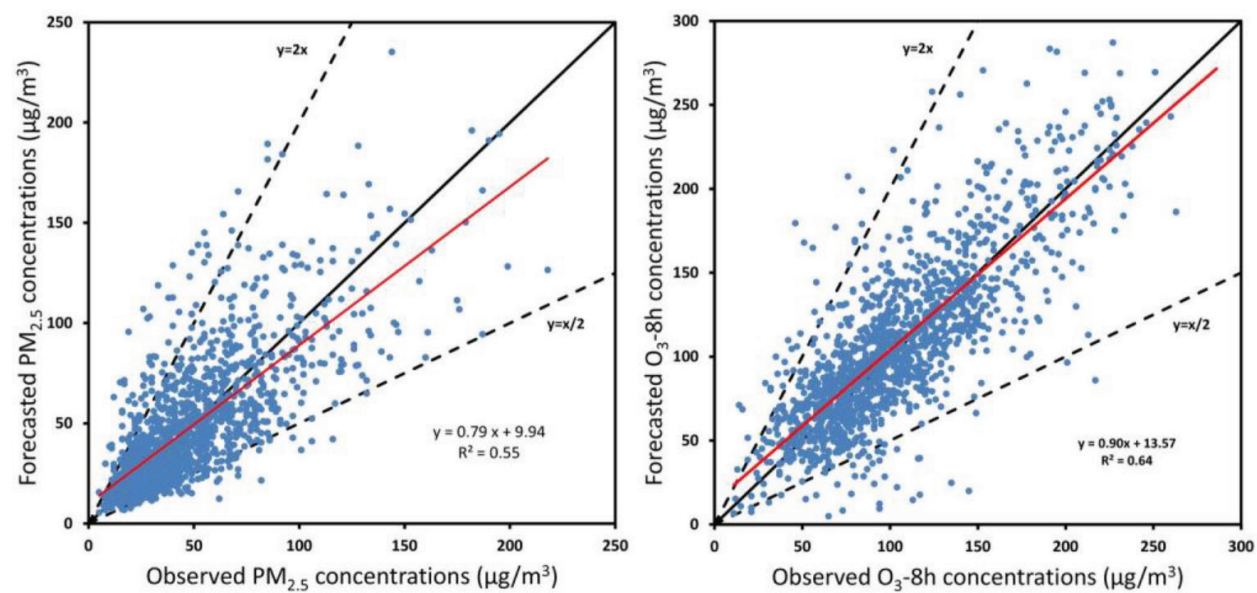


Figure 4. Scattering plot of 48-h forecasted and observed daily mean PM_{2.5} and O₃-8h for shanghai during 2014–2017.

The performances for different years were generally consistent for both PM_{2.5} and O₃-8h (Table 2). For example, the values of FAC2 were around 0.89 for PM_{2.5} and 0.93–0.97 for O₃-8h, respectively. RMSEs were within 20.8–23.9 µg/m³ for PM_{2.5} and 28.2–32.9 µg/m³ for O₃-8h, respectively. Correlation coefficients agreed well with each other. But MBs and NMBs had some difference. MBs showed that the concentration of PM_{2.5} was underestimated in 2014 and 2015 while overestimated in 2016 and 2017 although the biases were not very large. O₃-8h was underestimated in 2015 and overestimated in the other 3 years. NMBs for PM_{2.5} in 2017 and for O₃-8h in 2014 were relatively larger. In general, most statistical indicators for different years were comparable with each other.

To evaluate the capability of RAEMS on forecasting pollution, the categorical performance was calculated using the definition referenced in [20, 38] and the results are listed in Table 3. Only one heavy pollution for O₃-8h (>265) occurred and therefore it was not included in the analysis. The exceedance limits were set using the criterion values for lightly, moderately, and heavily (PM_{2.5} only) polluted level in the technical regulation of CNAAQS2012. The results

| | R | MB | RMSE | NMB (%) | FAC2 | R | MB | RMSE | NMB (%) | FAC2 |
|------|------|------|------|---------|------|------|------|------|---------|------|
| All | 0.74 | 0.1 | 22.3 | 8.1 | 0.89 | 0.80 | 3.5 | 30.6 | 7.2 | 0.95 |
| 2014 | 0.75 | −0.7 | 23.9 | 4.4 | 0.89 | 0.80 | 15.8 | 32.0 | 21.3 | 0.96 |
| 2015 | 0.78 | −5.6 | 22.5 | −2.3 | 0.89 | 0.81 | −6.5 | 30.0 | −1.4 | 0.94 |
| 2016 | 0.73 | 1.3 | 22.1 | 13.3 | 0.89 | 0.76 | 2.1 | 32.9 | 5.9 | 0.93 |
| 2017 | 0.75 | 5.3 | 20.8 | 17.2 | 0.88 | 0.86 | 2.8 | 28.2 | 3.2 | 0.97 |

Table 2. Summarized statistics of forecast performance of daily PM_{2.5} (left panel) and O₃-8h (right) for different forecast length (units: µg/m³ for MB and RMSE).

| Exceedance limit ($\mu\text{g}/\text{m}^3$) | 75 | 115 | 150 | 160 | 215 |
|---|------|------|------|------|------|
| Accuracy (%) | 87.2 | 95.0 | 98.5 | 91.5 | 97.0 |
| Probability of detection (%) | 63.5 | 44.1 | 40.0 | 75.3 | 67.5 |
| Missed detection rate (%) | 36.5 | 55.9 | 60.0 | 24.7 | 32.5 |
| False alarm rate (%) | 43.5 | 60.6 | 68.4 | 42.3 | 52.6 |
| Critical success index (CSI) | 0.43 | 0.26 | 0.21 | 0.49 | 0.39 |
| Bias | 1.12 | 1.12 | 1.3 | 1.31 | 1.43 |

Table 3. Categorical performance evaluated with different exceedance limits for $\text{PM}_{2.5}$ (left panel) and O_3 -8h (right).

showed that the forecast performance decreases with increased exceedance limits for both $\text{PM}_{2.5}$ and O_3 -8h. The values probability of detection and critical success index decrease with higher exceedance limit, while those of missed detection rate and false alarm rate increase. The biases are relatively steady and show slight over-estimation for $\text{PM}_{2.5}$ and some for O_3 -8h. An interesting result is found for accuracy that it tends to increase with higher exceedance limits. Further analysis showed that this result is ascribed to the big percentage of the records under limits.

In general, RAEMS makes good performance on forecasting the major air pollutants over eastern China region. It also provides reliable products to support and promote the work on environmental meteorology and positive effects on increasing the ability to serve the decision-making and the public.

4. Uncertainty in forecasting air quality

The previous studies also showed shortage and uncertainty in several aspects in simulating and forecasting air quality using numerical models, although great improvements were achieved. The outputs of air pollutant concentrations from numerical models are more or less different from the observations in most cases. In other words, the bias of prediction and observation is usually more than 10%. If the forecast performances well, the bias could be even less than 10% (e.g. in [20, 32, 38]). For the ratio modeled value within between half and twice of observation, good performance could be around 90% in this work, while 70–80% [38, 39] or lower [58] were more recorded. Moreover, the temporal variation of model always varies from that of observation. This can be represented in correlation coefficient or ozone peak time as one often focused issue. High correlation coefficients could be greater than 0.7 or even 0.8 (in this work and [32, 38]), usually 0.5 or 0.6 (in [20, 32, 38, 39]) or lower (in [36]). A certain percentage of forecasted ozone peak time was several hours different from observed [32, 38]. The third aspect is that model performance is generally inconsistent in space, in other words, it may perform very well over some areas but poorly over some other areas in the same simulation using the same model. This phenomenon of inconsistency existed in results of all work. The models are not as satisfied in polluted situations as in usual or clean conditions while pollution always

takes more attention in many regions. For example, RAEMS did not provide enough satisfied forecast for air pollution, especially heavy pollution for Shanghai shown in former sections as well as in [20, 38] which showed unsatisfied results for high ozone in US. The performance on predicting aerosol components was worse than that on the integrated mass concentration (e.g. $PM_{2.5}$ and PM_{10}) (e.g. in [19, 20, 32]). This concerns to visibility and haze related forecast, which leads to lower capability of models in forecasting visibility and haze events.

Major components which caused the uncertainty on numerical air quality modeling and forecasting could be classified into the several following issues. First of all, emission inventories are important as they were always mentioned in many previous studies [21, 32, 38, 41]. Emissions can be classified into natural emissions and anthropogenic emissions. Natural emissions are from respiration and photosynthesis of plants, sea spray, forest fire, volcano explosion, etc. Many sources of deviation could be included in the model calculation because it's impossible for modelers to know all of the details that can influence emission. For example, it is hard to obtain the fully accurate information on the growing states and types of plants, ambient conditions such as temperature, humidity, radiance, etc. in the region and duration to be forecasted or modeled. In forecasting, it is also difficult to know exactly when, where or even whether a forest fire or volcano explosion will occur or not. There are also many kinds of uncertainties in calculating the anthropogenic emissions. The inventory is always 2 or 3 years delayed and supplies the total amount of emission for 1 month or 1 year. In most situations, the diurnal variations used in the modeling are solid in time and space and cannot describe the tempo-spatial change due to actual activities of industry, traffic, etc. Another gap is that basic monitoring data is not sufficient enough for producing anthropogenic emission inventory in chemical species and spatial resolution, and therefore many approaches are implemented in developing inventories. At the same time, inventories are also sufficient enough for modeling, e.g. the number and types of chemical species and the height of each power plant.

The second uncertainty came from model representation. While developing a model, scientists always endeavored to balance the scientific understanding and the goal of extremely "perfect" performance. But in fact, a perfect model is always idealized and being sought. The understanding of the chemical processes formatting or depleting air pollutants, the physical processes that transport or disperse air pollutants, the ambient conditions that influence chemical reactions is advancing. Forecast models usually introduce relatively mature technologies and keep them suitable for most situations. New technology is always developing to study or solve problems and be implemented into forecast model when it is validated. So, air quality models were in progress in the past and there is still some shortage or uncertainty in "current" model. Concerning RAEMS, its core model was developed several years ago and some elements were not included which were confirmed to influence the performance. For example, aerosol direct forcing in solar radiation was not considered in the model, which leads to more solar radiative flux to the air near ground and to ground surface. This deficiency results in higher near surface wind speed, PBL height and stronger vertical diffusion and thus lower primary pollutants and $PM_{2.5}$ [21, 41]. This model missed some heterogeneous uptake of sulfate under high relative humidity conditions. For example, Wang et al. [14] and Cheng et al. [25] found a new source from reactive nitrogen chemistry in aerosol water, which explained the missing of sulfate and particle matter in extreme pollution conditions in northern China region.

Bias may come from the treatments and inputs of initial and lateral boundary conditions. Usually, input data for initial and boundary conditions includes biases comparing with “real” atmosphere and is coarser than regional air quality model. More on this issue in meteorological predictions can be found in the other chapters and chemical aspects are analyzed here. Specific to RAEMS, the inputted meteorological data is 0.5 degree and much coarser than the model resolution of 6-km. The interval of 6-h may also involve bias in calculating the tendency of meteorological variables. The treatment of lateral boundary conditions in chemistry using historic mean field may make them far from reality. The missing of assimilation on both meteorological and chemical variables produced initial bias. The impact of such missing on air pollutants may exist in several hours since the model start over strong emitting regions but last for a long time over downwind regions, as the effect of chemical assimilation can be kept within 12–24 h [59]. Better initial chemical conditions are strongly needed for nowcasting of air quality.

The uncertainty in meteorological variables could be another important source. It is known that meteorological variables are drivers of CTMs. Some of them drive the processes of advection, convection, dispersion, turbulent mixing, etc. Some of them participate in chemical reactions such as vapor or decide the reactivity rate. This chapter will not focus on this for much discussion, however, this uncertainty can be found in other chapters which concern meteorology prediction. But one point we should emphasize is that the uncertainty in forecast of weak weather conditions will be paid more attention to because heavy air pollution often occurs under such conditions, although weak conditions are not so focused in meteorology for less extreme weather occurring.

5. Work in the future

To improve the performance of numerical air quality forecast, several types of work are taken into consideration in the future. As one important application of numerical meteorological prediction and the role of meteorological variables driving CTMs, introduction of better numerical forecast of weather is always one economical and effective way to improve air quality forecast. This way should be carried out indubitably if it is feasible in technology.

Update in emission inventory and its implementation in CTMs is another core action. It includes several aspects: (1) reduction of time delay; (2) increase in horizontal and vertical resolution; (3) improving the accuracy of emission inventory itself; and (4) improving the applicability in models. The former three aspects mainly require efforts of inventory community and the last one needs efforts of modelers. Specifically, one job is to improve on-line calculated emissions, such as biogenic volatile organic compounds. For example, biogenic emissions can be calculated using model meteorological variables and some inputted static data in many current CTMs (e.g. WRF-Chem and CMAQ). Better vegetation data (classification, leaf area, etc.) will benefit improvements of biogenic emissions and they can be retrieved from satellite data nearly real time. The other is to build one fast technology to adjust the emission data inputted into forecast system. The determination of indicators which may be used to adjust the emission data will be the first step and then develop a relatively fast evaluation system or technology to supply the result how the forecast performed in previous duration.

Based on the evaluation results, a fast adjustment technology is to be implemented to update emissions used in the coming forecasts. Besides the regular treatments, fast response to emergency or temporary emission control needs to be prepared based on relatively less detailed information.

To fit the extending needs, numerical air quality forecast is increasing its capability on longer predictable period, finer resolution, and better service for other interests. Long time length and fine scale is the two main aims or requirements of coming air quality prediction besides higher accuracy. Long prediction of over 1 week has been urgently needed and required by decision-making agencies during recent years. Under the strong requirements on improving air quality, environment protection agencies over eastern China often carry out or be demanded to carry out temporary emission control to reduce air pollution. This action usually needs a few days ahead of predicted pollution episode. Another important need is on macro-management of industrial production, electric power, etc. for long-term objectives such as the level of annual mean air pollutant concentrations and the level of days of pollution. It requires climate scale prediction of air quality, such as monthly or seasonally. The other aim is finer forecast in space and time. For example, tasks of air quality forecast for a specific community or a specific time point were required, which were far beyond the capability of current forecast service 3 times a day for the entire Shanghai. Many other interests, such as human health service, also need the support of numerical air quality forecast. These needs require supporting information beyond forecast results to promote their own goals.

Comparing with that in meteorological prediction, treatment and approach in initial and boundary layer conditions is rough and ongoing. Assimilation on air quality related variables or chemical assimilation is needed to improve initial conditions and forecast performance, especially in nowcasting of air quality. Of course, chemical assimilation is more difficult than meteorological assimilation due to insufficient monitoring data. Implementation of real time global forecast in boundary is another way to reduce bias from lateral input out of the model domain. This treatment will greatly benefit the forecasts near model lateral boundary and of long-term period.

Improvement in representation of CTMs such as involving the feedback and interaction between meteorological variables and air pollutants is one persistent work. This work will provide better models for numerical air quality forecast and is essential for improving model performance. But it depends on scientific understanding and technological maturity. Some nowadays jobs could focus on increasing model performance on near-surface wind, vertical diffusion of particles, aerosol species, and diurnal variation in operational forecast. We should show more desire to involve new technology into forecast system in the future.

6. Conclusion

Air pollution is focused because of its adverse effects, e.g. on human health. Numerous works were taken into action including scientific study, policy making, and emission control, etc. over eastern China due to the severe situation as one of the most polluted areas. This chapter illustrated the numerical forecast of air quality over the eastern China region, especially what has been done in Shanghai Meteorological Service.

Numerical air quality forecast has become truly profiting from the achievements on air quality models and computation technology during past decades. Three-dimensional chemical transport models were the major choice in studying and predicting air quality in both global and regional scale after entering the twenty-first century. In very recent years, online approach CTMs, which calculate meteorological and chemical variables in one model, prevent from the loss of information between two meteorological outputs, and benefit involving the interaction between meteorology and air pollution. The fully online coupled WRF-Chem was chosen to develop the Regional Atmospheric Environmental Modeling System for eastern China by SMS for its good performance in modeling the air quality/pollution over this region.

The operational RAEMS was certified by China Meteorological Administration in March 2013 and has been providing numerical forecast data and products from then on. This forecasts greatly promoted the air quality prediction, air pollution warning, and decision-making service in meteorological agencies as well as environmental protection agencies. A previous detailed evaluation validated the performance on forecasting the spatial distribution and temporal variation of major air pollutants over eastern China region during the 2 years of 2014–2015 [38]. For the two most important air pollutants of $PM_{2.5}$ and O_3 -8h for the city of Shanghai, RAEMS had excellent performance during 2014–2017 as analyzed in this chapter. At the same time, RAEMS showed relatively lower accuracy under polluted conditions than unpolluted conditions, and it even performed worse under heavier polluted conditions.

Further analysis showed that shortage or uncertainty in current numerical air quality forecast mainly came from four aspects of emission inventory or emission related inputs, model capability in chemical representation, biases in initial and lateral boundary layer conditions, and uncertainty in meteorological variables. These suggested ideas for improving performance of forecasts in the future. Longer predictable period and finer temporal and spatial resolution is also important goal and challenge for fitting the extending needs from application communities.

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Conflict of interest

The authors declared that they have no conflicts of interest to this work.

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