Application of an Adaptive Nudging Scheme in Air Quality Forecasting in China

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Submitted to

Journal of Applied Meteorology and Climatology

July 31, 2007

Revised January 8, 2008

ABSTRACT

A major challenge for air quality forecasters is to reduce the uncertainty of air pollution emission inventory. Error in the emission data is a primary source of error in air quality forecasts, much like the effect of error in the initial condition on the accuracy of weather forecasting. Data assimilation has been widely used to improve weather forecasting by correcting the initial conditions with weather observations. Similarly, observed concentrations of air pollutants can be used to correct the errors in the emission data. In this study, a new method is developed for estimating air pollution emissions based on a Newtonian relaxation and nudging technique. Case studies for the period of August 1-25, 2006 in 47 cities in China indicate that the nudging technique resulted in improved estimations of SO_2 and NO_2 emissions in majority of these cities. Predictions of SO_2 and NO_2 concentrations in January, April, August, and October using the emission estimations derived from the nudging technique showed remarkable improvements over those based on the original emission data.

Key words: Nudging, air pollution, emission, data assimilation, inverse modeling, Olympic game.

1. Introduction

As the date for the 2008 Olympic Summer Games approaches, one of the biggest issues facing the game's organizers is accurately forecasting the air quality in the host city, Beijing, China. Forecasters at Beijing Meteorological Bureau will rely on coupled numerical weather prediction (NWP) and atmospheric chemistry models, such as MODELS-3 (Dennis et al. 1996), a widely used operational air quality forecast system developed by the United States Environmental Protection Agency (EPA), to accomplish their task. MODELS-3 consists of three components: 1) a regional NWP model, 2) an air pollution source initialization model, and 3) a multi-scale atmospheric chemistry model (Community Multi-scale Air Quality Model or CMAQ). The modeling system has demonstrated skill in simulating and forecasting air quality at local, city, regional and continental scales in the United States (Byun 1999a,b). However, the forecast accuracy depends critically upon the accuracy of pollution emission inventory that the model uses as input. Thus, obtaining an accurate air pollution emission inventory is a prerequisite for improving air quality forecasts.

The results from the Beijing City Air Pollution Observation Experiment (BECAPEX) (Xu et al. 2003) showed that air pollution emissions change seasonally in Beijing and differed significantly from the annual values estimated by Streets and Waldhoff (2000). For example, SO_2 emission during winter heating periods is often twice as large as that observed during the summer. Thus, it is prudent that more accurate estimates of emissions which take into account their seasonal variability be used to initialize air quality forecast models. However, neither up-to-date nor seasonally-dependent emission inventory is available in China. Therefore, in order to depict the seasonal variability of emissions, inversely estimating the emissions prior to the forecast period is the only option.

Previous studies have demonstrated the effectiveness of using various inverse modeling methods to obtain the spatial distribution of pollution emissions, as well as to improve the forecast skill of air quality models (e.g., Hartley and Prinn 1993; Yienger and Levy 1995; Reich et al. 1999; Guenther et al. 1995, 1999; Bergamaschi et al. 2000; Bousquet et al. 1999; Hein et al. 1997; Houwelin et al. 1999; Martin et al. 2002). Inverse modeling of pollution emissions has also been used in air quality modeling in China. Zhu et al. (2002) applied a generic algorithm to inversely compute the emissions from point sources. Li et al. (2003) developed a simple two-dimensional dispersion model to invert the sources and sinks of atmospheric CO_2. Liu et al. (2005) proposed an optimization theory for selecting the sites of pollutant-emitting factories with a goal to minimize the impact of air pollution. Xu et al. (2005) combined dynamical and statistical approaches to improve air quality forecasts by correcting the bias of model forecasts statistically. However, the effectiveness of using an inverse modeling approach to correct the emissions in an entire forecast domain and then use the corrected emissions to improve the air quality forecast at a regional domain has not being quantified in China.

The purpose of this study is to demonstrate the effectiveness and value of correcting the error in emission inventory using a nudging-based inverse modeling approach. The nudging scheme is constructed by adding an array of adjustable “nudging terms” to the forecast equation to minimize the differences between the predicted and the observed values of air pollution concentration.

2. Description of Modeling System, Nudging Method and Data

2.1 Model Description

The multi-scale air quality forecasting system is comprised of the CMAQ air quality model, MM5 mesoscale weather forecast model and an inverse modeling scheme based on a four-dimensional data assimilation (FDDA) nudging scheme. CMAQ is the core of the air quality forecasting system, Models-3, developed by the U.S. Environment Protection Agency. In this study, the air quality forecasting system is configured for the China domain as illustrated in Figure 1. The MM5 mesoscale weather forecast model is configured for the larger domain (16° – 50°N, 70° – 135° E), whereas the CMAQ model is configured for the slightly smaller domain (17° – 49° N, 71° – 134° E) within the MM5 domain. The use of a smaller domain for CMAQ is for the purpose of reducing the impact of the lateral boundary condition on the air quality forecast. The horizontal resolution for both domains is set to a uniform 36 km grid size in both x and y directions. In the vertical direction, a non-uniform 13 level terrain-following sigma coordinate is used in CMAQ. Higher resolution is used near the lower boundary, with half the grids set within the lowest 2 km to better resolve the boundary layer processes. MM5 uses 27 levels with the top level at about 17km. Again, higher resolution is used within the lowest 2 km to better describe the boundary layer processes.

2.2 Data

The lateral boundary conditions and initial conditions for the weather forecast model (MM5) are derived from the reanalysis data from the operational weather forecast model of the National Meteorology Center of China Meteorological Administration. The data covers 31 vertical levels on 0.5625° x 0.5625° horizontal grids and the forecasts are updated every 6 hours. Nudging of meteorological data from 2500 surface weather stations and 300 upper air stations occurs twice daily at 08:00 and 20:00 Beijing local time.

The performance of the MM5 for the study region was evaluated by Xu et al. (2005). In their study, MM5 was run for the period of September 2004 through March 2005. Meteorological variables including surface and upper air temperature, humidity and wind fields simulated by MM5 were validated against observations from 2500 surface weather stations and 300 upper air stations. Xu et al. (2005) concluded that the meteorological variables simulated by the MM5 are reliable for driving air quality forecast models in the study region. Separately, Beijing Meteorological Bureau has carried out a mandated evaluation of the MM5 model before it was adopted for routine operational weather and air quality forecasting.

The emission inventory used to initialize the CMAQ model is from Streets et al. (2003), which describes the emissions in Asia for the year 2000. It is interpolated into the 36 km x 36 km CMAQ domain as shown in Fig. 1. This data set will be referred to as S2000 hereafter.

For model validation, two sources of datasets were used. The first is the pollution emissions and daily mean pollutant concentration observations from 47 surface monitoring stations across China as published by China Statistics Press (China Environment Year Book, 2004). This dataset will be referred to as China2004 hereafter. The second is the 2004 update of S2000 (personal communication). It will be referred to as S2004 hereafter.

In all calculations, CB-IV (Carbon Bond Mechanism version 4.0) is chosen as the chemical mechanism in CMAQ. Air quality nudging procedure is applied to selected fair weather dates prior to the validation periods as shown in Table 1. For example, for the forecast period of 8/1 – 8/25/2006, which represents the summer condition, nudging is applied for July 20 and 21, 2006. Similar procedure is used to produce the air quality forecasts for January, April, and October, 2006, representing winter, spring, and fall conditions, respectively. Note that except for August for which forecasts were for 25 days due to the lack of observations for August 26-31, full month forecasts were made for January, April and October.

2.2 Nudging Technique

The general form of a Newtonian relaxation nudging scheme can be expressed as

$$\frac{\partial \boldsymbol{\alpha}}{\partial \boldsymbol{t}} = \boldsymbol{F(\alpha, x, t)} + \boldsymbol{N} \tag{1}$$

where α is the array of variables to be predicted, ***F*** denotes the array of the forcing function, ***x*** for spatial dimensions, *t* for time, and ***N*** for the "nudging term". For the concentration of air quality parameter *P*, (1) can be rewritten as

$$\frac{\partial P_n}{\partial t} = F\left(P_n, x, t\right) + N(P_n, P^*, Q_n) \tag{2}$$

where subscript *n* indicates the number of iterations in the nudging process, P^* is the observed concentration, and Q_n is the estimated emission value after *n* iterations. Nudging can be carried out for multiple air quality parameters simultaneously. For *m* species of pollutants, the emissions at iteration *n+1* (Q_{1n+1}, Q_{2n+1}, …, Q_{mn+1}), can be estimated through the following array of nudging equations:

$$\begin{pmatrix} Q_{1n+1} \\ Q_{2n+1} \\ \vdots \\ Q_{Mn+1} \end{pmatrix} = \begin{pmatrix} Q_{1n} \\ Q_{2n} \\ \vdots \\ Q_{Mn} \end{pmatrix} \begin{pmatrix} \dfrac{P_1^* - \beta_1 (P_{1n} - P_{1n-1})}{P_{1n}} \\ \dfrac{P_2^* - \beta_2 (P_{2n} - P_{2n-1})}{P_{2n}} \\ \vdots \\ \dfrac{P_M^* - \beta_M (P_{Mn} - P_{Mn-1})}{P_{Mn}} \end{pmatrix} \qquad \text{n=1, 2, 3, …} \tag{3}$$

where P_{mn} is the concentration of the m^{th} pollutant at the n_{th} iteration, and β is the empirical nudging coefficients which are positive if $P_m^* > P_{mn,}$ and negative if $P_m^* < P_{mn}$.

The CMAQ model is used to compute the first guess field of P_{m1} from the original emission data Q_{m1} derived from S2000. The predicted concentration is used together with the observed concentration to derive the corrected emission estimation Q_{m2} through the iteration process described in (3). The new emission estimation is then used to predict the concentration P_{m2} using CMAQ. Next, P_{m1} and P_{m2} are used to estimate Q_{m3} using (3), and so on until a convergence is reached. This iterative scheme is referred to as "adaptive nudging" hereafter.

3. **Results**

In this section, we describe the results from twin SO_2 and NO_2 concentration forecasting experiments, one uses the nudging scheme described in Section 2 (referred to as the Nudging Experiment), and the other without nudging (referred to as the Control Experiment). The case used in this study is for the period of August 1-25, 2006. This period was chosen because it is approximately the same period for the Beijing Olympic Game in 2008, and the weather during this period was mostly stable. For the Nudging Experiment, observed SO_2 and NO_2 concentrations at 47 urban observing stations in China from July 20 and 21, 2006 (fair weather days) were used to correct the emissions through the iterative nudging process described in Section 2. For the Control Experiment, the original emission data (S2000) was used without correction.

3.1 Improvements in SO_2 and NO_2 concentration forecasts for August 1-25, 2006

Figures 2a,b show the comparison of the August 1-25 mean SO_2 and NO_2 Air Pollution Index (API) values among the Control Experiment, Nudging Experiment, and the observations. API is a classification of air pollution severity according to the concentration of air pollutants. The China National API values for urban area are described in Table 2 (Fan 1998). Larger API values correspond to more severe air pollution conditions.

The simulated API values of SO_2 and NO_2 are shown in Figure 2, where Panel a) depicts the SO_2 API index, and b) for the NO_2 API index. The API indexes are computed for 47 cities across China. It is obvious that the NO_2 and SO_2 API values from the Nudging Experiment (gray) are much closer to the observations (blue) than those from the Control Experiment (white) in nearly all cities. The forecasts from August 1-25 for all 47 cities (a total of 1122 forecast samples) from the Nudging Experiment are statistically similar to the observations as shown in Figures 3a and b. The R^2 values between the observed API values and those from the Nudging Experiment is 0.44 for SO_2 and 0.43 for NO_2, both exceeded the 99% significance level. In contrast, the R^2 values between the observations and the API indexes from the Control Experiment were only 0.026 for SO_2 and 0.055 for NO_2, neither passed the 90% significance test. Thus, it is evident that the Nudging Experiment showed remarkable improvement over the Control Experiment for both the SO_2 and the NO_2 forecasts.

The advantage of using "air quality nudging" is also evident when validated for different regions. Table 3 lists the differences between the average forecast API and that of the observed API in seven regions in China. It is shown that for all seven regions in China, the Nudging Experiment showed significant improvement in forecasting SO_2 and NO_2 API values, with error reductions ranging from 54% to 71% for NO_2 and 27% to 74% for SO_2.

3.2 Nudging-derived SO_2 and NO_2 emissions based on July 2006 SO_2 and NO_2 concentrations

The error reductions in SO_2 and NO_2 forecasts from the nudging experiment can presumably be attributed to the improvements made to the SO_2 and NO_2 emissions by nudging their simulated values toward the observed SO_2 and NO_2 concentrations. In this section, the changes of SO_2 and NO_2 emissions resulted from the nudging procedure will be analyzed. Because the Chinese government only publishes annual SO_2 emissions, emissions for NO_2 need to be derived from other sources. In this study, the S2004 NOx emissions will be used as the "observations".

The comparison between the derived NO_x emissions using the nudging procedure described in Section 2 and the 2004 "observations" of NO_x emissions (S2004) is shown in Figure 4. It is evident that the nudging procedure is clearly effective in improving the NO_x emissions. For example, on average, the difference between the S2000 and S2004 is 36%, the nudging procedure reduced the difference to approximately 10% on average, achieving an average improvement of 72%. In other words, if one does not have S2004, the nudging procedure employed here effectively led to an "update" of S2000 that is within 10% of the S2004 values.

For SO_2 emissions, the comparison between China2004 and the derived emissions is shown in Figure 5. The difference between the emissions derived by the nudging procedure using July 20-21, 2006 SO_2 concentration and the China2004 SO_2 emissions (white bars) is substantially smaller than that between the S2000 SO_2 emissions and China2004 (dark bars) at nearly all SO_2 emission data locations.

$$\begin{pmatrix} R_A \\ \\ R_B \end{pmatrix} = \begin{pmatrix} \dfrac{|EM_A - EM_G|}{EM_G} \\ \\ \dfrac{|EM_B - EM_G|}{EM_G} \end{pmatrix} \tag{3}$$

where *EMA* represents S2000 emissions, *EMB* the estimated emissions using July 20 and 21, 2006 observed concentrations and meteorology data, *EMG* the emissions published by the Chinese government (China2004), *RA* the percent departure between S2000 and China2004, and *RB* the percent departure between the derived emissions through the nudging procedure and China2004.

For the 47 air quality monitoring stations across China, *RB* is smaller than *RA* at majority (82.6%) of the stations. On average, *RA* (0.96) is almost twice as large as RB (0.49). Thus, if China2004 is considered more accurate than S2000, then it is evident that the nudging procedure is effective in substantially reducing the emission error for the majority of the 47 cities across China, and the average error reduction is approximately 50%.

3.3 Forecasting the seasonal values of SO_2 and NO_2 concentrations

To further quantify the effectiveness of nudging on the air quality forecasts in China, over 4000 data samples of NO_2 and SO_2 concentrations taken in 4 months (January, April, August and October) at 47 air quality monitoring stations across China and their corresponding forecast values are compared statistically. Figure 6 shows the correlation coefficients (R) between the data and the forecasts from the experiments without nudging (white bars) and those with nudging (dark bars). It is evident that in all seasons, nudging led to significant improvements in the correlation between the forecasts and the data for both NO_2 and SO_2.

For the four seasons in 2006, the observed SO_2 concentrations are more closely correlated with the forecasts using the derived emissions (R=0.44) than the forecasts using the original S2000 emissions (R=0.23). This is also true for NO_2, with correlation coefficients of 0.49 (for forecasts using the derived emissions) and 0.19 (for forecasts using the original 2000 emissions) (Fig. 6). Thus, one can conclude that the nudging procedure devised in this study is effective in reducing the SO_2 and NO_2 forecast error in all seasons.

4. Conclusions

Current three-dimensional dynamic air quality modeling and forecasting in China rely primarily on the use of an outdated air pollution emission inventory S2000. In this study, we demonstrated that by incorporating an adaptive nudging scheme into the CMAQ-based air quality forecast system, the error field in the emission data can be reduced effectively through an inverse modeling procedure using observed air pollution levels, and the improved emissions can further lead to significant improvement in air quality forecasts in all seasons.

A set of simulations and hindcasts for SO_2 and NO_2 API values for January, April, August and October, 2006 were carried out to quantify the effectiveness of the nudging scheme. The experiment for August 2006 is used to quantify the effectiveness of nudging in improving the estimation of emission sources. The emissions of SO_2 in 47 cities in China were actual SO_2 emission observations are available have been computed inversely using S2000 as the first guest field of the emissions and real-time SO_2 and NO_2 concentrations observed in late July 2006 to correct the first guest field. The experiments showed that the derived emissions are in better agreement with the corresponding observations than the original S2000 emissions, indicating that the nudging procedure was effective in reducing the error in the original emission inventory. The model results also show that using the derived emissions of SO_2 and NO_2 led to significant improvement in the forecasts of SO_2 and NO_2 concentrations.

An implication of the results presented above is that since air pollution emissions are quite uncertain in China, one should avoid using uncorrected emissions, such as S2000 in air quality forecasting. Using the observations of pollutant concentrations prior to the forecast period to correct the emission data shows a great promise for improving air pollution forecasts.

Finally, it should be noted that air quality forecast error can originate from multiple sources. Error in emission inventory is only one of several potential causes of forecast error. For example, error in meteorological forecasts and inaccuracy in the description of atmospheric chemistry in the model can all lead to air quality forecast error. Correcting the error field in the emissions represents only one of several approaches to improve emissions and air quality forecasts.

Acknowledgements This work is supported by the national key basic research plan (No. TG1999045700) and the key project of international cooperation in science and technology of the China Science and Technology Ministry (No. 2004DFA06100) and the national key research plan of National Natural Science Foundation of China (No. 90502003).

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Table 1. Description of Nudging Experiments

Experiment Cases	Period of Nudging	Period of Forecast	Correlation (r) with observations		Correlation (r) with observations	
			SO_2_cmaq	SO_2_NF	NO_2_cmaq	NO_2_NF
Winter	Dec. 14-15,2005	Jan. 1-31, 2006	0.34	0.43	0.15	0.37
Spring	Mar. 1-2,2006	Apr. 1-30, 2006	0.28	0.48	0.21	0.55
Summer	Jul. 20-21,2006	Aug. 1-25, 2006	0.13	0.39	0.24	0.48
Fall	Sept. 14-15,2006	Oct. 1-31, 2006	0.18	0.47	0.18	0.58

Table 2. API and Corresponding Concentration of Pollutants

API Levels	Pollutant Concentration（μg/m^3）				
API	SO_2	NO_2	PM_{10}	CO	O_3
50	0.050	0.080	0.050	5	0.120
100	0.150	0.120	0.150	10	0.200
200	0.800	0.280	0.350	60	0.400
300	1.600	0.565	0.420	90	0.800
400	2.100	0.750	0.500	120	1.000
500	2.620	0.940	0.600	150	1.200

Table 3 Comparison of NO_2 and SO_2 API index differences between Nudging Forecast (NF), observations (OBS) and CMAQ control experiments (CMAQ) from August 1-25, 2006.

Region	NO_2_cmaq —NO_2_obs	NO_2_NF-NO_2_obs	% Error Reduction	SO_2_cmaq-SO_2_obs	SO_2_NF-SO_2_obs	% Error Reduction
NE	-18	-8	56%	-11	-8	27%
N	-13	-6	54%	-14	-8	43%
E	-11	-5	55%	-16	-8	50%
S	-14	-4	71%	-23	-8	65%
C	-16	-6	63%	-35	-17	51%
NW	-17	-5	71%	-23	-6	74%
SW	-18	-8	56%	-41	-15	63%
Average	-15	-6	60%	-23	-10	55%

Figure Captions:

Figure 1. Study area. The outer domain depicts the simulation area for the meteorological variables using Mesoscale Model 5 (MM5). The inner domain depicts the area for the air quality (CMAQ) model.

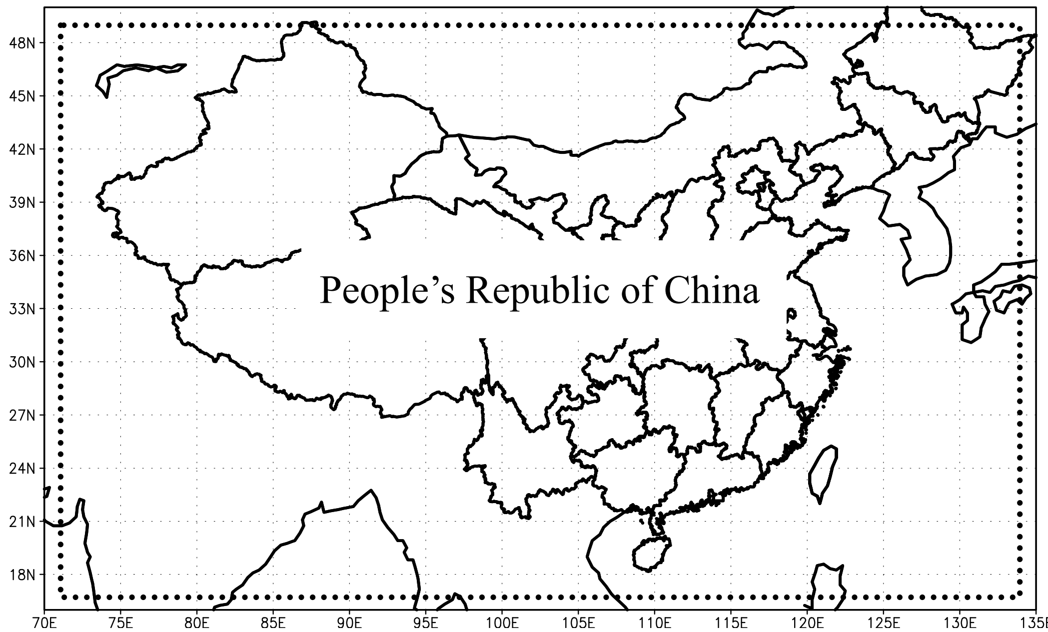
Figure 2. Comparison of the August 1-25 mean SO_2 and NO_2 API values among the Control Experiment, Nudging Experiment, and the observations. a) For SO_2 API index, and b) For NO_2 API index. The API indexes are computed for all 47 cities as shown in the figure. It is obvious that the NO_2 and the SO_2 API values from the Nudging Experiment (light shade) are closer to the observations (dark shade) than from the Control Experiment (white) in nearly all cities.

Figure 3. Scatter plots of the forecast data and the observed data from August 1-25 for all 47 cities (a total of 1122 forecast samples) from the nudging experiment. a) For SO_2 API values; b) For NO_2 API values.

Figure 4. NO_x emission inventory "error" measured in term of the percentage departure from the S2004 NO_x inventory. White bar is for the "error" of S2000 NO_x emission; Black is for the error of the derived emission using the nudging procedure.

Figure 5 Deviation ratio between the derived emissions and S2000 with respect to China2004 emissions. □ R_A: Deviation ratio between S2000 and China2004. ■ R_B: Deviation ratio between the derived emissions and China2004.

Figure 6. Seasonal change of correlation coefficients between forecast NO_2 and SO_2 values and corresponding observed concentrations. □ R_{cmaq}: Correlation coefficient for forecasts using S2000; ■ R_{NE} : Correlation coefficient for forecasts using the derived emissions.



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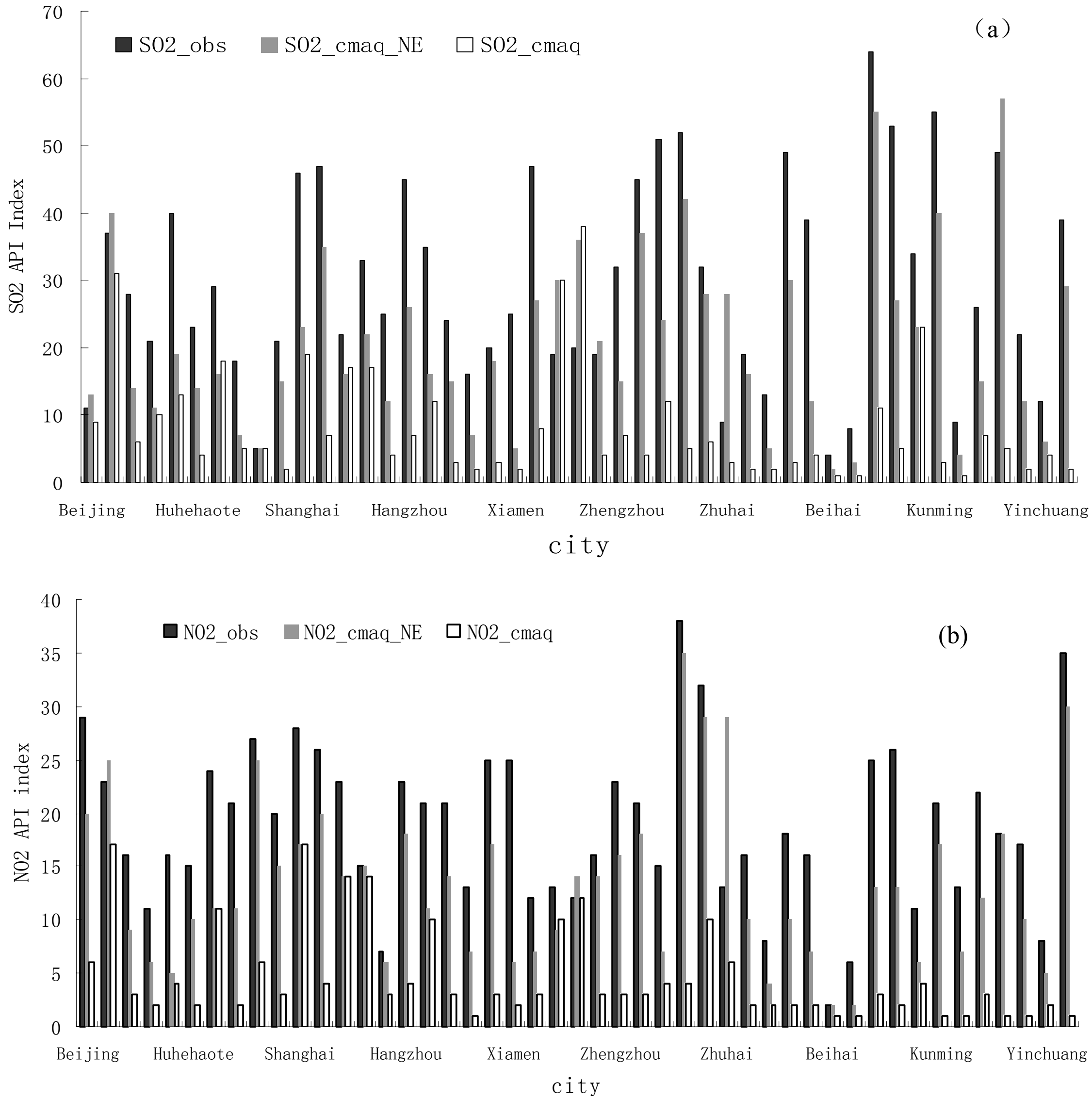

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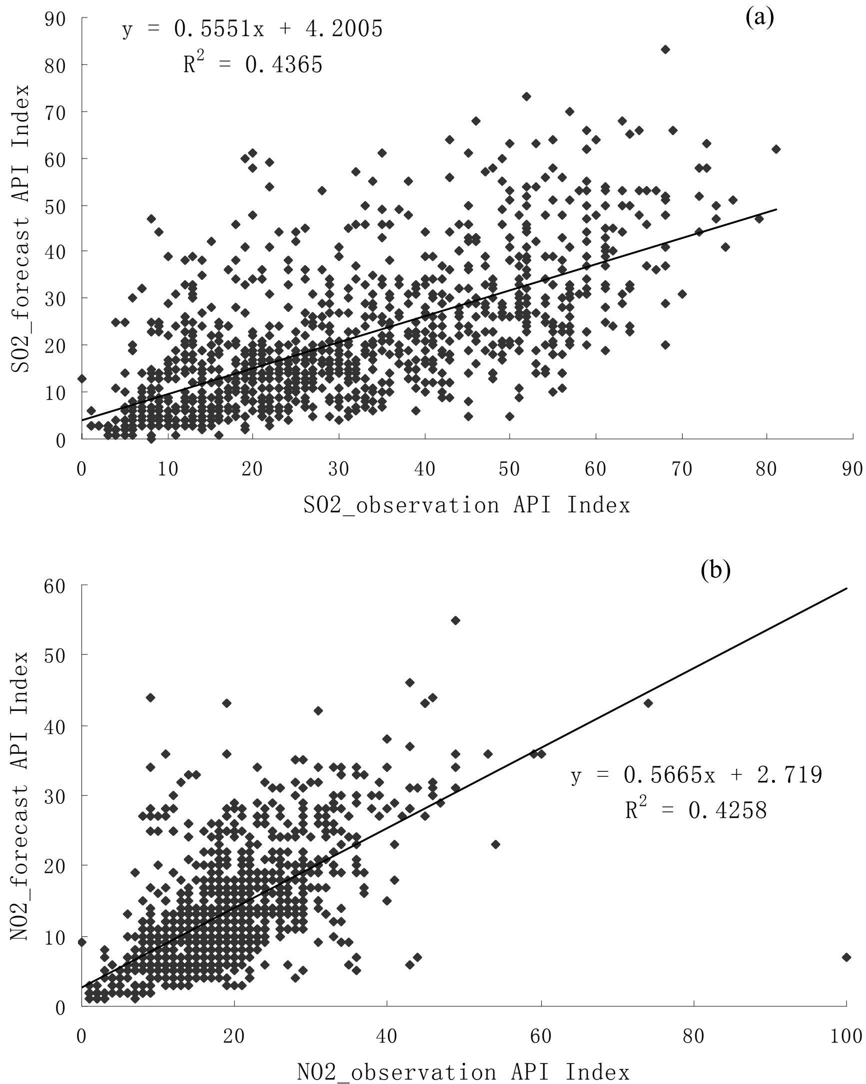

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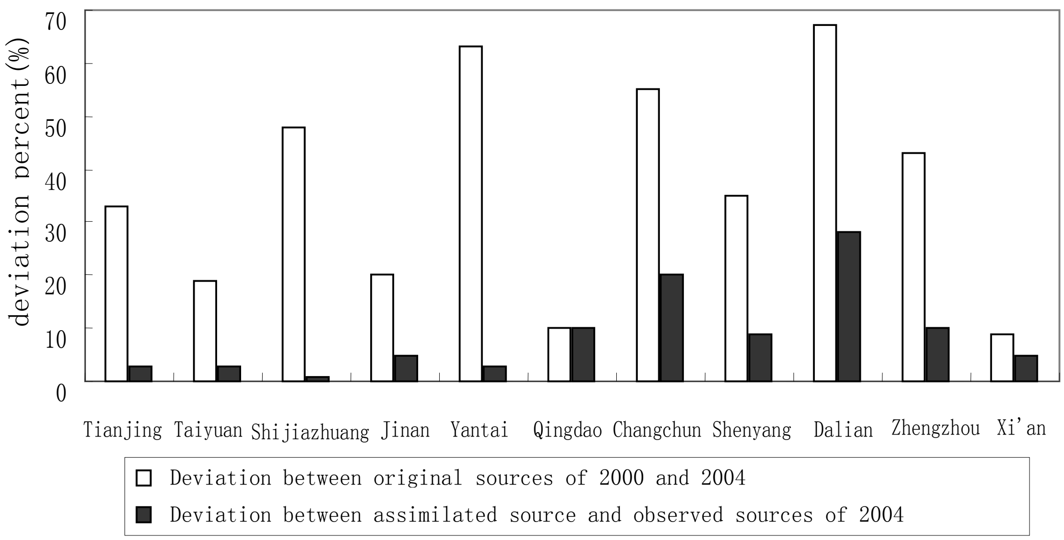

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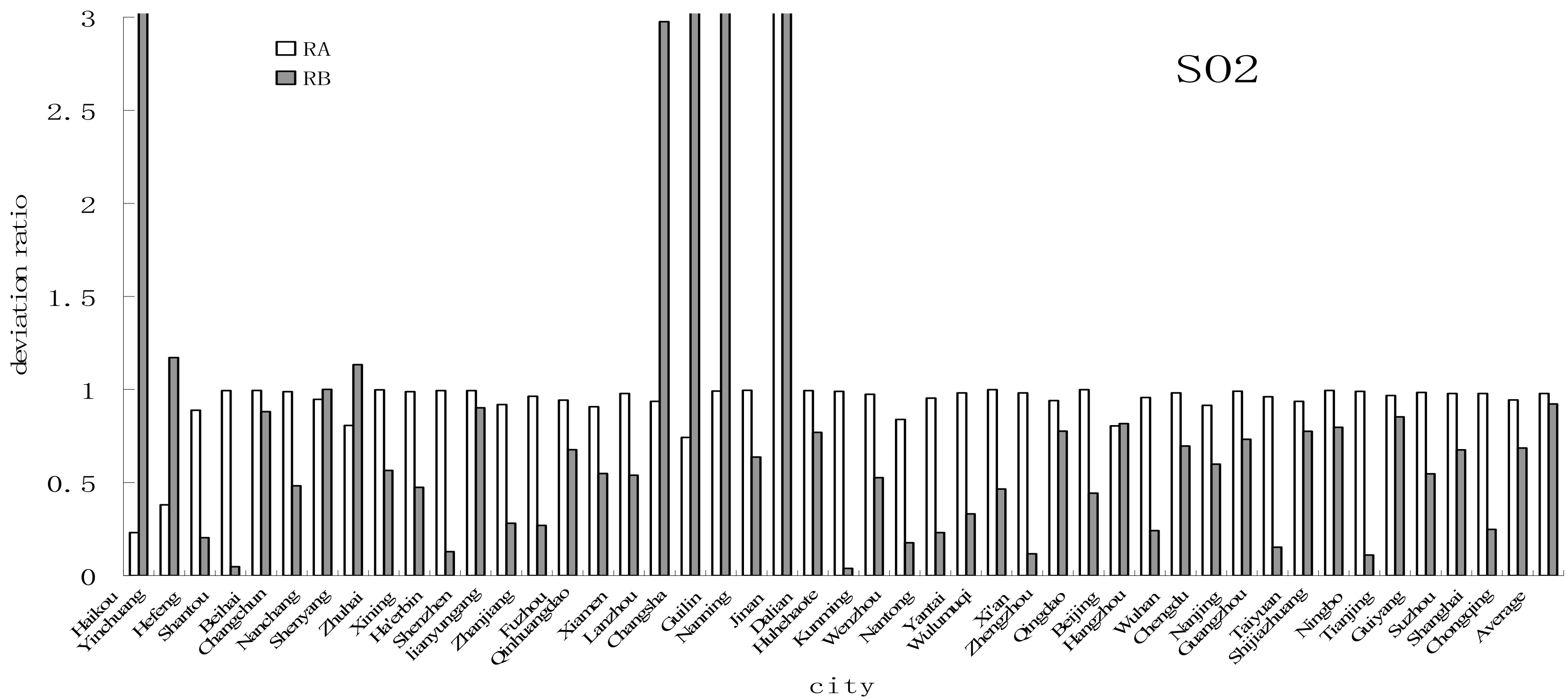

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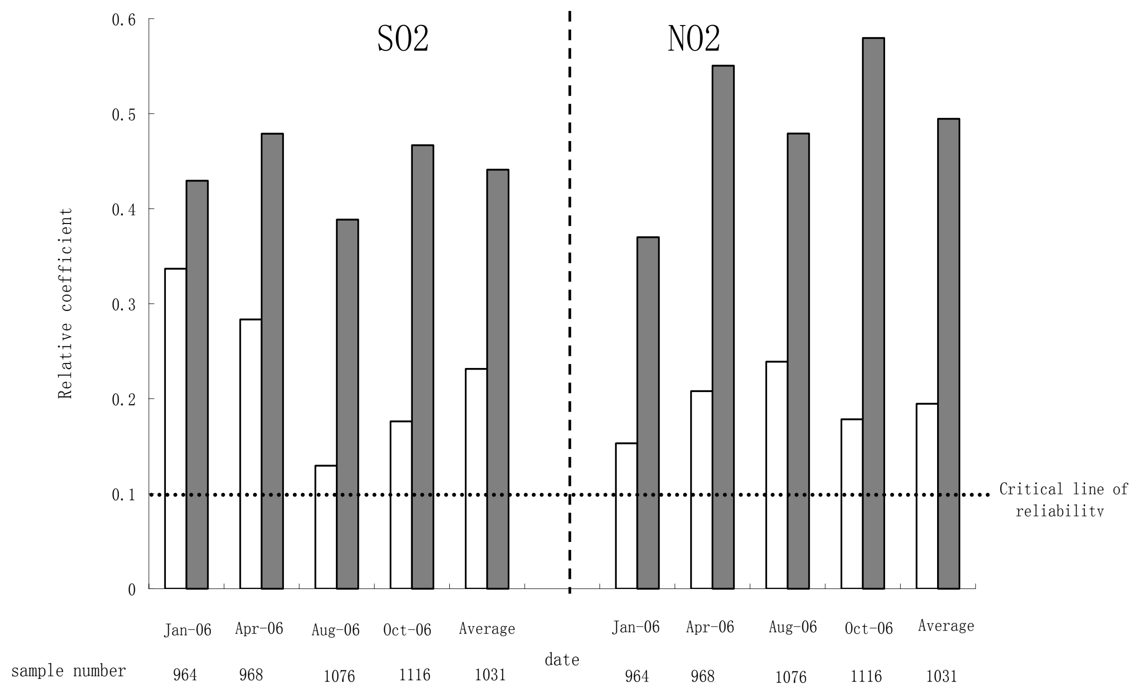

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