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AN AIR POLLUTION PREDICTION TECHNIQUE FOR URBAN DISTRICTS BASED ON MESO-SCALE NUMERICAL MODEL

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ABSTRACT: Taking Shenzhen city as an example, the statistical and physical relationship between the density of pollutants and various atmospheric parameters are analyzed in detail, and a space-partitioned city air pollution potential prediction scheme is established based on it. The scheme considers quantitatively more than ten factors at the surface and planetary boundary layer (PBL), especially the effects of anisotropy of geographical environment, and treats wind direction as an independent impact factor. While the scheme treats the prediction equation respectively for different pollutants according to their differences in dilute properties, it considers as well the possible differences in dilute properties at different districts of the city under the same atmospheric condition, treating predictions respectively for different districts. Finally, the temporally and spatially high resolution predictions for the atmospheric factors are made with a high resolution numerical model, and further the space-partitioned and time-variational city pollution potential predictions are made. The scheme is objective and quantitative, and with clear physical meaning, so it is suitable to use in making high resolution air pollution predictions.

Key words: city air pollution; potential prediction; district-partition; numerical model

1 INTRODUCTION

Since the 1930's, urban air pollution has caused increasing concerns across the world [1]. Various pollution prediction techniques have been put into use in the 1970's and significant results have been achieved^[2]. Air quality prediction has been operational over recent years in many parts of China owing to cooperation between meteorological and environmental protection departments [3-9]. The prediction is conducted via either numerical model, potential or stochastic approaches. Due to existing restraints of intensity of discharging sources, temporal and spatial density and accuracy of pollutants concentration watch, prediction directly using numerical models do not give accurate levels of pollution. With the current condition in China, potential prediction is still necessary and useful. Past insufficiency in data and model condition lead to coarse schemes for potential prediction, for they fail to differentiate pollutants, ignore the differences between parts of the city, taking no detailed account of diurnal variation of pollution potential nor linkages between meteorological parameters and pollutants concentration, etc. It is then impossible to make potential prediction that is more detailed and accurate than it is now unless other sophisticated means are employed to improve the physical content, objective quantity and temporal and spatial resolution to meet developmental needs. It is difficult to meet the needs if only conventional meteorological observation and forecast are used, because there are quite a large number of atmospheric processes (parameters) governing the dissipation and dilution of pollutants. It is just an area where general systems for potential prediction encounter their most difficulty. With physical and detailed statistic analysis of the relation between pollution

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concentration and meteorological parameters, the current study uses a sophisticated mesoscale to predict atmospheric parameters with high resolution in time and space, in which dynamic processes are introduced to potential prediction, to make objective, quantitative forecast that is district-partitioned and period-divided. Guangdong (in which Shenzhen sits) is a region that is densely populated with concentrated emission of industrial (including traffic) pollutants. It is why Shenzhen is taken to illustrate the technique.

2 DATA AND METHODS

According to a large number of previous studies, factors that play a major role in the potential pollution on the city scale include wind direction / speed, wind profiles, atmospheric stability, thickness of the mixing layer, precipitation, terrain and solar radiation, etc. It is then decided that the following types of data will be used in the work. They are the surface meteorological observations at the Shenzhen station, sounding data at the Hong Kong site (including mandatory and significant levels), and observed diurnal mean pollution concentration in Shenzhen, for the whole year of 1997. There are three pollutants in the observation, NOx, SO₂ and TSP. There are six sites of observation at the Lizhi Park, Hong Hu, Nan Hu Primary School, Nan Hai Oil, Lixiang Middle School and Huaqiao Cheng Primary School. The former three sites are within urban districts and the latter three suburban districts, the mean of which to represent respective concentration. The mean for all six sites stands for the mean concentration of the whole city. The number of days in which observations are sampled is 147 for NOx and SO₂ and 101 for TSP.

Data Merging from mandatory layers and significance layers (temperature and wind treated separately)

Intensity estimates of city heat-island effects (including diurnal variation)

Values of *Hm* are determined for individual time levels using *TM* and *TN* and data at 00Z and 12Z (hourly model predictions)

Vertical mean of individual parameters (including wind direction / speed, humidity) are determined for the *Hm* layer

Fig.1 Working flow for atmospheric parameters derivation. *TM*, *TN* and *Hm* are the maximum, minimum temperature and thickness of mixing layer.

Fig.1 gives the flow in which atmospheric parameters are sought. First of all, the mixing layer thickness (*Hm*) is determined. Requiring high accuracy, failures of potential prediction may be caused if its errors are more than 200 m. The following remedies are therefore adopted to ensure the quality. (1) A method conjoining data from both mandatory and significant levels is used for temperature and wind separately to nudge the vertical resolution to required accuracy. (2) To control the accuracy estimates of urban heat-island effect, the following empirical expression is used based on summaries on past experience in observation and research:

$$DT(t) = (A + B(t) \bullet (1 - A)) \bullet DDT \tag{1}$$

in which DT(t) is the intensity of heat-island effect at the time t and A is an adjusting factor relating with the diurnal range of temperature.

$$A = \max \left[\frac{\Delta Tm - \Delta T}{\Delta Tm}, \quad 0 \right]$$
 (2)

T is the diurnal difference of temperature and

Im is the critical diurnal difference with which the daytime heat-island effect disappears (by taking 10 to 15 degrees).

$$DDT = \begin{cases} dT - \frac{dT}{9} \bullet \overline{V} & (\overline{V} \le 3.5 \text{ m/s}) \\ \max \left[\frac{5.5}{9} dT - \frac{5.5 - 2}{10 - 3.5} (\overline{V} - 3.5) \bullet dT, 0 \right] & (\overline{V} > 3.5 \text{ m/s}) \end{cases}$$
(3)

in which dT is the maximum intensity of heat-island effect for the season in a city, which is related with the density and scale of urban architecture and time of the year, \overline{V} is the mean wind speed in urban districts and Eq.(3) reflects the effect of wind speed.

B(t) is the factor of diurnal range, which changes between 0 and 1, t is the local time (hour). B(t)=1 when it is four hours after sunset but B(t)=0 when temperature is the highest while it changes linearly over other periods of time.

3 ANALYSIS OF THE RELATIONSHIP BETWEEN POLLUTION CONCENTRATION IN SHENZHEN AND ATMOSPHERIC CONDITION

As shown in the data of 1997, NOx is the main source of pollution among the three pollutants in Shenzhen. It is above Level Two of the national standard, followed by SO_2 , which stays around the standard, and TSP, which goes above it occasionally. According to incomplete statistics for 1994, traffic mainlines amount to about 230 km in total in Shenzhen, topping all other cities in the province, with mean flows about 2000 vehicles per hour. The emission of automobile tail gas is so huge that the city is on the same magnitude of order as the capital Guangzhou as far as the diurnal mean concentration of NOx over the year is concerned. In contrast, the diurnal mean levels of SO_2 during the same course are almost a magnitude of order smaller than the latter and those of TSP are comparable with other cities in the province. The result is generally consistent with that concluded with the data covering $1986 - 1993^{[2]}$.

Tab.1 gives the relationship between the city mean concentration and concentration for individual sites and districts. It is seen that the latter has a significant positive correlation with the former (being much higher than the confidence level of 0.01). It suggests that the individual sites (districts) share consistent tendencies of variation, with TSP having the highest consistency in concentration changes. It should be noted, however, correlation does not show as well as it is supposed to be. For instance, the NOx concentration for the two districts is poorly correlated with the city mean while the urban SO_2 level is more poorly correlated with the city mean. It indicates that the city mean level of pollution cannot stand for variation in individual districts all by itself, saying nothing of individual sites. Pollution concentration does not follow exactly the same pattern across the city.

Tab.2 gives the correlation of pollution levels between the urban and suburban districts. It clearly shows that the correlation coefficient is quite small for all but TSP, which is lower than the confidence level of 0.1. In other words, pollutants change their levels of concentration inconsistently in the two districts. It is then necessary to deal with them separately to achieve optimal results in making potential prediction of pollution.

Tab.1 Coefficients of the correlation between the mean pollution levels of Shenzhen and individual sites and districts

	park	Nan Hu Primary school	Honghu	Urban district	Nan Hai .Oil	Hua Qiao primary school	Li Zhi Middle School	Suburban district	Sample size
NOx	0.58	0.56	0.67	0.80	0.41	0.57	0.66	0.83	147
SO_2	0.28	0.21	0.52	0.58	0.68	0.60	0.42	0.90	147
TSP	0.77	0.71	0.74	0.90	0.83	0.57	0.85	0.95	101

Tab.2 Coefficients of the correlation air pollution concentration between the urban and suburban districts

	NOx	SO_2	TSP
Correlation coefficients	0.125	0.094	0.544
sample	97	97	82

Tab.3 gives the mutual relation between pollutants concentration. The subscripts T, 1 and 2 in the table stand for the mean for the whole city, urban and suburban districts. It is clear that there is significant positive correlation among concentration of different pollutants in terms of the city mean, which gets near or obtains the confidence level of 0.05 with the exception of NO_{XT} and TSP_T, indicating consistent effects of atmospheric diffusion on the concentration of pollutants and account for reasons behind they are treated as a whole in general potential prediction systems. Low correlation coefficients remain the main concern. The problem is particularly obvious when viewed on a district basis — the correlation coefficients are generally small (like 0.02), being independent of various pollutants concentration. It is indicative that the concentration of pollutants varies by uneven, even complete different paces. In other words, the atmosphere affects the concentration change in a way that depends differently on districts of Shenzhen (being equivalent to local scales) and types of pollutants. It may be attributed to the difference in pollutants sources (e.g. NOx mainly comes from the surface – tail gas of automobiles, SO₂ is sought chiefly from industrial chimneys and TSP is largely made up of suspending dust — coal is consumed in little amount in Shenzhen area), the topographic features of the city (being next to the South China Sea with the south facing Hong Kong, north connecting with mainland and southwest and west reaching out to sea, see Fig.2) and the characteristics of the pollutants (e.g. gaseous pollutants are made easier to dissipate and bring about dust if surface winds are large, etc.). It is then necessary to carry out the potential prediction based on the districts and pollutants.

Tab.3 Coefficients of the correlation between pollutants concentration in Shenzhen

	SO_{2T}	SO_{21}	SO ₂₂	TSP _T	TSP 1	TSP 2
NO _{xT}	0.20			0.06		
NO_{x1}		0.07			0.17	
NO_{x2}			0.29			0.02
$\mathrm{SO}_{\mathrm{2T}}$				0.18		
SO_{21}					0.24	
SO_{22}						0.04

With the analyses above, we conducted potential predictions of three airborne pollutants for two districts of the Shenzhen city. Next is a discussion of the linkage between pollution concentration and atmospheric condition.

The atmospheric condition is analyzed first on the surface level. Tab.4 gives the correlation between meteorological elements at the Shenzhen station and pollutants. Specifically, *PS*, *RH*, *T*, *FF*, *R08* and *R20* stand for the diurnal mean of surface pressure, humidity, temperature and wind speed and 24-h accumulated amount of precipitation at 08:00 and 20:00 (L.T., same below), respectively, with the superscript "–1" indicating the value on the previous day. The followings can be seen by examining the table. (1) All levels of pollutants are positively correlated with pressure in large numbers, which is consistent with the fact that the atmosphere is so stable that it does not contribute to dissipation if pressure is high. (2) The concentration of pollutants are in obvious negative correlation with temperature, which runs odds with past findings that point out that temperature somehow affects the pollution potential on scales larger than 10 km while largely leaving it alone on sub-local scales. It is then inferred that it does not necessarily lead to physical causality so as to be used as an independent factor, for the high correlation shown in this

case is concluded to have been caused by that between temperature and pressure / humidity. Temperature may act as an independent factor considering the particular geographic location of Shenzhen (fugure omitted) — it may immediately affect the intensity of land / sea breeze to make the difference in pollution potential. The issue will not be discussed in more detail than what has been attempted so far as offshore sea temperature data are not sufficient enough to start with. (3) The significant negative correlation between pollutants concentration and humidity may be mainly attributed to the observation that the pollutants are dissolved and absorbed by moisture to change to substances like SO_4^{2-} and NO_3^{-} , which favors the descent of dust rather than raise it. (4) The two airborne pollutants' concentration levels do not significantly relate with surface wind speed, which goes contrarily with past arguments for possible reasons of (a) poor representation of surface wind speed in Shenzhen and (b) additional relevance with wind direction by concentration (which will be dealt with later in the work). The significant positive correlation of wind speed with the TSP concentration can be physically explained (through the relationship between wind speed and suspending dust). (5) All of the pollutants have significant negative correlation with precipitation, among which SO2 has the least correlation, and the effect of precipitation is somewhat lagging behind, which can be seen from the high correlation with R20⁻¹.

Tab.4 Coefficients of the correlation of surface meteorological elements at the Shenzhen station and mean pollution concentration

	PS	RH	T	FF	R08	R20	$R08^{-1}$	$R20^{-1}$	sample
NOx	0.26	-0.15	-0.18	0.05	-0.21	-0.15	-0.01	-0.12	197
SO_2	0.28	-0.23	-0.29	0.01	-0.04	-0.07	-0.06	-0.10	197
TSP	0.21	-0.13	-0.38	0.17	-0.16	-0.14	0.03	-0.10	153

Next we will discuss the atmospheric condition at upper levels. Tab.5 gives the correlation between a number of upper-level atmospheric parameters and individual pollutants levels. Specifically, Hm, Fm, RHm, Um and Vm are the thickness, wind speed and relative humidity of the mixing layer and the U and V components of the wind, and the subscript "m" stands for the mean of the mixing layer. Additionally, dT3 and dT8 are the maximum inversion intensity below 300 m and around 800 m, respectively, and F1, U1 and V1 are the wind speed at 1000 hPa and its U and V components, respectively. The table reveals the following points. (1) The diurnal mean concentration of NOx is much negatively correlated with Hm, Fm, RHm and Vm but much positively correlated with dT3 and Um. The correlation of Fm and Um (with opposite signs) jointly reflects the effect of wind speed on concentration (for the easterly is the prevailing climatological wind in Shenzhen), that of dT3 shows a close relationship between the NOx concentration and temperature inversion at the near-surface layer but a loose one between them at the upper-levels. It reflects on the characteristics of surface sources. In addition, each of the correlation pairs is usually higher at 12Z (for daytime) than at 00Z (for nighttime), indicating that the NOx pollution mainly comes from tail gas discharge from automobiles in the daytime. (2) The diurnal mean concentration of SO₂ is much negatively correlated with Fm, Fm, RHm, Vm and V1 but much positively correlated with dT8 and dT3, i.e. temperature inversion at both low and high levels is responsible for high SO₂ concentrations, but mildly related with Hm, which is associated with the fact that strong vertical mixing also carries upper-level pollutants downwards. Besides, wind direction is also a significant factor. While the east-west wind (U) poses weak effects, the north-south wind (V) has strong ones, for high winds from the south (over the ocean surface) tend to lower the concentration of SO₂. (3) Diurnal mean TSP levels are much negatively correlated with Um and U1 but much positively correlated with dT8, F1 and Fm, i.e. high lower-level winds and strong PBL temperature inversion are increasing the TSP concentration. The correlation between F1 and Fm is just the contrary to the other two pollutants, suggesting that high winds be a lifter of dust and the primary component of TSP be the flying dust.

Tab.5	Coefficients	of the	correlation	between	upper-level	atmospheric	parameters	and	mean
	pollution cor	ncentra	tion						

		Нт	Fm	RHm	dT3	dT8	Um	Vm	U1	V1	F1	Samples
	00Z	-0.10	-0.06	-0.12	0.04	0.10	0.20	-0.14	-0.09	-0.01	0.04	160
NOx	12Z	-0.23	-0.14	-0.17	0.31	0.02	0.12	-0.20	0.12	-0.15	-0.01	160
	Mean	-0.21	-0.07	-0.16	0.17	0.08	0.21	-0.19	0.07	-0.04	-0.00	150
	00Z	-0.00	-0.16	-0.22	0.09	0.20	-0.06	-0.23	0.01	-0.11	-0.06	160
SO_2	12Z	0.01	-0.19	-0.19	0.20	0.17	-0.03	-0.16	0.06	-0.12	-0.07	160
	Mean	0.05	-0.18	-0.20	0.13	0.21	-0.06	-0.20	0.08	-0.10	-0.11	150
	00Z	0.02	0.19	-0.12	-0.08	0.29	-0.22	-0.06	-0.18	-0.12	0.26	115
TSP	12Z	-0.07	0.16	-0.03	-0.01	0.48	-0.28	-0.03	-0.25	-0.04	0.27	115
	Mean	-0.07	0.19	-0.09	-0.06	0.49	-0.30	-0.09	-0.24	-0.04	0.30	105

Next, factors are analyzed that affect the difference in the variation of concentration between the urban and suburban districts. Tab.6 shows that the suburban district is much higher than the urban district in terms of the NOx correlation, which can be explained by the geographic location of Shenzhen (figure omitted). The suburban district faces the ocean to the west and south and winds originating there tend to decrease the concentration. Things are different in the urban district (the relatively high correlation with Um, Vm, Us and Vs and relatively low correlation with Fm and Fs show that wind direction plays a more important role than wind speed). Additionally, it may have bearings with intensity changes resulted from non-meteorological factors such as dense concentration of population and communications. For the case of SO₂, higher correlation is also found in the suburban district with the same cause as above. Additionally, a reversed-sign correlation between U1 and the concentration in the two districts suggests that east and west wind will carry suburban industrial pollutants either to the urban district in the leeward side or out of it, increasing or decreasing the pollution in the urban area (Figure omitted). The positive correlation between F1 and urban concentration can be attributed to the same cause (the easterly is the local annual mean wind). Although the TSP correlation is less significant between the two districts as the above two pollutants, it does differ to some extent. For instance, its correlation with Vs and V1 has just the reversed signs in the districts, which is associated with the fact that the urban district faces Hong Kong to the south while the suburban district borders with the ocean to the south. Combining the analysis of Tab.2 and Tab.3, we conclude that the aforementioned points must be taken into account in potential prediction.

Tab.6 Coefficients of the correlation between pollution concentration and wind direction (u, v) and speed in the districts

	Um	Vm	Fm	Us	Vs	Fs	U1	V1	<i>F</i> 1	Samples
NO_{x1}	-0.09	-0.10	-0.01	-0.05	-0.03	0.08	0.05	-0.09	0.06	100
NO_{x2}	-0.27	-0.23	-0.09	-0.24	-0.12	-0.06	0.04	-0.01	-0.06	100
SO_{21}	-0.05	-0.05	-0.03	0.00	0.06	-0.05	-0.20	0.03	0.19	100
SO_{22}	-0.09	-0.30	-0.23	-0.05	-0.26	-0.15	0.19	-0.23	-0.20	100
TSP_1	-0.25	0.04	0.09	-0.18	0.09	0.00	-0.24	0.16	0.24	90
TSP ₂	-0.29	-0.08	0.19	-0.22	-0.05	0.15	-0.24	-0.01	0.29	90

4 PREDICTION OF POTENTIAL POLLUTION FOR SHENZHEN

From the analysis above, we know that it is desirable to predict potential pollution for Shenzhen with approaches varying with pollutants and districts. Tab.7 lists the factors that need to be considered in making potential predictions based on different pollutants and districts.

Tab.7	Main factors	affecting the	prediction of	potential	pollution based	d on different districts and pol-	lutants

items	Main factors in play									
NO _{x1}	dT3 Hm Um Vm V1 RR Ps RH T									
NO_{x2}	dT3 Hm Um Vm Us Vs RR Ps RH T									
SO_{21}	dT8 U1 F1 dT3 RH RHm Ps RR T									
SO_{22}	Fm RHm T dT3 dT8 RH Ps RR Vm U1 V1 F1									
TSP_1	dT8 F1 RR U1 V1 RH Ps Um T									
TSP_2	dT8 F1 RR U1 RH Ps Um T									

The predictions are made using a rank division technique. The above factors are assigned additive indexes (with the values ranging from -2 to 2) based on their physical meanings and relative significance of correlation. The assignment is carried out by

In the dissignment is carried out by
$$I_{X} = \begin{cases}
-2 & X \leq \overline{X} - \alpha_{2} \delta_{X} \\
-1 & \overline{X} - \alpha_{2} \delta_{X} < X \leq \overline{X} - \alpha_{1} \delta_{X}
\end{cases}$$

$$0 & \overline{X} - \alpha_{1} \delta_{X} < X < \overline{X} + \beta_{1} \delta_{X}$$

$$1 & \overline{X} + \beta_{1} \delta_{X} \leq X < \overline{X} + \beta_{2} \delta_{X}$$

$$2 & X \geq \overline{X} + \beta_{2} \delta_{X}$$

$$(4)$$

Specifically, X is the atmospheric parameter, \overline{X} is its temporal mean, X is the variance of X and X, X, and X are the rank factors. X and X are the rank factors. X and X are the rank factors.

$$WI_i = \sum_{j=1}^{n_i} (I_j)_i$$
 $i=1, 2, \dots, 6$ (5)

 WI_i is the prediction of potential pollution index for the *i*th object to be predicted, $(I_j)_i$ is the additive index for factor *j* versus element *i*, n_i is the number of factors used in index prediction for element *i*. $i=1, 2, \ldots, 6$, standing for the three pollutants in the two districts.

Evolutions of hourly 3-D element fields from the mesoscale numerical model are used to determine the values of individual factors in Tab.7 so that time series of potential indexes is forecast and potential indexes are obtained for individual periods of time. The mesoscale model used in the current work is a modified version of German Weather Bureau's model with horizontal resolution of 0.25° and 20 vertical layers. Its PBL is divided into six layers and treated with a 2-order-matrix scheme [12]. The experiment shows that it meets the requirements for the determination of atmospheric parameters in the potential prediction system.

Tab.8 summaries historical fittings of 1997 potential pollution prediction for Shenzhen with the rank index method proposed in the work. The potential is divided into three ranks, large, normal and small. "Correct" means that the forecast index and actual pollution concentration are in the same rank, "basically correct" indicates that they are in the same rank or differ by only one rank, and "incorrect" refers to cases where the above situations do not exist. It is seen that correct fittings are quite high, about 0.5, basically correct fittings are very high, close to 0.9, and incorrect fittings are between 0.1 and 0.2, with those of TSP being especially high, due to complicated reasons that cause it and relatively large scattering distribution of concentration. The method is then considered effective and useful.

Tab.8 Historical fittings of potential pollution prediction for Shenzhen in 1997

	SO_{21}	SO_{22}	SO_{2T}	NO_{x1}	NO_{x2}	NO_{xT}	TSP 1	TSP 2	TSP _T
Correct	0.47	0.52	0.35	0.48	0.63	0.48	0.48	0.63	0.52
Basically correct	0.91	0.83	0.86	0.94	0.75	0.89	0.77	0.71	0.78
Incorrect	0.09	0.17	0.14	0.06	0.25	0.11	0.23	0.29	0.22

5 CONCLUDING REMARKS

In this work, a prediction technique for potential pollution is proposed. It takes into account inherent physical linkages between atmospheric parameters (condition for dissipation) and pollution concentration, differentiate individual characteristics of pollutants and reflect on the differences between different parts of cities (geographic locations). Observed data are used to derive linkages between relevant atmospheric parameters and pollution potentials and possible physical causes. Effects of atmospheric parameters on different pollutants and locations of the cities as well as their possible mechanisms are discussed. In the last portion of the work, the data analysis is based to formulate a scheme for prediction of air pollution potential in cities that treat districts and pollutants in a different way. On the basis of it, a method of air pollution potential prediction is then designed through high-resolution in both time and space of a mesoscale numerical model. The method includes both physical – statistic foundations and dynamic evolutions.

The principle of the method can be readily applied in other similar fields of research. In the meantime, it may be possible to develop other predictions of potential concentration by combining the idea with source intensity and concentration.

Main conclusions are as follows:

- a. Pollution concentration varies across different districts of a city. It must be differentiated in predicting pollution potential to achieve optimal results.
- b. With the same atmospheric condition, the atmosphere has different effects on city districts (being equivalent to local scales) and pollutants, and with respective explanation of physics. It is then necessary to conduct potential prediction according to the types of the districts and pollutants.
- c. The concentration of pollutants in Shenzhen is significantly and differently associated with surface pressure, temperature, humidity, precipitation, mixing layer thickness, the mean wind speed, direction and humidity of the mixing layer, the intensity of temperature inversion near 300 hPa and 850 hPa, wind direction and speed at the near-surface layer, etc. Having real physical meanings, these linkages reflect on the comprehensive influence from factors like atmospheric dissipation properties, geographic location, sources and characteristics of pollutants.
- d. Data with high resolution in time and space from numerical models are used not only to predict pollution potential to ensure high resolution in the dimensions but to have significant advantages by quantitative inclusion of dynamic processes needed in future atmospheric condition.
- e. The high historical fitting rates with the predictions by the current scheme implies that it is effective and useful.

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