Data assimilation experiment on SO_2 initial conditions in the Pearl River Delta

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Introduction

As the air pollution problem become more and more severe, many air quality models were developed and applied to research and forecast operation. However there are many uncertainties in the model, which affect the forecast result. Data assimilation is a state-of-the-art approach to reduce the uncertainties in input data, such as initial conditions or boundary conditions, by using observations. It can combine both advantages of model results and observations to improve the prediction.

In order to provide a more precise initial condition of SO_2 in the Pearl River Delta (PRD) region, data assimilation methods were introduced to the WRF-CMAQ model. Sensitivity experiments were carried out to exam the number of assimilation site and correlation scale. The comparative experiment on the optimal effect of different assimilation methods were conducted.

Methodology

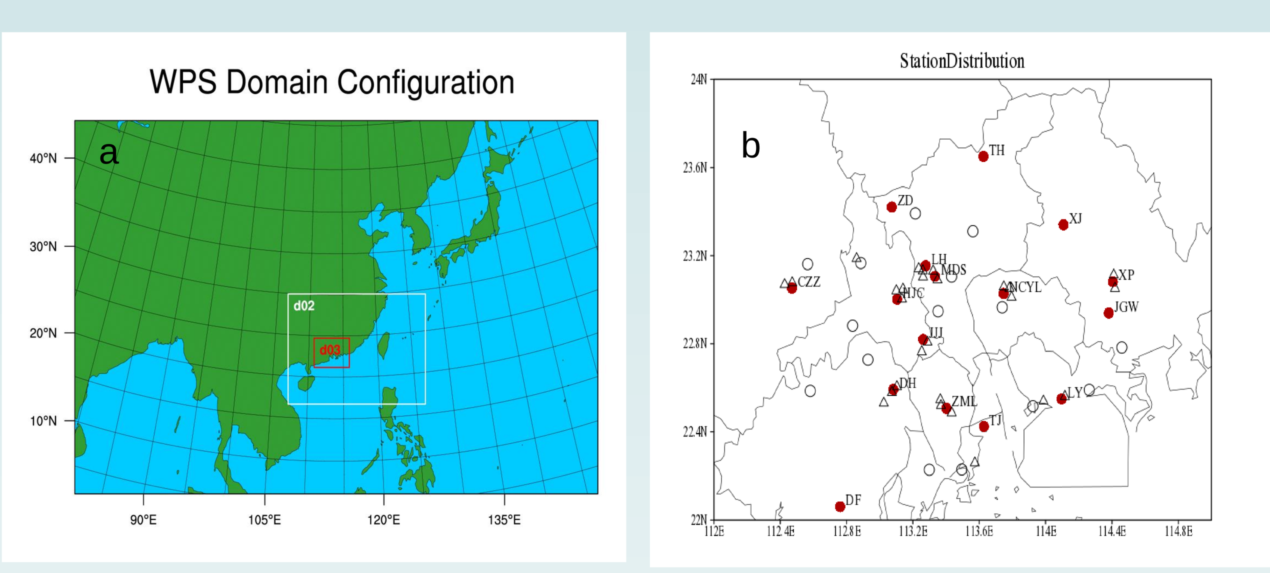

Fig.1(a) Nesting domain setting of the WRF-CMAQ model, domain 01(27x27km), domain 02 (9x9km) and domain 03 (3x3km); (b) Domain 03 shows the distribution of observation sites in the PRD region where we have the assimilation experiment.

The method used here is the Optimal Interpolation method (OI) and the Ensemble Square Root Filter method (EnSRF). The formula as follows:

OI

$$x^a = x^b + K(y^o - Hx^b)$$

$$K = B^b H^T \left(HB^b H^T + R\right)^{-1}$$

EnSRF

$$\bar{x}^a = \bar{x}^b + K(\bar{y}^o - H\bar{x}^b)$$

$$x'^a = x'^b - \tilde{K} H X'^b$$

$$K = B^b H^T \left(HB^b H^T + R\right)^{-1}$$

$$\tilde{K} = \alpha K, \quad B^b = \frac{x'^b x^{bT}}{N-1}$$

$$\alpha = \left(1 + \sqrt{\frac{R}{HB^b H^T + R}}\right)^{-1}$$

$$x^a = \bar{x}^a + x'^a$$

x^a :analysis field, x^b background field,

x^{12} and x^{24} :12h and 24h forecast fields

y^o: observation field, H: operator, B^b: background error covariance

R: observation error covariance, N: number of ensemble，here is 30

Superscript：T and -1, transpose and inversion of Matrix

- and ’average and bias of ensemble

Results and Discussion

Model Evaluation

Table 1 Statistical comparison of simulated and observed meteorological parameters

Guangzhou	T	RH	WS
Mean Bias (MB)	0.23	-2.96	1.70
Mean Absolute Gross Error (MAGE)	1.87	12.94	1.84
Normal Mean Bias (NMB)	3%	3%	70%
Normal Mean Error (NME)	0.18	0.23	0.74
Index of Agreement (IOA)	0.94	0.82	0.67
Correlation Coefficient (CORR)	0.88	0.72	0.70

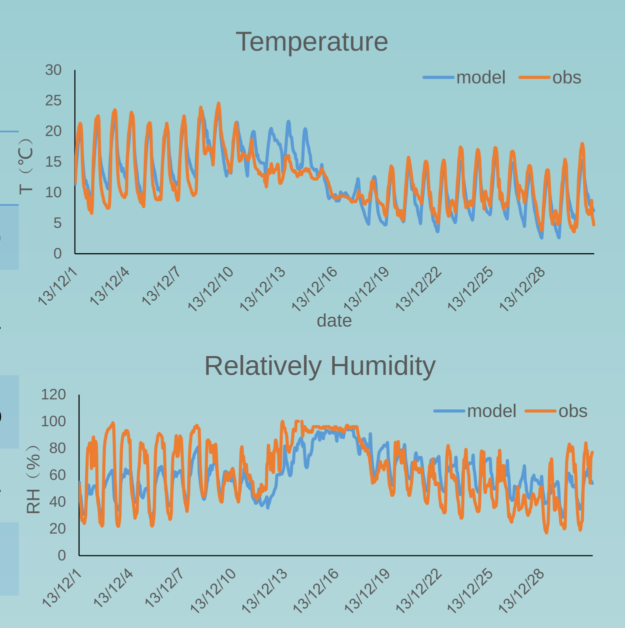

Fig. 2 Temporal variations of temperature and relatively humidity

Table 2 Statistical analyses of modelling performance on daily mean SO_2

SO_2	ave	max	min
MB	9.42	41.87	-34
MAGE	17.79	41.87	5.14
NMB	61.11%	389.00%	-50.00%
NME	84.13%	389%	17%
RMSE	20.93	45.96	7.15
CORR	0.75	0.93	0.34

- Generally, diurnal variations of temperature and relatively humidity are well captured by model, the simulation of wind speed and SO_2 are relatively high.

Background Analyses

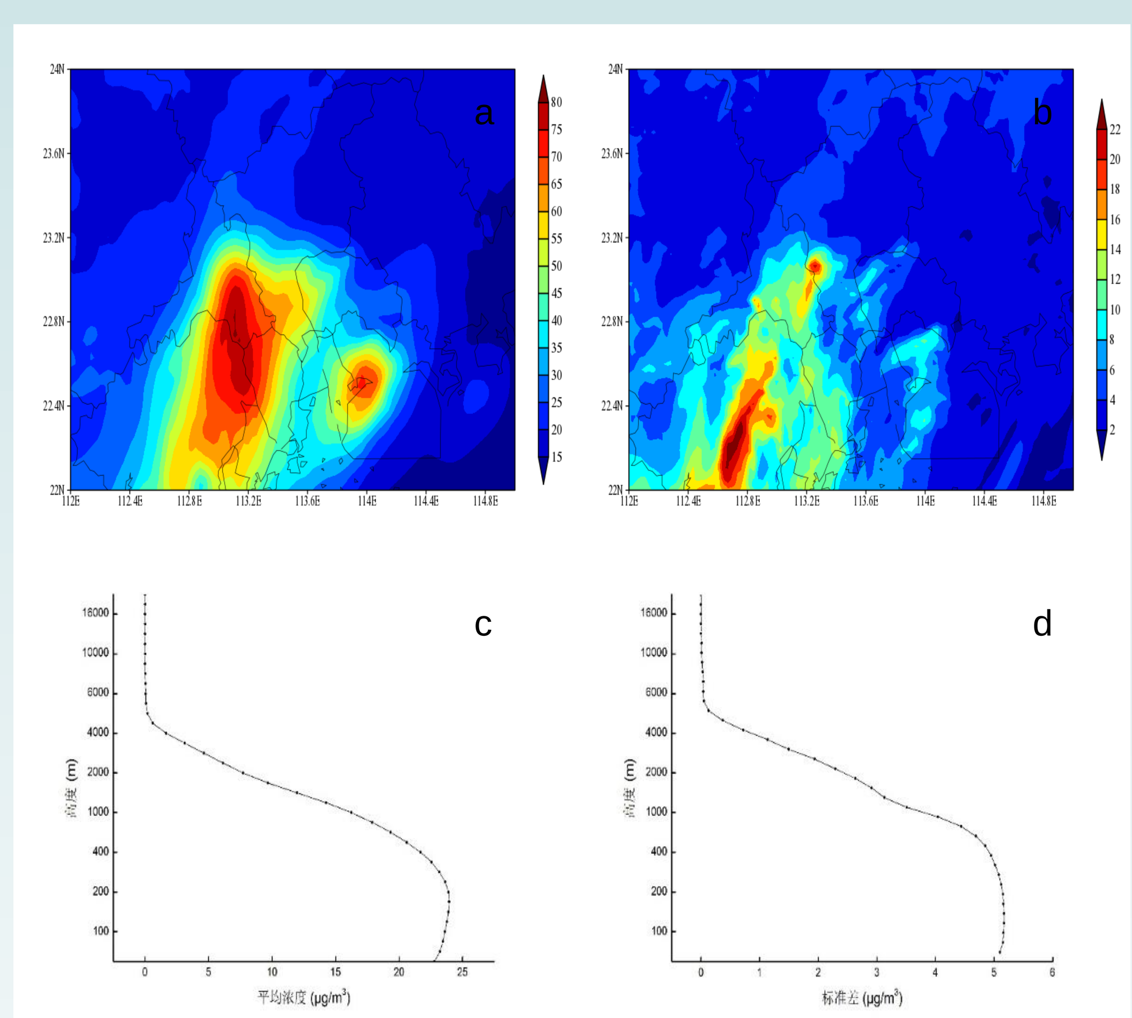

Fig.3(a)Distribution of the monthly average concentration of SO_2 at the first model level;(b) Distribution of the standard error of SO_2 at the first model level;(c) Vertical profile of monthly average concentration of SO_2;(d) Vertical profile of monthly average concentration of SO_2.

- Horizontally, the high value region of error didn’t fit the concentration well. Locate in southwest region;
- Vertically, the variation of error and concentration are similar. Constant below 400m,decrease above 400m.

Number of assimilation site

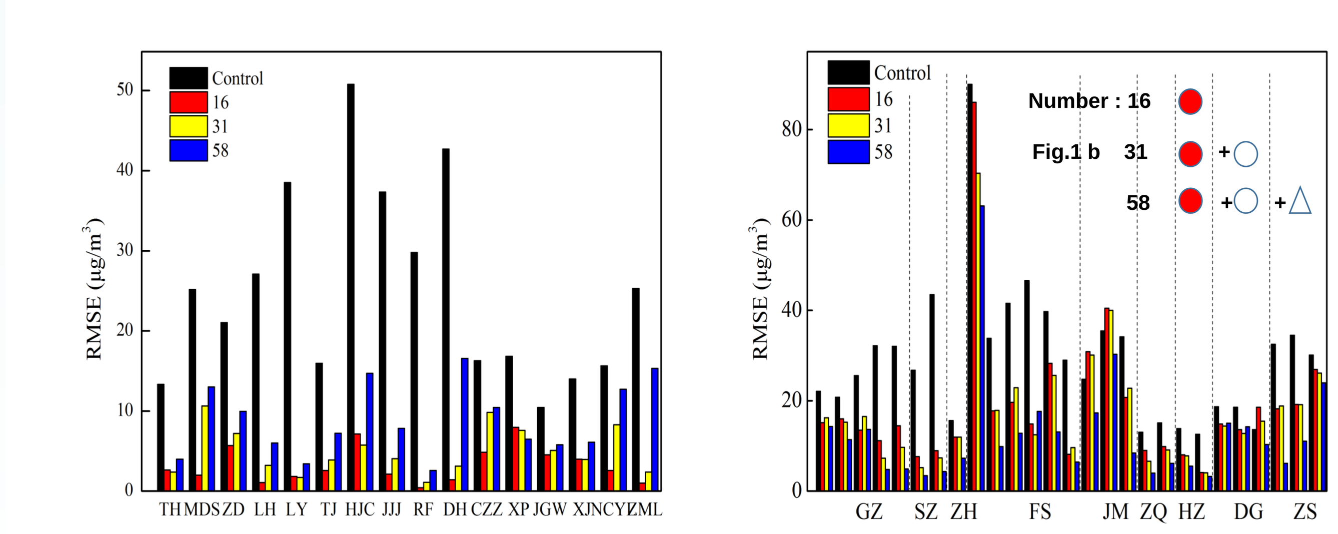

Fig.4 Comparisons of RMSE with assimilating different numbers of observations by OI

- Increasing the number is beneficial for broadening the coverage of site. But the optimal effect of the assimilation site decrease with the number of observations statistically.

Correlation Scale

Table3 Statistics of the result with different correlation scales of different methods

Sites		Control	Method	10km	20km	30km	40km	50km	60km	80km	100km
Assimilation	MAGE	21.39	OI	2.79	4.59	7.07	8.84	10.65	12.11	13.62	14.68
			EnSRF	1.68	2.55	3.40	4.16	4.87	5.51	6.31	6.81
	RMSE	27.08	OI	4.42	6.84	10.42	12.83	14.98	16.69	18.43	19.68
			EnSRF	3.30	4.65	5.92	6.94	7.90	8.99	10.16	10.88
Validation	MAGE	23.91	OI	12.95	13.05	13.18	13.19	12.99	13.30	14.14	14.79
			EnSRF	12.00	12.35	12.95	13.12	13.37	13.58	14.16	14.57
	RMSE	29.48	OI	17.81	17.60	17.82	18.20	18.42	18.94	20.02	20.75
			EnSRF	16.75	17.08	17.70	17.84	18.29	18.51	19.41	19.99

- Correlation scale decides the influence radius of the observation. The error of the analysis field increases with the correlation scale. Setting 20km will be more reasonable.

Different Methods

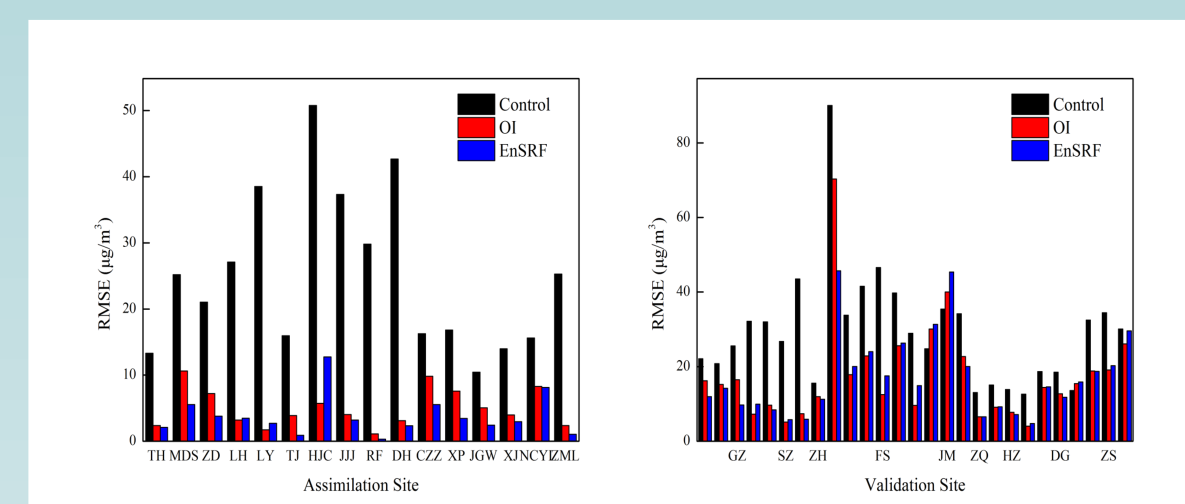

Fig.5 Comparisons of RMSE with and without assimilation using different methods（Assimilation sites 31, Correlation scale 20km）

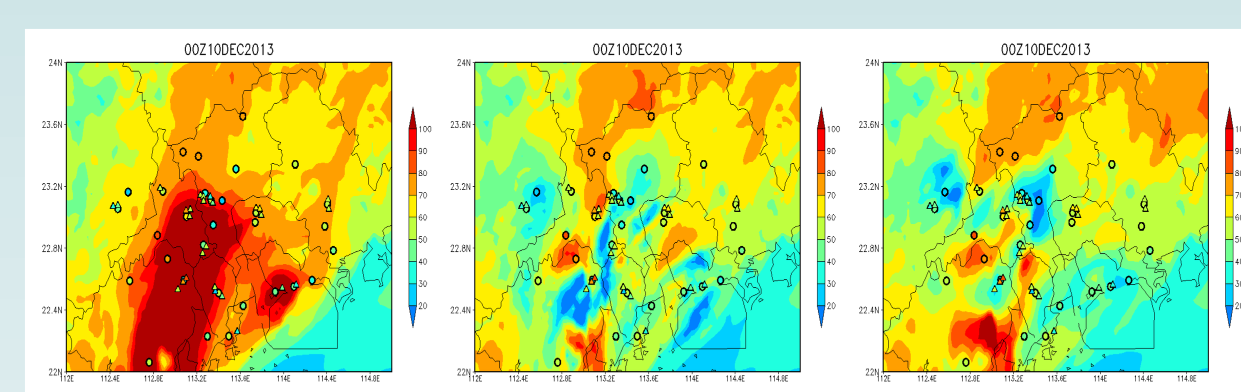

Fig.6 Distribution pattern of SO_2 concentration

- As a whole, both assimilation methods reduced the error, the optimal result of EnSRF is better than OI;
- Both methods adjusted the distribution pattern of SO_2 and make it more closed to the observation filed.

Conclusion

- The simulation of temperature and relative humidity were well, but higher for simulation of the wind speed and SO_2 is relatively high by WRF-CMAQ .
- The high values of the background error was mainly located in southwest region in horizontal direction. It was nearly constant below 400m and decreased with height above 400m.
- The sensitivity test showed that the optimal horizontal scale was 20km. With the number of the assimilation site increasing, the optimization of the assimilation site had a declining trend.
- Under the same conditions, the optimization of EnSRF method is better than that of OI method. Both methods can provide an analysis field closer to reality.

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