Inverse estimation of urban-scale CO emissions over Beijing and its surrounding areas: assimilating in-situ observation with Ensemble Kalman Filter

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Introduction

- As one of the biggest city-cluster in China, Beijing and its surrounding areas are suffering from high CO concentrations. However, accurate simulation or forecast of CO pollution is quite difficult currently because the bottom-up emission inventory highly relied on by air quality modeling is still largely uncertain (70% ~ 185%).
- Bottom-up estimation method provides another approach to estimate emissions through combining chemical transport model with observed concentrations of pollutants.
- The most frequently employed algorithm in previous inversion estimations of CO emissions is the four-dimensional variational algorithm, while the potential of EnKF in application for real emission inversion estimation problem is seldom investigated.
- Furthermore, very few studies focus on the urban-scale inversion estimation over Beijing and its surrounding areas, a region with high CO concentrations and undergoing rapid urbanization process and emission changes.

Aim

- The objective of this study is to do inverse estimation of urban-scale CO emissions over Beijing and its surrounding areas, and to investigate the potential of ensemble kalman fitler (EnKF) in emission inversion.
- Ground-based CO observations in 1h resolution and Nested Air Quality Prediction Modeling System (NAQPMS) are combined by EnKF to estimate CO emission rates over Beijing and its surrounding areas.
- Regional Emission inventory in Asia Version 1.1 (REAS1.1), as a widely used emission inventory, is employed as the priori emission inventory to be optimized. Optimizing simulated concentrations, as a potential way for reducing the uncertainty in emission inversion, is embedded into the emission inversion scheme.

Method: EnKF-based emission inversion method

EnKF employs a set of ensemble samples to represent the estimation of state variable and its error covariance. Emission-concentration sensitivity for inverse estimation is obtained through the statistic of the error covariance, and can evolve with highly nonlinear model integration. The emission inversion scheme based on EnKF is simply described as following.

- Perturbing state vector

$$x_0'(i) = x_0^b + \delta x_0(i),\ i = 1,2,\ldots,N$$

- Perturbing CO emissions and parameters

(a) CO emissions in EnKF perturbed with time-correlated noises

$$\eta_k'(i) = \eta_k^b + \delta\eta_k(i)$$

$$\delta\eta_k(i) = \alpha\delta\eta_{k-1}(i) + \sqrt{1-\alpha^2}\sigma w_{k-1}(i),\ i = 1,2,\ldots,N$$

(b) parameters in EnKF perturbed with white noises (model error)

$$\lambda_k'(i) = \lambda_k^b + \delta\lambda_k(i)$$

- Perturbing observations

$$y_k'(i) = y_k + \gamma_k(k),\ i = 1,2,\ldots,N$$

$$\gamma_k \in N(0, R_k)$$

- Adjusting CO emissions and concentrations

(a) ensemble forecast

$$x_k^f(i) = M_{k-1}\left(x_{k-1}'(i), \eta_{k-1}'(i), \lambda_{k-1}'(i)\right),\ i = 1,2,\ldots,N$$

(b) defining extended state vector

$$b_k^f(i) = \left|\begin{matrix} x_k^f(i) \\ \eta_k^f(i) \end{matrix}\right|,\ i = 1,2,\ldots,N$$

(c) estimating background error covariance

$$\mathbf{P}_k^f = \frac{1}{N-1}\sum_{i=1}^{N}\left(b_k^f(i) - \overline{b_k^f}\right)\left(b_k^f(i) - \overline{b_k^f}\right)^T$$

(d) updating the extended state vector

$$b_k^a(i) = b_k^f(i) + \mathbf{K}_k(y_k' - \mathbf{H}b_k^f(i)),\ i = 1,2,\ldots,N$$

$$\mathbf{K}_k = \mathbf{P}_k^f\mathbf{H}_k^T\left(\mathbf{H}_k\mathbf{P}_k^f\mathbf{H}_k^T + \mathbf{R}_k\right)^{-1}$$

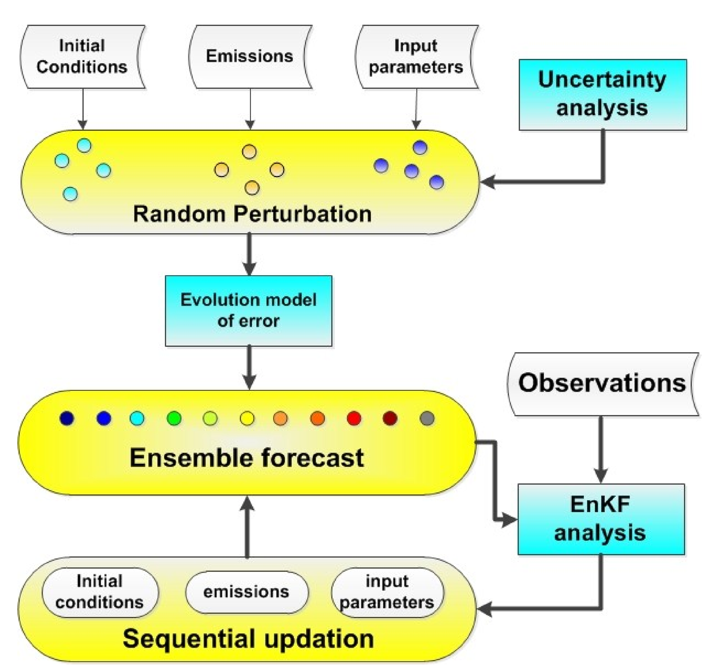

Fig. 1. The scheme of EnKF data assimilation system.

Experiment setting

- *The CTM used with EnKF is the Nested Air Quality Prediction Modeling System (NAQPMS).*
- *The hourly meteorological driver is provided by the Fifth-Generation NCAR/Penn State Mesoscale Model (MM5).*
- *CO emissions are hourly adjusted during 00:00 July 19 – 23:00 July 30, 2010.*

***Table 1.** Configurations of experiments.*
***ISI**: Inversion emission inventory*
***REAS1.1**: Regional Emission inventory in Asia Version 1.1*

Experiments	Initial emission inventory	Adjusted variable	
		CO concentrations	CO emissions
EXP1	REAS1.1	NO	NO
EXP2	REAS1.1	YES	YES
EXP3	IEI	NO	NO
EXP4	REAS1.1	NO	YES

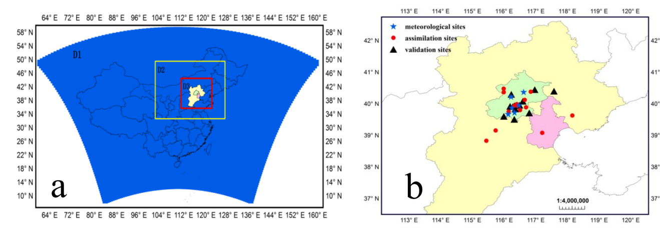

***Fig. 2.** (a) Model domains. The third domain includes Beijing and its surrounding areas with 9 km ×9 km resolution. (b) Monitoring stations.*

Results

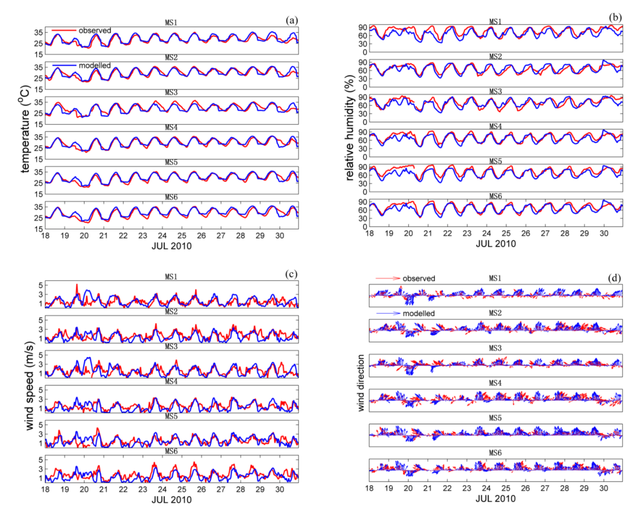

***Fig. 3.** Comparison of simulated and observed meteorological parameters at six meteorological stations (MS, shown in Fig. 2) during July 18-30, 2010 (Local Time). (a) temperature; (b) relative humidity; (b) wind speed; (d) wind direction.*

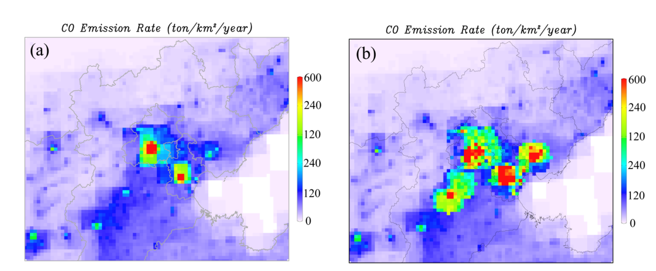

***Fig. 4.** CO emission rates in the third domains. (a) The estimates of CO emission rate in REAS1.1; (b) the inversion estimates of CO emission rates in IEI.*

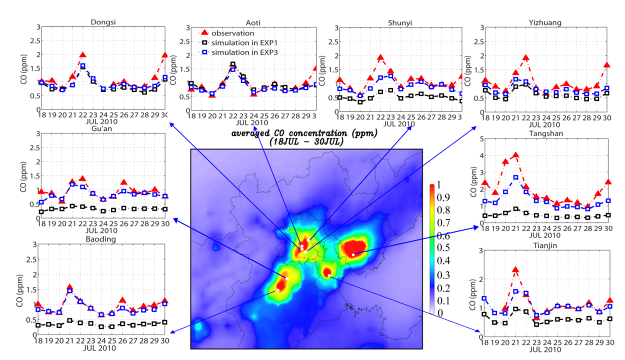

***Fig. 5.** Comparison of simulations and observations of daily CO. The shaded area represents the average CO concentrations over July 18-30, 2010 in EXP3.*

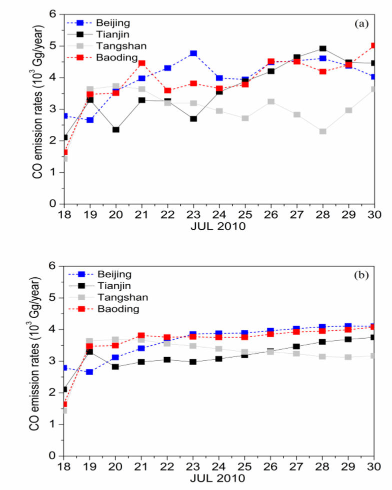

***Fig. 6.** Temporal variation of the estimates of CO emission rates in Beijing, Tianjin, Tangshan and Baoding in EXP2. **(a)** The estimate at one day is the average of the hourly estimates of CO emission rates within this day; **(b)** The estimate at one day is the average of the hourly estimates of CO emission rates from July 19, 2010 to this day.*

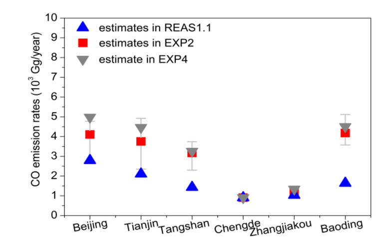

***Fig. 7.** A comparison of the CO emission estimations for Beijing, Tianjin, Tangshan and Baoding in EXP2 and EXP4.*

Cities	CO emission rates in REAS1.1 (Gg/year)	CO emission rates in IEI (Gg/year)
Beijing	2.8E+03	4.1E+03
Tianjin	2.1E+03	3.8E+03
Tangshan	1.4E+03	3.2E+03
Baoding	1.6E+03	4.1E+03

***Table 2.** Total emission rates of CO of Beijing, Tianjin, Tangshan and Baoding in IEI (inversion emission inventory) and those in REAS1.1.*

Conclusion

- A sequential emission estimation scheme based on EnKF was established with model error simulation and concentration field optimization embedded. The potential of EnKF in application for real emission inversion estimation problem has been exploited in this study.
- The CO emission rates over Beijing and its surrounding area in REAS1.1 and other inventories with similar CO emission level were found to be probably significantly underestimated. A new estimation of CO emissions over these areas was provided in urban scale resolution through assimilating surface CO observations.
- Our estimation is consistent with most of regional or global top-down estimations over East Asia region, and is partly validated by the recently updated CO emission estimations based on bottom-up method and independent surface CO observations.
- The inversion estimation results showed high sensitivities to post-processing of sequential adjusting coefficients and optimization of simulated concentrations. Adopting smoothing post-processing and simulated concentration optimization would be valuable for sequential emission inversion estimation.

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