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*Supplement of*

## **Numerical study of the effects of initial conditions and emissions on PM<sub>2.5</sub> concentration simulations with CAMx v6.1: a Xi'an case study**

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## Supplement

Table S1 shows the statistical results of the daily average PM<sub>2.5</sub> concentrations of 13 NSAQ Observation Stations during December 2016 in Xi'an. The correlation coefficients (R) of most urban stations can reach above 0.6, of which GYC is 0.73, while the R of XQ, QJ and XZ are low. Among the three stations in suburban counties, CAQ had the highest correlation coefficient of 0.68, and the other two stations are lower than 0.6. For bias, the model performances of stations in urban cities are better than that of the suburbs, and the simulated PM<sub>2.5</sub> concentrations in the suburbs are obviously underestimated. Except for CT, GYT and XZ, the FAC2 of the other 7 urban stations all reach more than 70%. Among the three suburban stations the CAQ has the best model performance, with FAC2 at 86%, while the other two stations are relatively low, especially the YLQ is only 31%. The average FAC2 of the urban cities is 74%, while the average FAC2 of the suburban counties is 62%, indicating that the model performance of the urban area is better than that of the suburban area in terms of total emissions.

**Table S1.** Verification statistics of PM<sub>2.5</sub> concentrations on December 2016 among all monitoring sites.

	Station	R	MB ( $\mu\text{g}/\text{m}^3$ )	ME ( $\mu\text{g}/\text{m}^3$ )	NMB %	NME %	RMSE	FAC2 %
urban	CT	0.70	-58.86	66.22	-38.08	42.84	89.99	64
	XQ	0.53	61.72	81.41	36.00	47.48	108.31	75
	JKQ	0.69	-76.00	84.91	-37.55	41.95	109.89	76
	TYC	0.66	75.46	89.90	45.98	54.78	108.49	77
	GYC	0.73	19.42	52.51	11.17	30.21	68.01	89
	QJ	0.59	14.79	71.73	8.06	39.11	89.90	76
	GYT	0.62	-31.46	69.01	-18.72	41.06	84.15	66
	FZC	0.67	3.11	60.68	1.79	35.01	76.42	78
	XZ	0.57	51.62	79.66	32.64	50.36	101.86	72
	GX	0.64	67.11	88.46	39.42	51.96	104.45	69
suburban	CAQ	0.68	8.51	54.49	5.36	34.29	72.26	86
	YLQ	0.60	-97.63	99.12	-57.67	58.55	120.78	31
	LTQ	0.57	-54.43	76.28	-33.53	46.98	97.49	69

Statistical parameters for the model evaluation:

Fraction of predictions within a factor of two of observations(FAC2):

$$0.5 \leq \frac{M_i}{O_i} \leq 2.0 \quad (\text{S1})$$