



## Supplement of

# **Development of WRF/CUACE v1.0 model and its preliminary application in simulating air quality in China**

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**Figure S1.** Schematic showing the flow of information within the WRF/CUACE v1.0 model. Gray boxes indicate the newly added modules to the WRF/Chem framework to build the WRF/CUACE v1.0 model. Dashed boxes are descriptions of each module.



**Figure S2.** The MEIC emissions of  $PM_{2.5}$  (a,e,i),  $NO_x$  (b,f,j),  $SO_2$  (c,g,k), and CO (d,h,l) in the three years of (a-d) 2012, (e-h) 2014, and (i-l) 2016. Emissions outside mainland China is from the MIX emission inventory. The unit is  $\mu g m^{-2} s^{-1}$  for PM<sub>2.5</sub>,  $NO_x$ , SO<sub>2</sub>, and is mg m<sup>-2</sup> s<sup>-1</sup> for CO.

#### Comparison of the simulation with Z01 and PZ10 deposition schemes

A winter month (January in 2015) was selected to simulate to show the model improvements with and without the updated dry deposition scheme. As shown in Fig. S3, the  $PM_{2.5}$  concentrations were commonly underestimated with the Z01 scheme (Fig. S3a), as it tends to overestimate the dry deposition velocity of fine particles (Petroff and Zhang, 2010). The underestimation was improved significantly when the Z01 scheme was updated to the PZ10 scheme (Fig. S3b).



**Figure S3.** Observed and simulated PM<sub>2.5</sub> concentrations on January 2015 with (a) Z01 and (b) PZ10 particle dry deposition schemes.

		Obs	Mod	R	MB	ME	NMB	RMSE
NCP	T2 (°C)	17.31	18.07	0.91	0.76	1.87	7.01 %	2.34
	RH2 (%)	62.88	51.10	0.80	-11.78	14.47	-18.94 %	17.91
	WS10 (m/s)	2.05	2.99	0.64	0.95	1.29	52.40 %	1.60
YRD	T2 (°C)	17.29	17.77	0.93	0.48	1.62	6.34 %	2.01
	RH2 (%)	70.74	64.51	0.82	-6.22	11.28	-8.55 %	13.95
	WS10 (m/s)	2.42	3.29	0.74	0.87	1.20	39.75 %	1.47
PRD	T2 (°C)	22.92	24.06	0.91	1.14	2.06	5.31 %	2.39
	RH2 (%)	75.74	67.20	0.78	-8.54	12.73	-10.72 %	14.88
	WS10 (m/s)	2.23	3.23	0.60	1.01	1.32	48.73 %	1.61
SCB	T2 (°C)	18.02	19.53	0.88	1.52	2.04	9.95 %	2.50
	RH2 (%)	74.17	59.87	0.73	-14.30	15.98	-19.00 %	18.77
	WS10 (m/s)	1.35	2.05	0.40	0.70	0.99	60.26 %	1.24

Table S1 Statistical metrics for meteorology fields in four haze contaminated areas (2013–2017).

**Table S2** Statistical metrics for hourly temperature at 2 m (T2), hourly relative humidity at 2 m (RH2) and hourly wind speed at 10 m (WS10), respectively in winter and summer in the NCP.

NCP region		Obs	Sim	R	MB	ME	RMSE
	T2 (°C)	1.59	2.01	0.85	0.42	1.67	2.14
Winter	RH2 (%)	62.65	53.17	0.75	-9.48	14.18	18.18
	WS10 (m s <sup>-1</sup> )	1.82	2.64	0.62	0.82	1.15	1.46
	T2 (°C)	27.48	28.88	0.89	1.40	1.89	2.38
Summer	RH2 (%)	72.79	59.61	0.84	-13.18	13.98	16.42
	WS10 (m s-1)	1.93	2.42	0.54	0.49	1.00	1.27

Table S3 Physical parameterization schemes used in the MM5/CUACE model.

Physical management	Parameterization		
Microphysics scheme	Mixed phase		
Radiation scheme	RRTM		
Land surface scheme	Noah		
Boundary layer scheme	MRF		
Cumulus scheme	Grell		

#### **Description of the index of agreement (IOA):**

The index of agreement (IOA) is based on Willmott et al. (1980), which spans between 0 (indicating "complete disagreement") to 1 (indicating "complete agreement"). It is defined as equation (S1)

$$IOA = 1 - \frac{\sum_{i=1}^{n} (P_i - O_i)^2}{\sum_{i=1}^{n} (|P_i - O| + |O_i - O|)} \quad ,$$
(S1)

where P, O and i represent simulation, observation and samples, respectively.

### **Reference:**

Willmott CJ, Wicks DE. An empirical method for the spatial interpolation of monthly precipitation within California. Physical Geography 1: 59–73, 1980.