

Supplementary Materials

Quantifying the Influence of a Burn Event on Ammonia Concentrations Using a Machine-Learning Technique

Jiabao Hu ^{1,2} Tingting Liao ^{3,4,*}, Yixuan Lü ^{1,5}, Yanjun Wang ¹, Yuexin He ¹, Weishou Shen ², Xianyu Yang ^{3,4}, Dongsheng Ji ¹ and Yuepeng Pan ^{1,5,6,*}

¹ State Key Laboratory of Atmospheric Boundary Layer Physics and Atmospheric Chemistry (LAPC), Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing 100029, China; hujiabao@nuist.edu.cn (J.H.); lvyixuan20@mails.ucas.ac.cn (Y.L.); 201842859@mail.sdu.edu.cn (Y.W.); heyuexin15@mails.ucas.ac.cn (Y.H.); jds@dq.cern.ac.cn (D.J.)

² Collaborative Innovation Centre of Atmospheric Environment and Equipment Technology, Jiangsu Key Laboratory of Atmospheric Environment Monitoring and Pollution Control, School of Environmental Science and Engineering, Nanjing University of Information Science & Technology, Nanjing 210044, China; wsshenn@nuist.edu.cn

³ The Plateau Atmosphere and Environment Key Laboratory of Sichuan Province/School of Atmospheric Science, Chengdu University of Information Technology, Chengdu 610225, China; xyang@cuit.edu.cn

⁴ Chengdu Plain Urban Meteorology and Environment Observation and Research Station of Sichuan Province, Chengdu 610225, China

⁵ University of Chinese Academy of Sciences, Beijing 100049, China

⁶ Artificial Intelligence Research Center for Atmospheric Science, Beijing 100029, China

* Correspondence: ltt2014@cuit.edu.cn (T.L.); panyuepeng@mail.iap.ac.cn (Y.P.)

Supporting information includes 4 figures and 5 tables.

Figures:

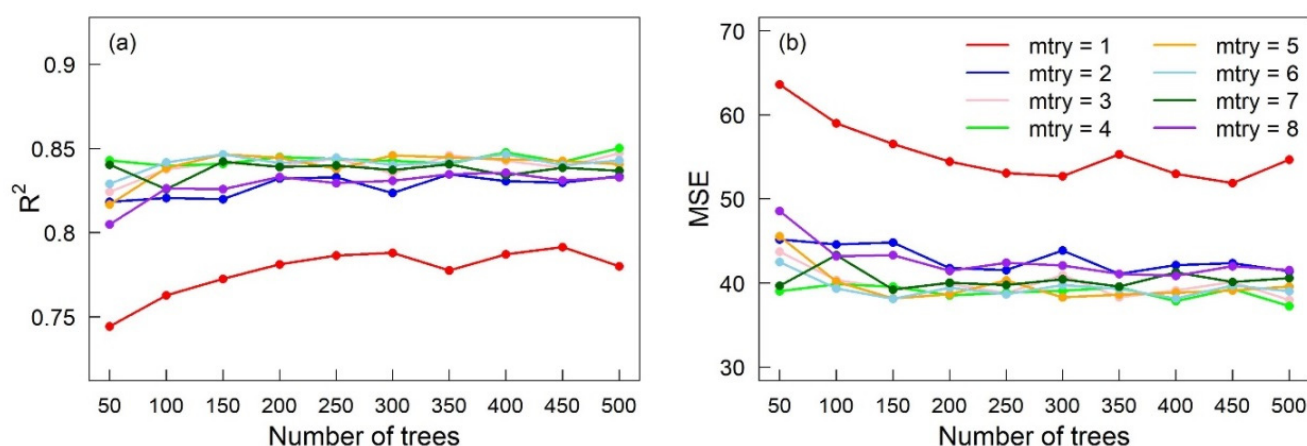


Figure S1. Influence of different *ntree* and *mtry* values on RF model.

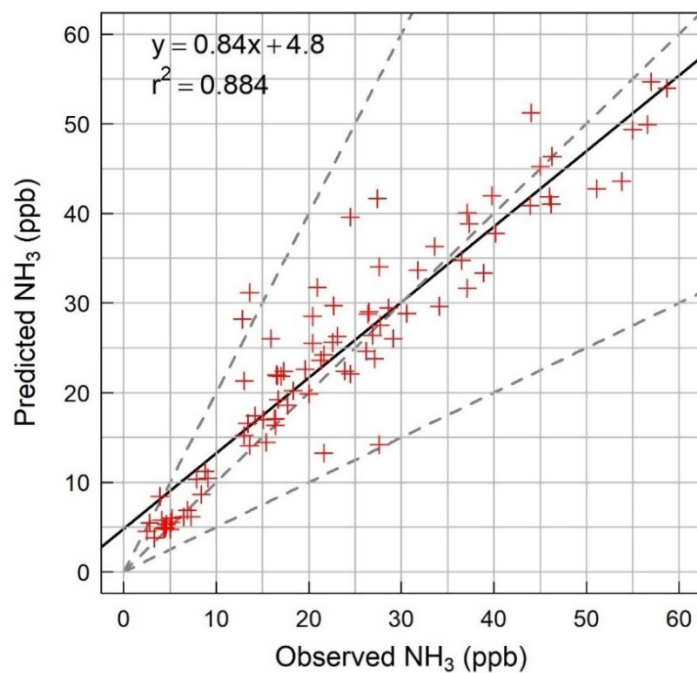


Figure S2. Performance of the RF model in predicting the NH_3 concentrations.

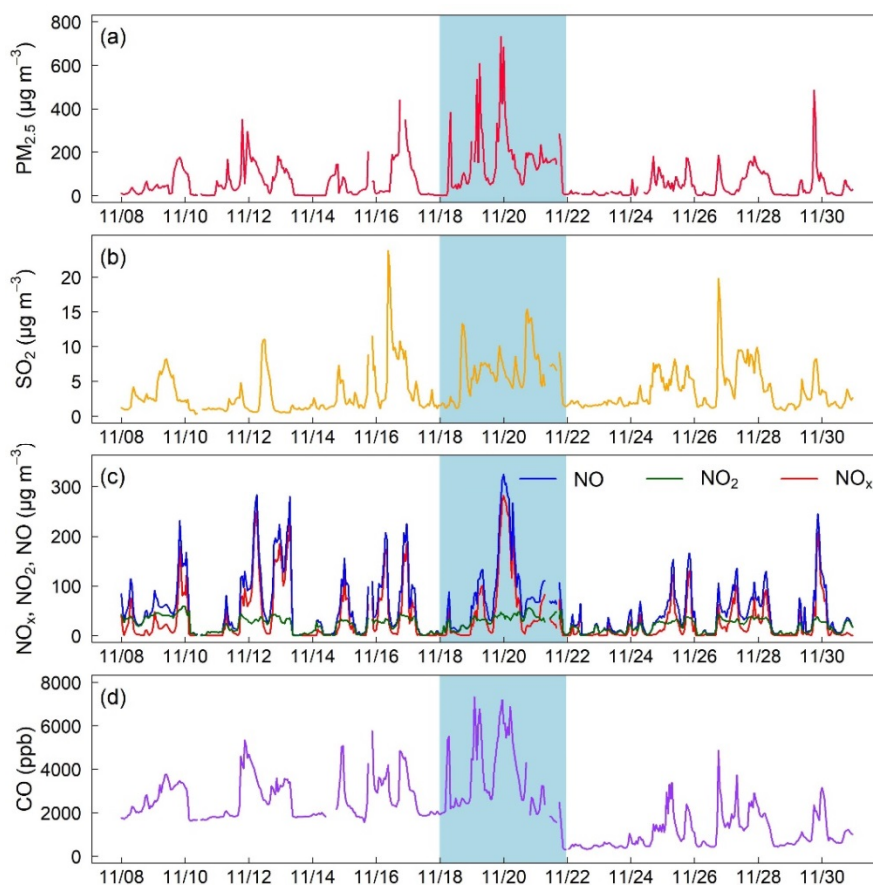


Figure S3. Temporal variation of hourly concentrations of $\text{PM}_{2.5}$, SO_2 , NO_x and CO .

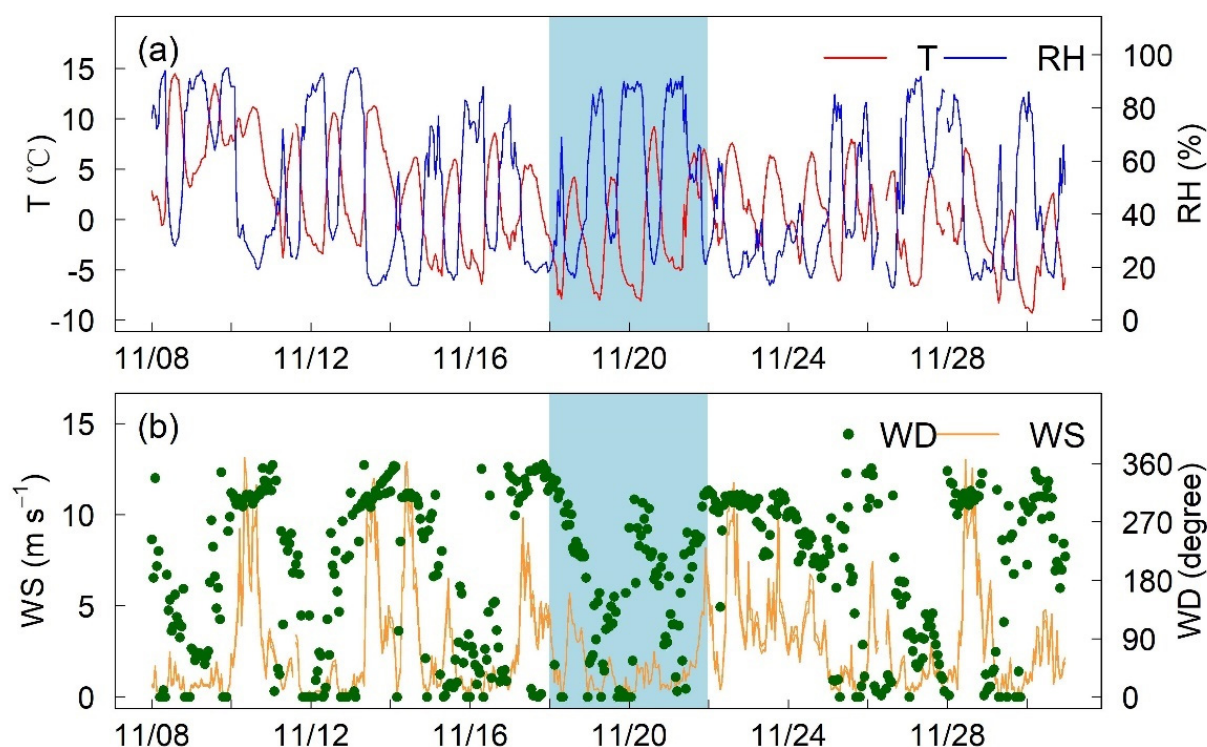


Figure S4. Hourly variation of meteorological parameters.

Tables:

Table S1. Summary of 11 RF models and their predictors in this study.

Name	Prediction variables
RF1	T, RH, WS, Pressure, cluster, day_julian, weekday, hour, WD
RF2	T, RH, WS, Pressure, day_julian, weekday, hour, WD
RF3	T, RH, WS, Pressure, cluster, day_julian, weekday, hour
RF4	T, RH, WS, Pressure, day_julian, weekday, hour
RF5	T, RH, WS, Pressure, day_julian, weekday, hour, PM _{2.5}
RF6	T, RH, WS, Pressure, day_julian, weekday, hour, NO _x
RF7	T, RH, WS, Pressure, day_julian, weekday, hour, CO
RF8	T, RH, WS, Pressure, day_julian, weekday, hour, SO ₂
RF9	T, RH, WS, Pressure, day_julian, weekday, hour, NO ₂
RF10	T, RH, WS, Pressure, day_julian, weekday, hour, NO
RF11	T, RH, WS, Pressure, day_julian, weekday, hour, CO, NO _x

Table S2. Model validation in 11 RF models in this study.

Name	R ²	FAC2	MB	NMB	RMSE	PCC
RF1	0.82	0.96	-0.23	-0.01	6.77	0.91
RF2	0.81	0.95	-0.07	0.00	6.79	0.91
RF3	0.83	0.96	-0.17	-0.01	6.50	0.92
RF4	0.83	0.95	-0.08	0.00	6.48	0.92
RF5	0.84	0.97	0.03	0.00	6.24	0.92
RF6	0.83	0.96	-0.02	0.00	6.56	0.91
RF7	0.84	0.97	-0.13	-0.01	6.37	0.92
RF8	0.83	0.97	-0.11	0.00	6.49	0.92
RF9	0.81	0.96	-0.12	0.00	6.89	0.90
RF10	0.83	0.95	-0.14	-0.01	6.56	0.92
RF11	0.82	0.98	-0.07	0.00	6.76	0.91

Table S3. Correlation matrix of NH₃, other air pollutants and meteorological parameters during the burning period.

Period	Species	NH ₃	PM _{2.5}	NO _x	NO ₂	NO	SO ₂	CO	T	RH	WS
Non-burning period	NH ₃	1									
	PM _{2.5}	0.48**	1								
	NO _x	0.58**	0.73**	1							
	NO ₂	0.58**	0.70**	0.91**	1						
	NO	0.57**	0.71**	0.94**	0.78**	1					
	SO ₂	0.42**	0.48**	0.40**	0.51**	0.36	1				
	CO	0.17**	0.55**	0.69**	0.66**	0.64**	0.24**	1			
	T	-0.15*	-0.16**	-0.43**	-0.22**	-0.42**	-0.09	-0.10*	1		
	RH	0.54**	0.60**	0.87**	0.83**	0.80**	0.29**	0.65**	-0.43**	1	
	WS	-0.42**	-0.58**	-0.78**	-0.75**	-0.70**	-0.33**	-0.61**	0.35**	-0.73**	1
Burning period	NH ₃	1									
	PM _{2.5}	0.52*	1								
	NO _x	0.72**	0.81**	1							
	NO ₂	0.62**	0.63**	0.74**	1						
	NO	0.73**	0.78**	0.97**	0.64**	1					
	SO ₂	0.20*	0.47**	0.40*	0.60**	0.31**	1				
	CO	0.74**	0.54**	0.70**	0.32**	0.71**	0.14	1			
	T	-0.33**	-0.53**	-0.52**	-0.08	-0.54**	0.02	-0.62**	1		
	RH	0.51*	0.79**	0.83**	0.58**	0.82**	0.39**	0.52**	-0.72**	1	
	WS	-0.57**	-0.61**	-0.64**	-0.45**	-0.62**	-0.21*	-0.57**	0.61**	-0.70**	1

* Significant at p<0.05 ** Significant at p<0.01

**Table S4.** Observed and predicted concentrations of NH₃ at the Xianghe site during the burning period.

Period	Date	Predicted	Observed
Before	2017/11/15	16.7±9.7	15.5±10.2
	2017/11/16	28.2±10.9	30.2±12.7
	2017/11/17	12.4±10.7	11.2±9.9
	All	19.1±12.3	19±13.6
During	2017/11/18	12.6±5.3	55±65.3
	2017/11/19	30.1±3.1	199.3±144.1
	2017/11/20	34.1±1.8	256.5±154.2
	2017/11/21	37.2±5	66.8±30.3
	All	28.5±10.4	144.4±139.7
After	2017/11/22	26.4±3.4	26.7±4.4
	2017/11/23	20.1±3.7	20.1±4.6
	2017/11/24	15.7±3.4	14.8±4.3
	All	20.7±5.6	20.5±6.6

The unit of NH₃ (ppb).

Table S5. Range and average of the ratio between NH₃ and other air pollutants before and during the burn event.

Period	Ratio	Range	Average
Before	NH ₃ /PM _{2.5}	0.0~14.1	1.2±2.1
	NH ₃ /NO _x	0.1~8.7	0.6±0.8
	NH ₃ /SO ₂	0.8~58.6	8.4±10.9
	NH ₃ /CO	0.001~0.050	0.008±0.005
During	NH ₃ /PM _{2.5}	0.1~66.3	1.9±6.9
	NH ₃ /NO _x	0.3~10.6	1.8±1.8
	NH ₃ /SO ₂	1.1~130.4	20.9±22.9
	NH ₃ /CO	0.001~0.170	0.043±0.037

The unit of NH₃/PM_{2.5}, NH₃/NO_x and NH₃/SO₂ (µg m⁻³/µg m⁻³)

The unit of NH₃/CO (ppb/ppb)