atmosphere

MDPI

Supplementary Materials

Establishment of a Combined Model for Ozone Concentration Simulation with Stepwise Regression Analysis and Artificial Neural Network

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Table S1. Performance of O_3 concentration simulation using SR and ANN models.

City	Model	Adjusted R2	RMSE	MAE
Shijiazhuang	SR	0.7837	28.62	21.90
	ANN	0.8619	22.87	16.59
Baoding	SR	0.7442	31.79	25.01
	ANN	0.8481	24.50	18.16
Cangzhou	SR	0.7431	27.54	21.80
	ANN	0.8199	23.05	17.34
Chengde	SR	0.6541	28.29	21.78
	ANN	0.8206	20.37	15.12
Handan	SR	0.7779	28.00	22.36
	ANN	0.8369	23.99	18.37
Hengshui	SR	0.7566	27.02	20.95
	ANN	0.8052	24.17	18.13
Langfang	SR	0.7352	29.80	23.42
	ANN	0.8366	23.41	17.23
Qinhuangdao	SR	0.6429	29.01	22.30
	ANN	0.7748	23.04	16.53
Tangshan	SR	0.7176	31.51	25.17
	ANN	0.8329	24.23	18.61
Xingtai	SR	0.7842	28.48	22.35
	ANN	0.8403	24.50	18.51
Zhangjiakou	SR	0.7205	22.09	16.42
	ANN	0.8268	17.40	12.17

Table S2. Input parameters for ANN in Shijiazhuang, Baoding, Cangzhou, Chengde, Handan, Hengshui, Langfang, Qinhuangdao, Tangshan, Xingtai and Zhangjiakou.

City	Input parameters
Shijiazhuang	T2M, SSR, WD, $PM_{2.5}$, NO_2, CO, WS
Baoding	T2M, SSR, WD, $PM_{2.5}$, NO_2, CO
Cangzhou	T2M, SSR, WD, $PM_{2.5}$, NO_2, CO
Chengde	T2M, SSR, WD, $PM_{2.5}$, NO_2, BLH, WS, TP
Handan	T2M, SSR, $PM_{2.5}$, NO_2, CO, SP
Hengshui	T2M, SSR, WD, $PM_{2.5}$, NO_2, BLH, WS
Langfang	T2M, SSR, WD, $PM_{2.5}$, NO_2, CO, BLH, WS
Qinhuangdao	T2M, SSR, WD, $PM_{2.5}$, NO_2, BLH, WS, PM_{10}
Tangshan	T2M, SSR, WD, $PM_{2.5}$, NO_2
Xingtai	T2M, SSR, WD, $PM_{2.5}$, NO_2, CO
Zhangjiakou	T2M, SSR, WD, $PM_{2.5}$, NO_2, CO, WS, PM_{10}, SP

Table S3. Performance of ANN on O_3 concentration simulation with different network structures.

City	Activation function	Number of nodes(hidden)	Adjusted R^2	RMSE	MAE
Hengshui	tanh	3	0.8026	24.33	18.21
		4	0.8041	24.24	18.25
		5	0.8052	24.17	18.12
	sigmoid	3	0.7912	25.03	18.73
		4	0.7997	24.51	18.44
		5	0.8002	24.48	18.28
Langfang	tanh	3	0.8279	24.02	17.35
		4	0.8284	23.99	17.47
		5	0.8366	23.41	17.23
	sigmoid	3	0.8211	24.49	18.03
		4	0.8376	23.34	17.02
		5	0.8297	23.90	17.67
Qinhuangdao	tanh	3	0.7463	24.45	17.73
		4	0.7749	23.03	17.03
		5	0.7752	23.04	16.53
	sigmoid	3	0.7465	24.44	18.36
		4	0.7621	23.68	17.11
		5	0.7637	23.60	16.95
Tangshan	tanh	3	0.8269	24.67	18.74
		4	0.8333	24.21	18.20
		5	0.8330	24.23	18.62
	sigmoid	3	0.8191	25.22	19.27
		4	0.8245	24.84	18.77
		5	0.8203	25.14	18.85
Xingtai	tanh	3	0.8356	24.86	18.93
		4	0.8458	24.08	17.99
		5	0.8403	24.50	18.51
	sigmoid	3	0.8376	24.70	18.77
		4	0.8385	24.64	18.72
		5	0.8366	24.78	18.81
Zhangjiakou	tanh	3	0.8092	18.25	13.14
		4	0.8308	17.19	12.32
		5	0.8268	17.40	12.17
	sigmoid	3	0.8076	18.33	13.14
		4	0.8157	17.94	13.02
		5	0.8214	17.66	12.40
Shijiazhuang	tanh	3	0.8513	23.73	17.24
		4	0.8541	23.51	17.08
		5	0.8619	22.87	16.59
	sigmoid	3	0.8512	23.74	17.20
		4	0.8498	23.85	17.49
		5	0.8535	23.56	17.27
Baoding	tanh	3	0.8252	26.28	19.44
		4	0.8352	25.51	18.81
		5	0.8481	24.50	18.16
	sigmoid	3	0.8286	26.02	19.38
		4	0.8200	26.66	20.17

		5	0.8433	24.88	18.40
Cangzhou	tanh	3	0.8040	24.05	18.20
		4	0.8143	23.41	17.47
		5	0.8199	23.05	17.34
	sigmoid	3	0.8033	24.09	18.25
		4	0.8115	23.59	17.77
		5	0.8121	23.55	17.94
Chengde	tanh	3	0.8077	21.09	15.38
		4	0.8352	19.53	13.98
		5	0.8198	20.37	15.12
	sigmoid	3	0.7991	21.56	15.74
		4	0.8118	20.87	15.29
		5	0.8028	21.37	15.42
Handan	tanh	3	0.8345	24.17	18.59
		4	0.8364	24.03	18.61
		5	0.8370	23.99	18.38
	sigmoid	3	0.8265	24.74	19.19
		4	0.8286	24.60	19.08
		5	0.8337	24.23	18.79

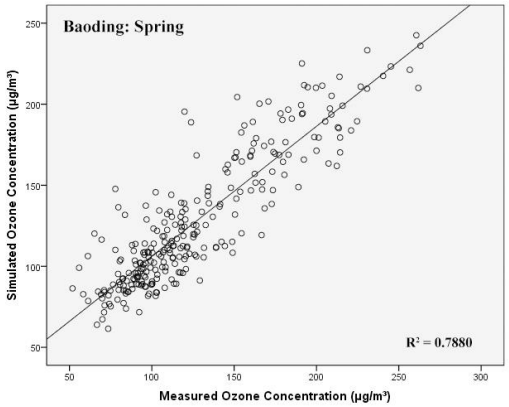
Table S4. Performance of ANN on O3 concentration simulation in different seasons using the optimal network structure.

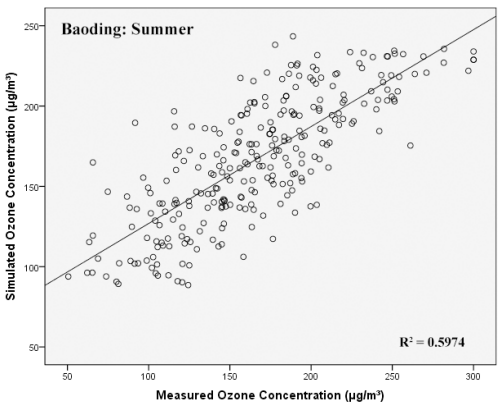
City	Season	Adjusted R^2	RMSE	MAE
Shijiazhuang	spring	0.6835	21.72	15.74
	summer	0.6862	27.38	21.09
	autumn	0.8368	19.80	14.31
	winter	0.7564	12.95	9.48
Baoding	spring	0.7880	20.59	15.51
	summer	0.5974	31.77	25.51
	autumn	0.8504	19.60	14.91
	winter	0.7845	12.73	9.57
Cangzhou	spring	0.6995	20.91	15.66
	summer	0.5712	30.30	24.21
	autumn	0.7713	20.76	14.65
	winter	0.6352	14.27	10.82
Chengde	spring	0.8084	16.29	12.46
	summer	0.6847	24.86	19.35
	autumn	0.7956	16.50	11.79
	winter	0.8748	7.68	5.92
Handan	spring	0.7210	19.94	15.47
	summer	0.6298	28.68	22.93
	autumn	0.7987	22.84	16.92
	winter	0.6276	17.29	13.26
Hengshui	spring	0.6597	21.92	16.79
	summer	0.5569	29.33	21.67
	autumn	0.7155	24.05	17.35
	winter	0.7277	14.09	10.46
Langfang	spring	0.7416	22.67	16.57
	summer	0.6408	29.19	22.33
	autumn	0.8131	20.18	14.65

	winter	0.7798	11.29	8.35
Qinhuangdao	spring	0.7308	18.89	14.70
	summer	0.4599	33.84	25.51
	autumn	0.8018	18.28	12.54
	winter	0.7444	9.11	6.69
Tangshan	spring	0.7545	22.14	16.90
	summer	0.5961	34.42	27.56
	autumn	0.8438	18.68	13.75
	winter	0.7642	10.12	7.98
Xingtai	spring	0.7494	19.14	14.66
	summer	0.6229	29.80	22.87
	autumn	0.7472	24.86	18.63
	winter	0.6005	17.56	13.18
Zhangjiakou	spring	0.7095	17.27	11.93
	summer	0.7165	19.61	15.29
	autumn	0.7860	13.85	10.29
	winter	0.7224	8.36	6.38

Table S5. Prediction performance using SR and ANN models.

City/Province	Model	POD	TS	FAR
Shijiazhuang	SR	0.7234	0.5842	0.2478
	ANN	0.7957	0.6727	0.1870
Baoding	SR	0.7080	0.5710	0.2532
	ANN	0.7560	0.6517	0.1747
Cangzhou	SR	0.6250	0.4874	0.3112
	ANN	0.7222	0.5865	0.2427
Chengde	SR	0.3250	0.3071	0.1522
	ANN	0.7000	0.5563	0.2696
Handan	SR	0.7531	0.5607	0.3130
	ANN	0.8075	0.6433	0.2402
Hengshui	SR	0.6835	0.5438	0.2732
	ANN	0.7798	0.6028	0.2735
Langfang	SR	0.6651	0.5909	0.1588
	ANN	0.8093	0.7045	0.1553
Qinhuangdao	SR	0.2443	0.2238	0.2727
	ANN	0.6183	0.5294	0.2136
Tangshan	SR	0.5742	0.4819	0.2500
	ANN	0.7177	0.6224	0.1758
Xingtai	SR	0.7613	0.5987	0.2629
	ANN	0.8025	0.6655	0.2041
Zhangjiakou	SR	0.3780	0.3529	0.1579
	ANN	0.6378	0.5294	0.2430


Baoding: Spring
R² = 0.7880
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)


Baoding: Summer
R² = 0.5974
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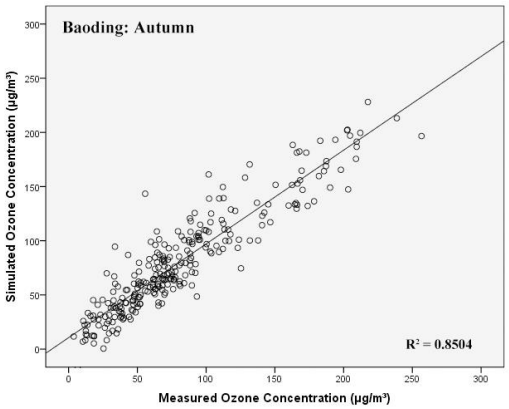
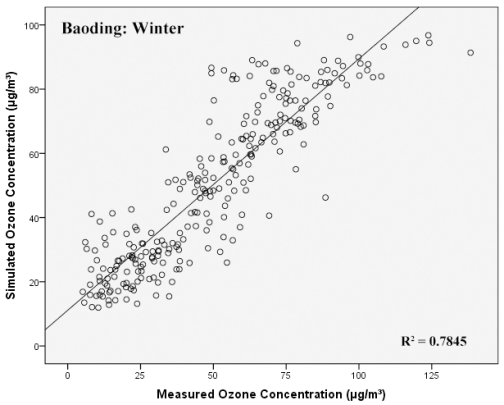
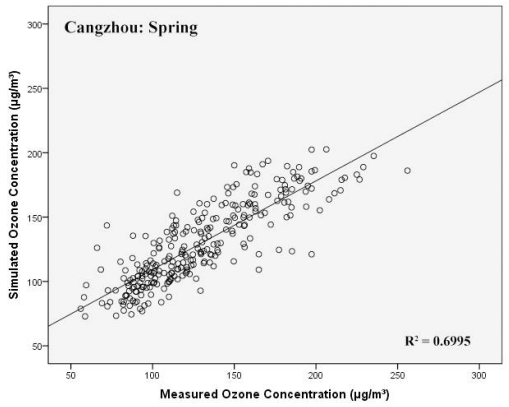
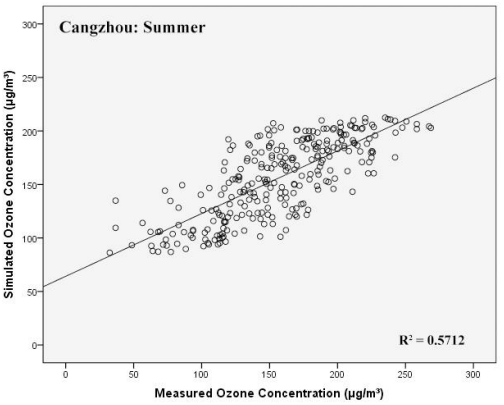
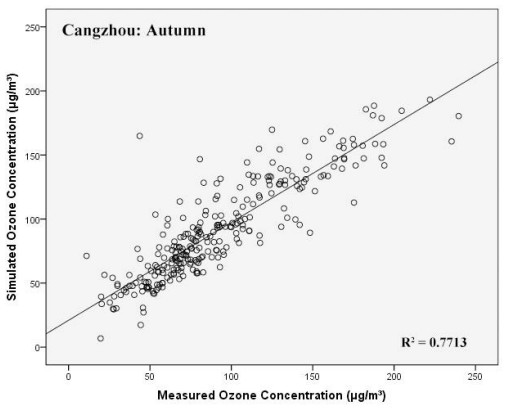
Measured Ozone Concentration (μg/m³)

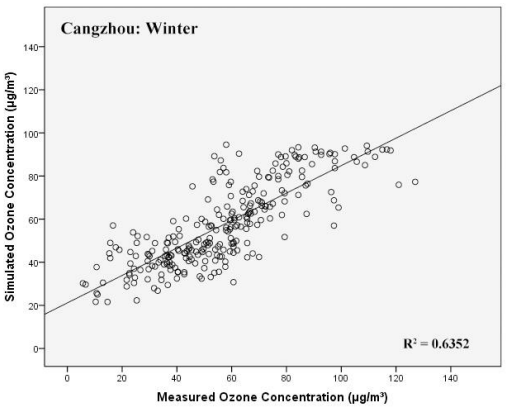

Baoding: Autumn
R² = 0.8504
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)

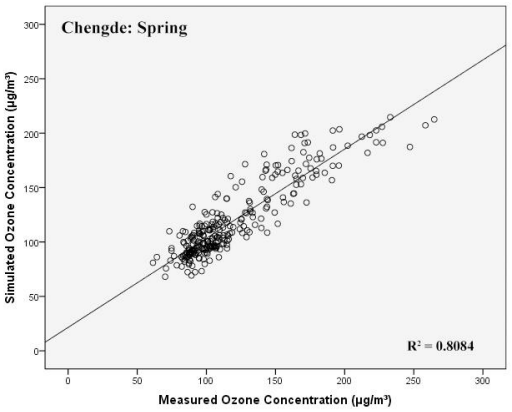

Baoding: Winter
R² = 0.7845
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)

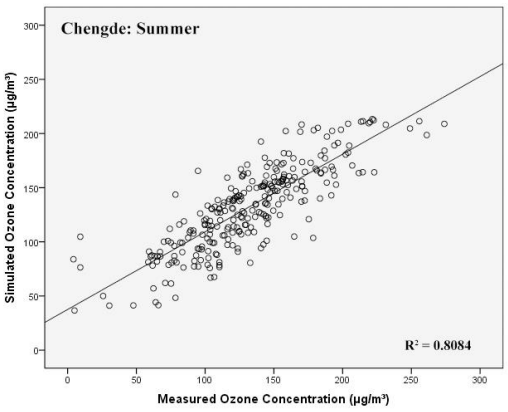

Cangzhou: Spring
R² = 0.6995
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)

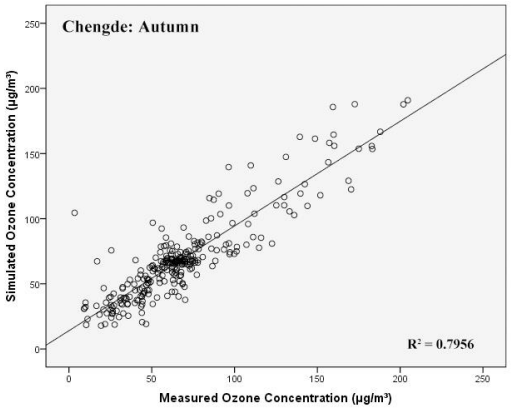

Cangzhou: Summer
R² = 0.5712
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)

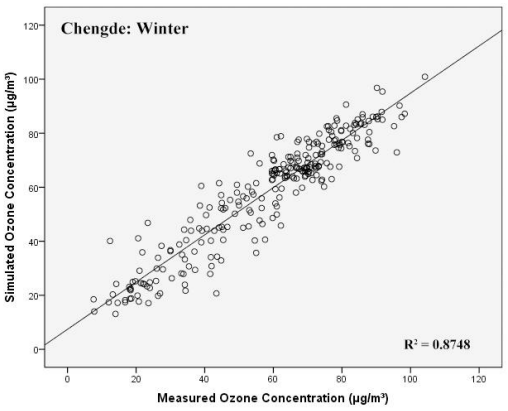

Cangzhou: Autumn
R² = 0.7713
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)

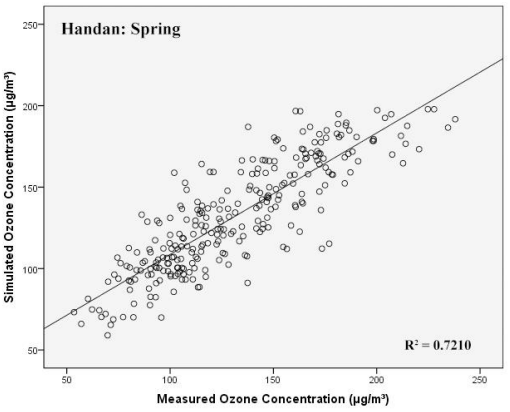

Cangzhou: Winter
R² = 0.6352
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)

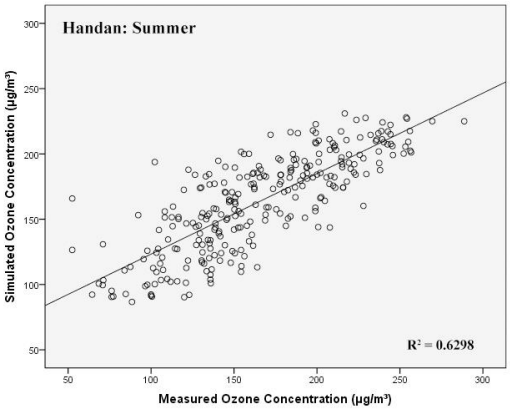

Chengde: Spring
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.8084

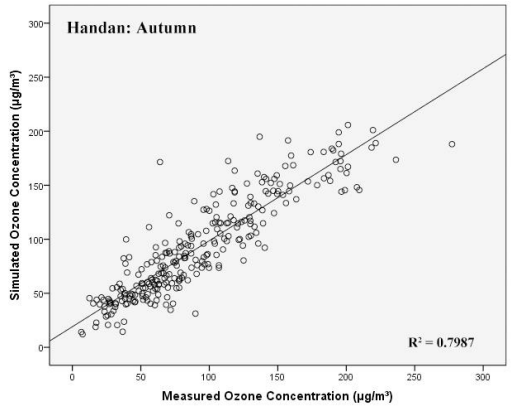

Chengde: Summer
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.8084

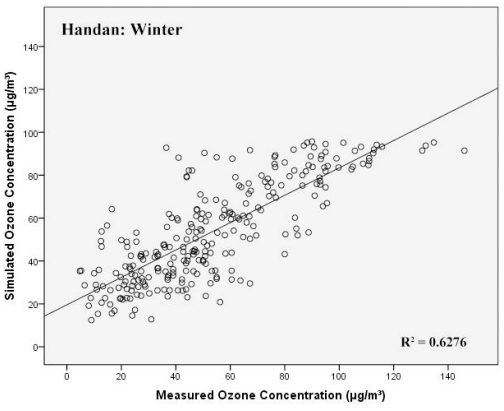

Chengde: Autumn
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.7956

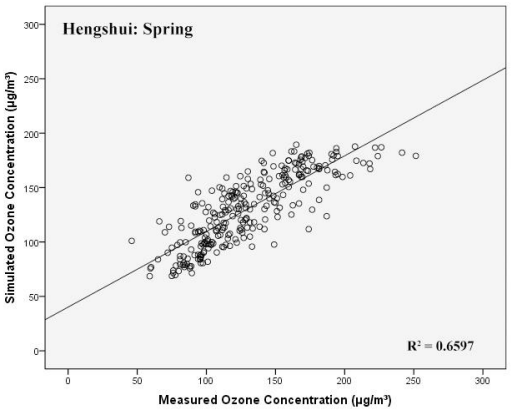

Chengde: Winter
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.8748

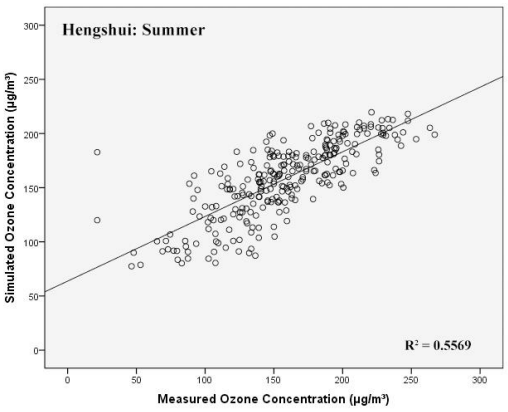

Handan: Spring
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.7210

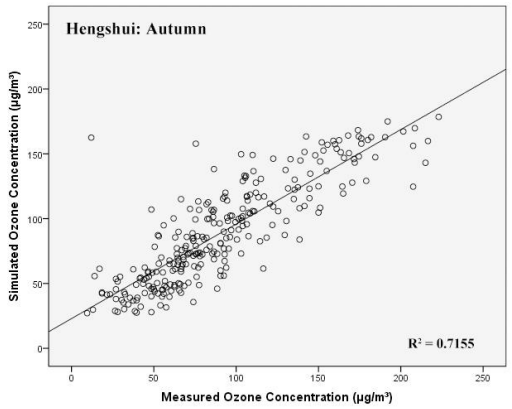

Handan: Summer
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.6298

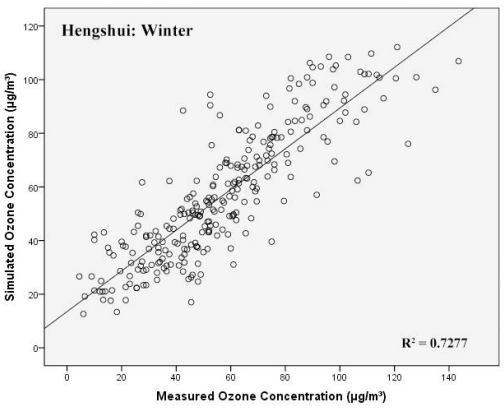

Handan: Autumn
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.7987

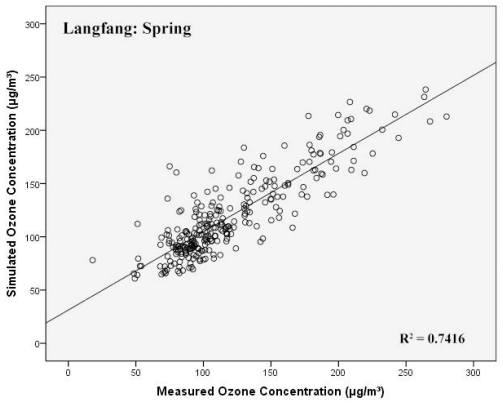

Handan: Winter
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.6276

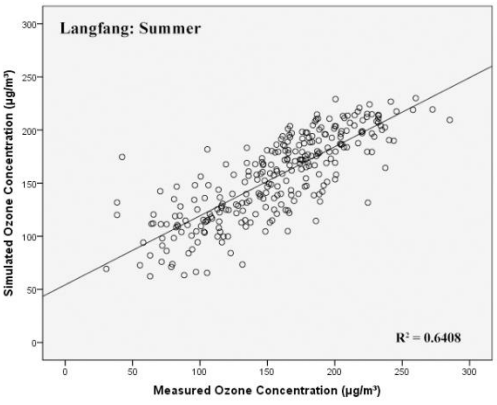

Hengshui: Spring
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.6597

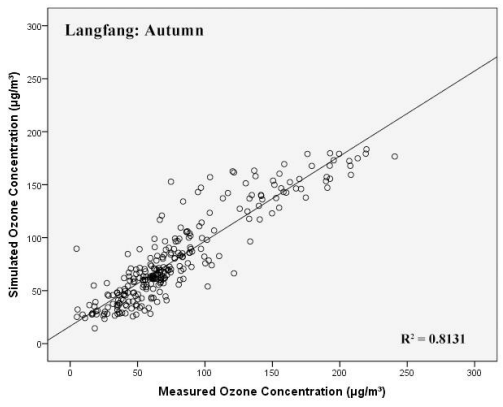

Hengshui: Summer
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.5569

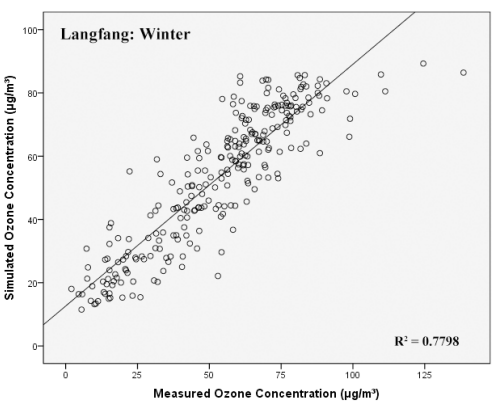

Hengshui: Autumn
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.7155

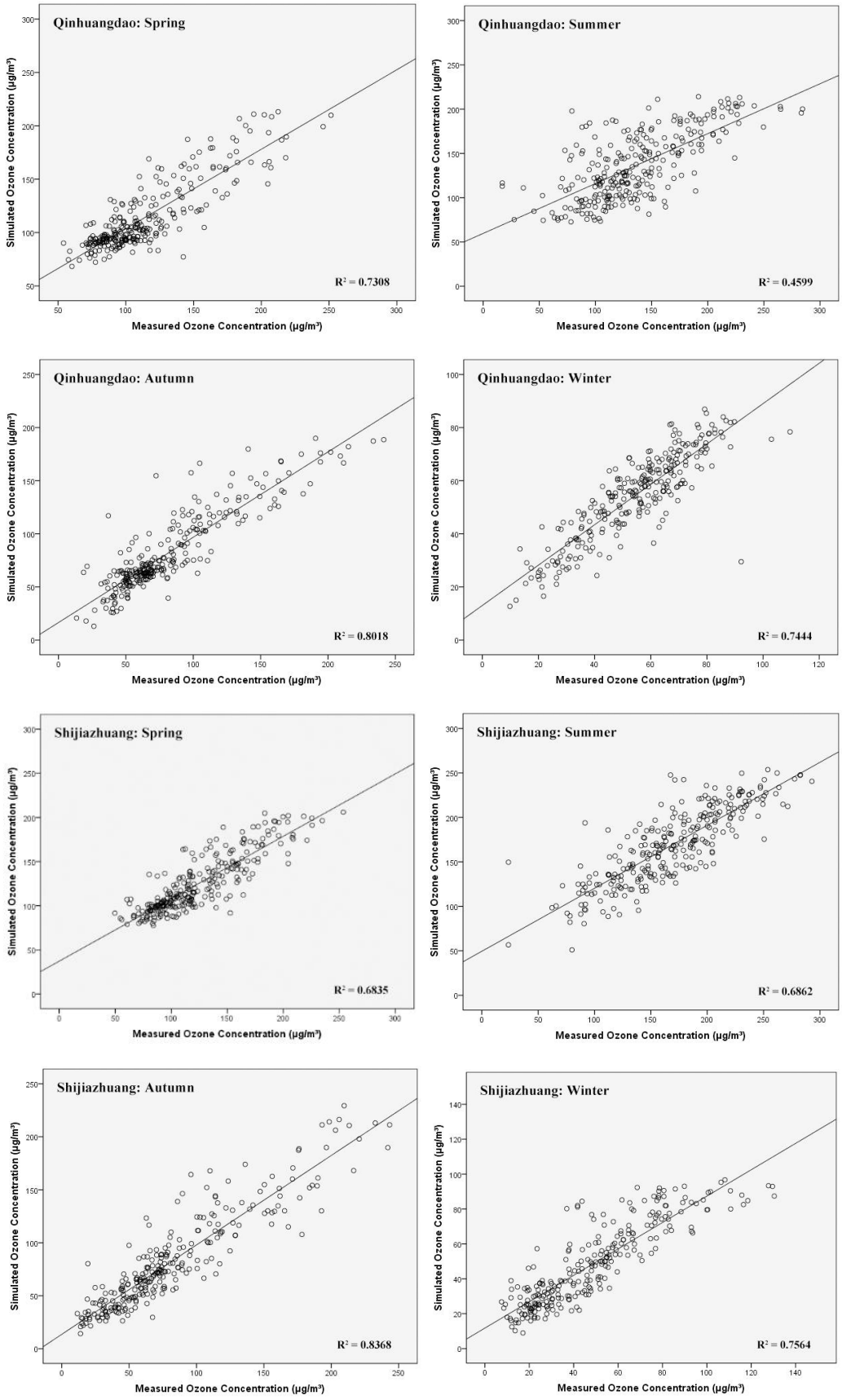

Hengshui: Winter
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.7277

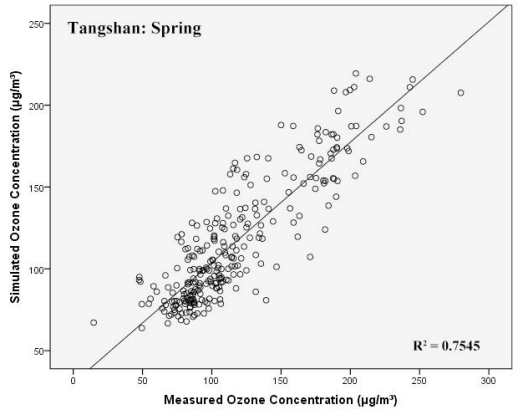

Langfang: Spring
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.7416

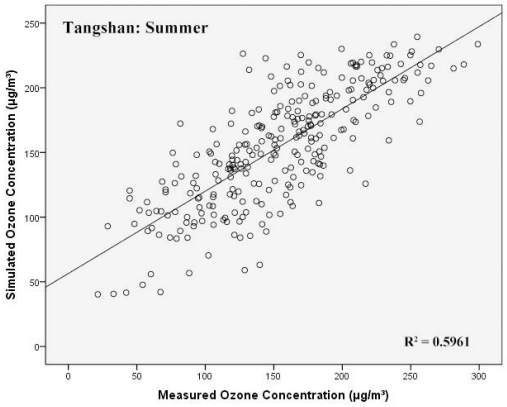

Langfang: Summer
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.6408

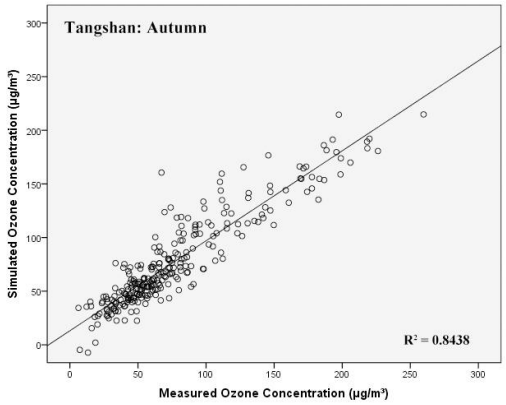

Langfang: Autumn
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.8131

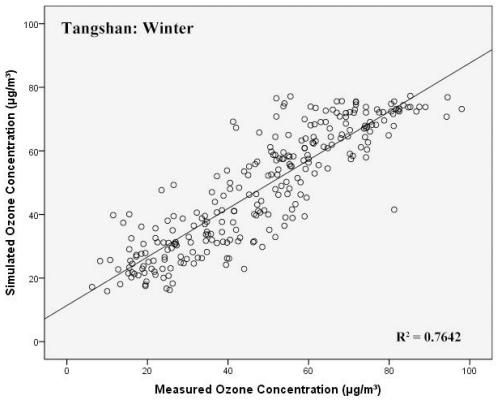

Langfang: Winter
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.7798

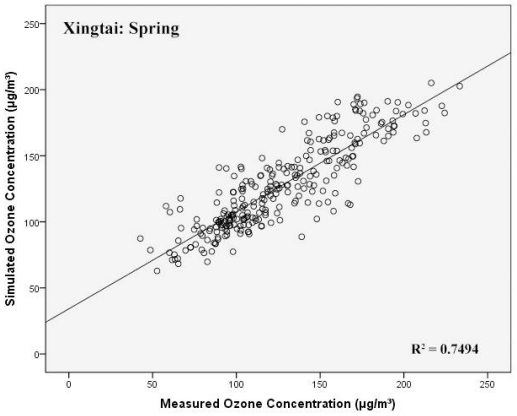

Qinhuangdao: Spring
R² = 0.7308
Qinhuangdao: Summer
R² = 0.4599
Qinhuangdao: Autumn
R² = 0.8018
Qinhuangdao: Winter
R² = 0.7444
Shijiazhuang: Spring
R² = 0.6835
Shijiazhuang: Summer
R² = 0.6862
Shijiazhuang: Autumn
R² = 0.8368
Shijiazhuang: Winter
R² = 0.7564
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)

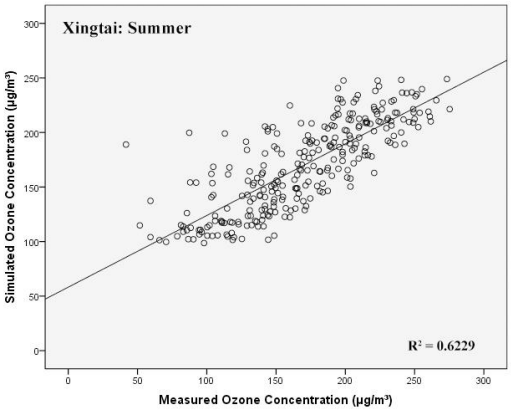

Tangshan: Spring
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.7545

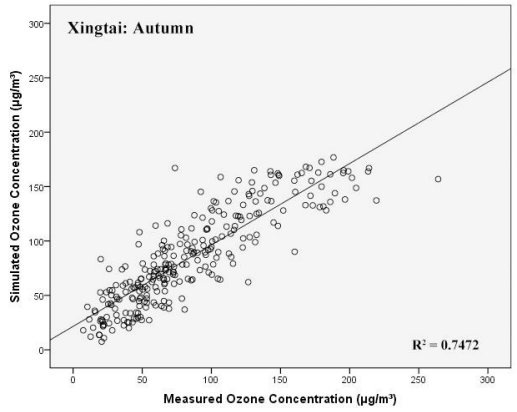

Tangshan: Summer
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.5961

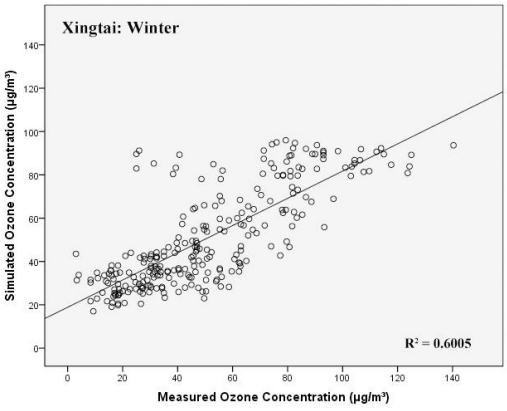

Tangshan: Autumn
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.8438


Tangshan: Winter
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.7642


Xingtai: Spring
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.7494


Xingtai: Summer
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.6229


Xingtai: Autumn
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.7472


Xingtai: Winter
Simulated Ozone Concentration (μg/m³)
Measured Ozone Concentration (μg/m³)
R² = 0.6005

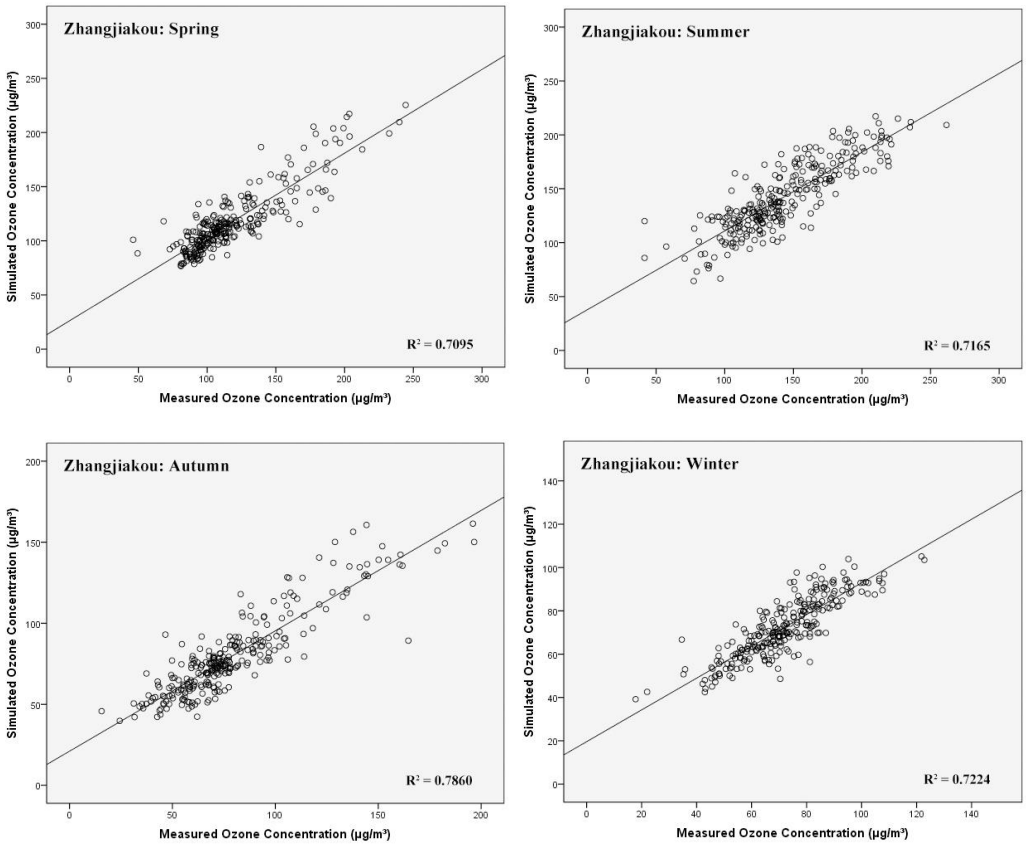


Figure S1. Relationship between the simulated value of O_3_8h and the actual monitored concentration of O_3_8h in each season based on the neural network model with activation function of tanh.