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Quantification of the enhanced effectiveness of NO_x control from simultaneous reductions of VOC and NH_3 for reducing air pollution in the Beijing–Tianjin–Hebei region, China

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Table S1. Control matrix of out-of-sample datasets

	Beijing					Tianjin					HebeiN					HebeiE					HebeiS				
#	NO_x	SO_2	NH_3	VOCs	POA	NO_x	SO_2	NH_3	VOCs	POA	NO_x	SO_2	NH_3	VOCs	POA	NO_x	SO_2	NH_3	VOCs	POA	NO_x	SO_2	NH_3	VOCs	POA
base	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Out-of-sample 100 (OOS100)																									
1	0.073	0.704	0.122	0.324	0.359	0.073	0.704	0.122	0.324	0.359	0.073	0.704	0.122	0.324	0.359	0.073	0.704	0.122	0.324	0.359	0.073	0.704	0.122	0.324	0.359
2	0.182	1.041	0.250	1.015	0.028	0.182	1.041	0.250	1.015	0.028	0.182	1.041	0.250	1.015	0.028	0.182	1.041	0.250	1.015	0.028	0.182	1.041	0.250	1.015	0.028
3	0.636	0.197	0.981	0.431	0.721	0.636	0.197	0.981	0.431	0.721	0.636	0.197	0.981	0.431	0.721	0.636	0.197	0.981	0.431	0.721	0.636	0.197	0.981	0.431	0.721
4	0.522	0.351	0.178	0.107	0.162	0.522	0.351	0.178	0.107	0.162	0.522	0.351	0.178	0.107	0.162	0.522	0.351	0.178	0.107	0.162	0.522	0.351	0.178	0.107	0.162
5	0.583	0.994	0.702	0.259	0.572	0.583	0.994	0.702	0.259	0.572	0.583	0.994	0.702	0.259	0.572	0.583	0.994	0.702	0.259	0.572	0.583	0.994	0.702	0.259	0.572
6	0.837	0.431	0.385	0.082	0.644	0.837	0.431	0.385	0.082	0.644	0.837	0.431	0.385	0.082	0.644	0.837	0.431	0.385	0.082	0.644	0.837	0.431	0.385	0.082	0.644
7	0.814	0.081	0.420	1.065	1.186	0.814	0.081	0.420	1.065	1.186	0.814	0.081	0.420	1.065	1.186	0.814	0.081	0.420	1.065	1.186	0.814	0.081	0.420	1.065	1.186
8	0.114	0.886	0.440	0.935	0.439	0.114	0.886	0.440	0.935	0.439	0.114	0.886	0.440	0.935	0.439	0.114	0.886	0.440	0.935	0.439	0.114	0.886	0.440	0.935	0.439
9	0.573	0.825	0.403	0.991	0.714	0.573	0.825	0.403	0.991	0.714	0.573	0.825	0.403	0.991	0.714	0.573	0.825	0.403	0.991	0.714	0.573	0.825	0.403	0.991	0.714
10	0.688	1.007	1.104	0.676	0.268	0.688	1.007	1.104	0.676	0.268	0.688	1.007	1.104	0.676	0.268	0.688	1.007	1.104	0.676	0.268	0.688	1.007	1.104	0.676	0.268
11	0.223	0.153	0.547	0.186	0.038	0.223	0.153	0.547	0.186	0.038	0.223	0.153	0.547	0.186	0.038	0.223	0.153	0.547	0.186	0.038	0.223	0.153	0.547	0.186	0.038
12	0.411	0.086	0.798	1.144	0.181	0.411	0.086	0.798	1.144	0.181	0.411	0.086	0.798	1.144	0.181	0.411	0.086	0.798	1.144	0.181	0.411	0.086	0.798	1.144	0.181
13	0.723	0.116	1.140	0.911	1.122	0.723	0.116	1.140	0.911	1.122	0.723	0.116	1.140	0.911	1.122	0.723	0.116	1.140	0.911	1.122	0.723	0.116	1.140	0.911	1.122
14	0.231	0.904	0.517	0.494	0.931	0.231	0.904	0.517	0.494	0.931	0.231	0.904	0.517	0.494	0.931	0.231	0.904	0.517	0.494	0.931	0.231	0.904	0.517	0.494	0.931
15	0.992	0.810	0.899	0.687	1.029	0.992	0.810	0.899	0.687	1.029	0.992	0.810	0.899	0.687	1.029	0.992	0.810	0.899	0.687	1.029	0.992	0.810	0.899	0.687	1.029
16	0.622	0.123	0.083	0.529	0.592	0.622	0.123	0.083	0.529	0.592	0.622	0.123	0.083	0.529	0.592	0.622	0.123	0.083	0.529	0.592	0.622	0.123	0.083	0.529	0.592
17	0.287	1.115	0.105	0.773	0.408	0.287	1.115	0.105	0.773	0.408	0.287	1.115	0.105	0.773	0.408	0.287	1.115	0.105	0.773	0.408	0.287	1.115	0.105	0.773	0.408
18	0.913	0.626	0.162	1.074	0.954	0.913	0.626	0.162	1.074	0.954	0.913	0.626	0.162	1.074	0.954	0.913	0.626	0.162	1.074	0.954	0.913	0.626	0.162	1.074	0.954
19	0.328	1.084	0.820	1.174	0.796	0.328	1.084	0.820	1.174	0.796	0.328	1.084	0.820	1.174	0.796	0.328	1.084	0.820	1.174	0.796	0.328	1.084	0.820	1.174	0.796
20	0.589	0.741	1.172	0.961	0.423	0.589	0.741	1.172	0.961	0.423	0.589	0.741	1.172	0.961	0.423	0.589	0.741	1.172	0.961	0.423	0.589	0.741	1.172	0.961	0.423
21	0.299	0.310	0.766	0.801	0.872	0.299	0.310	0.766	0.801	0.872	0.299	0.310	0.766	0.801	0.872	0.299	0.310	0.766	0.801	0.872	0.299	0.310	0.766	0.801	0.872
22	0.025	0.454	0.868	0.442	0.557	0.025	0.454	0.868	0.442	0.557	0.025	0.454	0.868	0.442	0.557	0.025	0.454	0.868	0.442	0.557	0.025	0.454	0.868	0.442	0.557
23	0.144	0.255	0.857	1.188	0.314	0.144	0.255	0.857	1.188	0.314	0.144	0.255	0.857	1.188	0.314	0.144	0.255	0.857	1.188	0.314	0.144	0.255	0.857	1.188	0.314
24	0.844	0.347	0.234	0.851	0.138	0.844	0.347	0.234	0.851	0.138	0.844	0.347	0.234	0.851	0.138	0.844	0.347	0.234	0.851	0.138	0.844	0.347	0.234	0.851	0.138
25	0.265	0.971	0.642	0.980	0.603	0.265	0.971	0.642	0.980	0.603	0.265	0.971	0.642	0.980	0.603	0.265	0.971	0.642	0.980	0.603	0.265	0.971	0.642	0.980	0.603
26	0.424	0.566	0.445	0.203	0.476	0.424	0.566	0.445	0.203	0.476	0.424	0.566	0.445	0.203	0.476	0.424	0.566	0.445	0.203	0.476	0.424	0.566	0.445	0.203	0.476
27	0.384	1.171	0.310	0.874	0.208	0.384	1.171	0.310	0.874	0.208	0.384	1.171	0.310	0.874	0.208	0.384	1.171	0.310	0.874	0.208	0.384	1.171	0.310	0.874	0.208
28	1.105	0.768	0.924	0.273	1.116	1.105	0.768	0.924	0.273	1.116	1.105	0.768	0.924	0.273	1.116	1.105	0.768	0.924	0.273	1.116	1.105	0.768	0.924	0.273	1.116
29	0.962	0.298	0.272	0.818	1.098	0.962	0.298	0.272	0.818	1.098	0.962	0.298	0.272	0.818	1.098	0.962	0.298	0.272	0.818	1.098	0.962	0.298	0.272	0.818	1.098
30	0.673	0.383	1.180	0.163	1.056	0.673	0.383	1.180	0.163	1.056	0.673	0.383	1.180	0.163	1.056	0.673	0.383	1.180	0.163	1.056	0.673	0.383	1.180	0.163	1.056
31	0.471	0.591	0.669	0.391	0.446	0.471	0.591	0.669	0.391	0.446	0.471	0.591	0.669	0.391	0.446	0.471	0.591	0.669	0.391	0.446	0.471	0.591	0.669	0.391	0.446
32	0.553	1.059	1.119	0.402	0.076	0.553	1.059	1.119	0.402	0.076	0.553	1.059	1.119	0.402	0.076	0.553	1.059	1.119	0.402	0.076	0.553	1.059	1.119	0.402	0.076
33	0.863	0.729	0.149	0.650	0.688	0.863	0.729	0.149	0.650	0.688	0.863	0.729	0.149	0.650	0.688	0.863	0.729	0.149	0.650	0.688	0.863	0.729	0.149	0.650	0.688
34	0.449	0.509	0.355	0.704	0.650	0.449	0.509	0.355	0.704	0.650	0.449	0.509	0.355	0.704	0.650	0.449	0.509	0.355	0.704	0.650	0.449	0.509	0.355	0.704	0.650
35	0.172	0.875	0.753	0.467	0.099	0.172	0.875	0.753	0.467	0.099	0.172	0.875	0.753	0.467	0.099	0.172	0.875	0.753	0.467	0.099	0.172	0.875	0.753	0.467	0.099
36	1.191	0.891	0.317	0.134	0.398	1.191	0.891	0.317	0.134	0.398	1.191	0.891	0.317	0.134	0.398	1.191	0.891	0.317	0.134	0.398	1.191	0.891	0.317	0.134	0.398
37	0.089	0.142	0.186	0.299	0.977	0.089	0.142	0.186	0.299	0.977	0.089	0.142	0.186	0.299	0.977	0.089	0.142	0.186	0.299	0.977	0.089	0.142	0.186	0.299	0.977
38	0.322	0.022	0.291	1.100	0.196	0.322	0.022	0.291	1.100	0.196	0.322	0.022	0.291	1.100	0.196	0.322	0.022	0.291	1.100	0.196	0.322	0.022	0.291	1.100	0.196
39	0.358	0.466	0.594	0.737	0.277	0.358	0.466	0.594	0.737	0.277	0.358	0.466	0.594	0.737	0.277	0.358	0.466	0.594	0.737	0.277	0.358	0.466	0.594	0.737	0.277

40	0.257	0.065	0.198	1.185	0.876	0.257	0.065	0.198	1.185	0.876	0.257	0.065	0.198	1.185	0.876	0.257	0.065	0.198	1.185	0.876	0.257	0.065	0.198	1.185	0.876
41	0.165	0.051	0.572	0.354	0.992	0.165	0.051	0.572	0.354	0.992	0.165	0.051	0.572	0.354	0.992	0.165	0.051	0.572	0.354	0.992	0.165	0.051	0.572	0.354	0.992
42	1.132	1.050	0.970	0.280	0.467	1.132	1.050	0.970	0.280	0.467	1.132	1.050	0.970	0.280	0.467	1.132	1.050	0.970	0.280	0.467	1.132	1.050	0.970	0.280	0.467
43	1.042	1.018	0.829	0.448	0.071	1.042	1.018	0.829	0.448	0.071	1.042	1.018	0.829	0.448	0.071	1.042	1.018	0.829	0.448	0.071	1.042	1.018	0.829	0.448	0.071
44	0.301	0.243	0.930	0.237	1.075	0.301	0.243	0.930	0.237	1.075	0.301	0.243	0.930	0.237	1.075	0.301	0.243	0.930	0.237	1.075	0.301	0.243	0.930	0.237	1.075
45	1.016	0.746	1.152	0.004	0.760	1.016	0.746	1.152	0.004	0.760	1.016	0.746	1.152	0.004	0.760	1.016	0.746	1.152	0.004	0.760	1.016	0.746	1.152	0.004	0.760
46	0.714	0.316	0.064	0.958	0.058	0.714	0.316	0.064	0.958	0.058	0.714	0.316	0.064	0.958	0.058	0.714	0.316	0.064	0.958	0.058	0.714	0.316	0.064	0.958	0.058
47	0.106	0.788	1.076	0.218	0.509	0.106	0.788	1.076	0.218	0.509	0.106	0.788	1.076	0.218	0.509	0.106	0.788	1.076	0.218	0.509	0.106	0.788	1.076	0.218	0.509
48	0.758	0.326	0.612	0.147	0.745	0.758	0.326	0.612	0.147	0.745	0.758	0.326	0.612	0.147	0.745	0.758	0.326	0.612	0.147	0.745	0.758	0.326	0.612	0.147	0.745
49	0.040	0.803	0.731	0.477	1.002	0.040	0.803	0.731	0.477	1.002	0.040	0.803	0.731	0.477	1.002	0.040	0.803	0.731	0.477	1.002	0.040	0.803	0.731	0.477	1.002
50	0.899	0.693	0.495	0.643	0.624	0.899	0.693	0.495	0.643	0.624	0.899	0.693	0.495	0.643	0.624	0.899	0.693	0.495	0.643	0.624	0.899	0.693	0.495	0.643	0.624
51	0.530	0.983	0.537	0.579	0.364	0.530	0.983	0.537	0.579	0.364	0.530	0.983	0.537	0.579	0.364	0.530	0.983	0.537	0.579	0.364	0.530	0.983	0.537	0.579	0.364
52	0.511	0.520	0.772	0.242	0.805	0.511	0.520	0.772	0.242	0.805	0.511	0.520	0.772	0.242	0.805	0.511	0.520	0.772	0.242	0.805	0.511	0.520	0.772	0.242	0.805
53	0.023	0.758	0.780	0.366	0.768	0.023	0.758	0.780	0.366	0.768	0.023	0.758	0.780	0.366	0.768	0.023	0.758	0.780	0.366	0.768	0.023	0.758	0.780	0.366	0.768
54	0.950	0.651	0.911	1.030	1.088	0.950	0.651	0.911	1.030	1.088	0.950	0.651	0.911	1.030	1.088	0.950	0.651	0.911	1.030	1.088	0.950	0.651	0.911	1.030	1.088
55	0.791	0.927	0.879	0.116	0.855	0.791	0.927	0.879	0.116	0.855	0.791	0.927	0.879	0.116	0.855	0.791	0.927	0.879	0.116	0.855	0.791	0.927	0.879	0.116	0.855
56	0.933	0.231	0.951	1.127	0.221	0.933	0.231	0.951	1.127	0.221	0.933	0.231	0.951	1.127	0.221	0.933	0.231	0.951	1.127	0.221	0.933	0.231	0.951	1.127	0.221
57	0.550	0.362	0.045	0.490	0.524	0.550	0.362	0.045	0.490	0.524	0.550	0.362	0.045	0.490	0.524	0.550	0.362	0.045	0.490	0.524	0.550	0.362	0.045	0.490	0.524
58	0.780	0.035	1.193	0.069	0.682	0.780	0.035	1.193	0.069	0.682	0.780	0.035	1.193	0.069	0.682	0.780	0.035	1.193	0.069	0.682	0.780	0.035	1.193	0.069	0.682
59	0.011	0.394	0.514	0.590	0.542	0.011	0.394	0.514	0.590	0.542	0.011	0.394	0.514	0.590	0.542	0.011	0.394	0.514	0.590	0.542	0.011	0.394	0.514	0.590	0.542
60	0.482	0.407	0.029	0.213	0.232	0.482	0.407	0.029	0.213	0.232	0.482	0.407	0.029	0.213	0.232	0.482	0.407	0.029	0.213	0.232	0.482	0.407	0.029	0.213	0.232
61	1.100	0.945	0.712	0.310	0.841	1.100	0.945	0.712	0.310	0.841	1.100	0.945	0.712	0.310	0.841	1.100	0.945	0.712	0.310	0.841	1.100	0.945	0.712	0.310	0.841
62	1.031	0.620	0.673	0.612	0.740	1.031	0.620	0.673	0.612	0.740	1.031	0.620	0.673	0.612	0.740	1.031	0.620	0.673	0.612	0.740	1.031	0.620	0.673	0.612	0.740
63	1.060	1.093	0.485	0.129	0.244	1.060	1.093	0.485	0.129	0.244	1.060	1.093	0.485	0.129	0.244	1.060	1.093	0.485	0.129	0.244	1.060	1.093	0.485	0.129	0.244
64	0.945	0.713	0.218	0.035	0.829	0.945	0.713	0.218	0.035	0.829	0.945	0.713	0.218	0.035	0.829	0.945	0.713	0.218	0.035	0.829	0.945	0.713	0.218	0.035	0.829
65	0.663	0.046	0.998	1.080	1.066	0.663	0.046	0.998	1.080	1.066	0.663	0.046	0.998	1.080	1.066	0.663	0.046	0.998	1.080	1.066	0.663	0.046	0.998	1.080	1.066
66	0.816	0.546	0.985	0.834	0.480	0.816	0.546	0.985	0.834	0.480	0.816	0.546	0.985	0.834	0.480	0.816	0.546	0.985	0.834	0.480	0.816	0.546	0.985	0.834	0.480
67	1.149	0.670	0.654	0.523	0.092	1.149	0.670	0.654	0.523	0.092	1.149	0.670	0.654	0.523	0.092	1.149	0.670	0.654	0.523	0.092	1.149	0.670	0.654	0.523	0.092
68	0.877	1.030	0.287	1.005	0.177	0.877	1.030	0.287	1.005	0.177	0.877	1.030	0.287	1.005	0.177	0.877	1.030	0.287	1.005	0.177	0.877	1.030	0.287	1.005	0.177
69	0.748	0.538	0.340	0.505	1.014	0.748	0.538	0.340	0.505	1.014	0.748	0.538	0.340	0.505	1.014	0.748	0.538	0.340	0.505	1.014	0.748	0.538	0.340	0.505	1.014
70	0.982	0.101	1.092	0.946	0.148	0.982	0.101	1.092	0.946	0.148	0.982	0.101	1.092	0.946	0.148	0.982	0.101	1.092	0.946	0.148	0.982	0.101	1.092	0.946	0.148
71	0.141	0.213	1.086	1.040	0.613	0.141	0.213	1.086	1.040	0.613	0.141	0.213	1.086	1.040	0.613	0.141	0.213	1.086	1.040	0.613	0.141	0.213	1.086	1.040	0.613
72	0.502	0.415	0.844	1.128	0.373	0.502	0.415	0.844	1.128	0.373	0.502	0.415	0.844	1.128	0.373	0.502	0.415	0.844	1.128	0.373	0.502	0.415	0.844	1.128	0.373
73	1.049	1.123	0.331	0.732	0.946	1.049	1.123	0.331	0.732	0.946	1.049	1.123	0.331	0.732	0.946	1.049	1.123	0.331	0.732	0.946	1.049	1.123	0.331	0.732	0.946
74	0.438	1.147	0.382	0.889	1.155	0.438	1.147	0.382	0.889	1.155	0.438	1.147	0.382	0.889	1.155	0.438	1.147	0.382	0.889	1.155	0.438	1.147	0.382	0.889	1.155
75	0.216	0.846	0.210	0.542	1.173	0.216	0.846	0.210	0.542	1.173	0.216	0.846	0.210	0.542	1.173	0.216	0.846	0.210	0.542	1.173	0.216	0.846	0.210	0.542	1.173
76	1.181	1.074	0.613	0.750	0.888	1.181	1.074	0.613	0.750	0.888	1.181	1.074	0.613	0.750	0.888	1.181	1.074	0.613	0.750	0.888	1.181	1.074	0.613	0.750	0.888
77	0.631	0.857	1.035	0.326	1.191	0.631	0.857	1.035	0.326	1.191	0.631	0.857	1.035	0.326	1.191	0.631	0.857	1.035	0.326	1.191	0.631	0.857	1.035	0.326	1.191
78	1.081	0.917	0.010	0.665	1.042	1.081	0.917	0.010	0.665	1.042	1.081	0.917	0.010	0.665	1.042	1.081	0.917	0.010	0.665	1.042	1.081	0.917	0.010	0.665	1.042
79	0.462	1.194	0.022	0.919	0.699	0.462	1.194	0.022	0.919	0.699	0.462	1.194	0.022	0.919	0.699	0.462	1.194	0.022	0.919	0.699	0.462	1.194	0.022	0.919	0.699
80	0.909	0.267	0.473	0.711	0.120	0.909	0.267	0.473	0.711	0.120	0.909	0.267	0.473	0.711	0.120	0.909	0.267	0.473	0.711	0.120	0.909	0.267	0.473	0.711	0.120
81	0.866	0.679	1.031	0.343	0.533	0.866	0.679	1.031	0.343	0.533	0.866	0.679	1.031	0.343	0.533	0.866	0.679	1.031	0.343	0.533	0.866	0.679	1.031	0.343	0.533
82	0.699	0.471	0.052	0.863	0.021	0.699	0.471	0.052	0.863	0.021	0.699	0.471	0.052	0.863	0.021	0.699	0.471	0.052	0.863	0.021	0.699	0.471	0.052	0.863	0.021
83	0.124	0.642	0.261	0.756	0.498	0.124	0.642	0.261	0.756	0.498	0.124	0.642	0.261	0.756	0.498	0.124	0.642	0.261	0.756	0.498	0.124	0.642	0.261	0.756	0.498
84	1.116	0.004	0.629	0.045	0.310	1.116	0.004	0.629	0.045	0.310	1.116	0.004	0.629	0.045	0.310	1.116	0.004	0.629	0.045	0.310	1.116	0.004	0.629	0.045	0.310

85	0.061	0.838	0.113	0.603	0.825	0.061	0.838	0.113	0.603	0.825	0.061	0.838	0.113	0.603	0.825	0.061	0.838	0.113	0.603	0.825	0.061	0.838	0.113	0.603	0.825
86	0.606	0.176	0.694	0.058	0.300	0.606	0.176	0.694	0.058	0.300	0.606	0.176	0.694	0.058	0.300	0.606	0.176	0.694	0.058	0.300	0.606	0.176	0.694	0.058	0.300
87	0.242	0.157	0.143	0.018	0.262	0.242	0.157	0.143	0.018	0.262	0.242	0.157	0.143	0.018	0.262	0.242	0.157	0.143	0.018	0.262	0.242	0.157	0.143	0.018	0.262
88	0.996	0.558	0.092	0.885	0.960	0.996	0.558	0.092	0.885	0.960	0.996	0.558	0.092	0.885	0.960	0.996	0.558	0.092	0.885	0.960	0.996	0.558	0.092	0.885	0.960
89	1.162	0.181	0.946	1.053	0.906	1.162	0.181	0.946	1.053	0.906	1.162	0.181	0.946	1.053	0.906	1.162	0.181	0.946	1.053	0.906	1.162	0.181	0.946	1.053	0.906
90	0.360	0.957	0.742	0.373	1.143	0.360	0.957	0.742	0.373	1.143	0.360	0.957	0.742	0.373	1.143	0.360	0.957	0.742	0.373	1.143	0.360	0.957	0.742	0.373	1.143
91	1.073	0.609	1.160	0.629	0.119	1.073	0.609	1.160	0.629	0.119	1.073	0.609	1.160	0.629	0.119	1.073	0.609	1.160	0.629	0.119	1.073	0.609	1.160	0.629	0.119
92	0.401	1.154	0.560	0.094	0.791	0.401	1.154	0.560	0.094	0.791	0.401	1.154	0.560	0.094	0.791	0.401	1.154	0.560	0.094	0.791	0.401	1.154	0.560	0.094	0.791
93	0.344	0.485	0.414	0.575	0.667	0.344	0.485	0.414	0.575	0.667	0.344	0.485	0.414	0.575	0.667	0.344	0.485	0.414	0.575	0.667	0.344	0.485	0.414	0.575	0.667
94	0.795	0.499	0.579	0.807	0.342	0.795	0.499	0.579	0.807	0.342	0.795	0.499	0.579	0.807	0.342	0.795	0.499	0.579	0.807	0.342	0.795	0.499	0.579	0.807	0.342
95	0.054	0.584	1.016	1.161	0.324	0.054	0.584	1.016	1.161	0.324	0.054	0.584	1.016	1.161	0.324	0.054	0.584	1.016	1.161	0.324	0.054	0.584	1.016	1.161	0.324
96	0.648	1.139	0.369	0.417	0.009	0.648	1.139	0.369	0.417	0.009	0.648	1.139	0.369	0.417	0.009	0.648	1.139	0.369	0.417	0.009	0.648	1.139	0.369	0.417	0.009
97	0.381	0.225	1.053	1.111	0.919	0.381	0.225	1.053	1.111	0.919	0.381	0.225	1.053	1.111	0.919	0.381	0.225	1.053	1.111	0.919	0.381	0.225	1.053	1.111	0.919
98	0.197	0.437	1.062	0.787	0.581	0.197	0.437	1.062	0.787	0.581	0.197	0.437	1.062	0.787	0.581	0.197	0.437	1.062	0.787	0.581	0.197	0.437	1.062	0.787	0.581
99	1.174	0.286	0.465	0.562	0.388	1.174	0.286	0.465	0.562	0.388	1.174	0.286	0.465	0.562	0.388	1.174	0.286	0.465	0.562	0.388	1.174	0.286	0.465	0.562	0.388
100	0.737	1.183	0.815	0.170	1.131	0.737	1.183	0.815	0.170	1.131	0.737	1.183	0.815	0.170	1.131	0.737	1.183	0.815	0.170	1.131	0.737	1.183	0.815	0.170	1.131
Out-of-sample 15 (OOS15)																									
1	0.1	0.1	0.1	0.1	0.1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	0.5	0.5	0.5	0.5	0.5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
3	1.15	1.15	1.15	1.15	1.15	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
4	1	1	1	1	1	0.1	0.1	0.1	0.1	0.1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	1	0.5	0.5	0.5	0.5	0.5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
6	1	1	1	1	1	1.15	1.15	1.15	1.15	1.15	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
7	1	1	1	1	1	1	1	1	1	1	0.1	0.1	0.1	0.1	0.1	1	1	1	1	1	1	1	1	1	1
8	1	1	1	1	1	1	1	1	1	1	0.5	0.5	0.5	0.5	0.5	1	1	1	1	1	1	1	1	1	1
9	1	1	1	1	1	1	1	1	1	1	1.15	1.15	1.15	1.15	1.15	1	1	1	1	1	1	1	1	1	1
10	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.1	0.1	0.1	0.1	0.1	1	1	1	1	1
11	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.5	0.5	0.5	0.5	0.5	1	1	1	1	1
12	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1.15	1.15	1.15	1.15	1.15	1	1	1	1	1
13	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.1	0.1	0.1	0.1	0.1
14	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.5	0.5	0.5	0.5	0.5
15	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1.15	1.15	1.15	1.15	1.15

Table S2. Performance of $PM_{2.5}$ and O_3 prediction using pf-RSM across grid cells

		MaxNE	MeanNE						
$PM_{2.5}$			Pollution levels						All
			<25	25-50	50-75	75-100	100-125	>125	
	Case1	0.88%	0.16%	0.16%	0.08%	0.07%	0.06%	0.03%	0.12%
	Case2	5.64%	0.76%	0.71%	0.79%	1.12%	2.22%	1.73%	0.90%
		MaxNE	MeanNE						
O_3			Pollution levels						All
			<60	60-70	70-80	80-90	90-100	>100	
	Case1	0.79%	0.02%	0.05%	0.08%	0.09%	0.08%	0.16%	0.07%
	Case2	1.95%	0.08%	0.26%	0.30%	0.29%	0.22%	0.29%	0.26%

*$PM_{2.5}$ and O_3 concentrations are calculated based on monthly averaged concentrations at each grid cell

Table S3. Performance of $PM_{2.5}$ and O_3 prediction using pf-RSM across days

			MaxNE	MeanNE						
				Pollution levels						All
				<25	25-50	50-75	75-100	100-125	>125	
$PM_{2.5}$	Case1	Beijing	0.69%	0.23%	0.32%	0.21%	0.23%	0.36%	0.44%	0.28%
		Tianjin	1.23%	-	0.37%	0.13%	0.37%	0.37%	0.31%	0.30%
		Hebei N	0.65%	0.19%	0.24%	0.34%	-	-	-	0.23%
		Hebei E	0.51%	-	0.28%	0.13%	0.15%	0.20%	0.29%	0.21%
		Hebei S	0.40%	-	0.40%	0.17%	0.10%	0.10%	0.14%	0.14%
	Case2	Beijing	12.69%	0.52%	0.36%	1.66%	3.37%	4.86%	6.74%	3.00%
		Tianjin	10.12%	-	0.95%	3.25%	4.46%	3.51%	3.63%	3.64%
		Hebei N	3.91%	1.61%	1.80%	1.00%	-	-	-	1.63%
		Hebei E	7.47%	-	0.58%	2.81%	2.65%	2.89%	3.62%	3.00%
		Hebei S	7.40%	-	0.48%	2.11%	3.42%	3.48%	3.29%	3.19%
			MaxNE	MeanNE						
				Pollution levels						All
				<60	60-70	70-80	80-90	90-100	>100	
O_3	Case1	Beijing	2.40%	0.29%	0.10%	1.39%	0.04%	0.85%	0.32%	0.46%
		Tianjin	5.32%	1.26%	0.12%	0.52%	0.18%	0.48%	1.55%	0.59%
		Hebei N	0.31%	0.03%	0.07%	0.07%	0.09%	0.17%	-	0.07%
		Hebei E	0.87%	0.52%	0.34%	0.15%	0.16%	0.18%	0.50%	0.26%
		Hebei S	0.54%	0.29%	0.19%	0.12%	0.23%	0.15%	0.38%	0.20%
	Case2	Beijing	6.42%	0.68%	1.06%	4.00%	0.42%	1.25%	1.06%	1.24%
		Tianjin	4.72%	1.74%	0.45%	1.12%	0.22%	1.01%	1.00%	0.93%
		Hebei N	1.03%	0.21%	0.35%	0.05%	0.33%	0.54%	-	0.26%
		Hebei E	2.86%	1.83%	0.84%	0.93%	0.55%	0.52%	1.40%	0.87%
		Hebei S	2.61%	0.70%	0.27%	0.50%	0.46%	0.61%	1.17%	0.60%

*$PM_{2.5}$ and O_3 concentrations are calculated based on daily averaged concentrations at averages of urban sites in each region

Table S4. Fitting coefficients of terms for $PM_{2.5}$ and O_3 in BTH

Pollutant	Month	Region	1*	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$PM_{2.5}$	January	Beijing	-70.66	-75.01	-5.53	-1.34	2.48	-24.33	22.29	-1.16	-2.14	5.44	20.42	13.94	3.96	6.06	13.40
		Tianjin	-60.70	-58.47	-8.04	-10.03	3.21	-10.58	-8.51	-15.22	0.02	10.22	36.62	29.14	9.56	10.77	22.70
		HebeiN	-12.13	-9.79	-0.37	-0.58	1.14	-6.68	3.76	-1.06	-0.37	2.00	8.93	6.52	2.97	2.09	5.26
		HebeiE	-95.99	-95.56	-3.52	-1.65	2.08	-31.97	29.28	-1.03	-2.94	4.74	28.76	19.70	5.57	7.46	24.03
		HebeiS	-82.06	-84.44	-3.53	-3.27	1.95	-28.66	28.79	-0.94	-4.58	4.72	27.26	17.01	4.41	8.58	26.72
	July	Beijing	-27.64	-29.09	-10.51	6.73	8.17	-6.41	5.11	4.55	-0.86	4.57	10.98	2.85	6.60	7.10	3.75
		Tianjin	-31.62	-30.77	-6.49	5.69	6.96	-8.64	6.99	2.69	-1.07	6.13	10.83	2.52	7.58	5.00	4.32
		HebeiN	-10.24	-14.19	-5.66	5.58	4.20	-1.70	2.09	2.30	-0.68	2.49	1.12	-2.45	3.18	4.40	1.91
		HebeiE	-27.35	-27.96	-10.04	6.70	5.78	-2.86	-1.68	1.59	-0.09	5.93	30.63	20.87	8.03	6.76	5.25
		HebeiS	-33.85	-37.48	-12.03	4.76	6.85	-8.76	6.88	2.02	-1.46	5.15	10.19	1.93	5.75	5.90	6.71
O_3	January	Beijing	164.46	213.89	53.32	12.99	-15.10	28.82	36.10	-1.19	-1.87	0.29	-0.57	4.00	0.50	-2.67	0.16
		Tianjin	114.98	149.97	41.72	12.94	-17.77	22.77	21.12	-4.47	-0.58	0.17	-0.12	5.03	0.50	-2.19	-0.04
		HebeiN	21.80	11.73	-4.78	3.92	-6.01	12.43	8.14	-1.29	-1.11	-0.04	0.00	2.39	0.23	-1.01	-0.05
		HebeiE	130.94	167.06	48.38	12.69	-15.04	25.45	24.37	-1.12	-2.85	0.13	-0.32	5.36	-0.32	-3.34	0.02
		HebeiS	109.76	134.7	34.02	12.16	-17.35	24.55	21.26	-4.56	-2.21	0.18	-0.18	5.81	-0.08	-3.09	-0.08
	July	Beijing	102.76	138.300	62.14	-12.18	-10.61	10.05	-9.88	2.29	-1.41	0.17	-0.31	18.37	-3.78	-1.93	-0.05
		Tianjin	-2.30	-38.89	-13.37	-3.60	-16.67	9.17	-9.03	0.06	-3.53	0.27	-0.31	14.05	-1.70	-1.84	-0.05
		HebeiN	28.07	44.95	27.48	-2.94	2.87	1.87	-4.84	1.39	-2.21	-0.05	-0.29	6.19	-1.03	-1.29	0.01
		HebeiE	24.69	23.24	14.04	-6.69	-5.32	7.83	-3.72	3.74	-0.76	0.14	-0.26	11.77	-3.05	-2.32	-0.07
		HebeiS	59.88	74.92	35.79	-8.14	-12.52	4.75	-7.62	1.55	-0.84	0.14	-0.28	11.80	-1.72	-0.91	-0.04

*The orders of terms are followed as Figure 4.

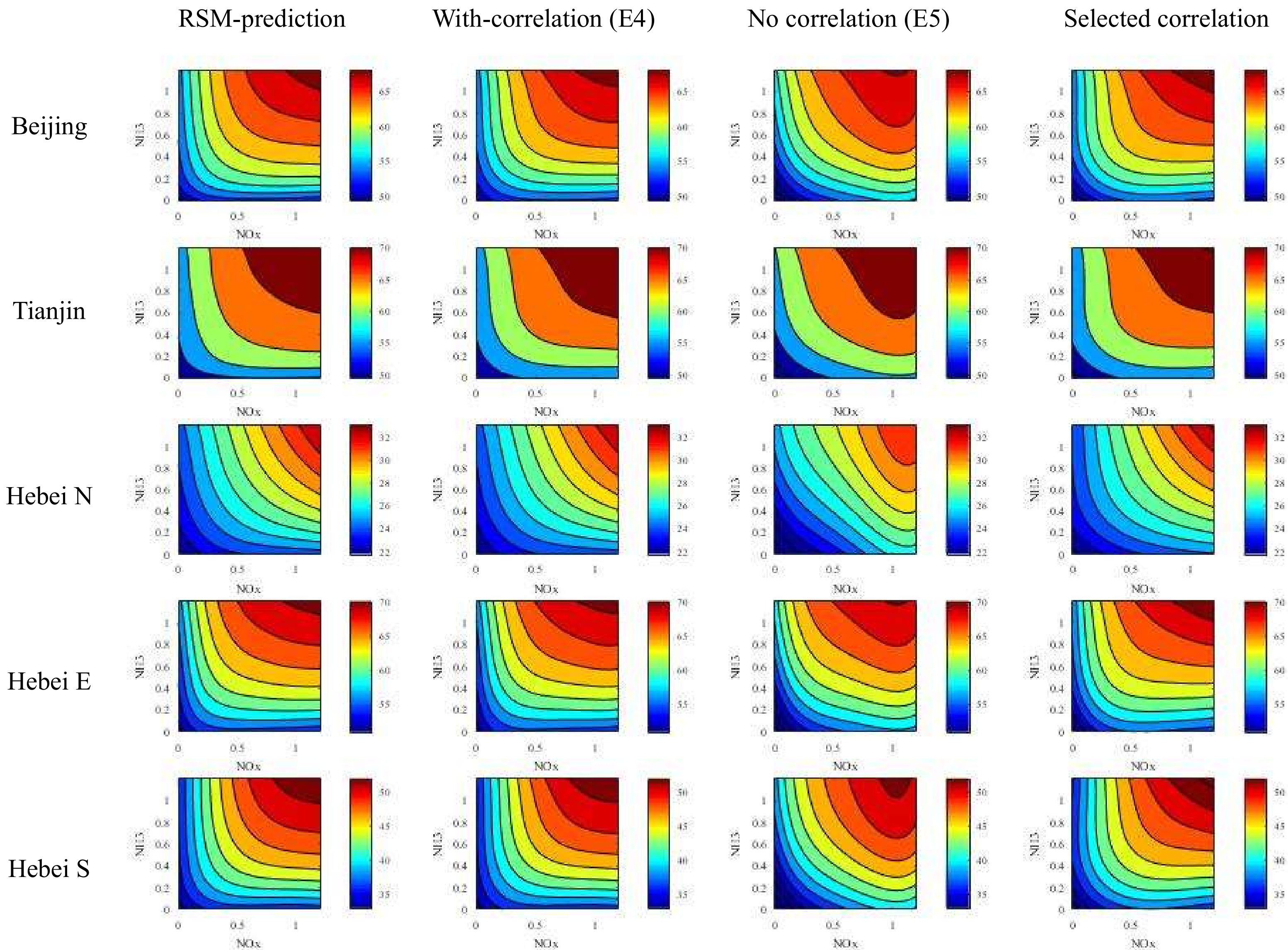


Figure S1. Interaction examination between NO_x and NH_3 for $PM_{2.5}$ (monthly averages in July 2014, The x and y axes shows $1+E_{NOx}$ and $1+E_{NH3}$, The different colors represent $PM_{2.5}$ concentrations, unit: μg m^{-3})

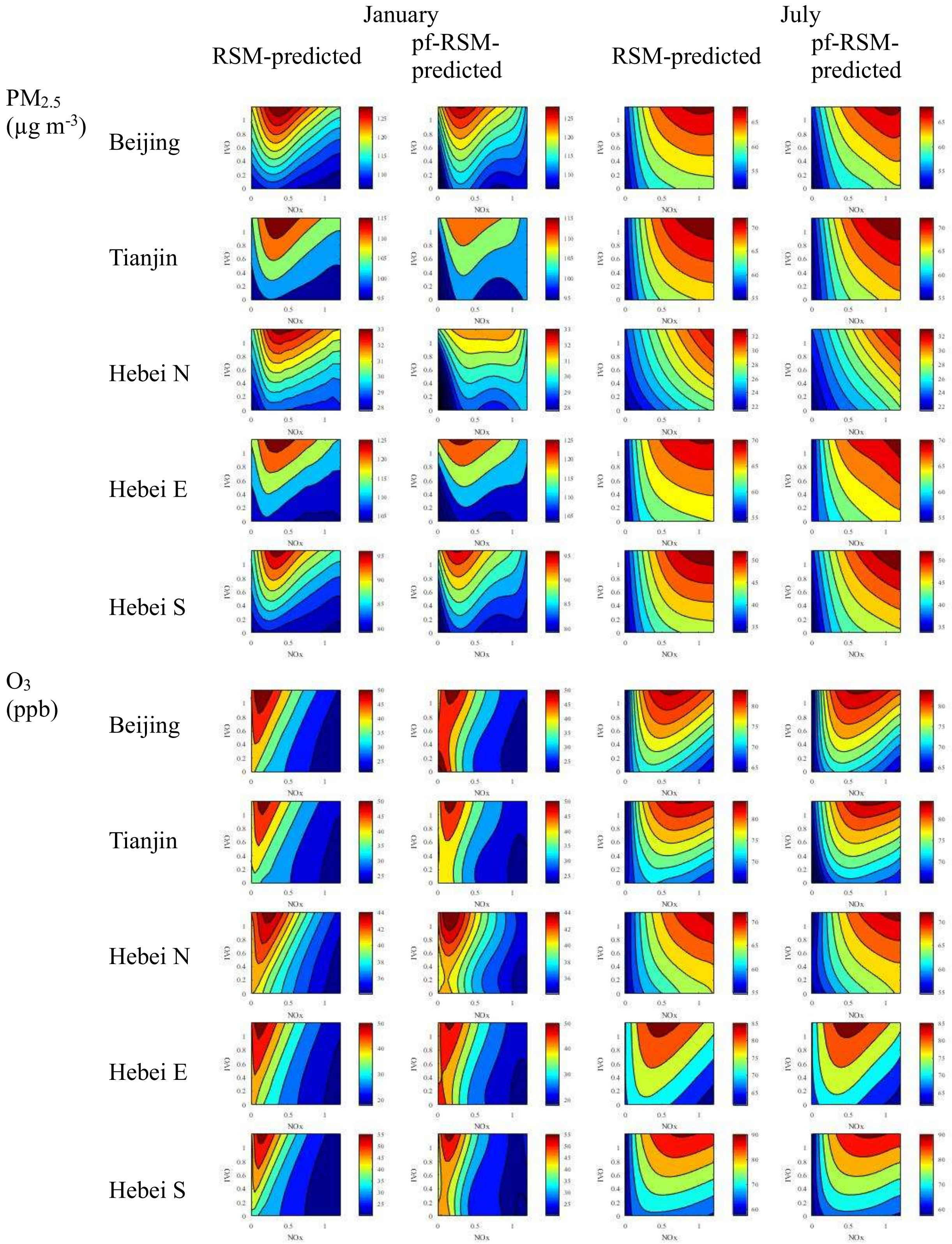


Figure S2. Isopleth validation of polynomial function with 20 training samples and even distributions (The x and y axes shows $1+E_{NOx}$ and $1+E_{VOCs}$, The different colors represent $PM_{2.5}$ or O_3 concentrations)

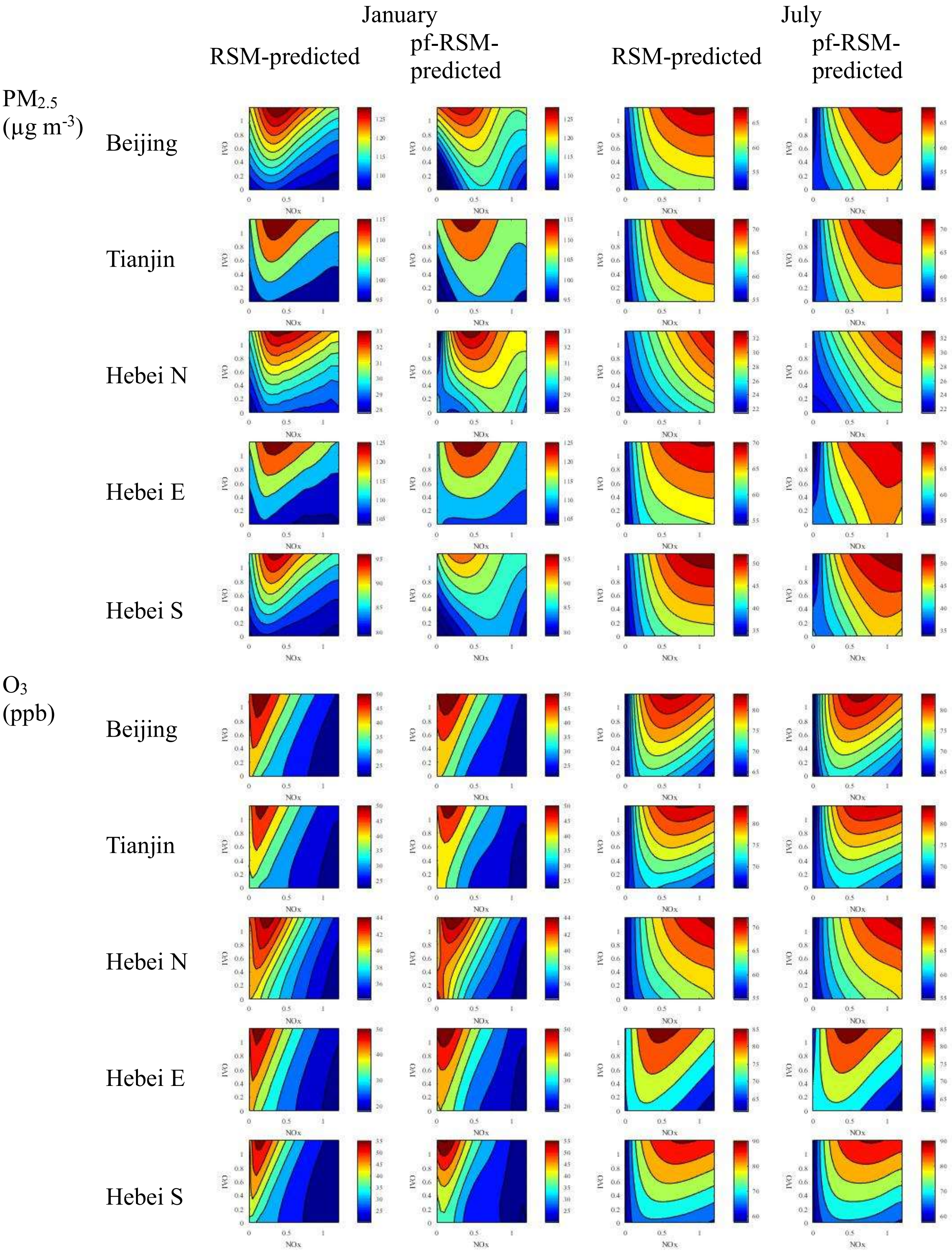


Figure S3. Same as Figure S1, for 20 training samples and marginal distributions

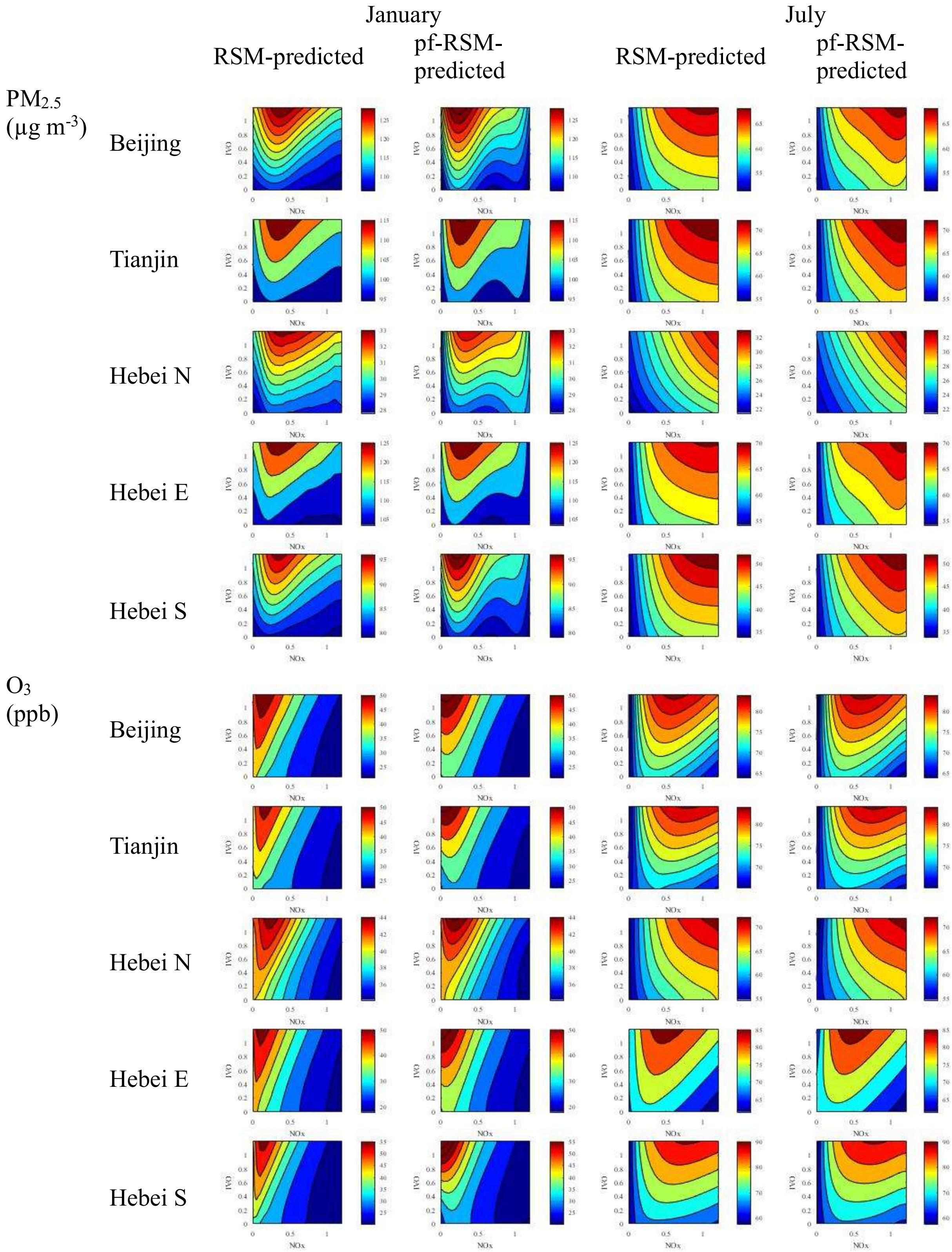


Figure S4. Same as Figure S1, for 30 training samples and even distributions

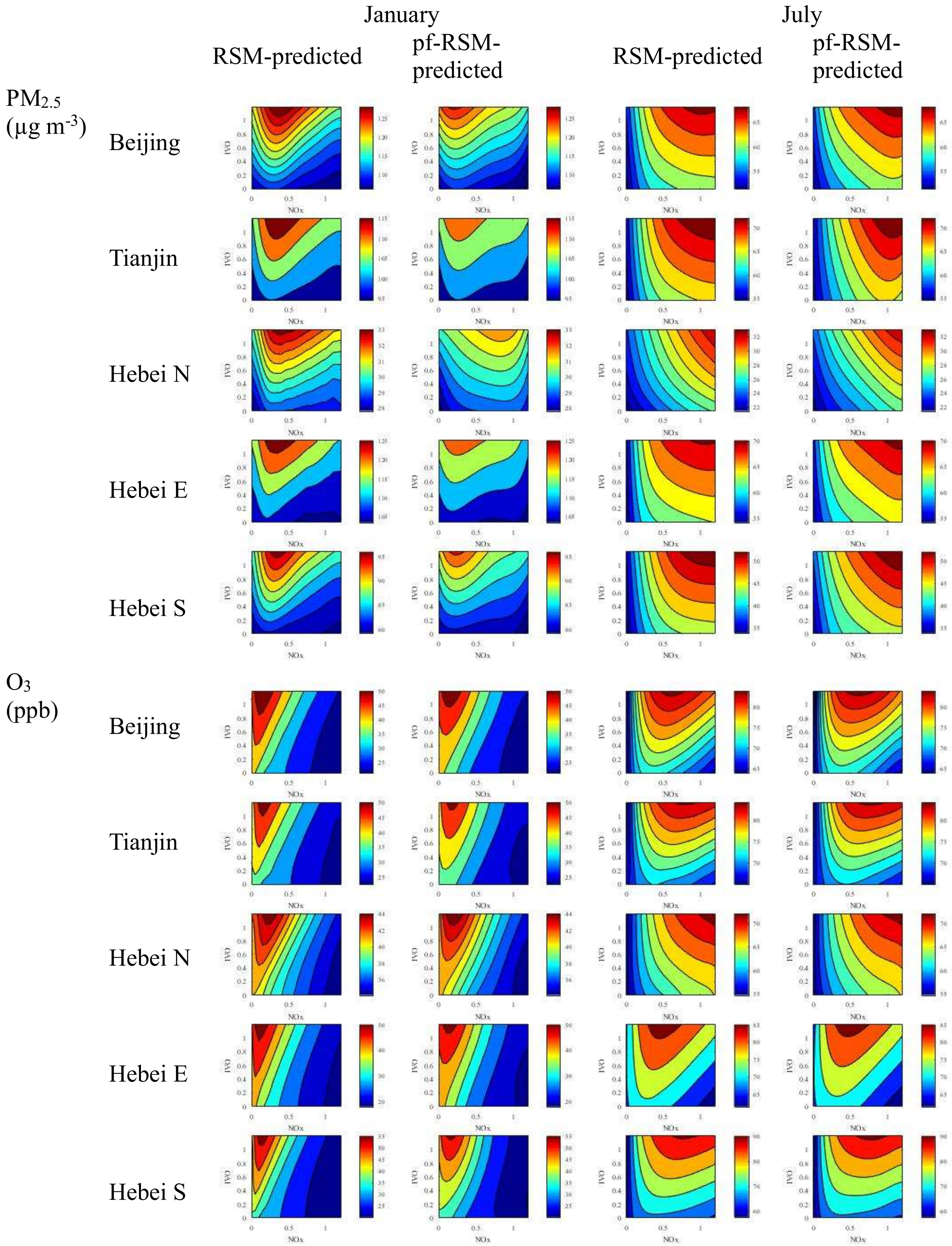


Figure S5. Same as Figure S1, for 30 training samples and marginal distributions

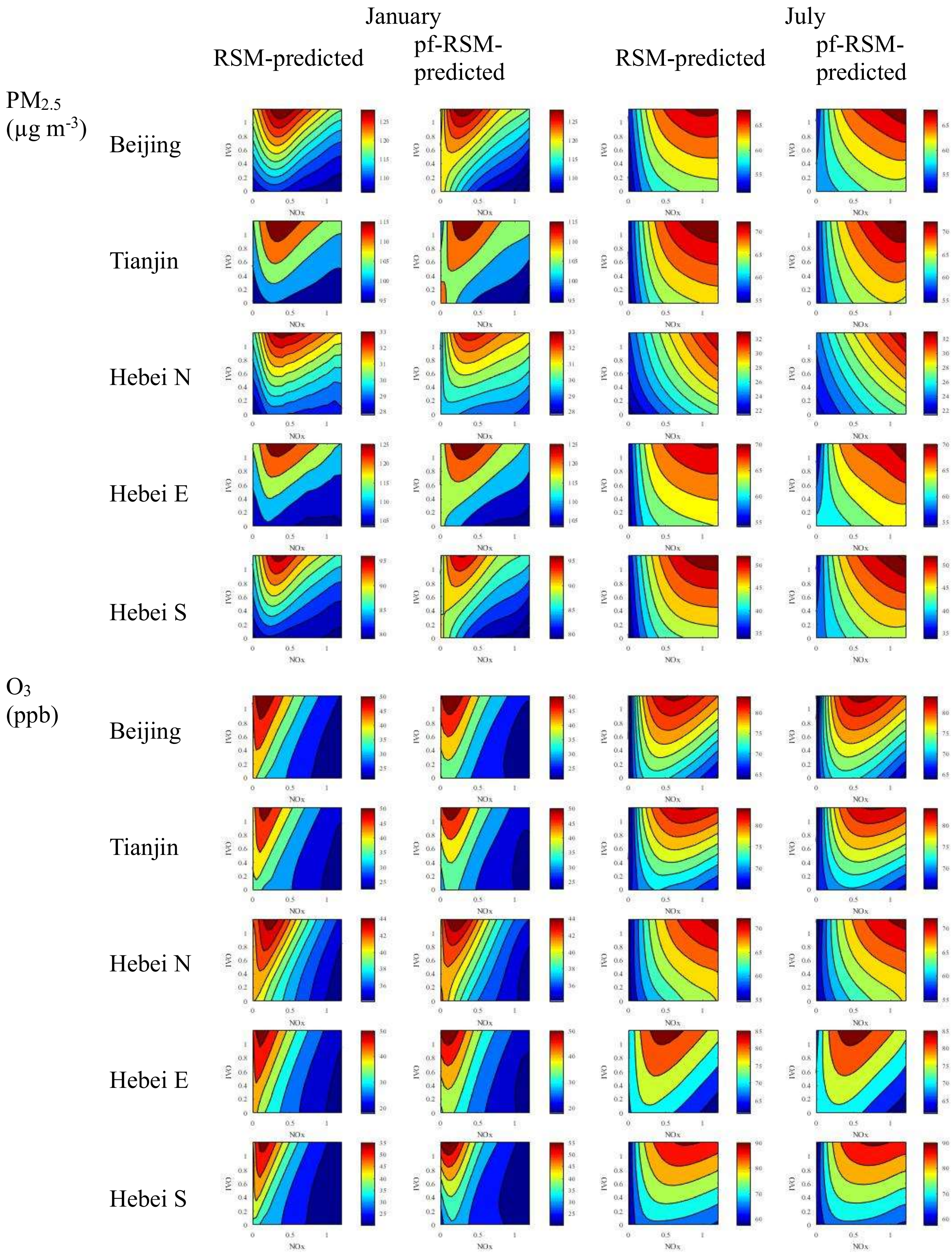


Figure S6. Same as Figure S1, for 40 training samples and even distributions

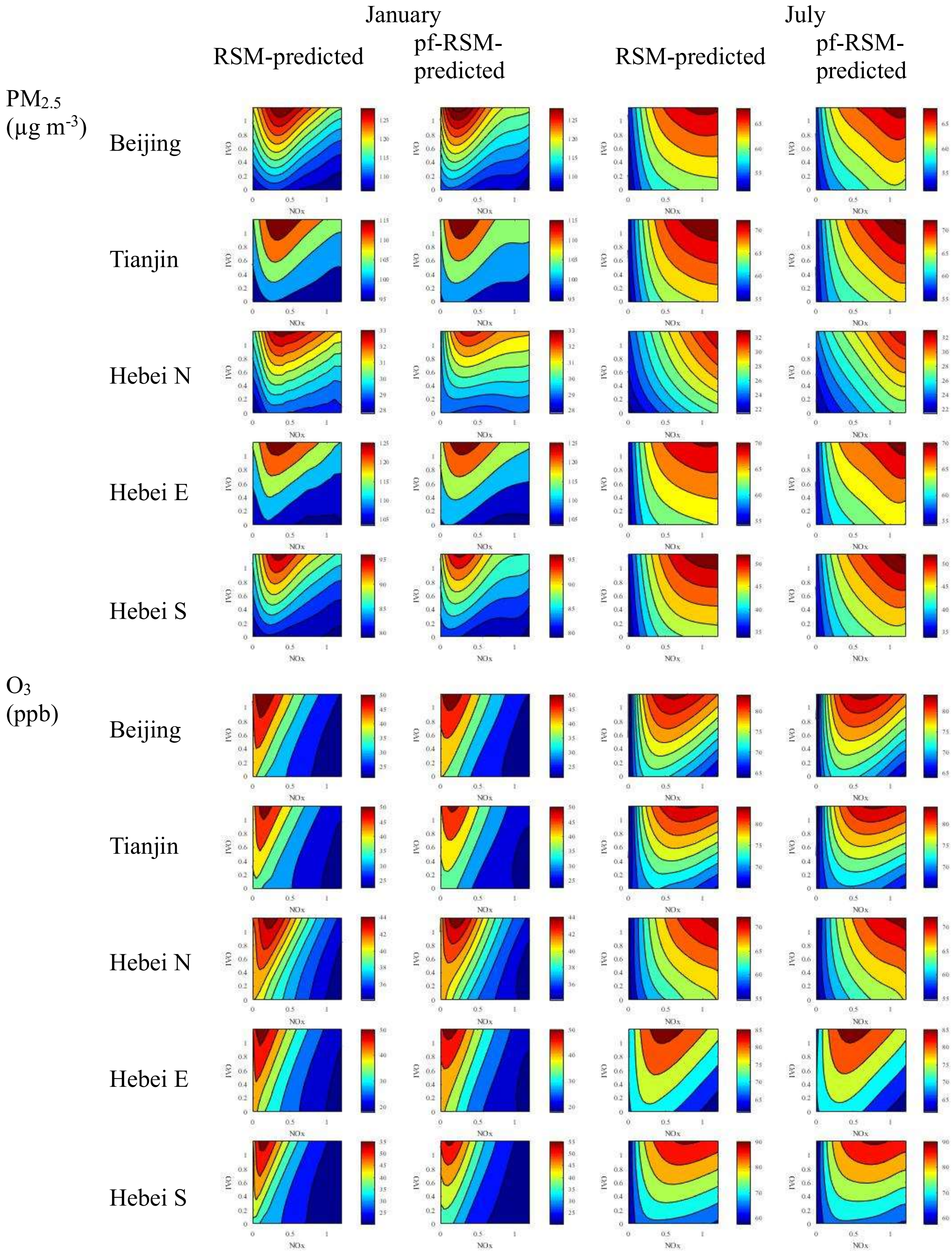


Figure S7. Same as Figure S1, for 40 training samples and marginal distributions

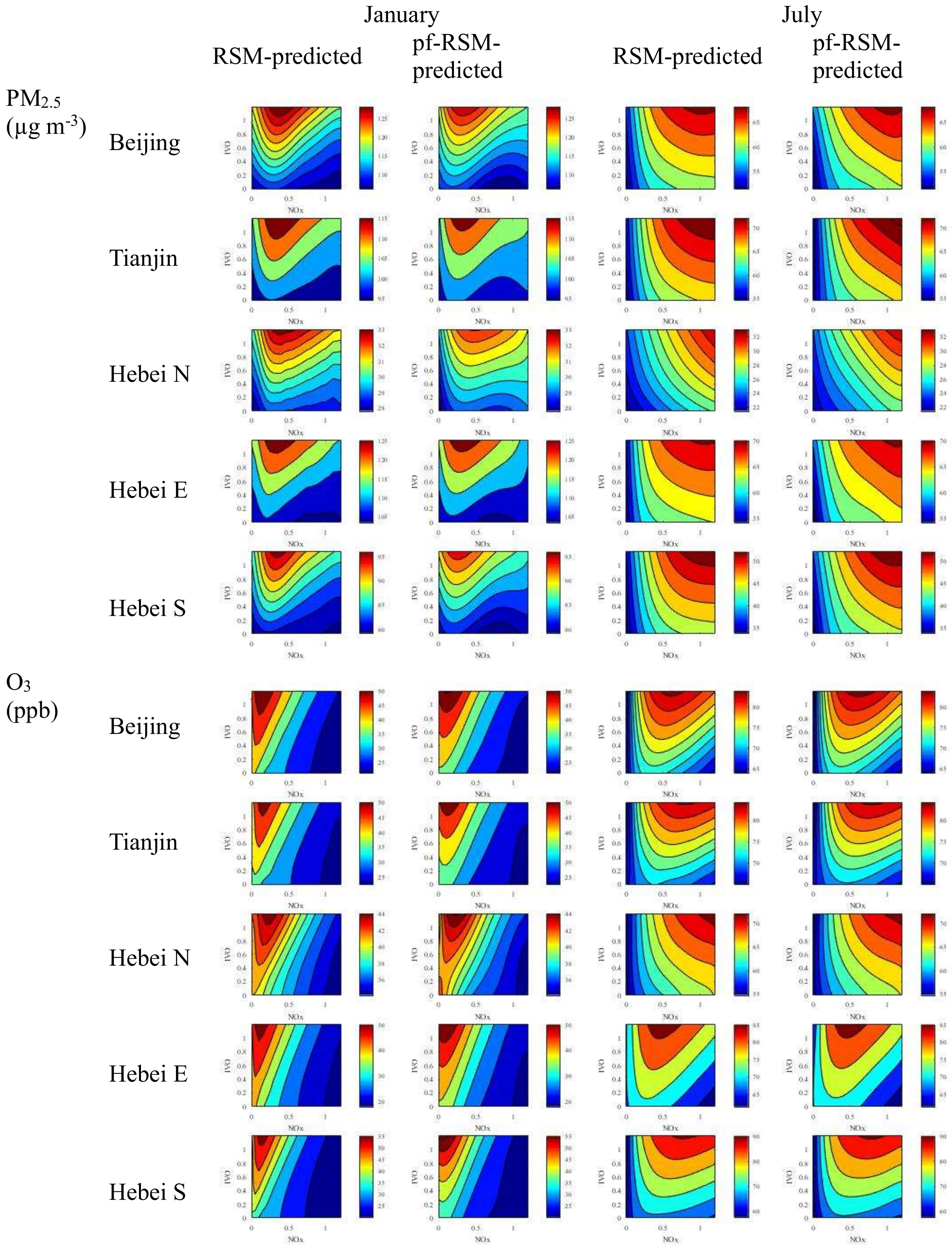


Figure S8. Same as Figure S1, for 50 training samples and even distributions

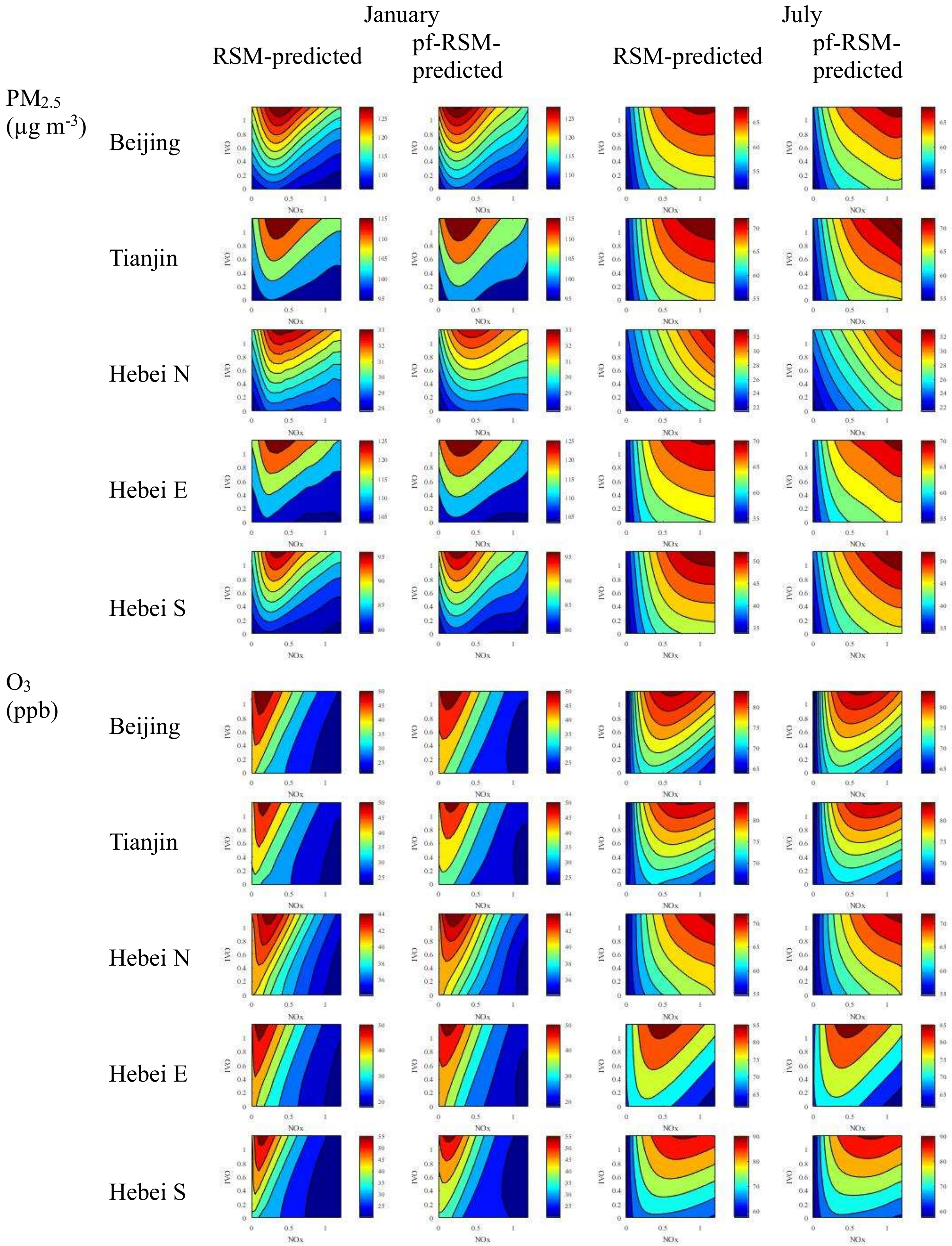
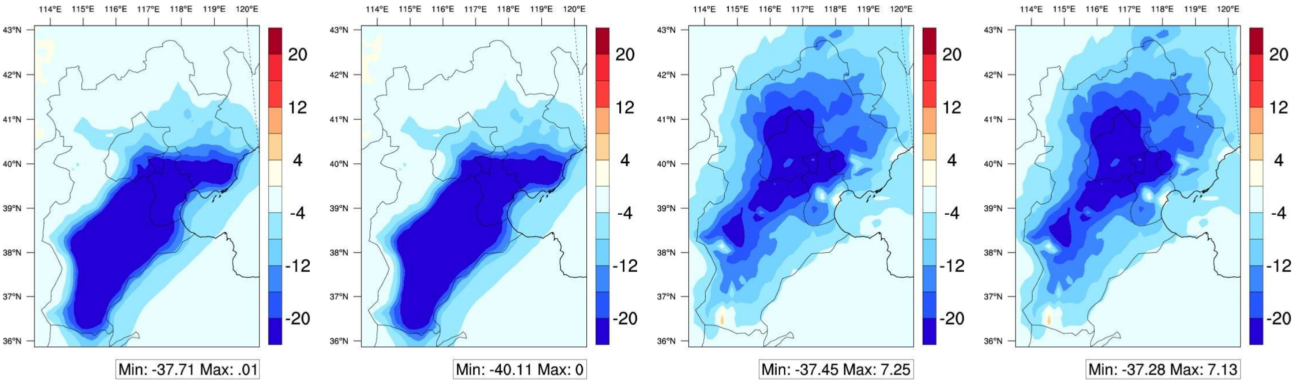


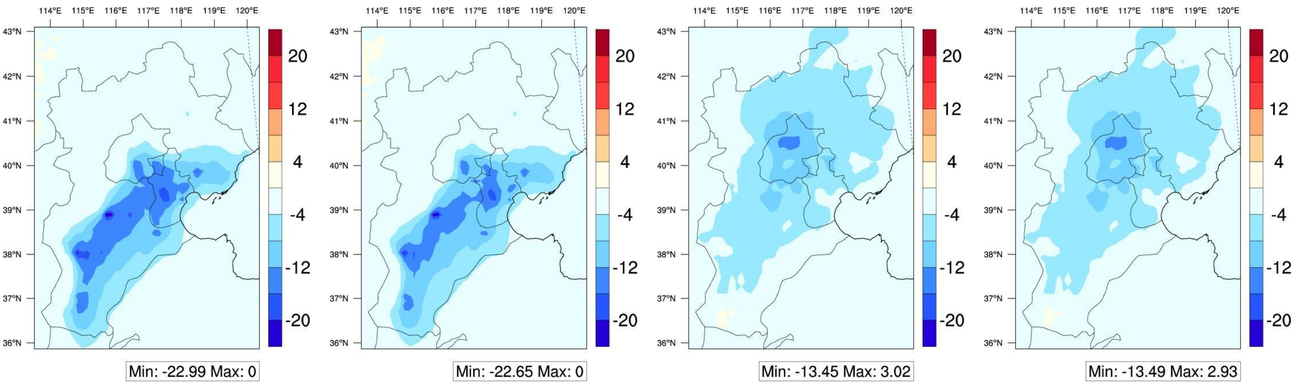
Figure S9. Same as Figure S1, for 50 training samples and marginal distributions

CMAQ-$\Delta PM_{2.5}$ pfRSM- $\Delta PM_{2.5}$ CMAQ-ΔO_3 pfRSM-ΔO_3

Case S1: E_{NOx}, E_{SO2}, E_{NH3}, E_{VOCs} and E_{POA} are 93%, 30%, 88%, 68%, and 64% respectively



Case S2: E_{NOx}, E_{SO2}, E_{NH3}, E_{VOCs} and E_{POA} are 36%, 80%, 2%, 57%, and 28% respectively



Case S3: E_{NOx}, E_{SO2}, E_{NH3}, E_{VOCs} and E_{POA} are 48%, 65%, 82%, 89%, and 84% respectively

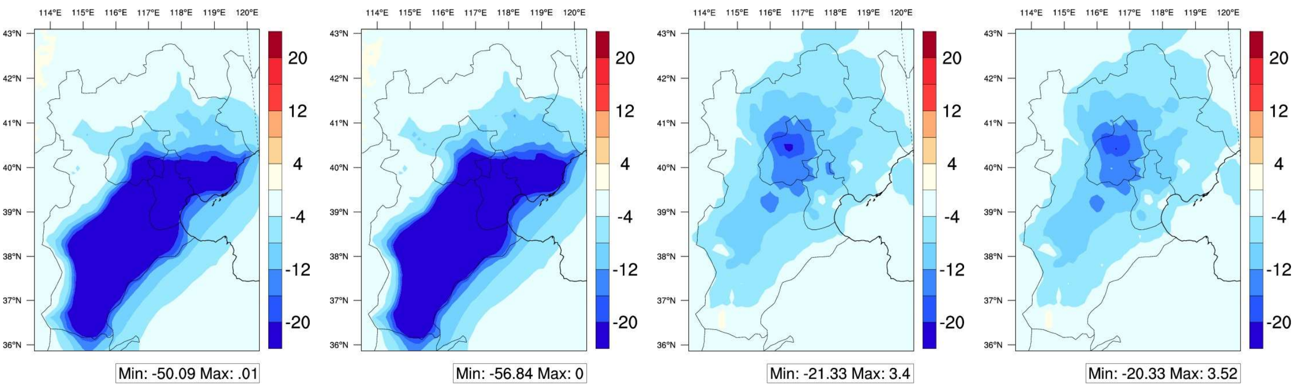
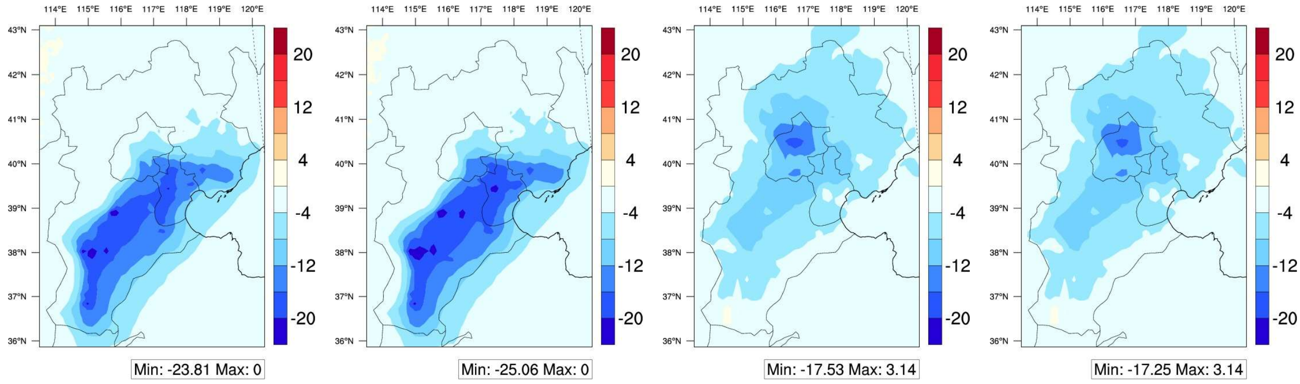


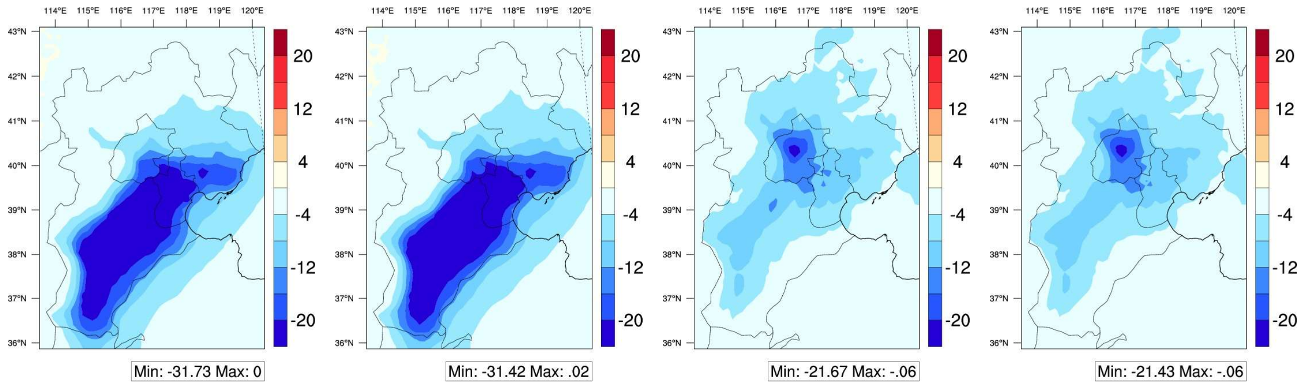
Figure S10. Spatial distribution of CMAQ-simulated and pf-RSM-predicted O_3 in baseline and O_3 responses in two control scenarios (monthly averages of daily 1-hour maxima O_3 in July 2014, unit: ppb)

CMAQ-$\Delta PM_{2.5}$ pfRSM- $\Delta PM_{2.5}$ CMAQ-ΔO_3 pfRSM-ΔO_3

Case S4: E_{NOx}, E_{SO2}, E_{NH3}, E_{VOCs} and E_{POA} are 42%, 1%, 30%, 74%, and 43% respectively



Case S5: E_{NOx}, E_{SO2}, E_{NH3}, E_{VOCs} and E_{POA} are 16%, 57%, 61%, 92%, and 36% respectively



Case S6: E_{NOx}, E_{SO2}, E_{NH3}, E_{VOCs} and E_{POA} are 89%, 11%, 56%, 6%, and 56% respectively

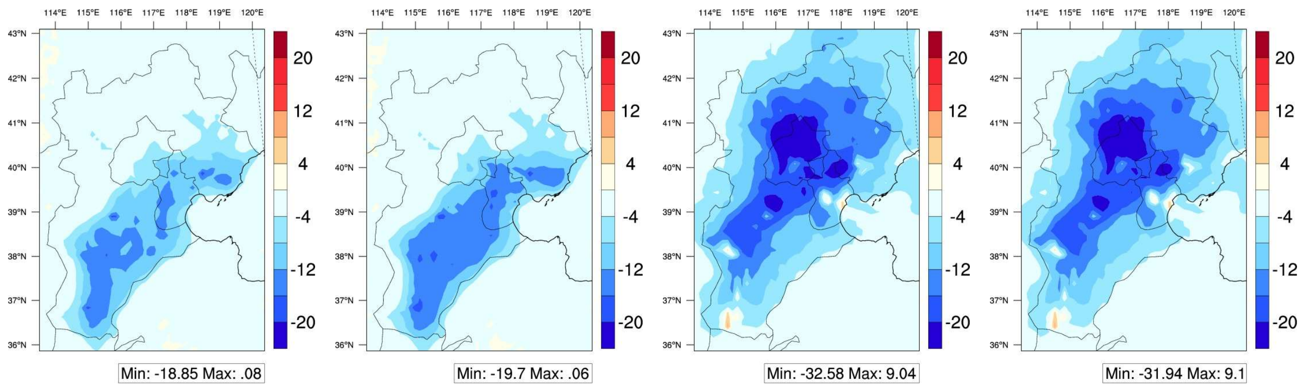
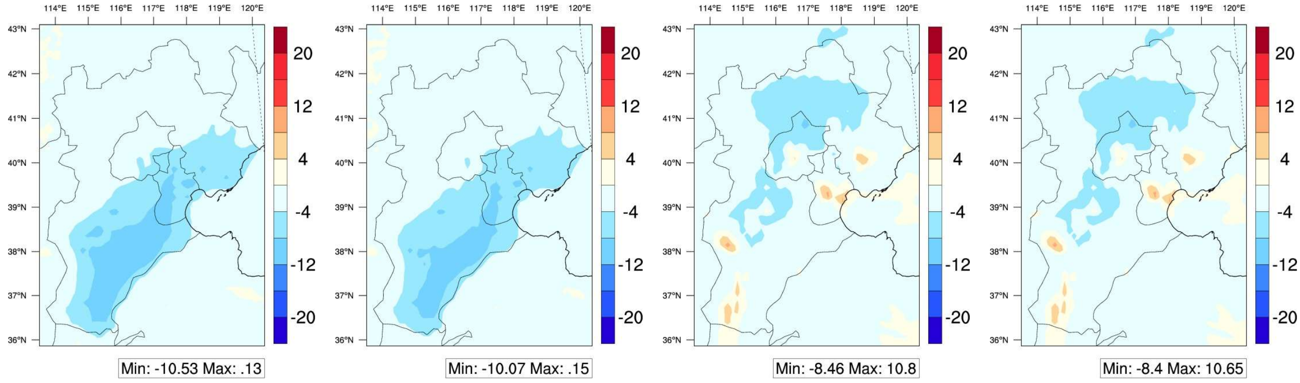


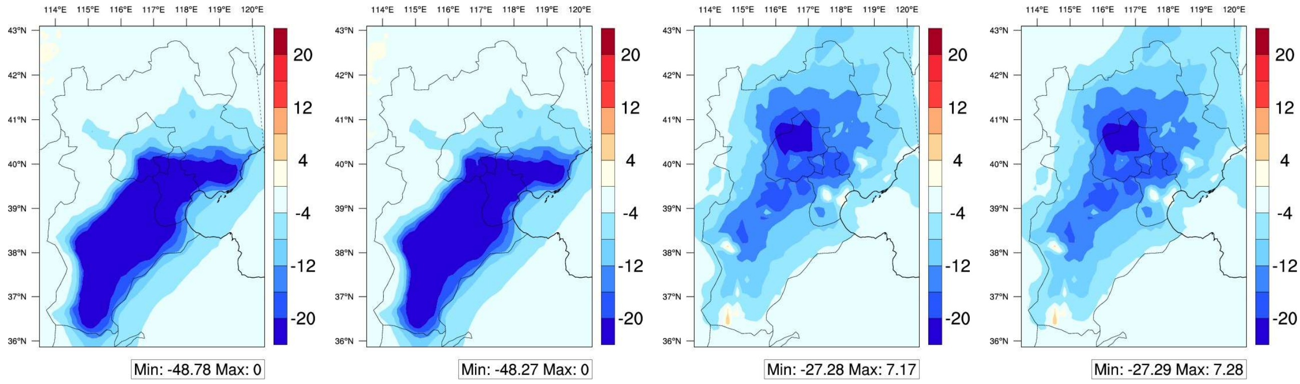
Figure S10. (cont.)

CMAQ-$\Delta PM_{2.5}$ pfRSM- $\Delta PM_{2.5}$ CMAQ-ΔO_3 pfRSM-ΔO_3

Case S7: E_{NOx}, E_{SO2}, E_{NH3}, E_{VOCs} and E_{POA} are 43%, 17%, 60%, 1%, and 29% respectively



Case S8: E_{NOx}, E_{SO2}, E_{NH3}, E_{VOCs} and E_{POA} are 78%, 85%, 45%, 81%, and 96% respectively



Case S9: E_{NOx}, E_{SO2}, E_{NH3}, E_{VOCs} and E_{POA} are 77%, 10%, 48%, 51%, and 7% respectively

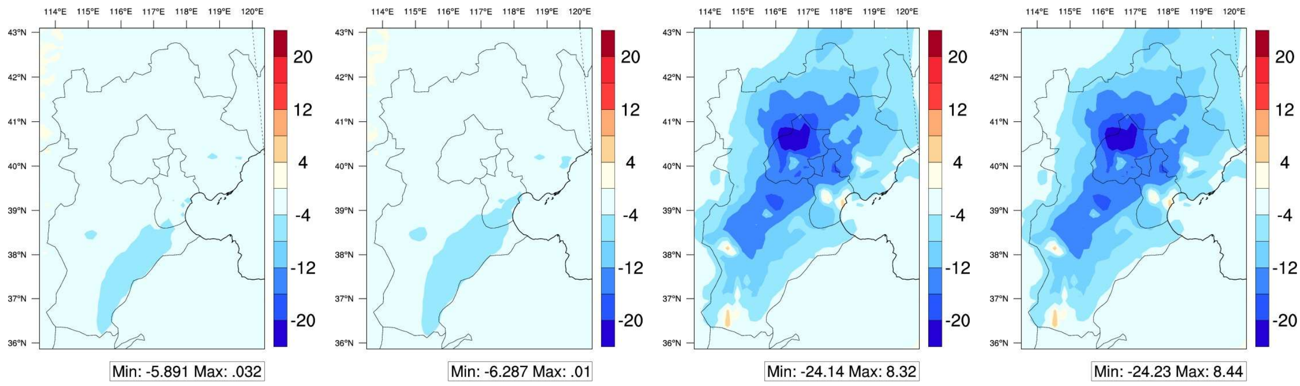


Figure S10. (cont.)