Supplement of Atmos. Chem. Phys., 15, 3045–3062, 2015
http://www.atmos-chem-phys.net/15/3045/2015/
doi:10.5194/acp-15-3045-2015-supplement

Atmospheric Chemistry and Physics Open Access

Supplement of

Impact of pollution controls in Beijing on atmospheric oxygenated volatile organic compounds (OVOCs) during the 2008 Olympic Games: observation and modeling implications

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Table S1. Comparison of the observed and predicted values of median ln([VOC]) and their corresponding concentrations before 21 July and the outputs P(t) from the T-test for the two datasets, where P(t)<0.05 implies that the difference in the two datasets is statistically significant at the confidence level of 95%.

	Median_ ln([VOC])			Concentration (ppbv)		Deviation of concentrations	
	observation	prediction	P(t)	observation	prediction	(%)	R
Benzene	0.247	0.249	0.573	1.280	1.282	-0.23	0.85
Toluene	0.664	0.671	0.995	1.943	1.956	-0.65	0.90
C8-aromatics	0.884	0.881	0.860	2.422	2.414	0.31	0.82
C9-aromatics	0.075	0.084	0.702	1.078	1.088	-0.90	0.84
Acetonitrile	-1.261	-1.255	0.575	0.283	0.285	-0.64	0.79
HCHO	1.880	1.882	0.804	6.554	6.570	-0.24	0.84
Acetaldehyde	0.999	0.986	0.277	2.716	2.680	1.37	0.93
Acetone	1.375	1.352	0.086	3.957	3.866	2.34	0.90
MEK	0.149	0.148	0.900	1.161	1.160	0.11	0.94
Methanol	2.705	2.757	0.064	14.959	15.752	-5.04	0.87
Isoprene	0.284	0.260	0.162	1.328	1.296	2.42	0.84
MVK+MACR	0.320	0.335	0.235	1.377	1.398	-1.52	0.93

Table S2. Emission ratios (ERs) of NMHCs relative to CO in Beijing during the summer of 2008 and 2005, compared with those measured in U.S. (Warneke et al., 2007; Borbon et al., 2013)

Compounds	ERs, ppbv[ppmv CO]$^{-1}$			
	Beijing, Aug, 2008	Beijing, Aug, 2005	New England, 2004	Los Angeles, 2010
Acetylene	5.61±0.19	4.87±0.18	3.60	5.87
Ethane	4.58±0.16	3.37±0.12	11.62	18.4
Propane	3.59±0.17	3.30±0.13	7.73	11.2
n-Butane	3.16±0.14	2.63±0.10	1.69	4.42
i-Butane	3.35±0.13	2.37±0.10	1.01	3.08
n-Pentane	0.82±0.04	1.65±0.06	1.55	3.26
i-Pentane	2.72±0.10	4.07±0.18	3.99	8.69
Ethylene	3.70±0.23	4.37±0.16	4.56	10.35
propene	0.90±0.07	1.23±0.05	1.36	3.74
trans-2-butene	0.64±0.04	0.50±0.03	0.05	0.10
1-butene	1.42±0.07	1.23±0.06	0.14	0.34
i-butene	0.54±0.03	0.72±0.03		
cis-2-butene	0.52±0.03	0.43±0.03	0.06	0.09
1-pentene	0.18±0.09	0.14±0.01	0.11	
trans-2-pentene	0.22±0.01	0.22±0.01	0.10	
cis-2-pentene	0.12±0.01	0.13±0.01	0.05	
Benzene	1.26±0.06	1.04±0.04	0.62	1.30
Toluene	3.57±0.13	3.69±0.12	2.62	3.18
Ethylbenzene	1.18±0.05	1.10±0.04	0.31	0.57
m,p-Xylene	1.77±0.08	2.43±0.10	1.16	1.79
o-Xylene	0.63±0.03	1.10±0.04	0.46	0.67

Table S3. Observed and modelled concentrations of OVOCs in different model scenarios during the full control period (average ± s.d.)

Compounds	Observed	M0	M1	M2	M3	M4
Formaldehyde (ppbv)	6.16±2.37	16.21±3.87	10.24±4.34	10.21±3.82	3.44±3.11	5.59±3.20
Acetaldehyde (ppbv)	2.38±1.13	4.98±1.85	3.54±1.30	3.36±1.31	1.23±0.72	3.03±0.94
Acetone (ppbv)	4.12±1.39	6.41±1.38	2.73±1.35	2.46±0.96	2.33±0.90	3.79±1.10
MEK (ppbv)	0.98±0.50	0.43±0.11	0.20±0.12	0.19±0.08	0.18±0.07	0.95±0.32
MVK+MACR (ppbv)	0.91±0.55	1.22±0.73	1.06±0.78	1.16±0.70	1.14±0.69	1.15±0.69
OH (molecule/cm^3)	3.33e+06*	3.61e+06	3.49e+06	3.43e+06	3.17e+06	3.26e+06
HO_2 (molecule/cm^3)		3.02e+08	2.47e+08	2.36e+08	1.91e+08	2.09e+08

*the calculated OH from the empirical relation between OH and $J(O^1D)$

Table S4. The average of production rates and percentage from main precursors to HCHO during the full control period (M4), compared to uncontrolled scenario (M5)

	the full control period (M4)			uncontrolled scenario (M5)	
Precursors	$P_{HCHO,}$ ppbh^{-1}	Percentage, %	Precursors	$P_{HCHO,}$ ppbh^{-1}	Percentage, %
Isoprene	1.263	37.46	Isoprene	1.348	35.89
Propene	0.478	14.18	Propene	0.539	14.35
2-Butenes	0.396	11.74	2-Butenes	0.440	11.70
Ethylene	0.216	6.41	Ethylene	0.261	6.96
2-Pentenes	0.206	6.12	2-Pentenes	0.230	6.12
Xylenes	0.138	4.09	Xylenes	0.154	4.10
Toluelne	0.133	3.95	Toluelne	0.148	3.95
Trimethylbenzenes	0.130	3.87	Trimethylbenzenes	0.145	3.85
i-Butene	0.126	3.75	1-Butene	0.151	4.01
1-Butene	0.124	3.67	i-Butene	0.150	3.99

Fig S1. The precision of typical species measured by PTR-MS during the CAREBEIJING-2008

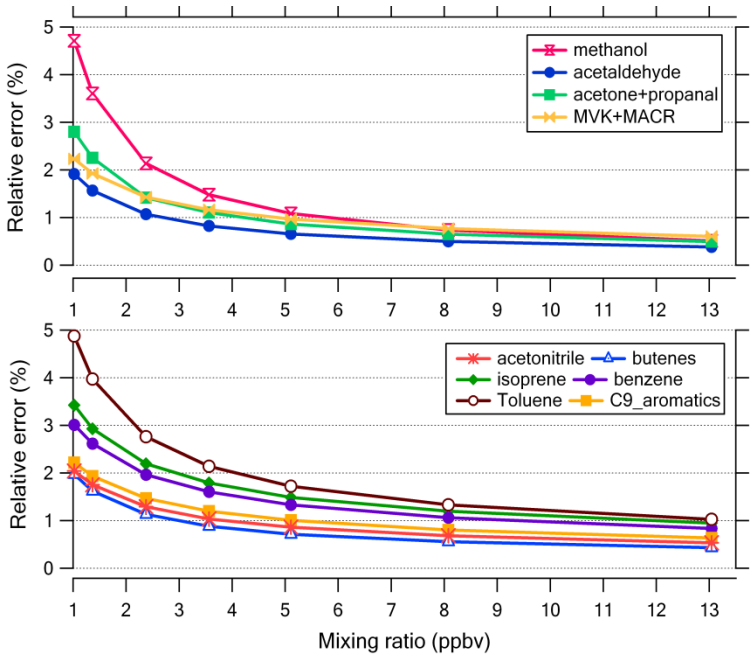

Fig S2a. Comparison between the PTR-MS and GC-MS data for benzene, toluene, C8-aromatics and C9-aromatics obtained during CAREBEIJING-2008, the PTR-MS data points were averaged over the sampling periods of the GC-MS measurements

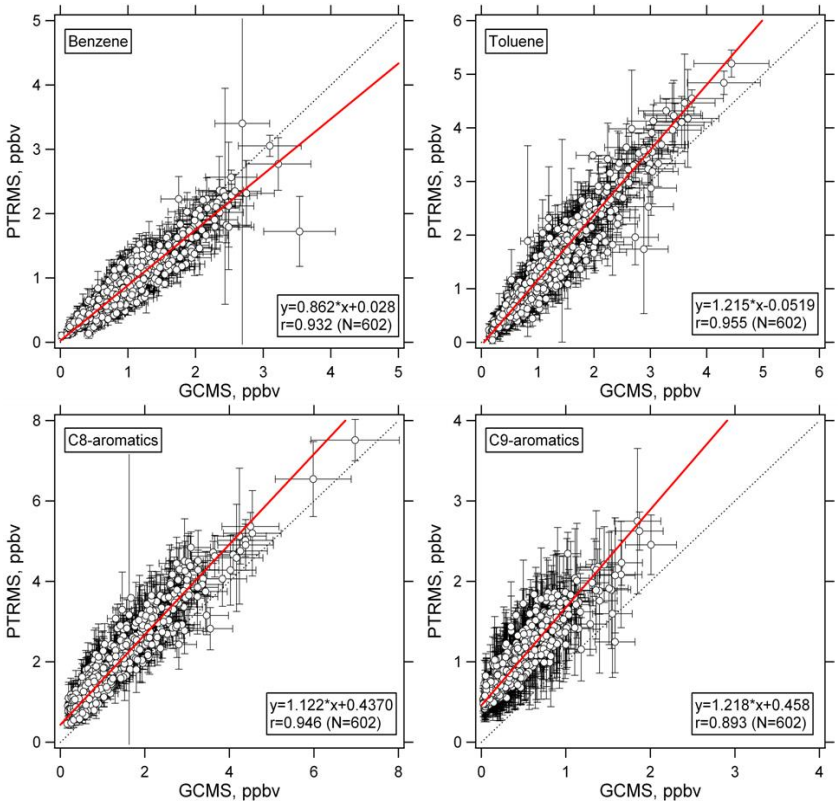

Fig S2b. Comparison between the PTR-MS and GC-MS data for isoprene during CAREBEIJING-2008, the PTR-MS data points were averaged over the sampling periods of the GC-MS measurements

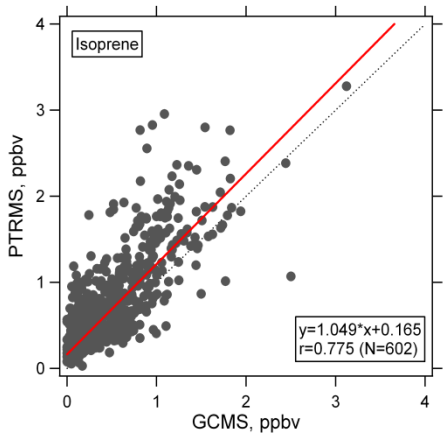

Fig S3. The observed and predicted values of ln(VOC) and their corresponding concentrations in the validation data (i.e. before 21 July) in MLP simulation: a) benzene, b) toluene, c) methanol, d) acetaldehyde, e) acetone and f) MEK.