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Impacts of biogenic and anthropogenic emissions on summertime ozone formation in the Guanzhong Basin, China

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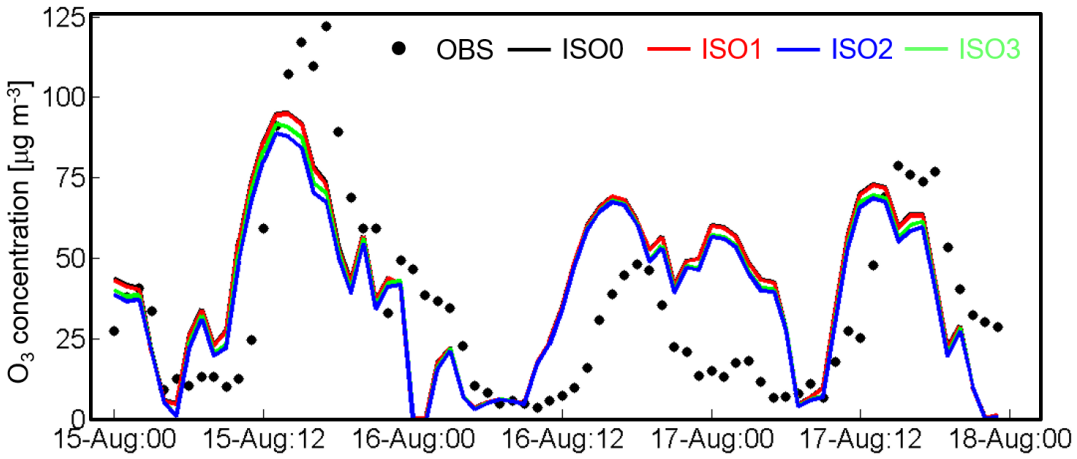

Figure S1. O_3 concentrations changes due to updated isoprene chemistry at Xi'an Jiaotong University for the period of 15th to 17th August 2011.

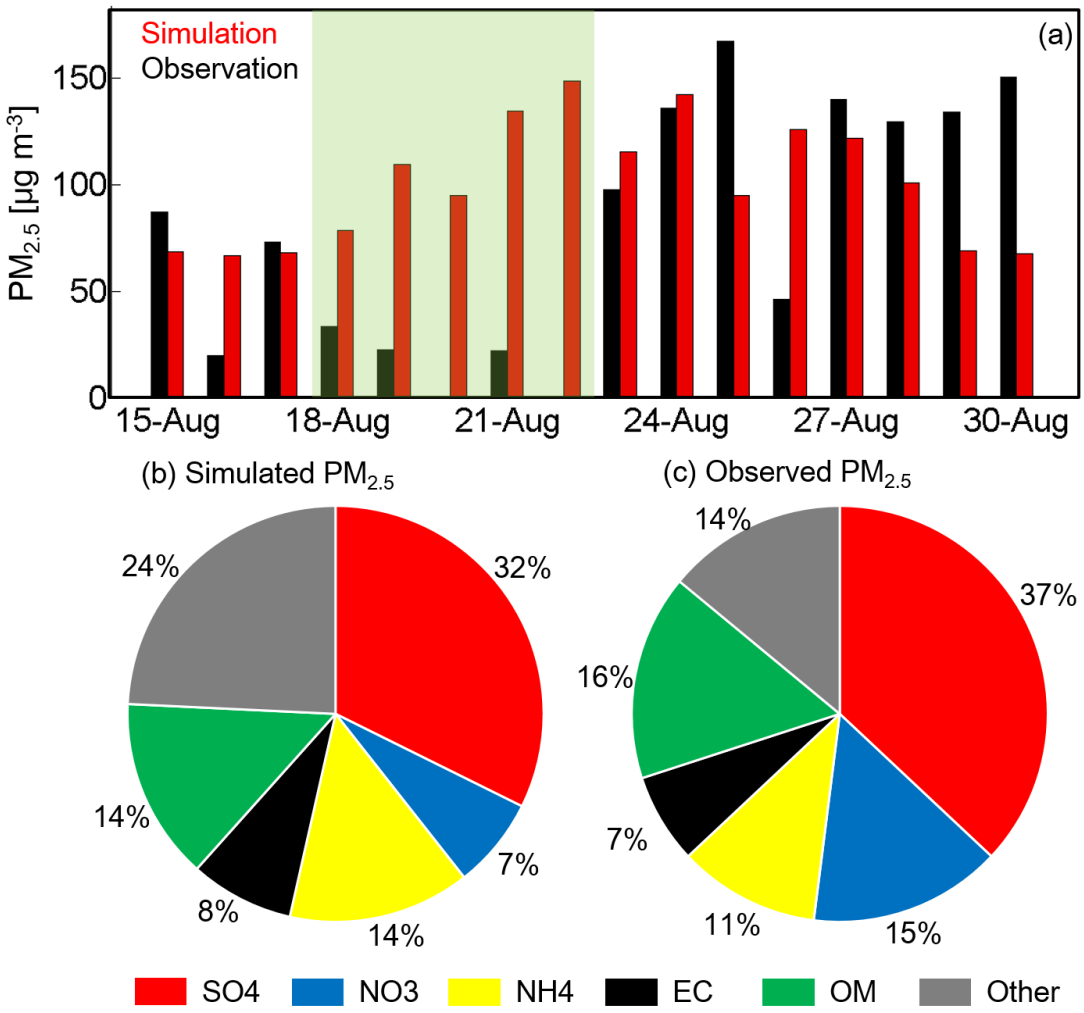

Figure S2. Observed and simulated $PM_{2.5}$ concentrations (a) and compositions (b and c) at Xi'an Jiaotong University in August 2011. The components are calculated during the periods excluding the rainy days (the green shadow).

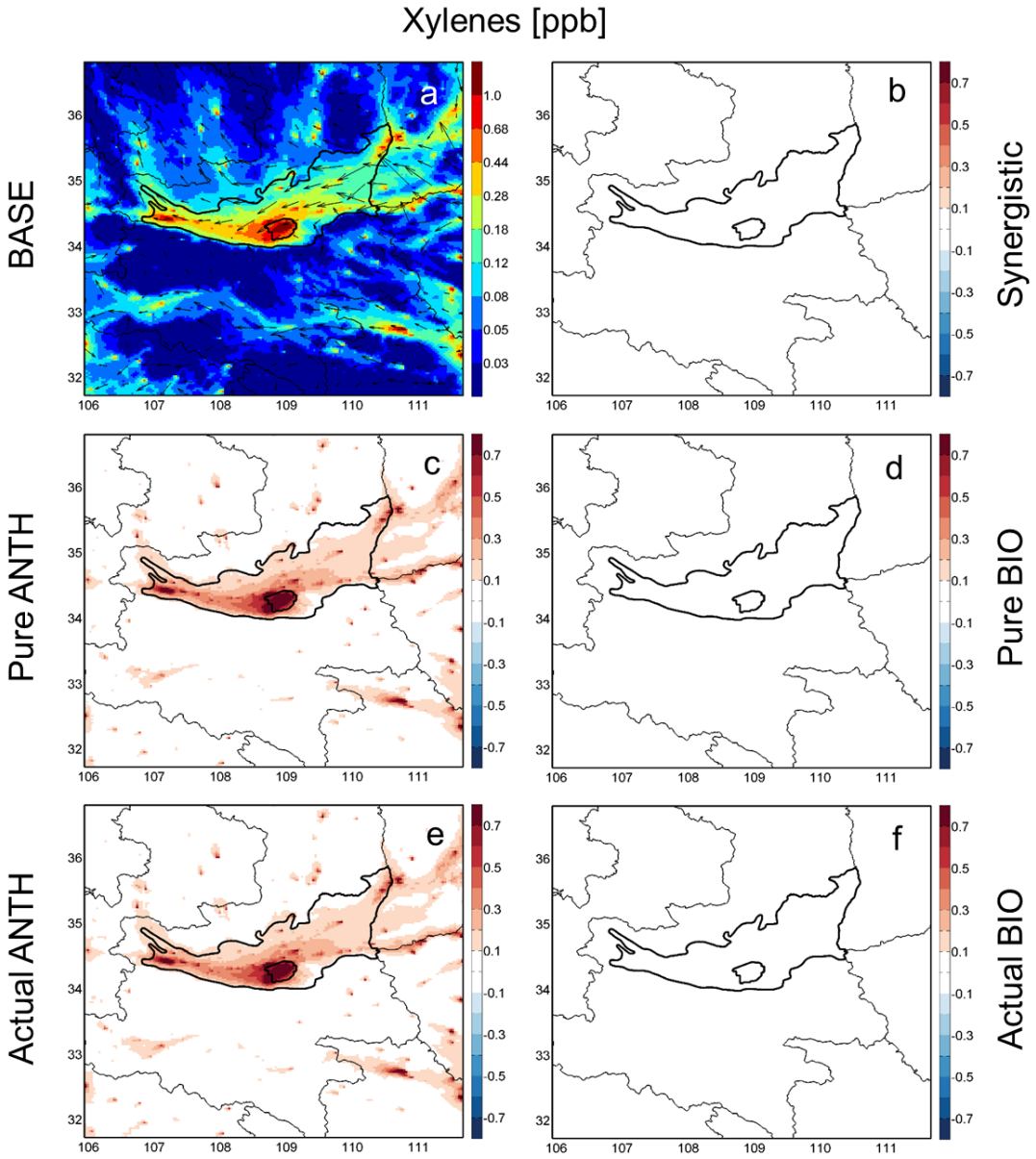

Figure S3. Spatial distributions of monthly mean concentrations of xylenes in August 2011. (a) is the result from the BASE simulation, overlaid with simulated wind vectors. (b)-(f) are simulated xylenes concentrations contributed from synergistic anthropogenic and biogenic, pure anthropogenic, pure biogenic, actual anthropogenic and actual biogenic sources, respectively.

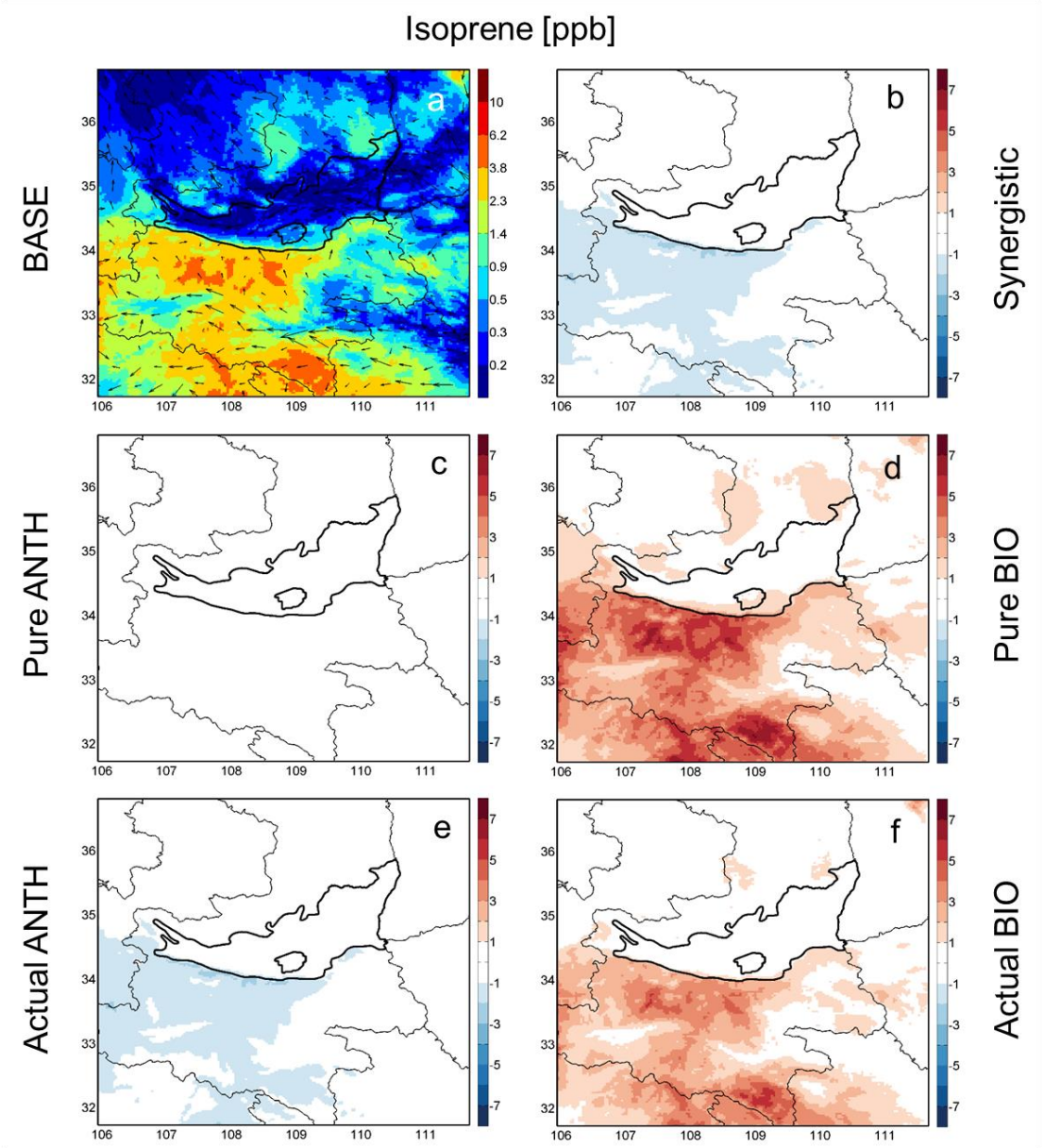

Figure S4. Spatial distributions of monthly mean concentrations of isoprene in August 2011. (a) is the result from the BASE simulation, overlaid with simulated wind vectors. (b)-(f) are simulated isoprene concentrations contributed from synergistic anthropogenic and biogenic, pure anthropogenic, pure biogenic, actual anthropogenic and actual biogenic sources, respectively.

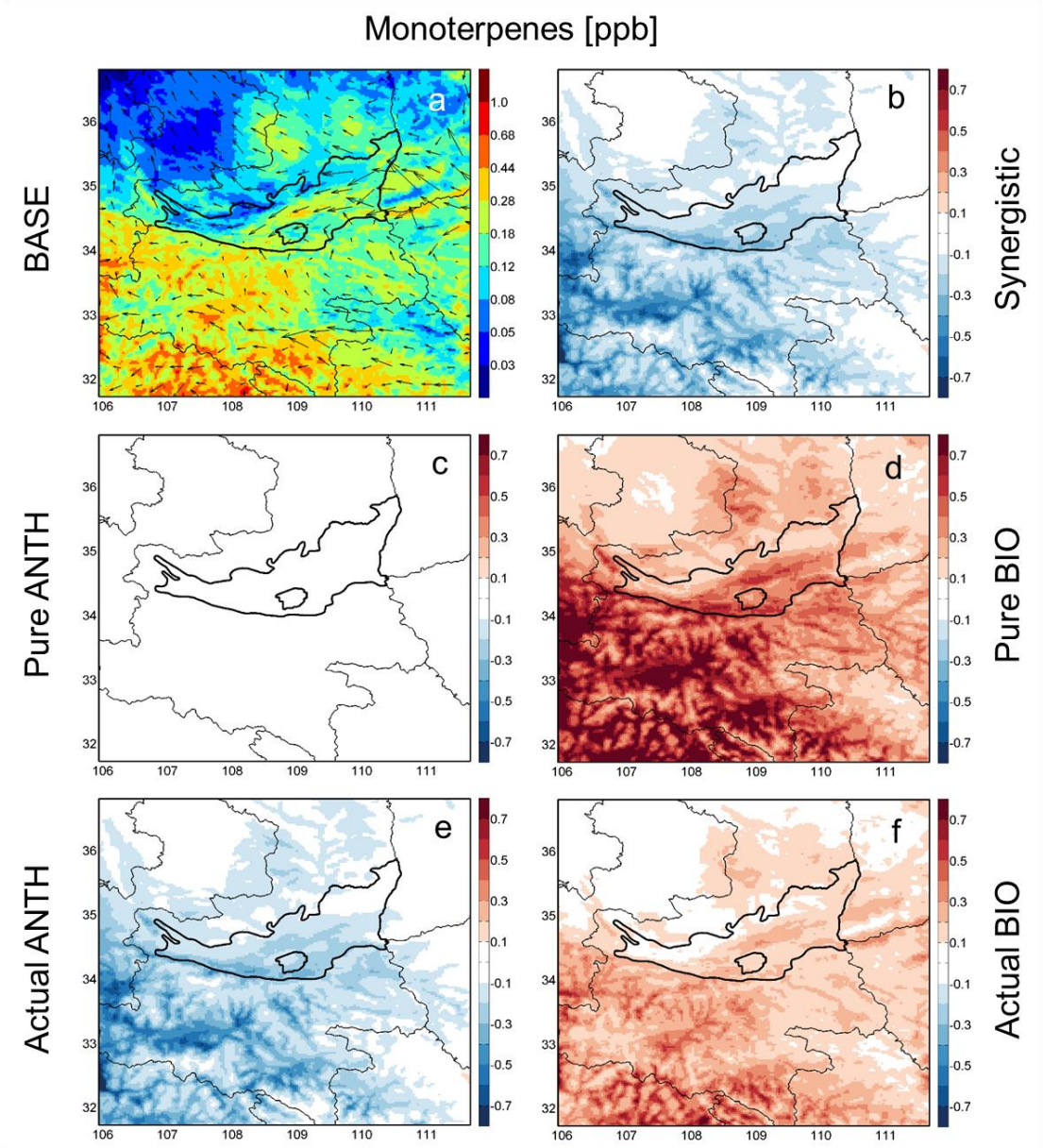

Figure S5. Spatial distributions of monthly mean concentrations of monoterpenes in August 2011. (a) is the result from the BASE simulation, overlaid with simulated wind vectors. (b)-(f) are simulated monoterpenes concentrations contributed from synergistic anthropogenic and biogenic, pure anthropogenic, pure biogenic, actual anthropogenic and actual biogenic sources, respectively.

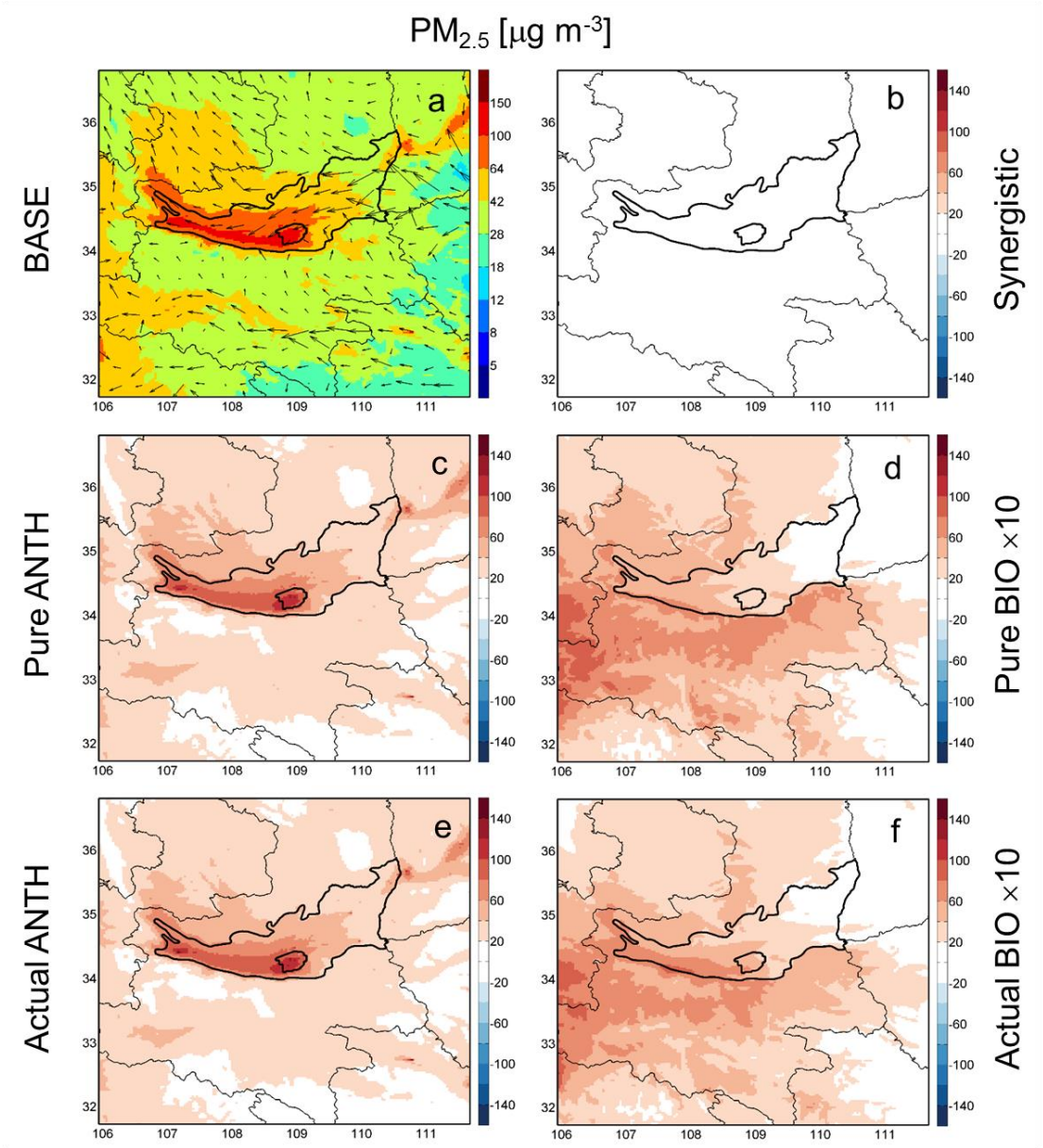

Figure S6. Spatial distributions of monthly mean concentrations of $PM_{2.5}$ in August 2011. (a) is the result from the BASE simulation, overlaid with simulated wind vectors. (b)-(f) are simulated $PM_{2.5}$ concentrations contributed from synergistic anthropogenic and biogenic, pure anthropogenic, pure biogenic, actual anthropogenic and actual biogenic sources, respectively.

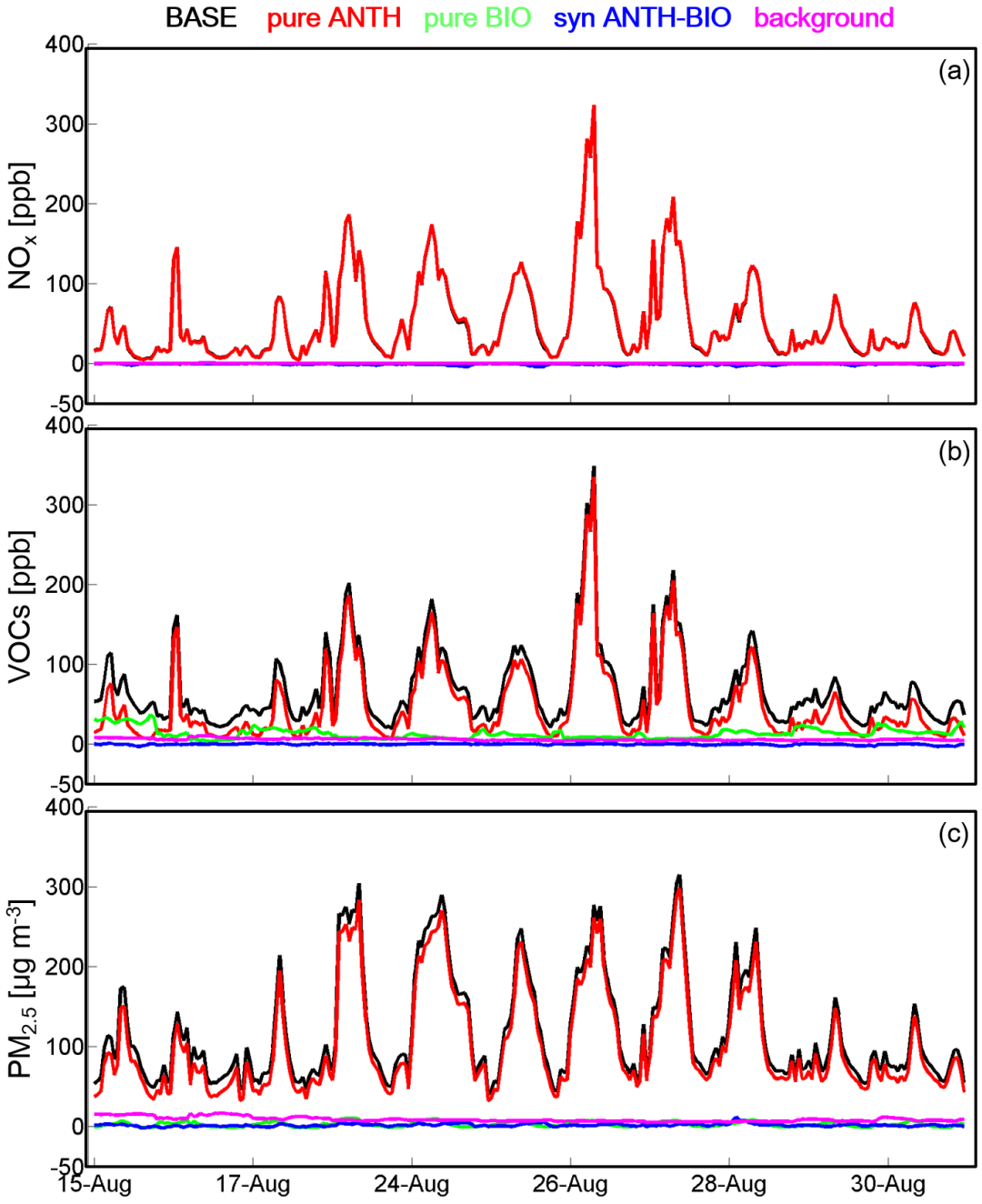

Figure S7. Temporal patterns of the simulated concentrations of NO_x, VOCs and $PM_{2.5}$ and the various contribution components during the period from 15th to 30th August 2011, excluding the rainy days (18th -22nd August).

Table S1. Updated isoprene oxidation chemistry (unit for reaction rate is molecule^{-1} cm^{3} s^{-1})

Reactions	**Reaction rates**
ISOPO2+NO > ALD+HCHO+HO2+0.96*NO2+0.04*ISOPN	2.7×10^{-12} ×exp(350/T)
ISOPO2 > 2*HO2+HCHO+0.33*MGLY+0.5*GLYALD+0.25*GLYX+1.5*HACET	4.07×10^{8} ×exp(-7694/T)

Species name	**Description**
T	Temperature (K)
NO	Nitric oxide
NO2	Nitrogen dioxide
HO2	Hydroperoxy radical
ISOPO2	Hydroperoxy radicals from isoprene oxidation by OH
ISOPN	Organic nitrate
HCHO	Formaldehyde
ALD	Acetaldehyde and higher aldehydes
HACET	Hydroxyacetone
MGLY	Methylglyoxal
GLYALD	Glycolaldehyde
GLYX	Glyoxal

Table S2. O_3 concentration changes due to updated isoprene chemistry averaged for urban Xi'an

O_3 concentration (ppb)	ISO1 [b]-ISO0 [a]	ISO2 [c]-ISO0	ISO3 [d]-ISO0
Daily peak	-0.47	-4.6	-2.9
24h average	-0.27	-2.9	-2.0

[a] ISO0: simulation using standard RADM2 mechanism

[b] ISO1: same as ISO0, but add isomerization of radicals from isoprene oxidation by OH

[c] ISO2: same as ISO0, but add formation of hydroxynitrates

[d] ISO3: same as ISO0, but with revisions in both ISO1 and ISO2.

Table S3. Domain-wide amount of emissions in August 2011

	Anthropogenic (Gg mon^{-1})	Biogenic (Gg mon^{-1})	Total (Gg mon^{-1})
SO_2	358 (±31%) [a]	-	358
NO_x	110 (±37%) [a]	2.1	112
NH_3	69.0 (±153%) [a]	-	69.0
$PM_{2.5}$	163 (±133%) [a]	-	163
VOCs	72.2 (±78%) [a]	204	276
Isoprene	<0.1	157	157
Monoterpenes	-	22.8	22.8
Alkanes	34.4	5.4	39.8
Alkenes	21.3	4.9	26.2
Aromatic	11.5	-	11.5
Carbonyls	4.5	12.1	16.6
Organic acids	0.5	1.5	2.0

[a] Uncertainty in emission estimates (95 % confidence intervals).

Table S4. Simulated O_3 and VOC concentrations in urban Xi'an during 15th-17th August 2011.

Species [ppb]	VOC0 [a]	VOC1 [b]	VOC2 [c]
O_3	**40.7**	**41.9**	**39.8**
Ethane	13.1	18.7	9.5
C>2 alkanes	11.2	16.1	8.9
HCHO	7.4	5.5	5.0
Acetaldhyde	5.4	4.7	4.2
Toluene	2.9	4.3	2.2
Ethene	2.8	4.2	2.3
Organic nitrogen	2.7	1.7	1.5
Organic peroxides	2.1	2.0	1.9
C>2 alkenes	2.0	3.2	1.7
Ketones	1.6	1.6	1.2
Xylenes	1.2	1.9	0.8
Organic acids	1.0	1.2	1.1
Total VOC	**53.3**	**64.9**	**40.3**

[a] VOC0: Base simulation using emission estimates from MEIC.

[b] VOC1: Same as Base, but with an increase of anthropogenic VOC emission by 50%

[c] VOC2: Same as Base, but with an decrease of anthropogenic VOC emission by 33%