



Supplement of

Physicochemical uptake and release of volatile organic compounds by soil in coated-wall flow tube experiments with ambient air

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Supplemental Information

Table S.1. Determined VOC desorption rate coefficient and desorption lifetime on the soil sample, during flushing with VOCs-free N₂.

	VOC species												
	A	B	C	D	E	F	G	H	I	J	K	L	M
Desorption rate coefficient (×10 ⁻³ s ⁻¹)	-	0.8	-	-	1.6	4.3	3.7	3.0	4.1	5.6	4.8	-	3.1
Desorption lifetime (min)	-	22.2	-	-	10.8	3.9	4.5	5.7	4.1	3.0	3.5	-	5.4

A: styrene, B: formaldehyde, C: toluene, D: isoprene, E: acetic acid, F: MVK+MACR, G: acetaldehyde, H: methanol, I: MEK, J: acetone, K: acetonitrile, L: benzene, M: formic acid. The symbol “-” means no detected emissions of this compound from the soil.

Table S.2. Integrated total amount and average surface flux of each adsorbed or emitted VOC species on soil for the whole measurement period.

	VOC species												
	A	B	C	D	E	F	G	H	I	J	K	L	M
Integrated total amount (μg)	0.54	11.86	2.08	0.75	2.51	0.58	1.18	9.54	0.37	1.98	0.15	0.34	-2.29
Average surface flux ($\text{nmol m}^{-2} \text{s}^{-1}$)	0.001	0.047	0.003	0.001	0.005	0.001	0.003	0.036	0.001	0.004	0.0004	0.001	-0.006

A: styrene, B: formaldehyde, C: toluene, D: isoprene, E: acetic acid, F: MVK+MACR, G: acetaldehyde, H: methanol, I: MEK, J: acetone, K: acetonitrile, L: benzene, M: formic acid. Positive values mean soil uptake and negative values mean soil emission.

Table S.3. Basic physicochemical parameters (at 298 K) of the measured VOC species.

	VOC species													
	A	B	C	D	E	F ₁	F ₂	G	H	I	J	K	L	M
$k_w \times 10^3$ (cm s ⁻¹)	7.6	10	4.4	4.6	4.7	3.6	3.6	3.4	3.8	1.7	1.8	2.1	1.3	-2.0
$k_{OH} \times 10^{12}$ (cm ³ molecule ⁻¹ s ⁻¹)	58	9.4	5.6	100	0.74 ^a	20	29	15	0.94	1.2	0.17	0.049 ^b	1.2	0.37 ^a
$k_{O_3} \times 10^{18}$ (cm ³ molecule ⁻¹ s ⁻¹)	17	< 0.01	< 0.01	13	N ^c	5.2	1.2	< 0.01	< 0.01	N	< 0.01	≤ 0.15 ^b	< 0.01	N ^c
$H \times 10^2$ (mol m ⁻³ Pa ⁻¹)	0.33	3200	0.15	0.013	5000	30	6.0	15	220	18	25	50	0.18	7000
P (mm Hg)	6.4	3.89	28.4	550	15.7	152	155	902	127	90.6	231	88.8	94.8	42.6
log K_{ow}	3.05	0.35	2.73	2.42	-0.17	0.41	0.59 ^d	0.45	-0.74	0.29	-0.24	-0.34	2.13	-0.54

A: styrene, B: formaldehyde, C: toluene, D: isoprene, E: acetic acid, F₁: MVK, F₂: MACR, G: acetaldehyde, H: methanol, I: MEK, J: acetone, K: acetonitrile, L: benzene, M: formic acid. k_w : surface reaction (or wall loss) rate coefficient, k_{OH} : rate coefficient of VOCs reaction with OH radicals in gas phase, k_{O_3} : rate coefficient of VOCs reaction with O₃, H : Henry's law constant, P : vapor pressure, K_{ow} : octanol-water partition coefficient. Both k_{OH} and k_{O_3} data refer to Atkinson and Arey (2003), H data refer to Sander (2015), P and K_{ow} data are from <https://pubchem.ncbi.nlm.nih.gov/> and Sangster (1989), unless otherwise noted by a: (Dagaut et al., 1988), b: (Harris et al., 1981), c: (Chebbi and Carlier, 1996) and d: (Barratt, 1996). Positive values of k_w mean soil uptake and negative values mean soil emission. N means the values are negligible.

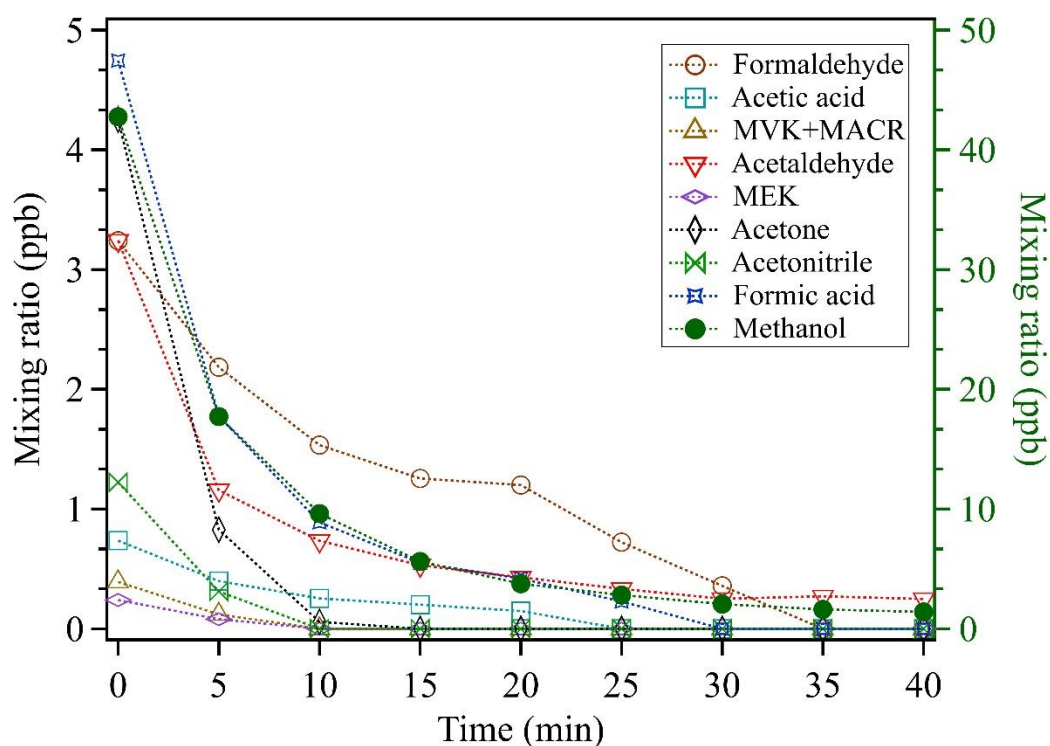
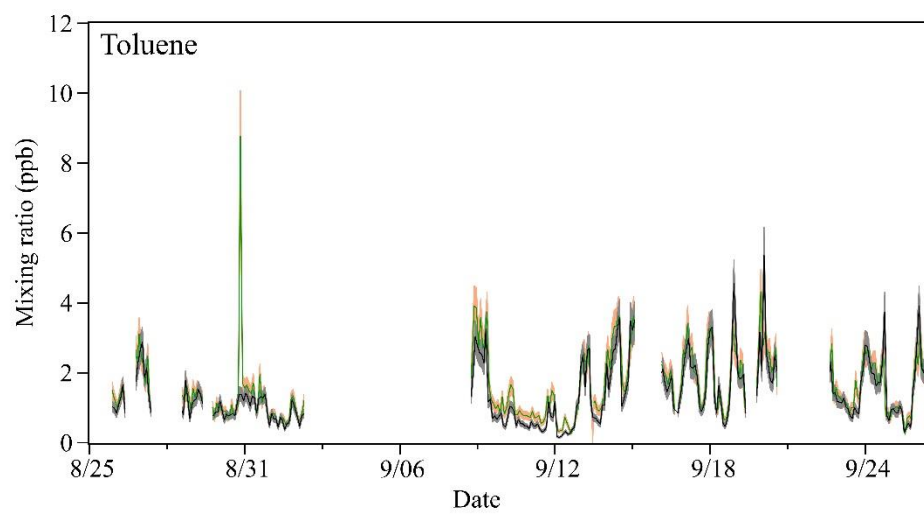
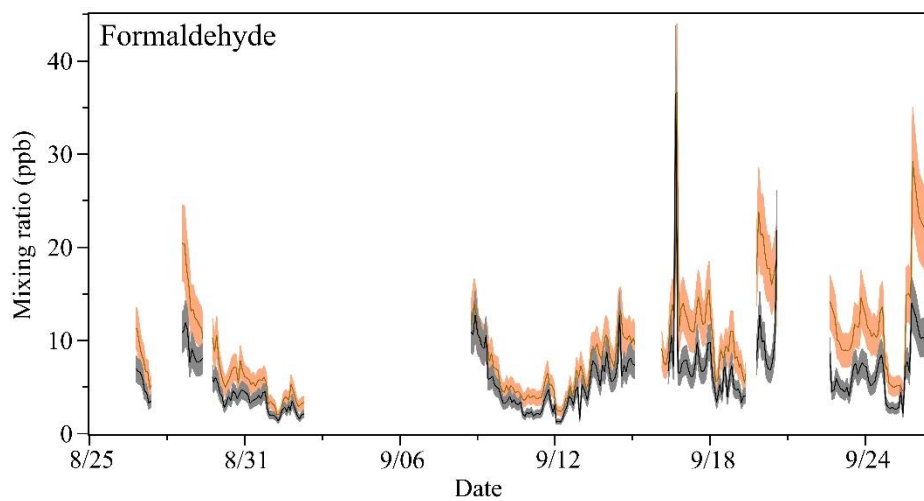
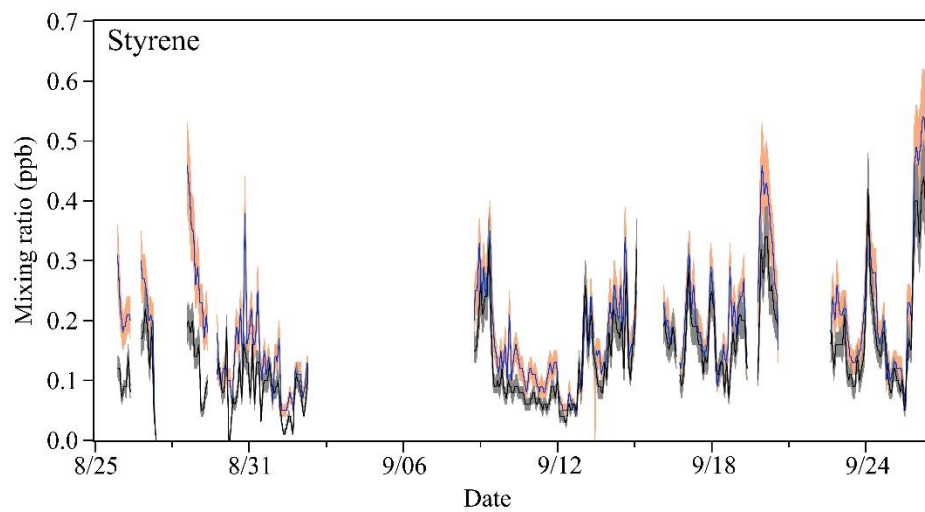
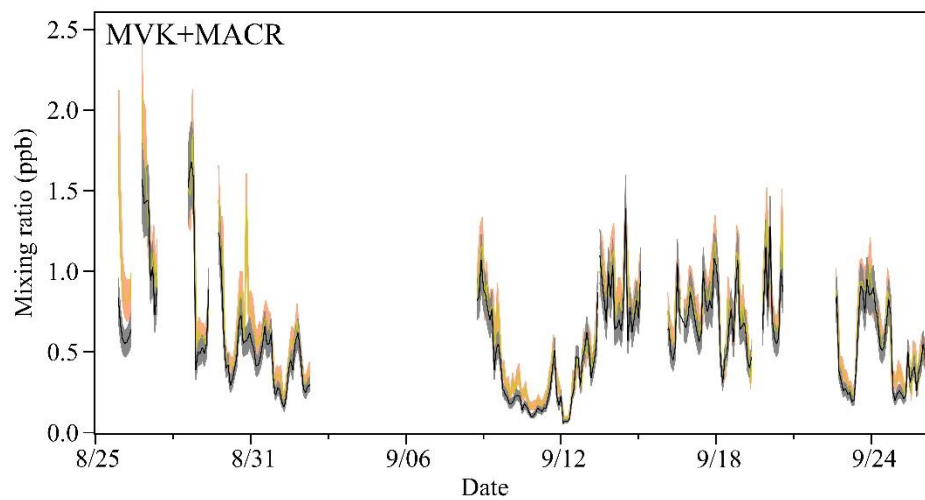
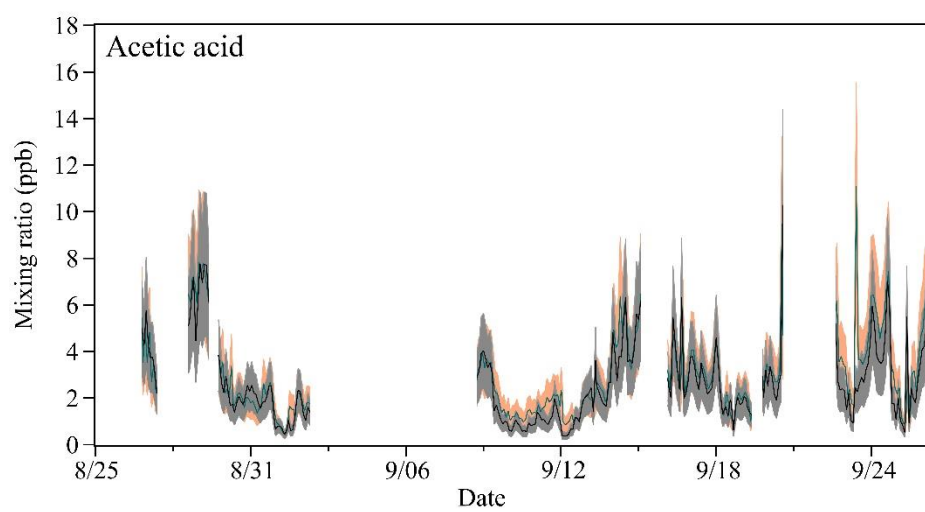
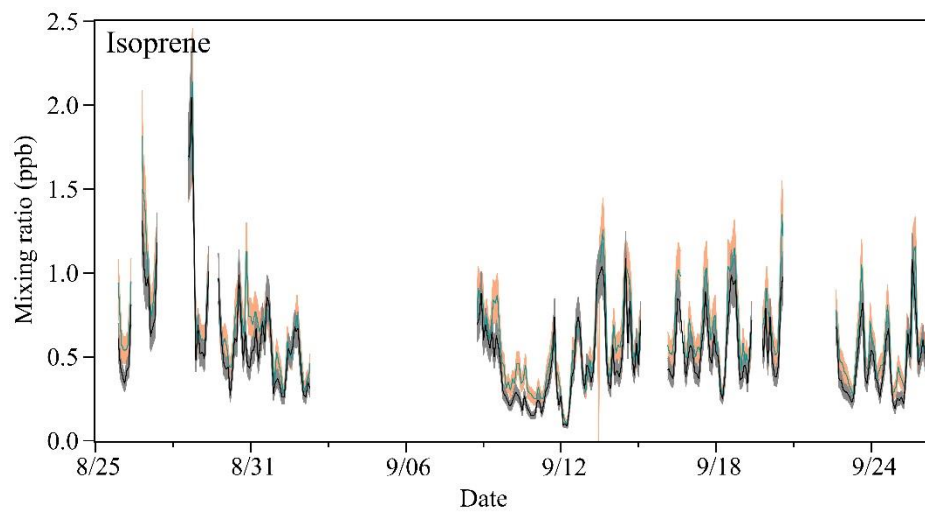
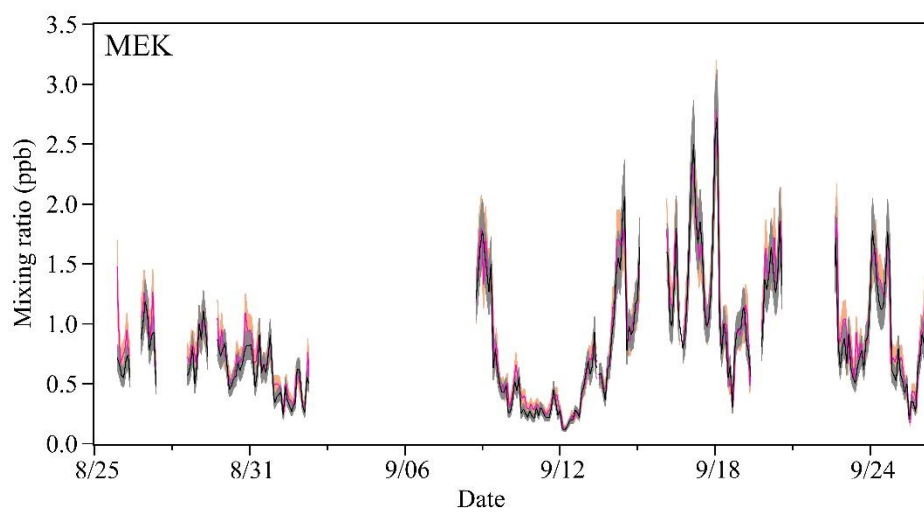
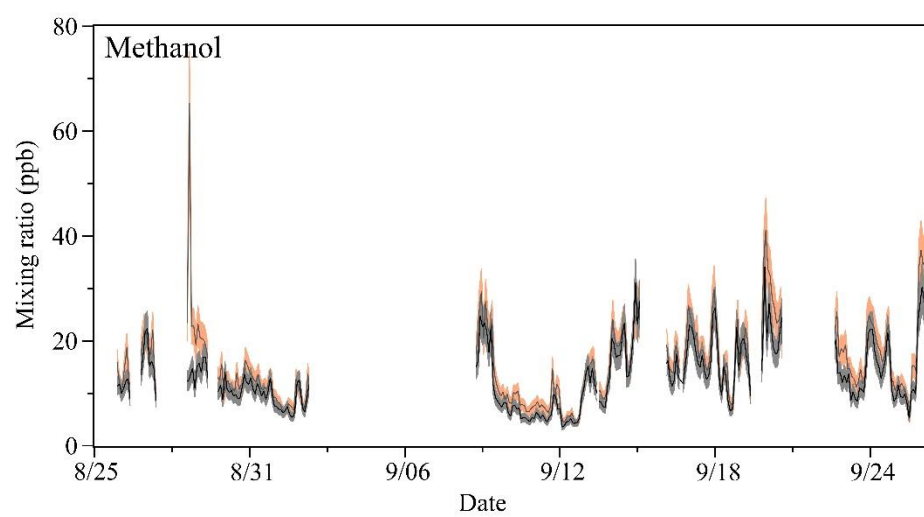
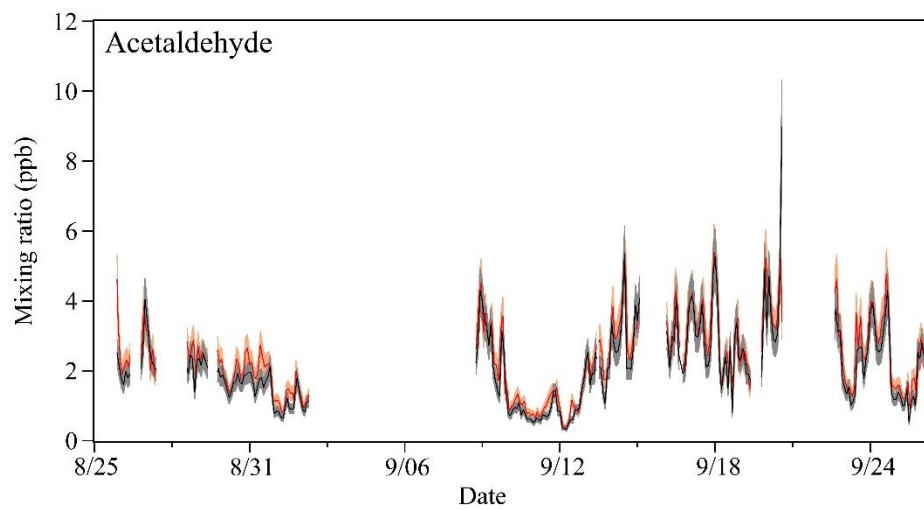
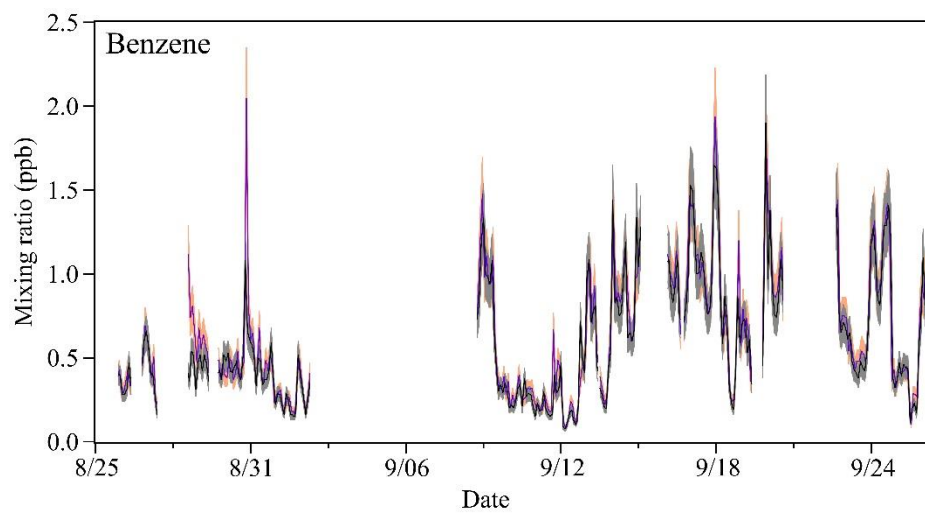
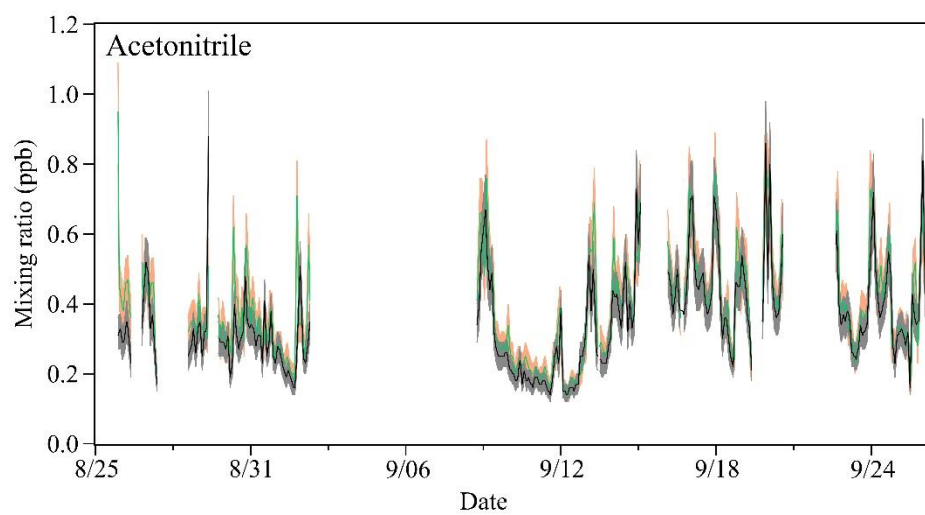
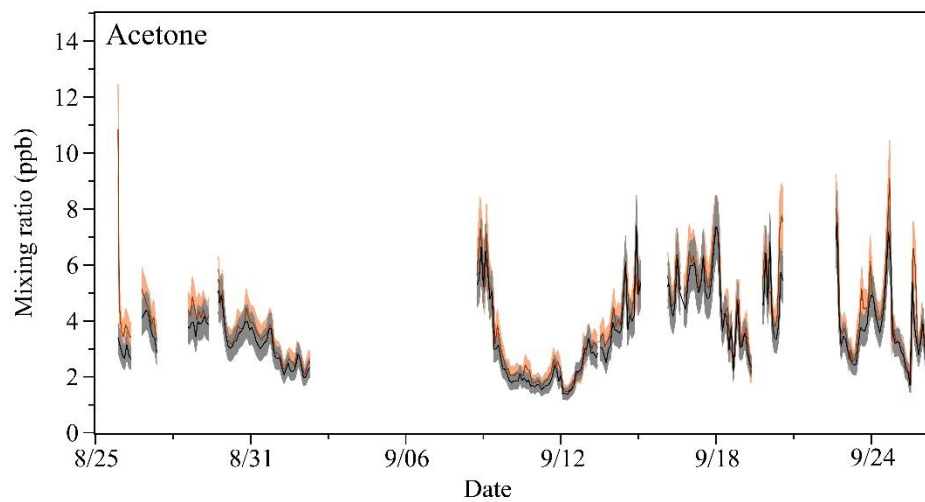


Figure S.1. Time course of VOC mixing ratios at the outlet of the freshly coated sample tube flushed with VOCs-free N_2 , prior to the ambient air uptake experiment. Methanol mixing ratios are referred to the right vertical axis and the other species are referred to the left.









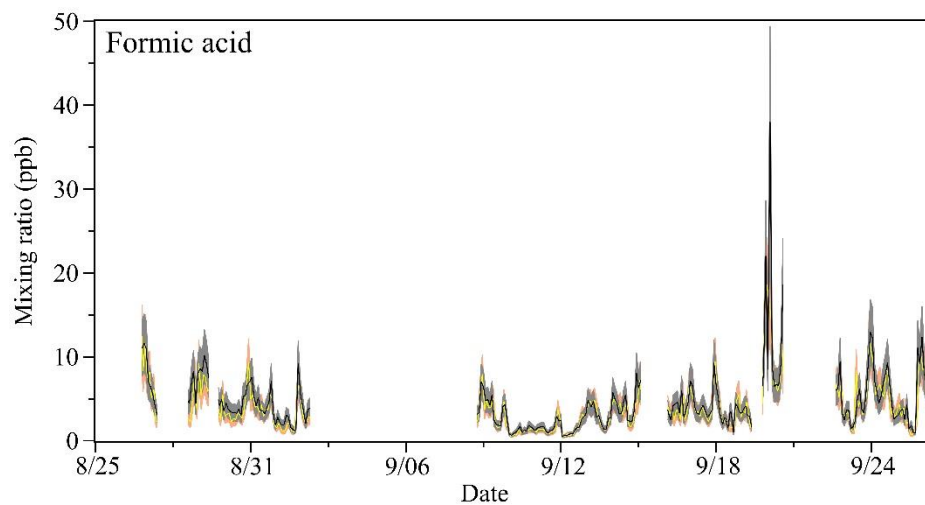


Figure S.2. Time series of ambient air mixing ratios of the examined VOCs. The lines mean the best estimation by the PTR-MS: colorful lines denote C_r and black lines denote C_s . The confidence bands (best estimate \pm measurement uncertainties) are shown as the orange shaded areas (for C_r) and gray shaded areas (for C_s).

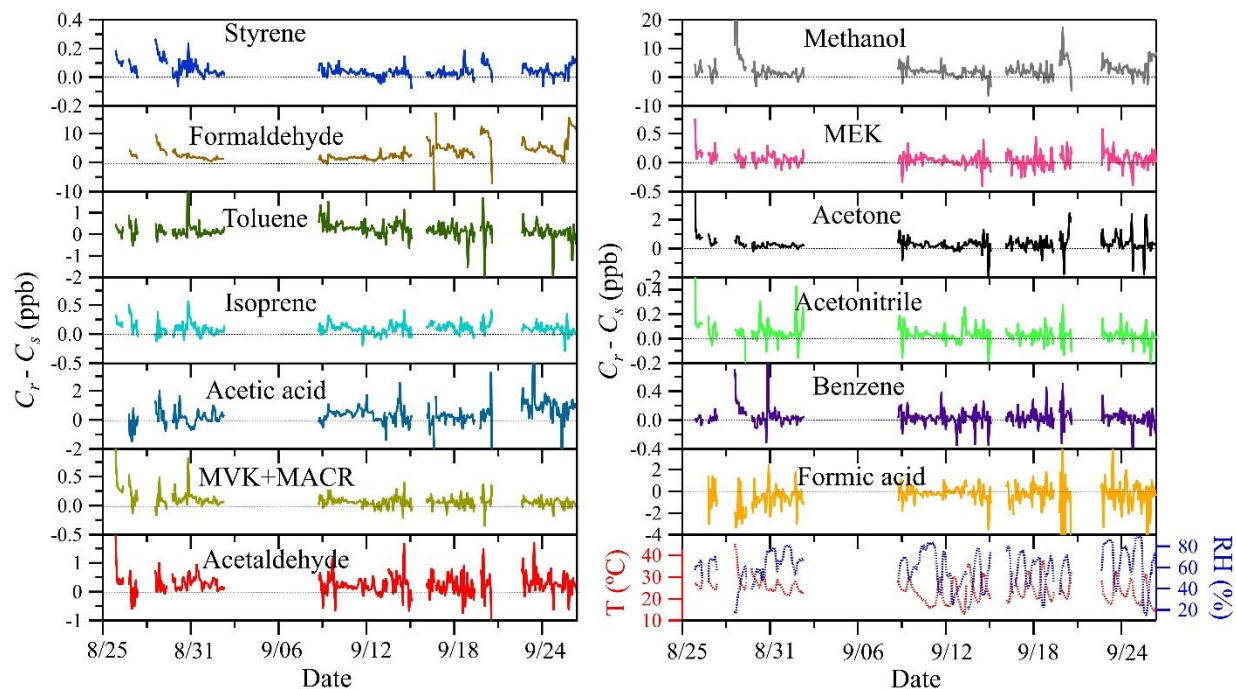


Figure S.3. Time series of the measured VOC mixing ratio differences between the reference channel and the sample channel: $C_r - C_s$. The lines are plotted using hourly averaged data.

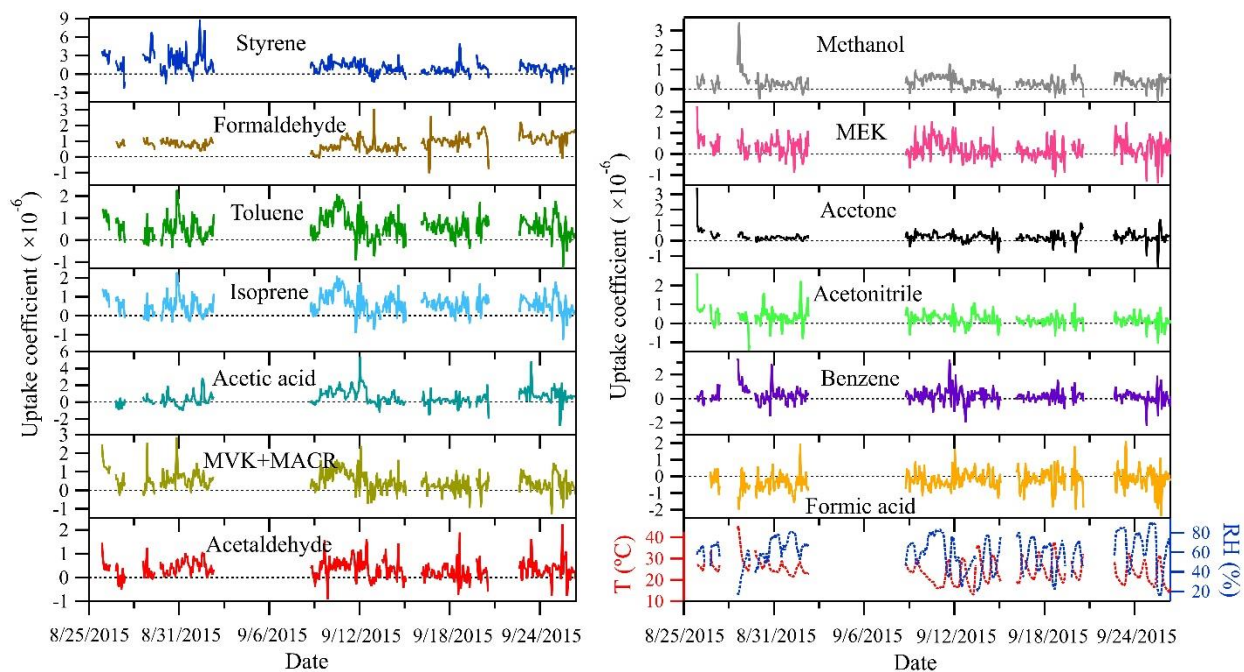


Figure S.4. Time series of the uptake coefficients of measured VOC species. The lines are plotted using hourly averaged data.

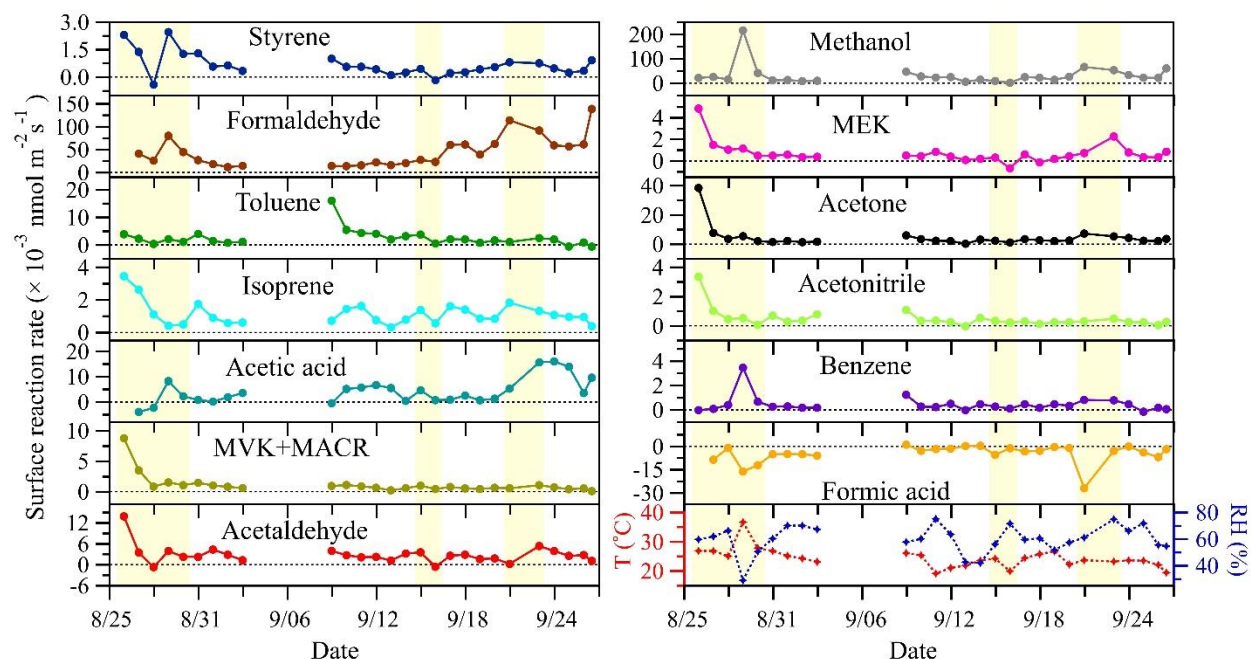


Figure S.5. Time series of the soil surface reaction rate of measured VOC species and air temperature (T) and relative humidity (RH). Each symbol represents daily averaged data and the yellow shaded areas indicate the days when measurements were not continuously running all day long. Positive values mean soil uptake and negative values mean soil emission. At the first three days of the measurement date, the significant decrease of the surface reaction rate for most of the VOC species can be rationalized by combined effect of soil surface adsorption/desorption equilibrium and bulk (soil pores) absorption saturation.

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