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# Seasonal dynamics and strategic mitigation of volatile Sulfur compounds emissions from an urban wastewater treatment plant: a long-term monitoring and AERMOD simulation

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## Legends

**Text S1.** Detailed information on the sample collection methods, sampling information, analytical techniques, and emission rate calculations.

**Fig. S1.** Process flow schematic diagram of the A/O WWTP. Abbreviations are as follows: Aerated grit tank (AGT), primary sedimentation tank (PST), anaerobic areas (ANA), oxic areas (OX), secondary sedimentation tank (SST), and sand-water separation unit (SWSU).

**Fig. S2.** Annual and seasonal wind directions and speeds in the study area.

**Fig. S3.** (a) Monthly wastewater temperatures; (b) Monthly influent wastewater volumes.

**Fig. S4.** (a) Proportional VSCs emission rates by treatment unit; (b) Proportional emission contributions by VSCs type.

**Fig. S5.** VSCs dispersion patterns (1-hour values); panels (a), (c), (e), (g), (i), (k) for scenario 1, panels (b), (d), (f), (h), (j), (l) for scenario 2.

**Fig. S6.** Contribution rates of VSCs at sensitive points; panels (a), (c), (e), (g), (i) for scenario 1, panels (b), (d), (f), (h), (j) for scenario 2.

**Fig. S7.** Layout of sensitive points.

**Fig. S8.** Enclosure status of grill and SWSU.

**Fig. S9.** VSCs concentrations at the WWTP boundary before and after enclosure of grill and SWSU; panels (a), (c), (e), (g), (i) show the concentrations before enclosure and panels (b), (d), (f), (h), (j) show the concentrations after enclosure.

**Fig. S10.** VSCs concentrations at sensitive points before and after enclosure of grill and SWSU.

**Fig. S11.** Odor pollution ranges before and after enclosure of the grill and SWSU under Scenario 2; panels (a), (c), (e) show the ranges before enclosure and panels (b), (d), (f) show the ranges after enclosure.

**Fig. S12.** Simulated deodorization facility site selection.

**Fig. S13.** Relationship between office area VSCs concentrations and simulated

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deodorization facility locations.

**Fig. S14.** Odor pollution ranges for original and #6 site selections; panels (a), (c), (e) show the ranges at the original site and panels (b), (d), (f) show the ranges at site #6.

**Fig. S15.** Relationship between office area VSCs concentrations and exhaust stack height.

**Fig. S16.** Odor pollution ranges with original exhaust stack height (15m) and increased height (40m); panels (a), (c), (e) show the odor pollution ranges with the exhaust stack at the original height of 15m and panels (b), (d), (f) show the ranges with the stack height increased to 40m.

**Fig. S17.** Relationship between office area VSCs concentrations and deodorization fan volume.

**Fig. S18.** Odor pollution ranges with original deodorization fan volume ( $10,000 \text{ m}^3 \cdot \text{h}^{-1}$ ) and increased volume ( $20,000 \text{ m}^3 \cdot \text{h}^{-1}$ ); panels (a), (c), (e) show the ranges with the deodorization fan volume at  $10,000 \text{ m}^3 \cdot \text{h}^{-1}$  and panels (b), (d), (f) show the ranges with the fan volume increased to  $20,000 \text{ m}^3 \cdot \text{h}^{-1}$ .

**Table S1** Correspondence between VSCs concentration and odor intensity.

**Table S2** Times and locations of maximum ground-level VSCs concentrations.

**Table S3** Times and locations of maximum ground-level TVSC concentrations by season.

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## *Supplementary Text*

### **Text S1. Detailed information on the sample collection methods, sampling information, analytical techniques, and emission rate calculations**

#### **1 Sample collection**

VSCs samples were collected monthly for ten months. All samples were collected between 9:30 a.m. and 2:30 p.m. and during non-extreme weather conditions.

Detailed sampling information is shown in **Table 1**.

**Table 1** Sample collection date, time, weather and WWTP influent quality.

Sampling date	Sampling time	Weather	Influent quality (mg/L)			
			COD	TN	NH <sub>3</sub> -N	TP
July 26th, 2021	10:00 am - 2:00 pm	sunny	450.00	56.79	50.89	5.97
August 16th, 2021	11:00 am - 2:30 pm	sunny	447.00	64.25	53.00	6.24
September 9th, 2021	10:00 am - 2:00 pm	sunny	262.00	47.35	38.92	4.39
October 6th, 2021	10:00 am - 2:00 pm	sunny	440.00	57.35	49.49	6.01
November 16th, 2021	9:30 am - 2:00 pm	sunny	307.00	53.85	50.18	5.28
December 7th, 2021	10:00 am - 2:00 pm	sunny	445.00	56.25	49.20	5.72
January 14th, 2022	10:00 am - 2:00 pm	sunny	254.00	52.78	49.62	4.81
February 18th, 2022	10:00 am - 2:00 pm	sunny	400.00	59.82	57.77	5.81

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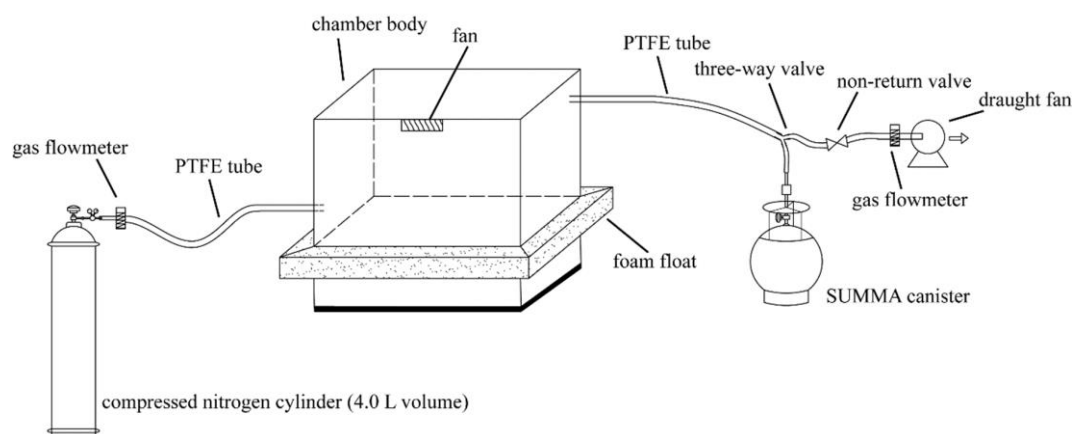
March 10th, 2022	10:00 am - 2:00 pm	sunny	488.00	59.05	53.42	5.72
April 12th, 2022	10:00 am - 3:00 pm	sunny	521.00	68.76	53.23	7.75

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## 2 VSCs sampling in non-aerated regions

A dynamic chamber was used to collect VSCs from the non-aerated units of the PST, ANA, and SST. The dynamic chamber was rectangular and made of plexiglass with a height of 0.2 m and a collection area of 0.063 m<sup>2</sup> (Fig. 1). Foam was fixed to the outside of the chamber so that it floated on the surface of the water column. Two polytetrafluoroethylene (PTFE) tubes were connected to the chamber, one to connect the chamber to a compressed nitrogen cylinder, the other to the output flow meter, and then to a SUMMA canister (negative pressure) and pump via a three-way valve. When collecting samples, the chamber was placed on the water surface, the nitrogen cylinder was opened, and the nitrogen input flow rate was adjusted to 400 ml·min<sup>-1</sup>. The pump was then switched on depending on the output flowmeter so that the output flow rate was equal to the input flow rate. The chamber was in dynamic equilibrium to avoid pressure changes affecting the natural release of VSCs and was purged for 40 min. When the air remaining in the chamber was completely replaced and the input and output flow rates were stable, the SUMMA canister valve was opened to collect the gas sample from the nitrogen purge. The gas sample in the SUMMA canister (3.0 L volume) was stored at room temperature and analyzed within 12 hours. It is important to note that the time needed for the air remaining in the chamber to be

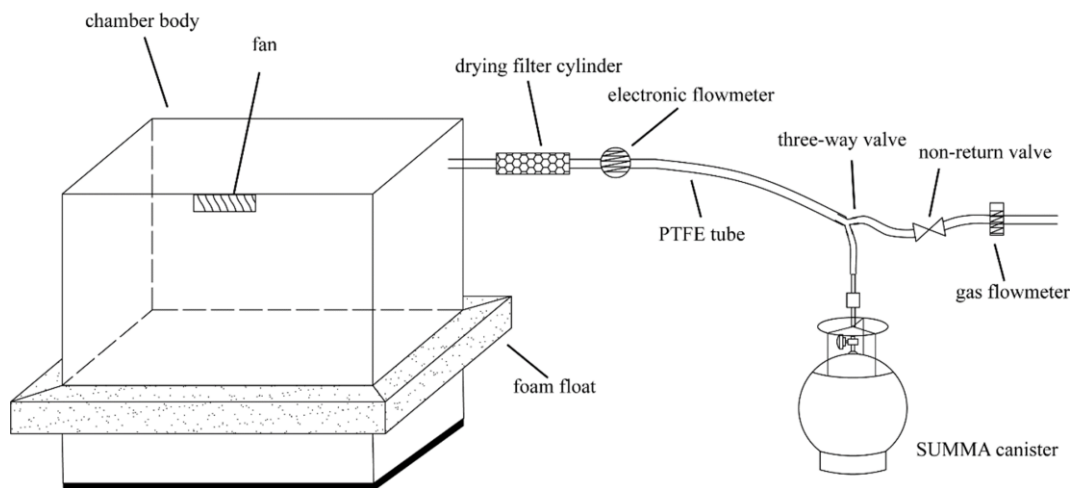
completely replaced needs to be investigated in advance.



**Fig. 1** the sampling method of VSCs in non-aerated regions

### 3 VSCs sampling in aerated regions

A static chamber was used to collect VSCs from the oxic areas. The static chamber was the same size and material as the dynamic chamber (**Fig. 2**). A PTFE tube was connected to the chamber, and the gas samples collected in the chamber were passed through an electronic flow meter (which measured the volume and cumulative flow of gas passing through it) and then connected to the SUMMA canister via a three-port-valve. The chamber was placed on the water surface when the sample was collected. The three-port-valve was opened and kept in contact with the ambient air for 10 min. After the air remaining in the chamber had been completely replaced, the electronic flow meter was cleared, the clock was started, and the valve of the SUMMA canister was opened to collect the gas sample released from the aeration water surface. The gas sample (3.0 L volume) in the SUMMA canister was stored at room temperature and analyzed within 12 hours.



**Fig. 2** the sampling method of VSCs in aerated regions.

#### 4 VOCs analytical methods

VOCs were collected and measured using SUMMA canister-gas chromatography. The SUMMA canister (3L, Hangzhou Tianjing Testing Technology Co., Ltd.) was used to collect and preserve gas samples. Gas chromatography (GC7890B, Agilent Technologies) equipped with a flame photometric detector (FPD) was used to determine VOCs concentrations. The VOCs were quantified using an external standard curve of peak area versus concentration. The chromatographic column was a Gas Pro (60 m × 320 μm), and the GC column chamber ramp-up procedure was as follows: initial temperature of 50 °C for 5 min, ramp-up to 120 °C at 20 °C·min<sup>-1</sup> for 4 min, and ramp-up to 180 °C at 25 °C·min<sup>-1</sup> for 16 min.

A linear standard curve was established between the concentration of the target compound and the peak area response value using an external standard method. The standard VOCs gases used were at ppm level. Standard VOCs gases consisted of H<sub>2</sub>S,

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MT, DMS, CS<sub>2</sub>, DMDS, provided by the Sichuan Zhong Ce Biao Wu technology Co., LTD, China. Standard gas gradient dilution was performed by Entech 4600 Dynamic Diluter (1ppm, 0.8ppm, 0.5ppm, 0.2ppm, 0.1ppm, 0.05ppm, 0.01ppm). Mixed standard samples were prepared in the same container (SUMMA canister) as the experimental samples to calibrate FPD. The quadratic curve equation was used to regress the obtained peak areas and VSCs contents to obtain the standard curve equation. Detection limits (ppm) of the VSCs were: H<sub>2</sub>S ( $9.94 \times 10^{-3}$ ), MT ( $8.2 \times 10^{-3}$ ), DMS ( $4.2 \times 10^{-3}$ ), CS<sub>2</sub> ( $2.4 \times 10^{-3}$ ), DMDS ( $2.6 \times 10^{-3}$ ).

### 5 VSCs emission rates calculation

The VSCs emission rates of PST, ANA, SST  $R_{na}$  ( $\text{mg}\cdot\text{m}^{-2}\cdot\text{h}^{-1}$ ) were calculated as shown in Eq. (1).

$$R_{na} = \frac{0.00006 \times c_1 \times q_1}{a_1} \times A \quad (1)$$

Where: 0.00006 is the conversion factor from ( $\text{ml}\cdot\text{min}^{-1}$ ) to ( $\text{m}^3\cdot\text{h}^{-1}$ ),  $c_1$  ( $\text{mg}\cdot\text{m}^{-3}$ ) is the concentration of VSCs collected through the dynamic chamber,  $q_1$  ( $\text{ml}\cdot\text{min}^{-1}$ ) is the nitrogen purge flow rate in the dynamic chamber,  $a_1$  ( $\text{m}^2$ ) is the collection area of the sampling unit (dynamic chamber), and  $A$  ( $\text{m}^2$ ) is the exposed area of the treatment unit.

The VSCs emission rates of OX  $R_a$  ( $\text{mg}\cdot\text{m}^{-2}\cdot\text{h}^{-1}$ ) were calculated as shown in Eq. (2).

$$R_a = \frac{3.6 \times c_2 \times V}{a_2 \times t} \times A \quad (2)$$

Where: 3.6 is the conversion factor from (s) to (h),  $c_2$  ( $\text{mg}\cdot\text{m}^{-3}$ ) is the concentration of

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VSCs collected through the static chamber,  $V$  (L) is the volume of gas passing through the electronic flow meter,  $a_2$  ( $m^2$ ) is the collection area of the sampling unit (static chamber), and  $t$  (s) is the time to collect the gas sample.

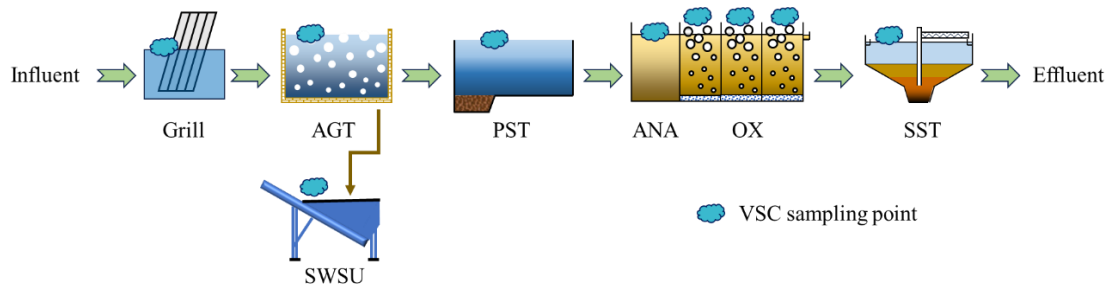
The VSCs emission rates of Grill, AGT, and SWSU  $R_2$  ( $mg \cdot h^{-1}$ ) were calculated as shown in Eq. (3).

$$R_2 = c_3 \times q_2 \quad (3)$$

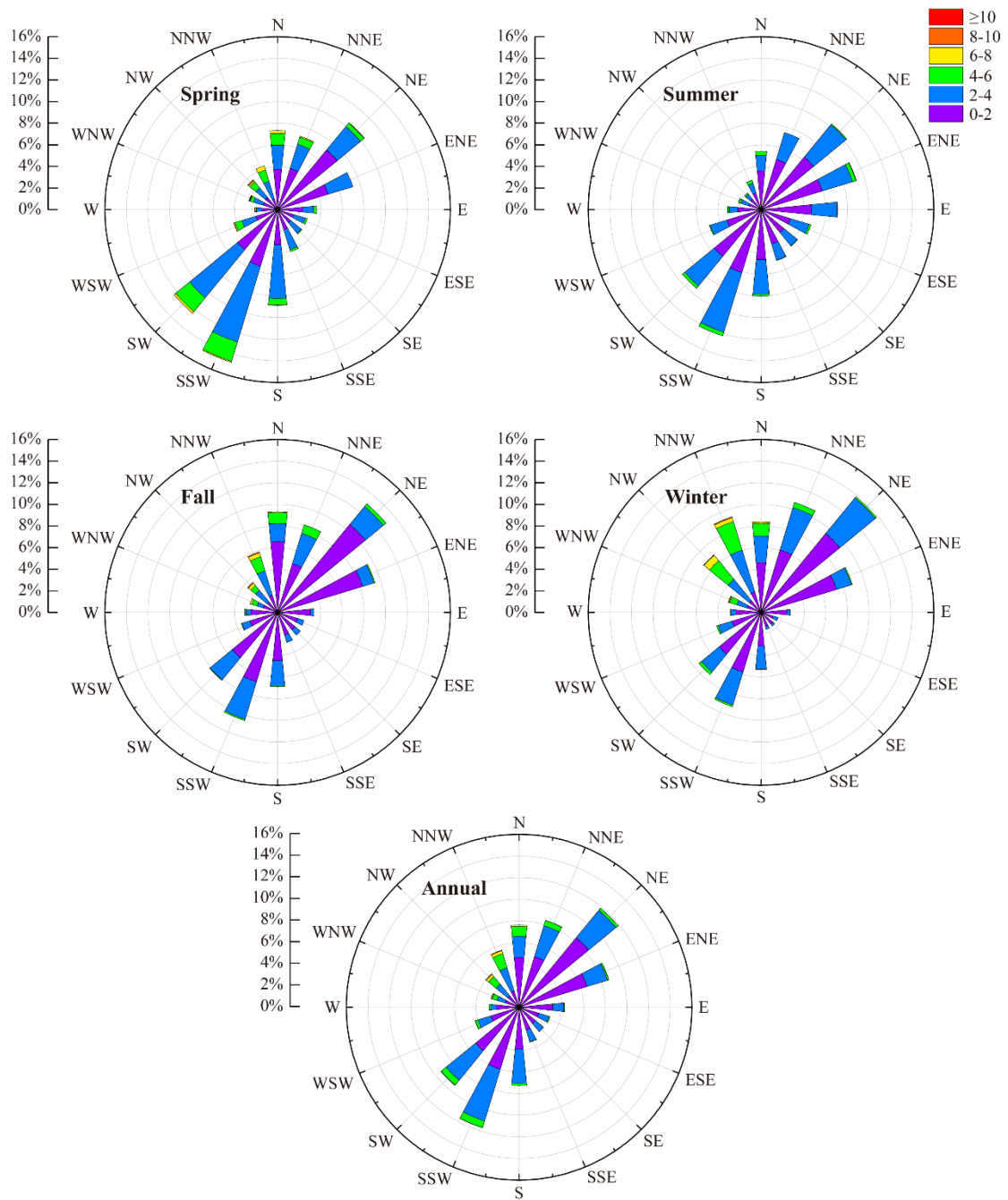
Where:  $c_3$  ( $mg \cdot m^{-3}$ ) is the concentration of VSCs collected at the collection port of the odor duct, and  $q_2$  ( $m^3 \cdot h^{-1}$ ) is the collection air volume at the collection port of odor duct.

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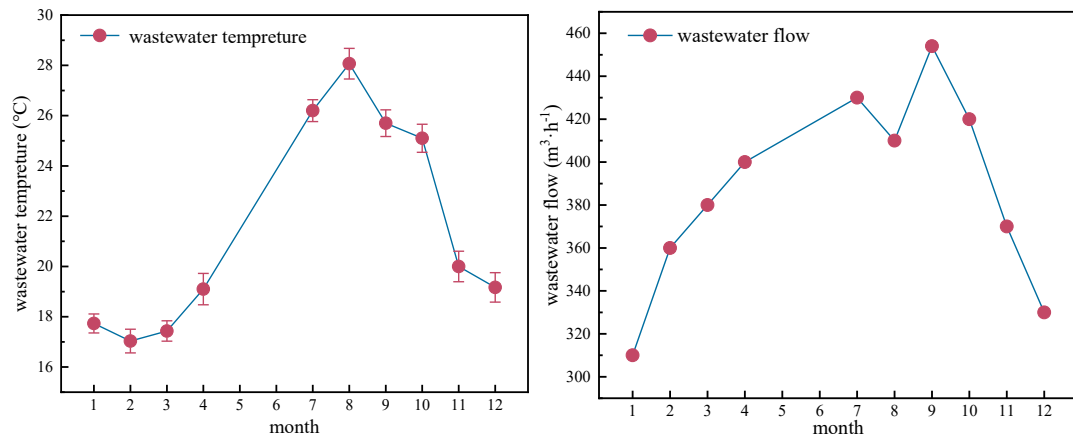
## Supplementary Figures



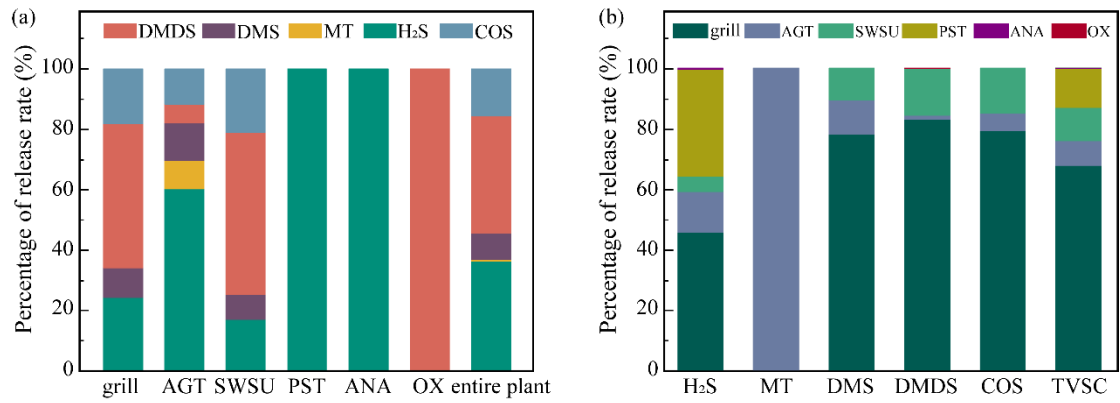
**Fig. S1** Process flow schematic diagram of the A/O WWTP. Abbreviations are as follows: Aerated grit tank (AGT), primary sedimentation tank (PST), anaerobic areas (ANA), oxic areas (OX), secondary sedimentation tank (SST), and sand-water separation unit (SWSU).



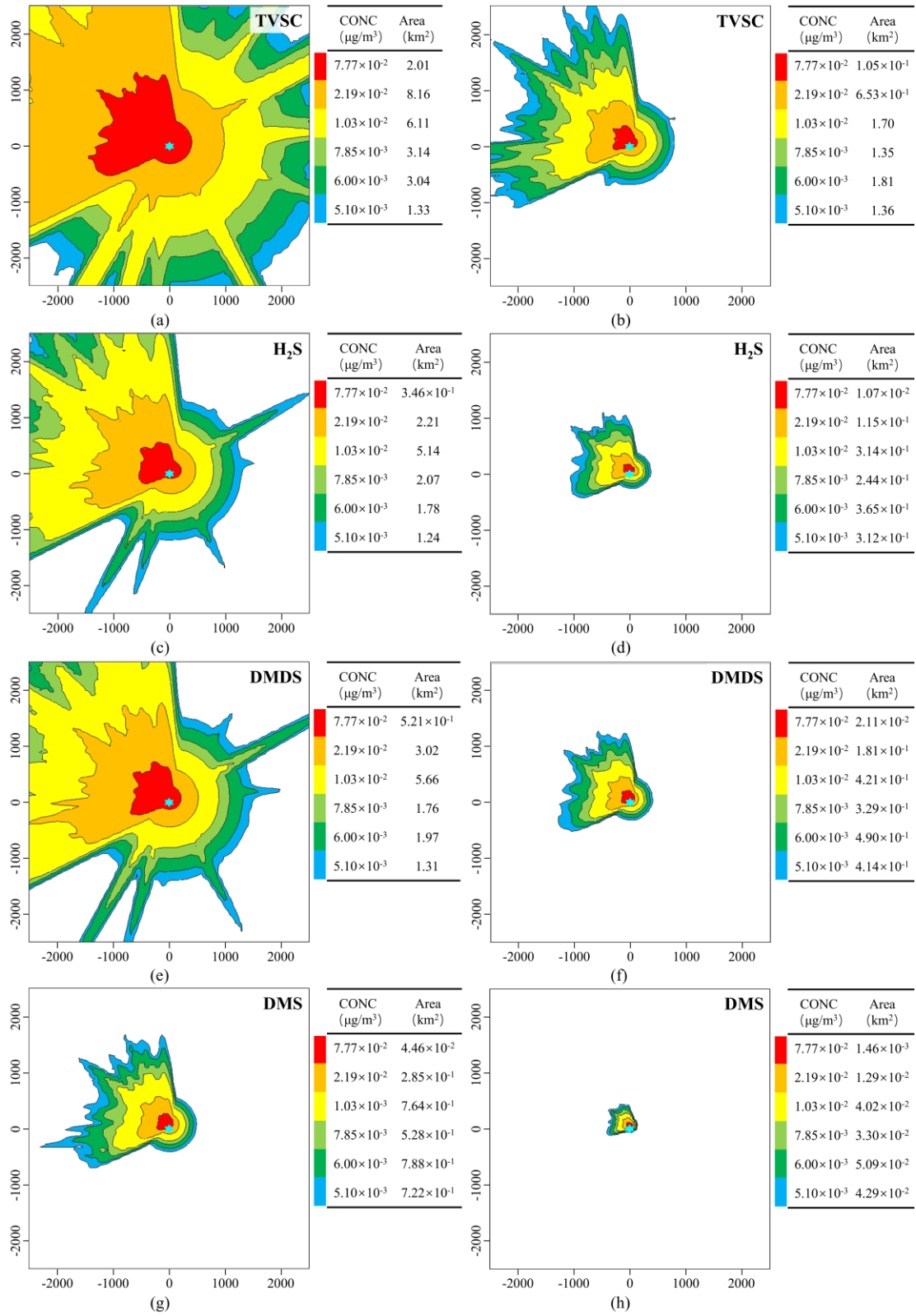
**Fig. S2** Annual and seasonal wind directions and speeds in the study area.

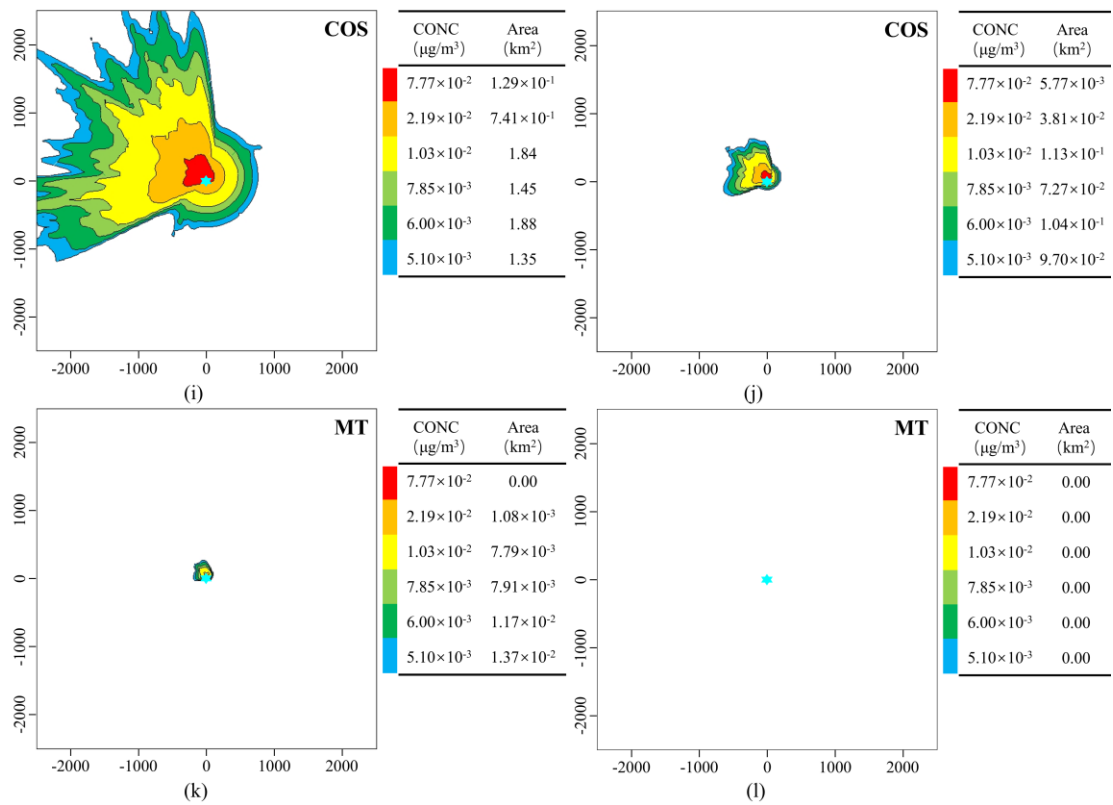


**Fig. S3** (a) Monthly wastewater temperatures; (b) Monthly influent wastewater volumes.

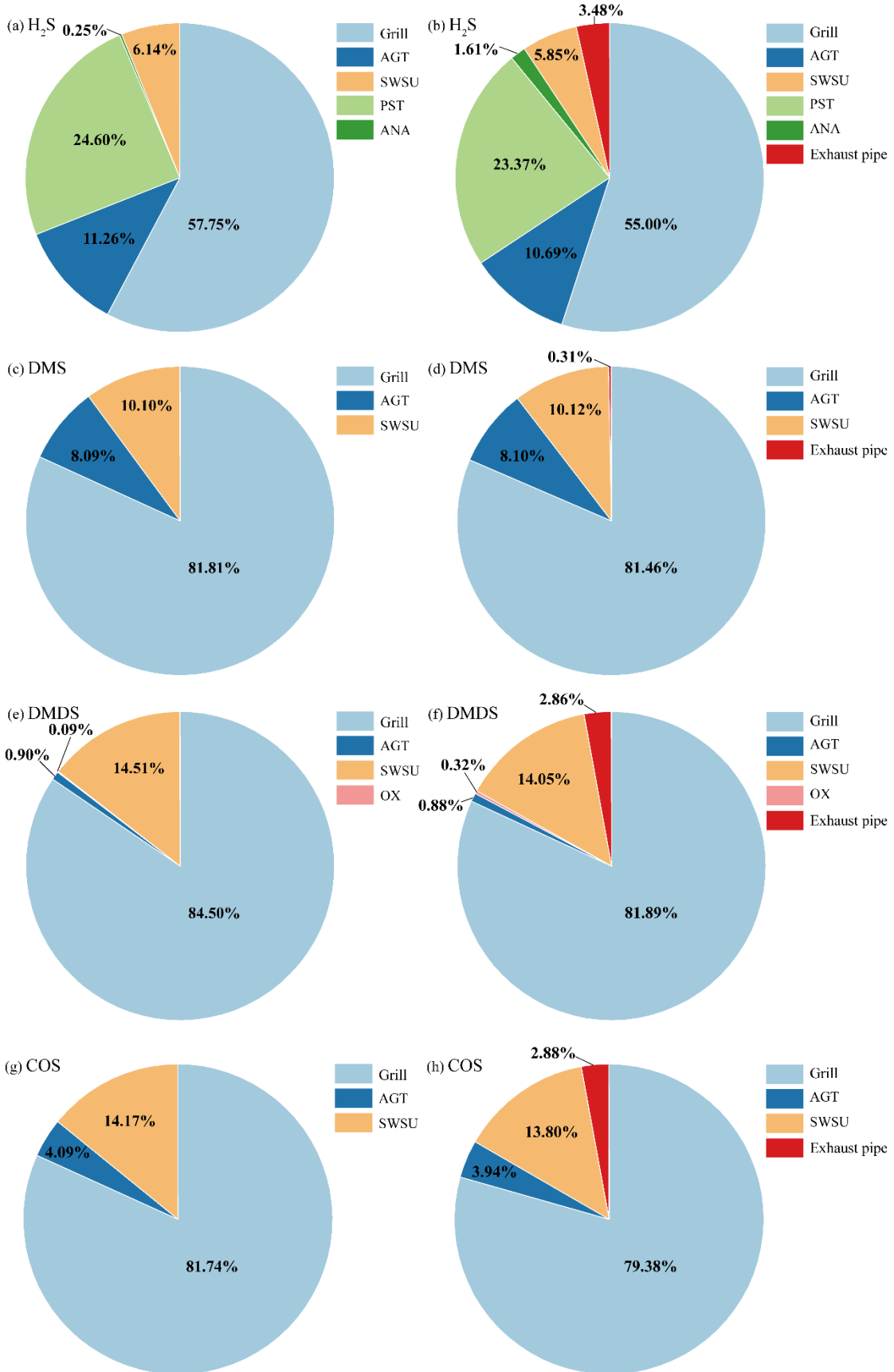


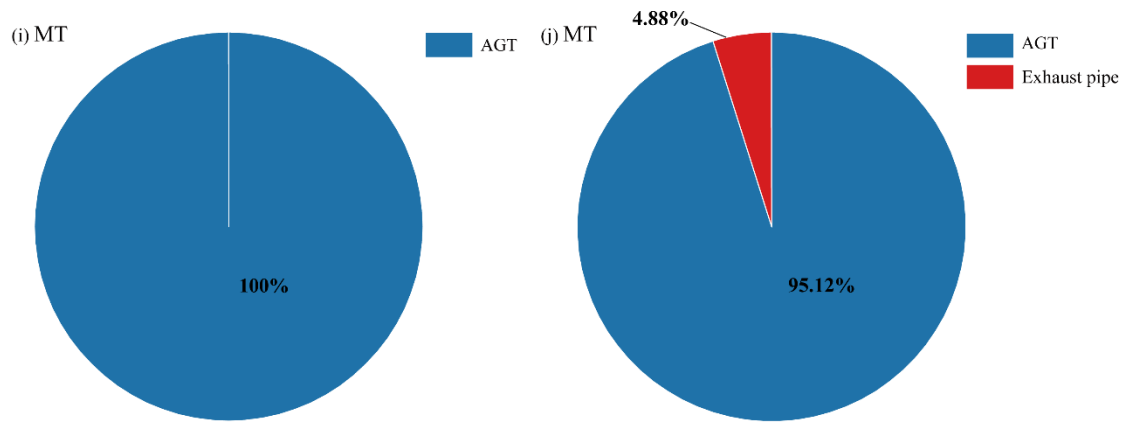
**Fig. S4** (a) Proportional VSCs emission rates by treatment unit; (b) Proportional emission contributions by VSCs type.



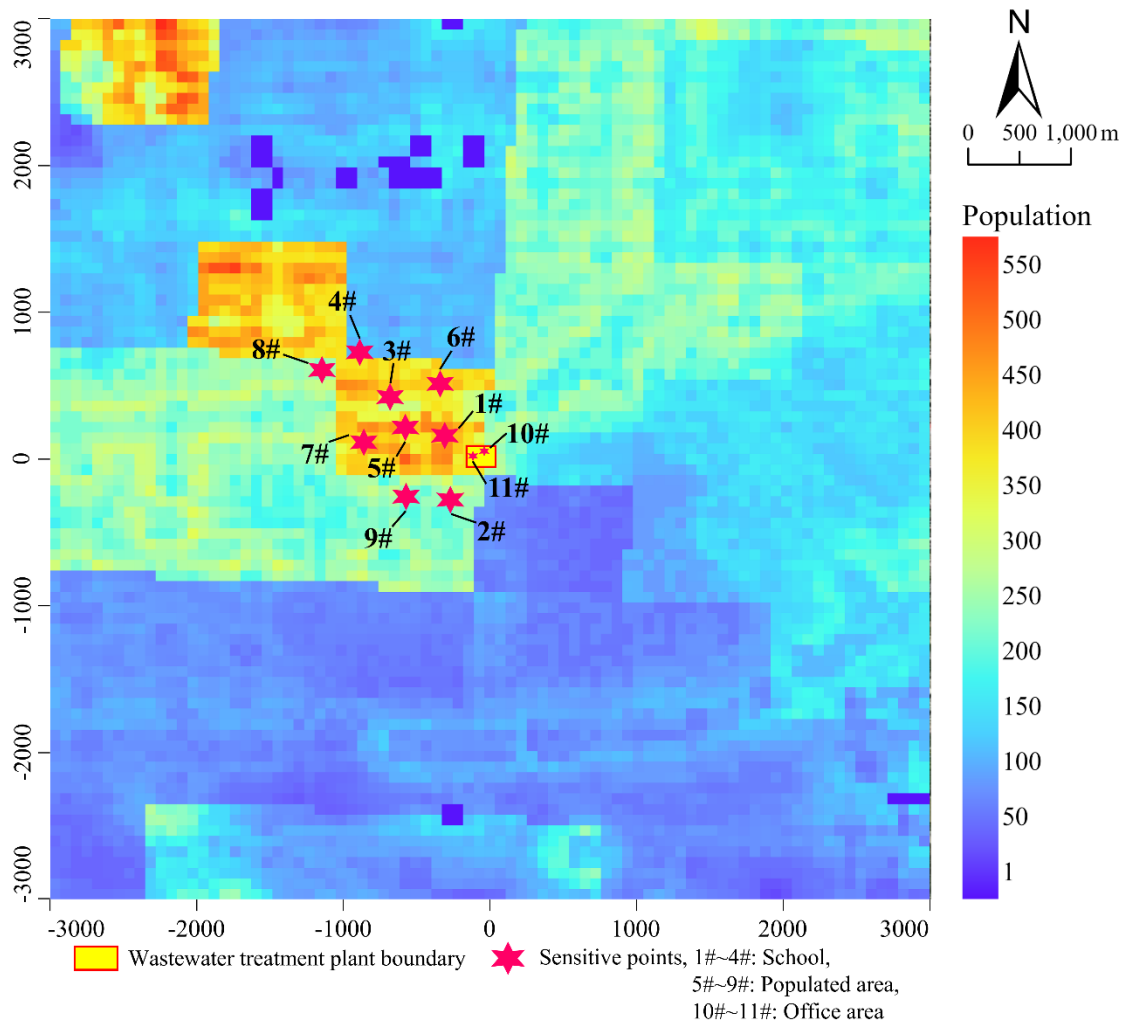


**Fig. S5** VSCs dispersion patterns (1-hour values); panels (a), (c), (e), (g), (i), (k) for scenario 1, panels (b), (d), (f), (h), (j), (l) for scenario 2.

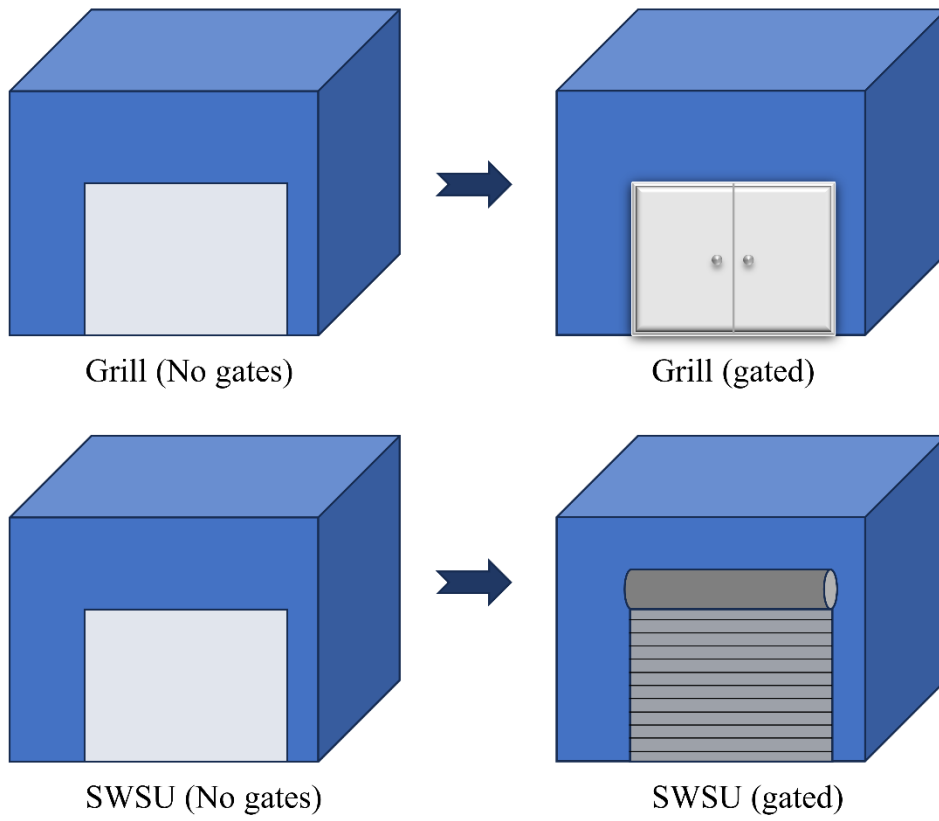




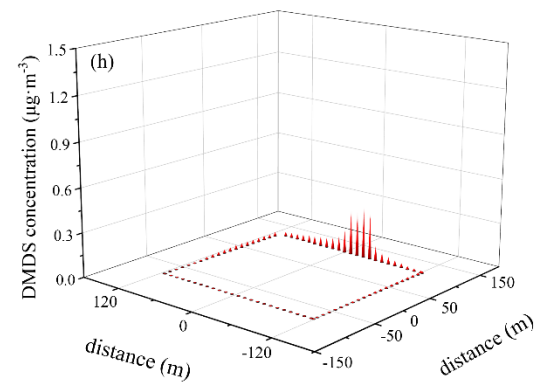
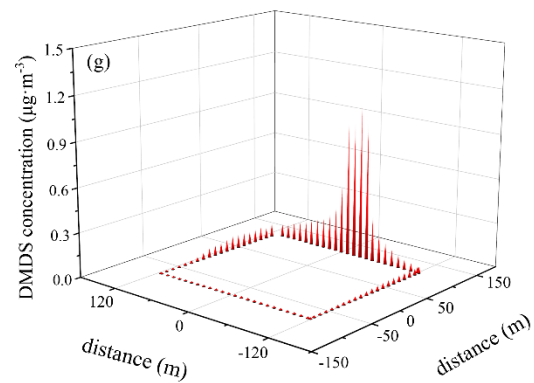
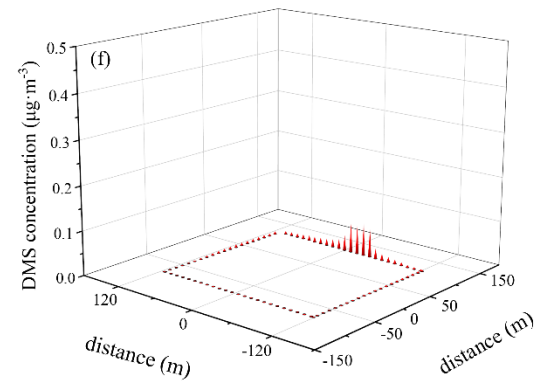
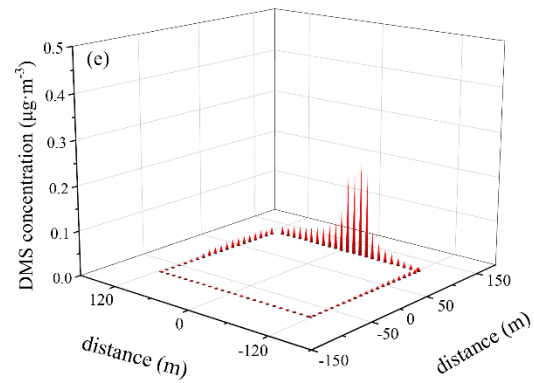
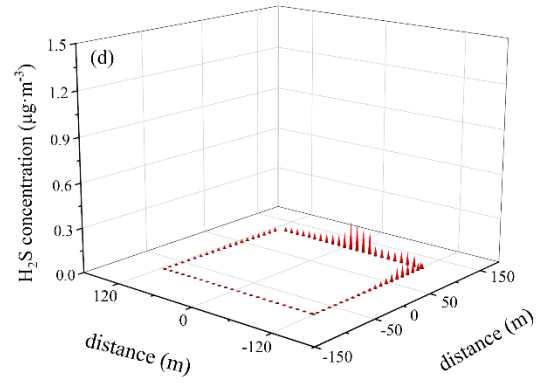
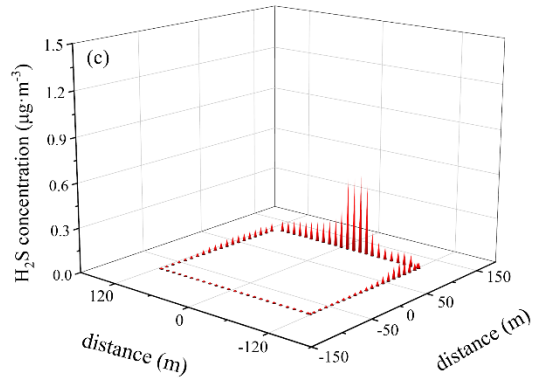
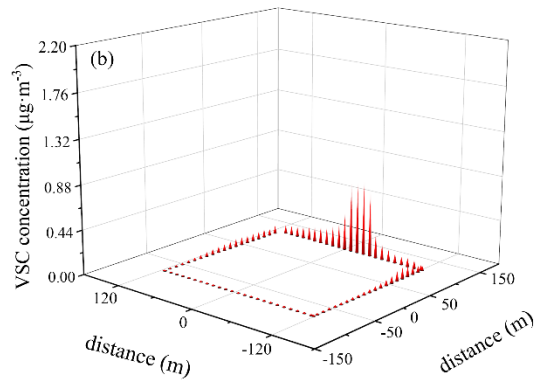
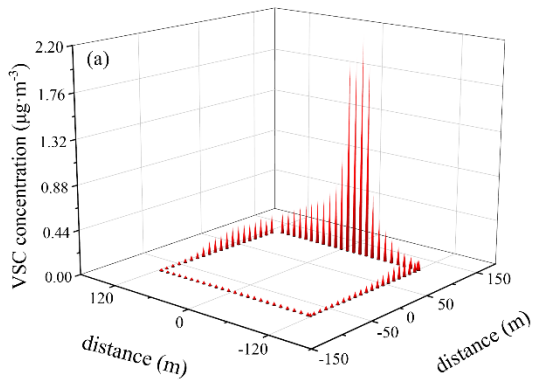
**Fig. S6** Contribution rates of VSCs at sensitive points; panels (a), (c), (e), (g), (i) for scenario 1, panels (b), (d), (f), (h), (j) for scenario 2.

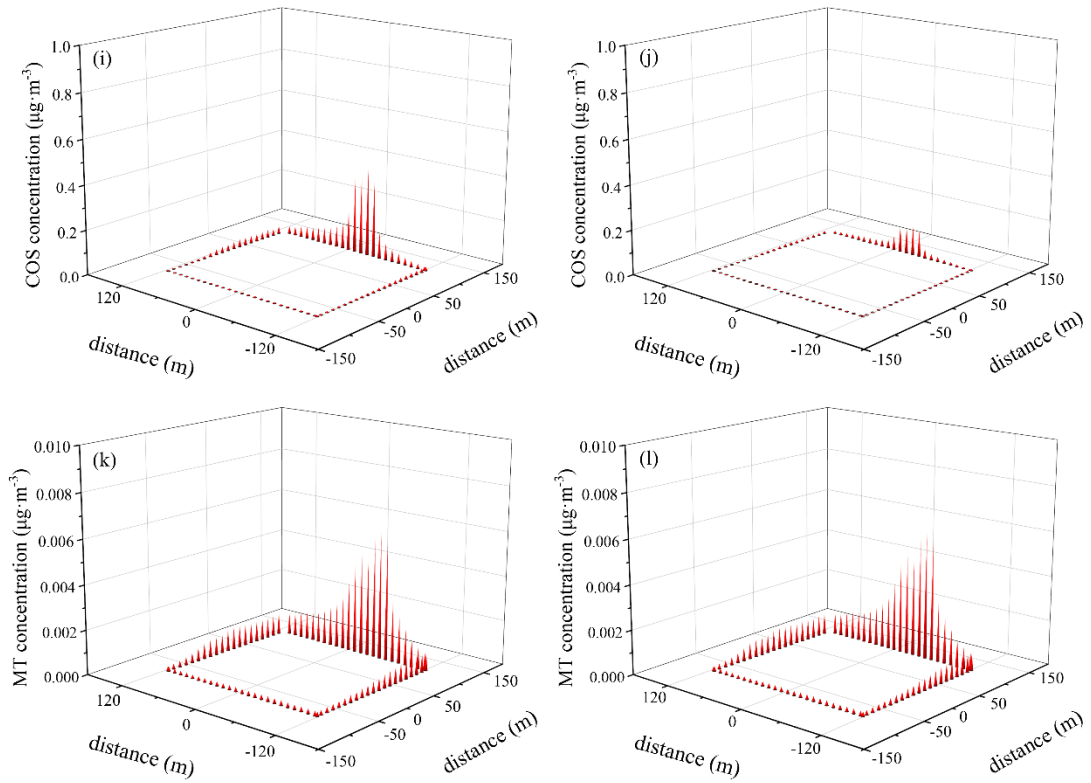


**Fig. S7** Layout of sensitive points.

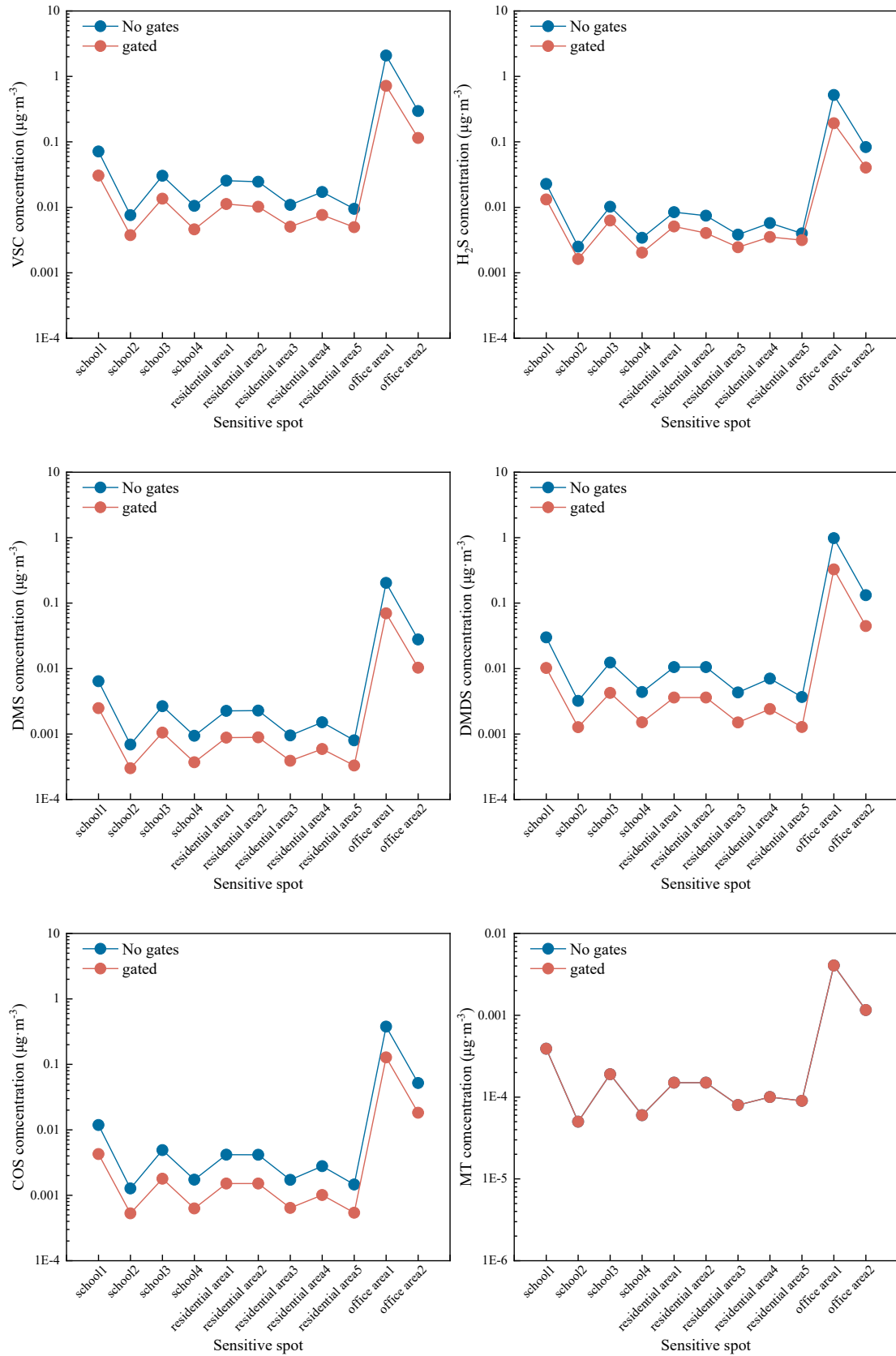


**Fig. S8** Enclosure status of grill and SWSU.

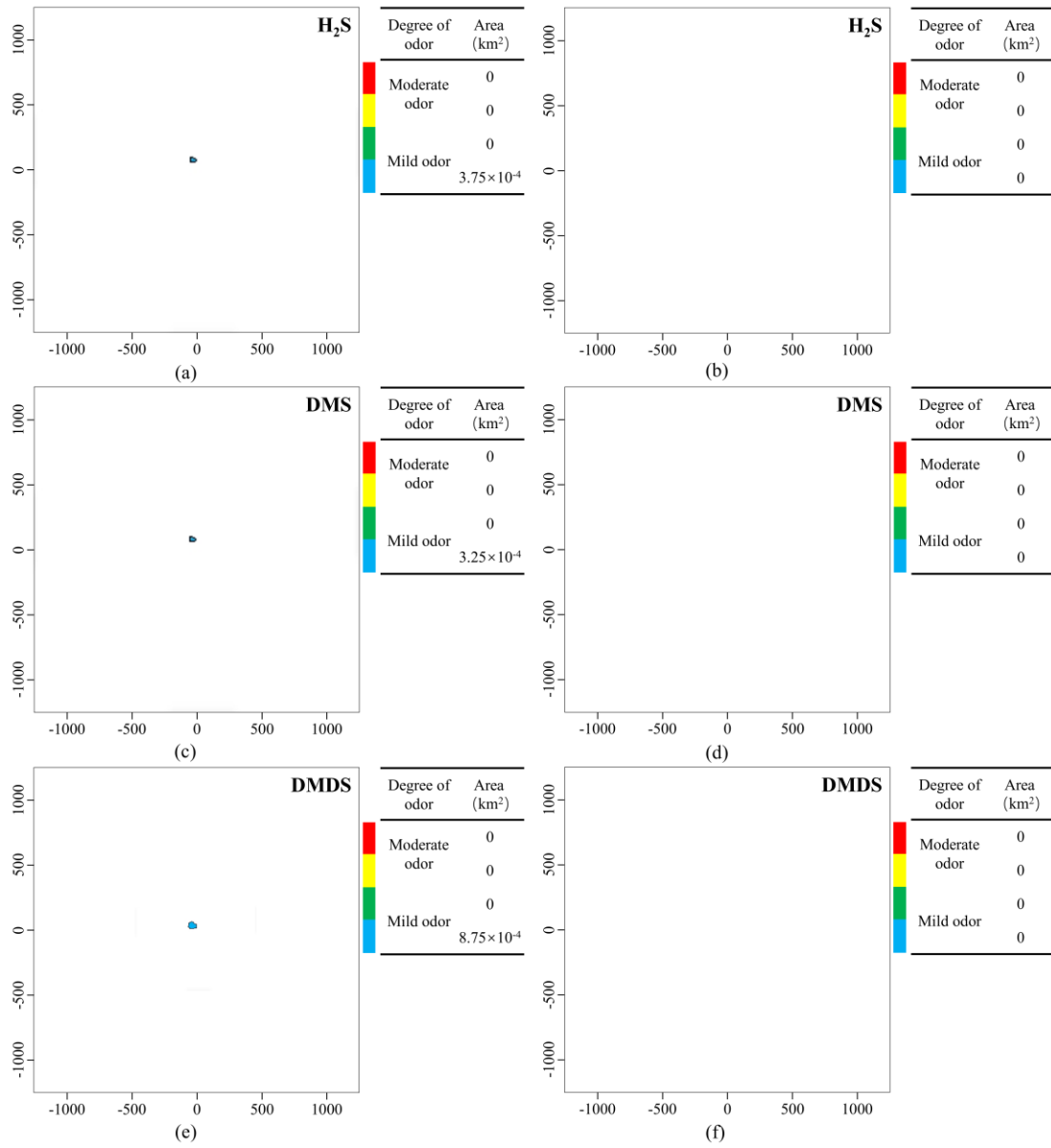




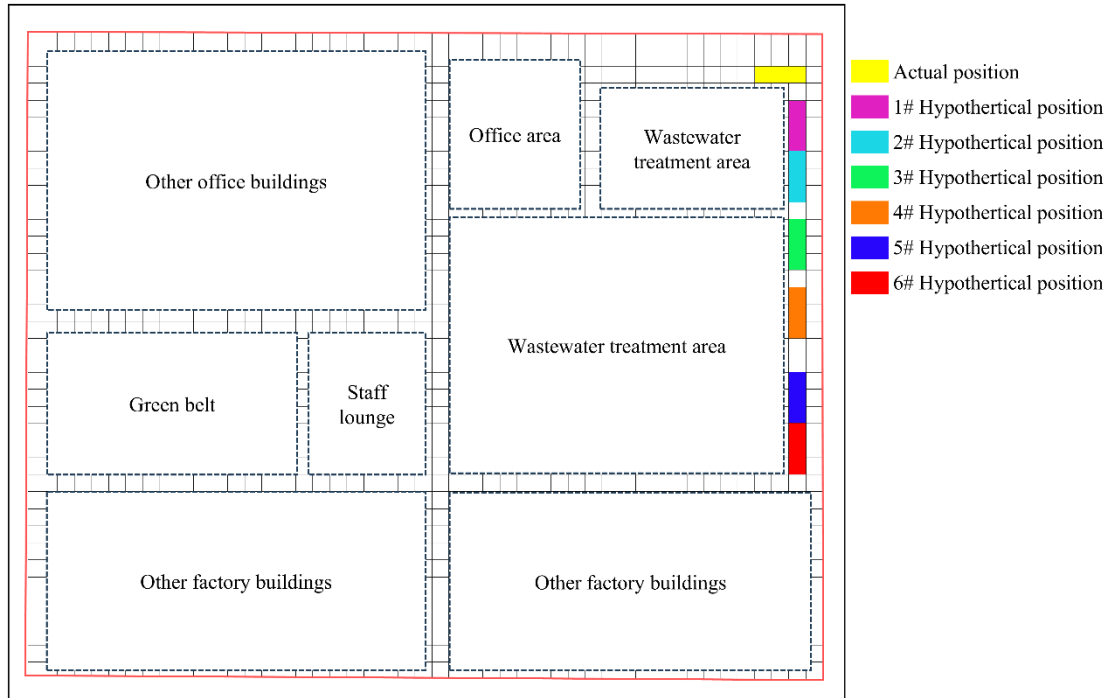
**Fig. S9** VSCs concentrations at the WWTP boundary before and after enclosure of grill and SWSU; panels (a), (c), (e), (g), (i) show the concentrations before enclosure and panels (b), (d), (f), (h), (j) show the concentrations after enclosure.



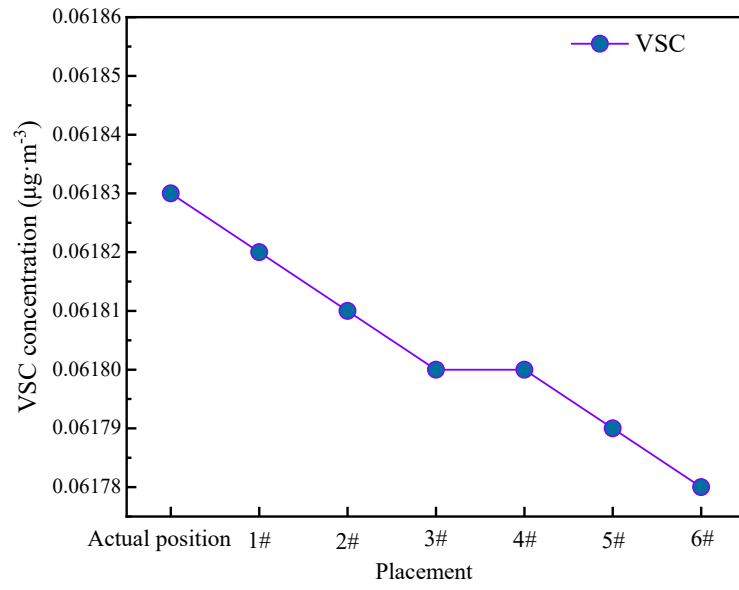
**Fig. S10** VSCs concentrations at sensitive points before and after enclosure of grill and SWSU.



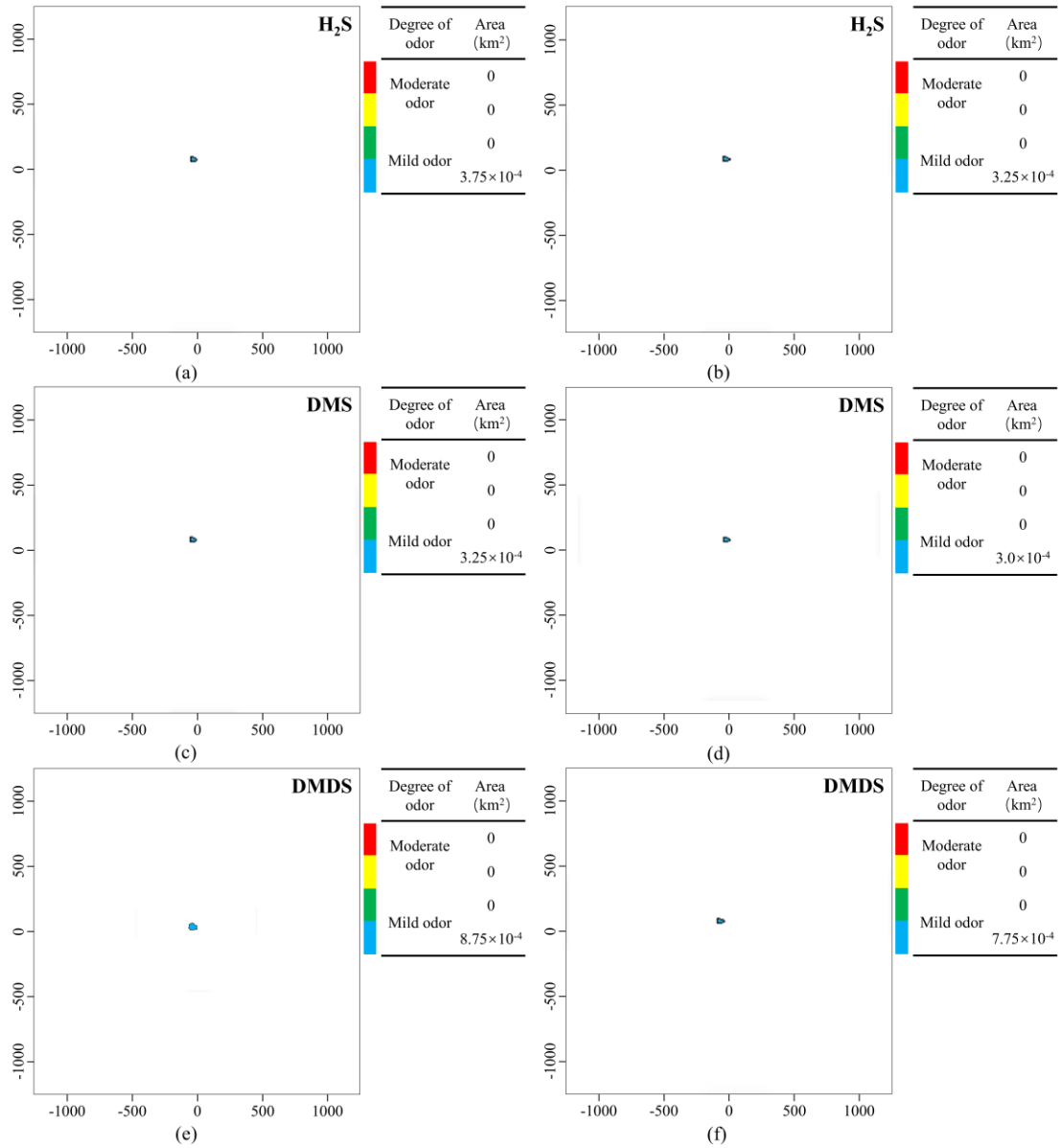
**Fig. S11** Odor pollution ranges before and after enclosure of the grill and SWSU under Scenario 2; panels (a), (c), (e) show the ranges before enclosure and panels (b), (d), (f) show the ranges after enclosure.



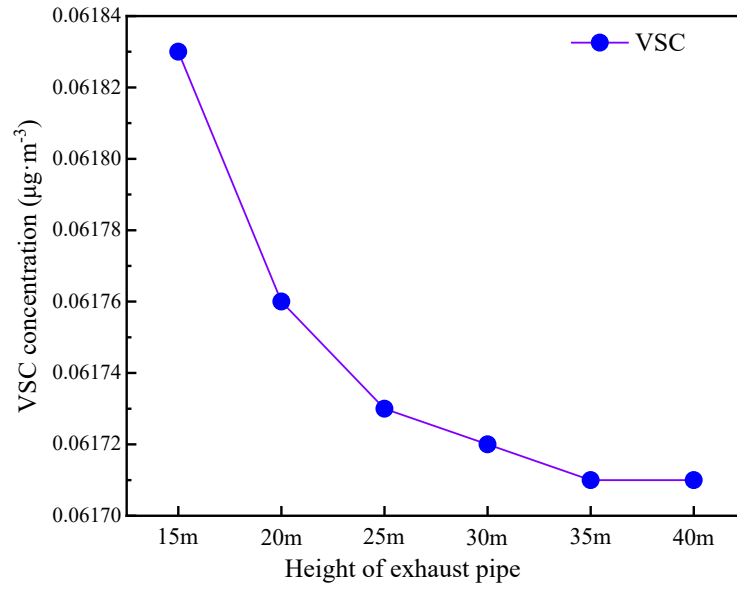
**Fig. S12** Simulated deodorization facility site selection.



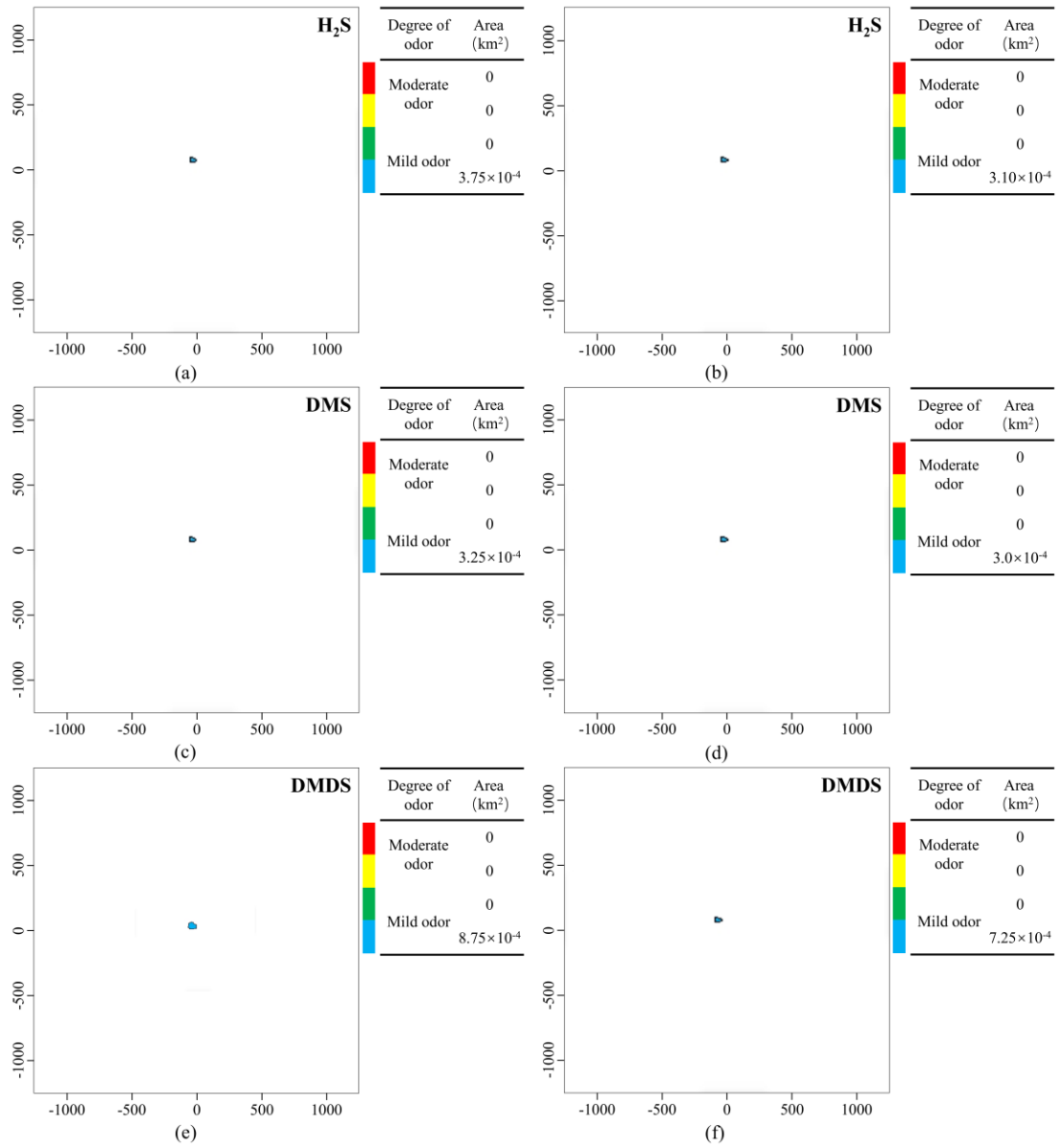
**Fig. S13** Relationship between office area VSCs concentrations and simulated deodorization facility locations.



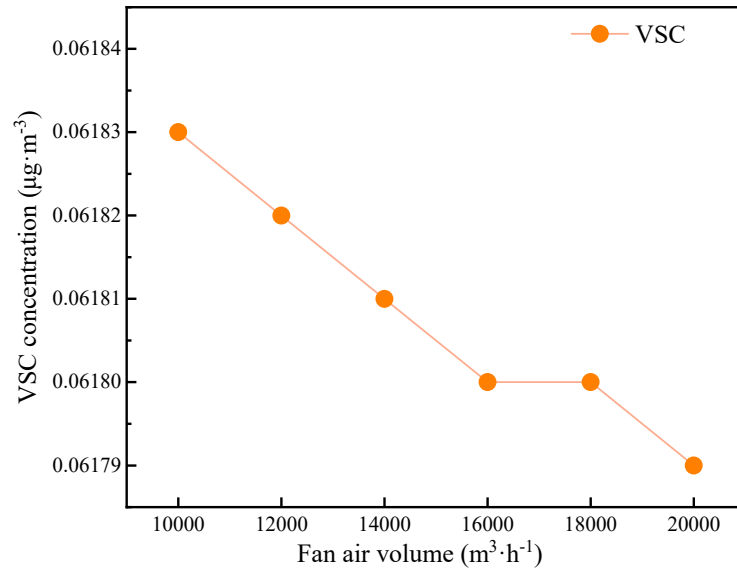
**Fig. S14** Odor pollution ranges for original and #6 site selections; panels (a), (c), (e) show the ranges at the original site and panels (b), (d), (f) show the ranges at site #6.



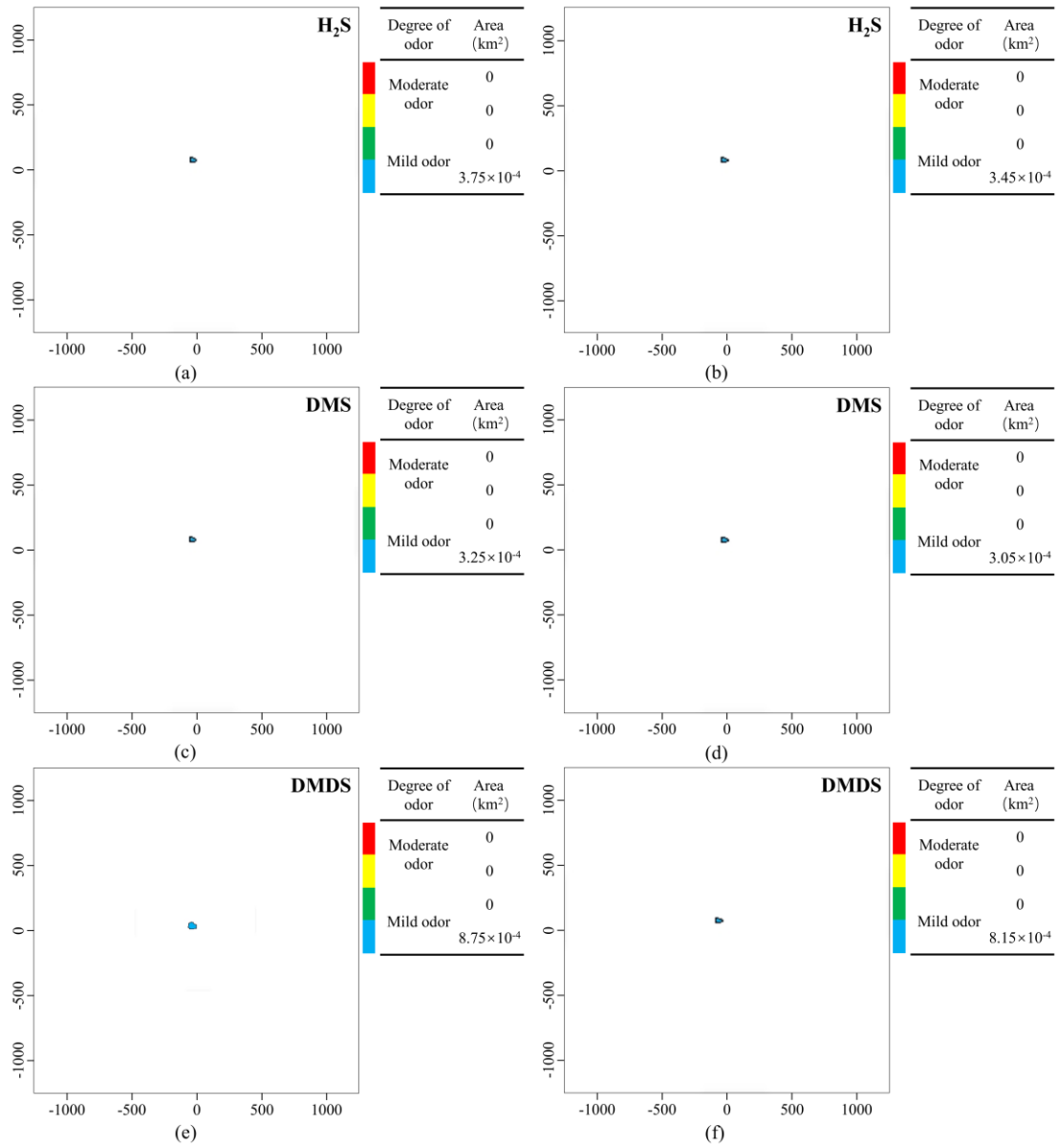
**Fig. S15** Relationship between office area VSCs concentrations and exhaust stack height.



**Fig. S16** Odor pollution ranges with original exhaust stack height (15m) and increased height (40m); panels (a), (c), (e) show the odor pollution ranges with the exhaust stack at the original height of 15m and panels (b), (d), (f) show the ranges with the stack height increased to 40m.



**Fig. S17** Relationship between office area VSCs concentrations and deodorization fan volume.



**Fig. S18** Odor pollution ranges with original deodorization fan volume (10,000 m<sup>3</sup>·h<sup>-1</sup>) and increased volume (20,000 m<sup>3</sup>·h<sup>-1</sup>); panels (a), (c), (e) show the ranges with the deodorization fan volume at 10,000 m<sup>3</sup>·h<sup>-1</sup> and panels (b), (d), (f) show the ranges with the fan volume increased to 20,000 m<sup>3</sup>·h<sup>-1</sup>.

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**Supplementary Table**

**Table S1** Correspondence between VSCs concentration and odor intensity.

Odor Intensity	Status	Odor Concentration (ppm)			
		H <sub>2</sub> S	MT	DMS	DMDS
0	Odorless	< 0.0005	< 0.0001	< 0.00012	< 0.00027
1	Slight Odor	0.0005	0.0001	0.00012	0.00027
1.5		0.0017	0.00026	0.00054	0.00088
2	Moderate Odor	0.0056	0.00065	0.0024	0.0028
2.5		0.019	0.0016	0.01	0.0091
3	Strong Odor	0.063	0.0041	0.044	0.029
3.5		0.21	0.01	0.19	0.094
4	Very Strong	0.72	0.026	0.84	0.31
4.5	Odor	2.39	0.064	3.64	0.98
5	Intolerable Odor	8.1	0.16	15.8	3.2

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**Table S2** Times and locations of maximum ground-level VSCs concentrations.

Type of VSCs	Scenario	Coordinates		Time	Concentration( $\mu\text{g}\cdot\text{m}^{-3}$ )
		X	Y		
TVSC	Scenario 1	-2	96	22.02.08.23	35.64354
	Scenario 2	-2	96	22.02.08.23	5.34654
H <sub>2</sub> S	Scenario 1	-2	96	22.02.08.23	8.70442
	Scenario 2	-2	96	22.02.08.23	1.30861
DMDS	Scenario 1	-2	96	22.02.08.23	16.93131
	Scenario 2	-2	96	22.02.08.23	2.53970
DMS	Scenario 1	-2	96	22.02.08.23	3.51682
	Scenario 2	-2	96	22.02.08.23	0.52747
COS	Scenario 1	-2	96	22.02.08.23	6.48758
	Scenario 2	-2	96	22.02.08.23	0.97314
MT	Scenario 1	-2	96	21.10.28.24	0.03964
	Scenario 2	-2	96	21.10.28.24	0.00595

**Table S3** Times and locations of maximum ground-level TVSC concentrations by season.

Season (TVSC)	Scenario	Coordinates		Time	Concentration( $\mu\text{g}\cdot\text{m}^{-3}$ )
		X	Y		
Spring	Scenario 1	-2	96	22.04.16.02	34.36904
	Scenario 2	-2	96	22.04.16.02	5.15537
Summer	Scenario 1	-2	96	21.08.01.21	30.59115
	Scenario 2	-2	96	21.08.01.21	4.58872
Fall	Scenario 1	-2	96	21.11.17.19	34.07931
	Scenario 2	-2	96	21.11.17.19	5.11192
Winter	Scenario 1	-2	96	22.02.08.23	35.64353
	Scenario 2	-2	96	22.02.08.23	5.34653

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**Table S4** Differential analysis of VSCs emission rates in different seasons

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Factor	Mean $\pm$ standard deviation				F-value	p-value
	Spring	Summer	Autumn	Winter		
value	918.87 $\pm$ 55.69	999.18 $\pm$ 32.	932.93 $\pm$ 40.	852.51 $\pm$ 7.74	7.106	0.021
		29	31			

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