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Supplement of

Glass plate sampling efficiency for trace gases in the sea surface microlayer

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S1 Experiment A—Preliminary test

Experiment A was conducted on three consecutive days between 13—15 March 2023, using one of our incubation baths (transparent plastic) as tank, filled with ultrapure water. We did these preliminary tests to learn about handling, measurements, mixing in the tank and sampling efficiency calculation from PA. As no glass plate had been available, we used a mesh screen. Targeted sample volume was $60\,\mathrm{mL}$. Figure S1 depicts the ratios of PA/PA_{ref} in experiment A, analogous to Fig. 3 of the main text (experiment B and C). Figure S2 depicts the resulting sampling efficiency. 9 of 16 points lie within the uncertainty range for DMS-d3 and isoprene-d5, and 4 of 9 for $^{13}\mathrm{CS}_2$. Therefore, it seems the tank was overall less well-mixed than in experiment B and C. However, no points are excluded from calculation of sampling efficiency, as experiment A serves as a test. This results in average ratios (± standard deviation) of PA/PA_{ref} of 0.98 ± 0.21, 0.99 ± 0.32, and 1.03 ± 0.29 for DMS-d3, isoprene-d5, and $^{13}\mathrm{CS}_2$ respectively. Sampling efficiency is 0.30 ± 0.08 ($n = 13$), 0.27 ± 0.09 ($n = 13$), and 0.26 ± 0.09 ($n = 10$) for DMS-d3, isoprene-d5, and $^{13}\mathrm{CS}_2$ respectively. Mean sampling efficiency and its standard deviation are, thus, larger here than with the glass plate in experiment B and C (compare with FW in Table 4 of the main text). The preliminary test with the mesh screen was less well constrained, which might explain the larger variation. The mesh screen might be more efficient, since wiping is not required. Also, the mesh screen captures more volume per dip, reducing the overall sampling duration. Furthermore, the mechanisms that contain the sample (fine mesh vs glass surface) might inherently be different physically and interact with the samples' properties. In field studies, the mesh screen samples are often associated with more dilution from ULW, as it samples a larger thickness than the glass plate. We do not expect this to have caused the differences in sampling efficiency during our experiment, as the ULW and SML should have been well-mixed. Finally, we did not remove any data points, thereby assuming that the tank was well-mixed at all times, though Fig. S1 indicates otherwise. An extended QC would presumably change the results and likely decrease the variation, but potentially maintain a similar mean sampling efficiency. We conclude from this preliminary test, that our experimental design seems suited to repeat the sampling efficiency estimation for mesh screen sampling.

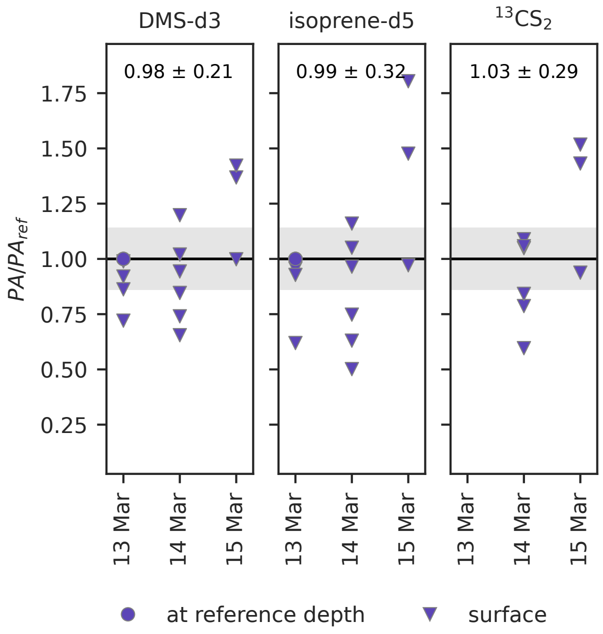

Figure S1. Test for uniform trace gas concentration in the tank (i.e., well-mixed) in experiment A with mesh screen. The ratios PA/PA_{ref} ($n = 16$ for DMS-d3 and isoprene-d5, $n = 9$ for $^{13}\mathrm{CS}_2$) are shown against date for DMS-d3 (left), isoprene-d5 (middle) and $^{13}\mathrm{CS}_2$ (right). Black horizontal line depicts $PA = PA_{ref}$ (i.e., well-mixed). Grey shaded area indicates $\pm 14.1\,\%$ uncertainty. Mean and standard deviation for PA/PA_{ref} is indicated in upper right of each subplot (including all shown points).

S2 Calibration curve examples gas chromatography-mass spectrometry

In order to use peak area normalized by sample volume (PA) instead of actual concentrations (i.e., skip calibration for the sake of more sample measurements per lab day), it is necessary that the gas chromatography–mass spectrometry (GC–MS) (1) behaves linear and (2) shows a (rela-

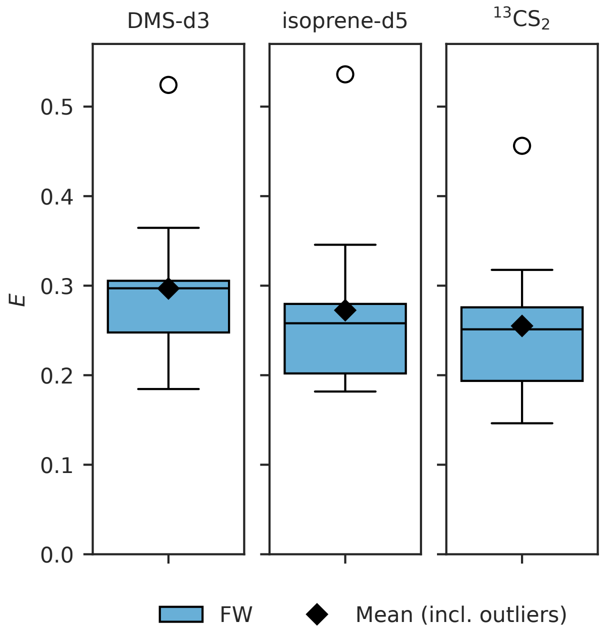

Figure S2. Sampling efficiency (E) for DMS-d3 (left), isoprene-d5 (middle) and $^{13}\mathrm{CS}_2$ (right) in experiment A with the mesh screen in treatment fresh water (FW). Box width shows 25 to 75 percentile, centre line denotes the median, diamonds denote the mean, open circles denote outliers, and whiskers show minimum and maximum. The number of data points in experiment A is $n = 13$ ($n = 10$ for $^{13}\mathrm{CS}_2$).

tively) low variation of the intercept (in relation to the lowest PAs measured). Figure S3 presents examples of calibration curves for DMS, isoprene, and CS2 (as analogues to DMS-d3, isoprene-d5, and $^{13}\mathrm{CS}_2$), accompanied by the respective statistics of the linear fits in Table S1. The presented calibration curves were recorded in the course of a 5 week long campaign that started about five weeks after our experiment B. This data set was chosen as (1) it contains daily calibrations over 5 weeks, nicely depicting sensitivity drifts, and (2) because unnaturally high concentrations were reached, which match the range of PAs presented in the main text better than our usual sea-going field studies. Each standard measurement was prepared as $10\,\mathrm{mL}$ ultrapure water with different amounts of liquid standard added to it (containing all three compounds). Measurements were performed as described in Sect. 2.3 of the main text. Raw peak area (PA_{raw}) was corrected by the respective blank and normalized by the volume used for standard preparation, yielding PA, to enable comparison between the PAs reported in the main text and the ones presented in Fig. S3. The PAs presented here have not been corrected for spectral fragmentation, as (different to experiment A, B, and C) no isotopically labelled substances had been added. Three calibration curves were selected for each compound, that match the ranges of PA presented in the main text. Usually the amount of substance (n_{gas}) in mol is used for the calibration curves. Here we calculated the corresponding concentration in the water-standard mixture as $n_{gas}/10\,\mathrm{mL}$. In the absence of actual calibrations during our experiments A, B, and C those values can serve as an indication of the order of magnitude of the concentrations achieved. Note, that not all samples in our experiments were $10\,\mathrm{mL}$ samples, i.e., in treatment AS with surfactants in experiment C $15\,\mathrm{mL}$ were used. Figure S3 shows that the GC–MS behaves linear (all $R2 > 0.996$) over the measured range in our experiments.

S3 Additional quality control using mass 91 applied in the context of Fig. 3 of the main text

Prior to assessing whether the tank was well-mixed (Sect. 3.2 of the main text), an additional step of quality control was performed on all ULW samples on each of the isotopes. PA of ULW samples that were far from the linear fit between PA of the respective isotope and mass 91 (e.g., grey point in Fig. S4) were flagged as poor-quality measurements and consequently removed from analysis. We assume that the poor-quality is caused by errors in measurement handling or short-term sensitivity drifts in the instrument. If the removed ULW sample was a reference sample, it was replaced with another ULW sample from the same sample set or, in the absence of more ULW samples, the sample set was discarded completely. SML samples formed a different cluster, due to the systematically lower PA compared to ULW (caused by decreased sampling efficiency) and, therefore, this step was not applied to SML samples. The sample indicated as being removed in Fig. S4 (mass spectrum ID “BULK_13CM_CC_06”) was the only ULW sample that was removed from the data set this way. It will be indicated with use_for_analysis_flag=False in the published data set.

S4 Effect of purging on surface activity measurements

Due to the limited surface area of the tank used in experiment C (“AZ crate”) two SML samples taken after each would not have been appropriate replicates of each other. Therefore, it was tested if the GC–MS sample could be reused for voltammetry analysis. The main differences for a reused GC–MS sample in voltammetry analysis are (1) longer standing time of sample before freezing and (2) being purged with helium for $10\,\mathrm{min}$. These differences could lead to contamination due to the added handling. Figure S5 shows the data points used in the statistics of purged vs non-purged SA (Sect. 3.1.2 of the main text). Only ULW samples were used, as we could safely assume that purging is the only source of error. Additionally, we took six subsamples (three for control, three were purged) from a beaker filled with ULW from the tank to specifically test the effect of purging. Surface activity is not affected by purging.

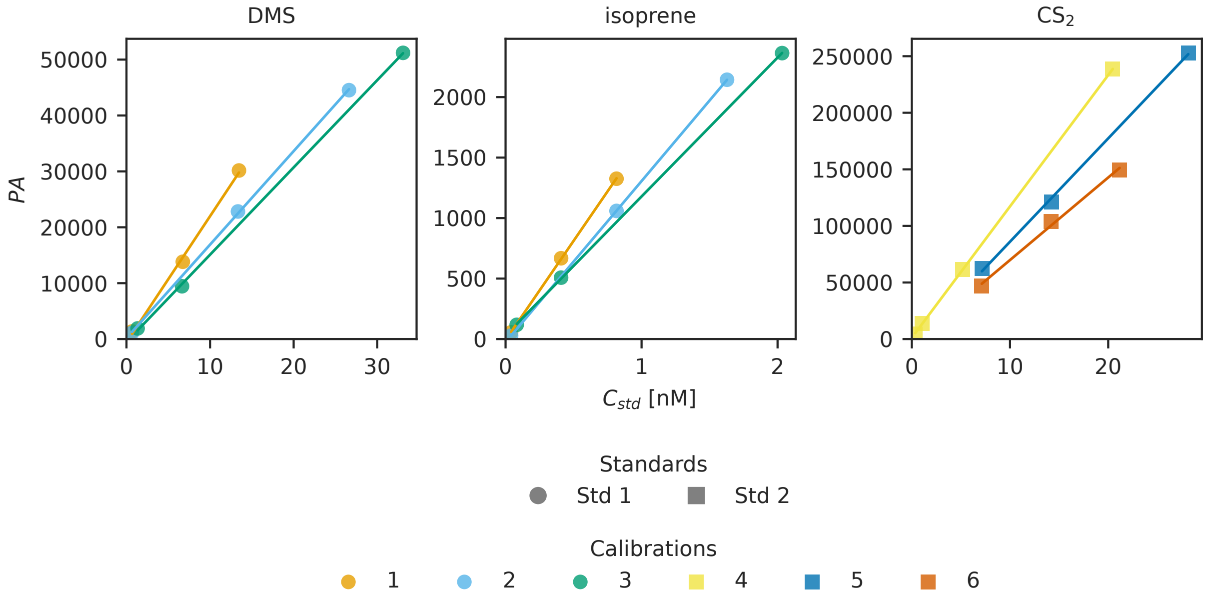

Figure S3. Example calibration curves of PA over concentration in the prepared standard (C_{std}) for GC–MS. Linear fit is shown as straight line (see Table S1 for details). Two mixtures of liquid standard in ultrapure water were used with different concentrations for the individual compounds, indicated by circles and squares.

Table S1. Linear regression of PA and C_{std} for DMS, isoprene, and CS_2 for the calibration curves shown in Fig. S3

	Linear Regression (OLS)				
Trace gas	slope	intercept	R^2	n	PAs
DMS	1561	-515	0.9998	3	1903; 9447; 51204
	2256	-575	0.9978	3	1362; 13830; 30160
	1672	172	0.9998	3	1112; 22826; 44530
isoprene	1148	31	>0.9999	3	117; 508; 2364
	1638	-8	>0.9999	3	56; 668; 1325
	1332	-26	>0.9999	3	29; 1059; 2143
CS_2	11607	1182	>0.9999	4	4658; 13828; 61602; 238659
	9132	-5269	0.9990	3	62239; 121095; 252953
	7293	-3082	0.9964	3	47104; 103852; 149452

S5 Results linear and multiple linear regressions in fresh water and artificial seawater from Sect. 3.4 of the main text

Linear regression of sampling efficiency against water temperature, salinity, spike volume per litre, and number of dips is shown for DMS-d3, isoprene-d5, and $^{13}CS_2$ in Fig. S6. Output from the multiple linear regression run in python is shown in Table S2, Table S3, and Table S4 for DMS-d3, isoprene-d5, and $^{13}CS_2$ respectively.

S6 Results linear and multiple linear regressions with an artificial surfactant from Sect. 3.5 of the main text

Linear regression of sampling efficiency against water temperature, salinity, spike volume per litre, and number of dips is shown for DMS-d3, isoprene-d5, and $^{13}CS_2$ in Fig. S7, and against SA in Fig. S8, Output from the multiple linear regression runs in python is shown in Table S5, Table S6, and Table S7 for DMS-d3, isoprene-d5, and $^{13}CS_2$ respectively.

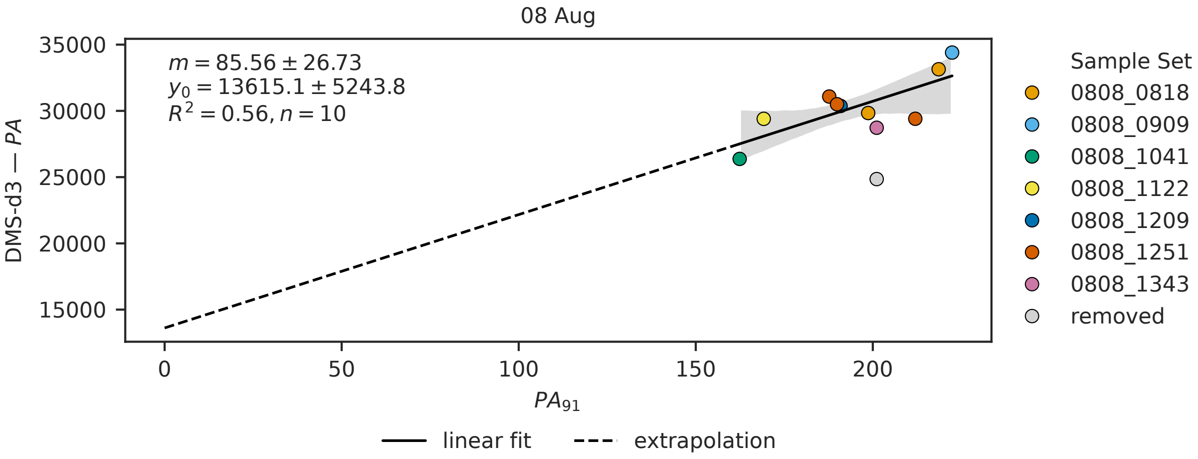

Figure S4. Example from 8 August of linear fit between PA of DMS-d3 and mass 91 to identify poor-quality measurements. All samples are ULW samples. Linear fit excludes grey point.

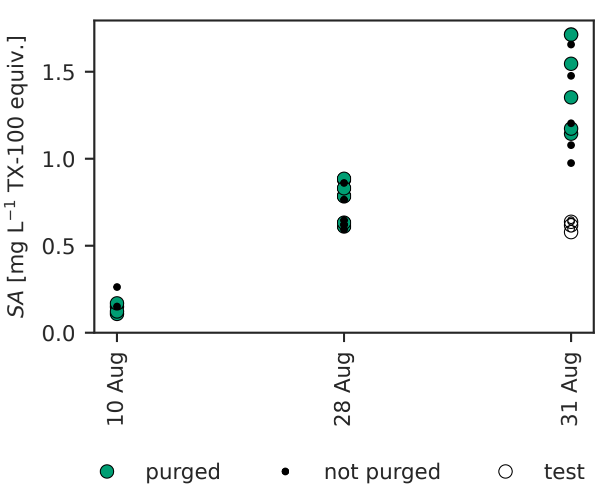

Figure S5. Measured surface activity (SA) of purged and non-purged samples. ULW samples in treatment AS with surfactants ($n = 30$, green and black) are shown and a test sample set ($n = 6$, empty circles).

S7 Calculations for diffusive boundary layer from Sect. 4.1.2 of the main text

A simple box model was used to assess the effect of the diffusive boundary layer (DBL) on C_{SML}. A mass balance (Eq.(S1)) was set up for the complete tank with flux (Neumann boundary condition) only through the surface (i.e., no-flux Neumann boundary conditions on all other sides).

$$\frac{dn(t)}{dt} = -J_{surface}(t) \cdot A \tag{S1}$$

where n is the moles as (absolute) PA (proportional to mol), t is time in s after mixing stopped, J is the flux in $\mathrm{mol\,m^{-2}\,s^{-1}}$ through the surface (defined as positive going inward), and A is the surface area of the tank in m^2. The flux through the surface is derived using Fick's first law of diffusion (Eq. (S2)). This assumes that the water in the tank was quiescent, $C_{air} \approx 0\,\mathrm{mol\,L^{-1}}$, and the air is a perfect sink.

$$J_{surface}(t) = \frac{C_0}{\sqrt{\pi D t}} = \frac{n_0}{V_{tank}\sqrt{\pi D t}} \tag{S2}$$

where $C_0 = n_0/V_{tank}$ is the initial concentration at $t = 0\,\mathrm{s}$ in $\mathrm{mol\,L^{-1}}$, D is the diffusivity in $\mathrm{m^2\,s^{-1}}$, n_0 are the initial moles in mol, $V_{tank} = AH$ is the volume of the water in the tank in m^3, and H is the depth of the water in the tank in m. The concentration in the ULW is used as initial condition, i.e., $C_0 = C_{ULW}$. Analytical solution of the ordinary differential equation (ODE) in Eq. (S1) by integrating is given in Eq. (S3).

$$n(t) = n_0 \exp\left(-\frac{2A}{V_{tank}}\sqrt{\frac{Dt}{\pi}}\right) \tag{S3}$$

where $n(t)$ are the moles left in the tank at time t, and t is time in s after mixing stopped. We calculate n_0 from mean PA per experiment by multiplying with the respective volume of the tank. Water volume in experiment B was $34\,\mathrm{cm} \times 78\,\mathrm{cm} \times 26\,\mathrm{cm}$, and $42\,\mathrm{cm} \times 61\,\mathrm{cm} \times 31\,\mathrm{cm}$ in experiment C. Diffusivity of DMS(-d3) ranged from 0.0000111–0.0000129 $\mathrm{cm^2\,s^{-1}}$ for the temperature range in this study. For this calculation we use $D = 1.29 \times 10^{-9}\,\mathrm{m^2\,s^{-1}}$ ($T = 20\,°\mathrm{C}$, $S_P = 0$, calculated for DMS according to Saltzman et al. (1993)). Due to missing diffusivity values for isoprene(-d5) and $^{(13)}\mathrm{CS}_2$, these two are skipped in the calculation. As time we (conservatively) set $t = 120\,\mathrm{s}$, though

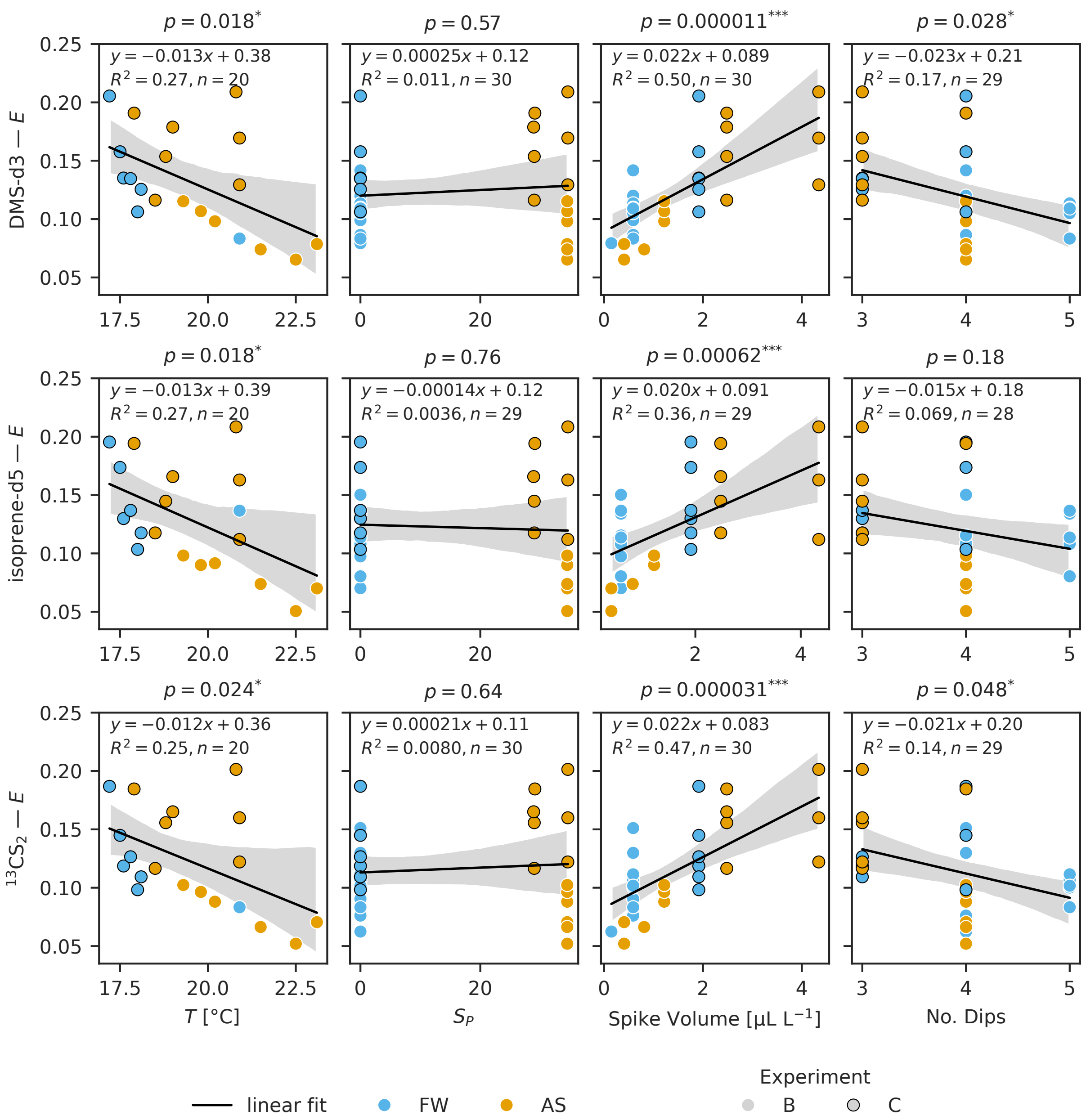

Figure S6. Linear regressions of sampling efficiency (E) for DMS-d3 (top), isoprene-d5 (middle) and ^{13}CS$_2$ (bottom) against water temperature, salinity, spike volume per litre and number of dips in fresh water (FW) and artificial seawater (AS) treatment. Linear fit, R^2 and number of samples (n) are given in top corner of each subplot. *, ** and *** mark where the null hypothesis was rejected, with p-values <0.05, <0.01 and <0.001 respectively.

the formation of a quasi-steady DBL only starts after the turbulent motion from the mixing has subsided, which is expected to take about 1 min. Finally, $n(t = 120\,\mathrm{s})$ yields that $n(t)/n_0 = 99.9\,\%$ of the moles are still left within the box (i.e., water volume) after 120 s. To estimate the dilution from the DBL on the glass plate, we partition this $n(t = 120\,\mathrm{s})$ between ULW and DBL. Under the assumption that within this short time C_{ULW} did not change, i.e., $C_{ULW} = C_0$, we calculate how many moles of $n(t)$ are present in the DBL with Eq. (S4).

$$n_{DBL} = n(t) - C_0 V_{ULW} \tag{S4}$$

where n_{DBL} are the moles in the DBL, $V_{ULW} =$ is the volume of the water below the DBL in the tank in m^3 calculated as $A(H - h_{DBL})$, and h_{DBL} is the thickness of the DBL in

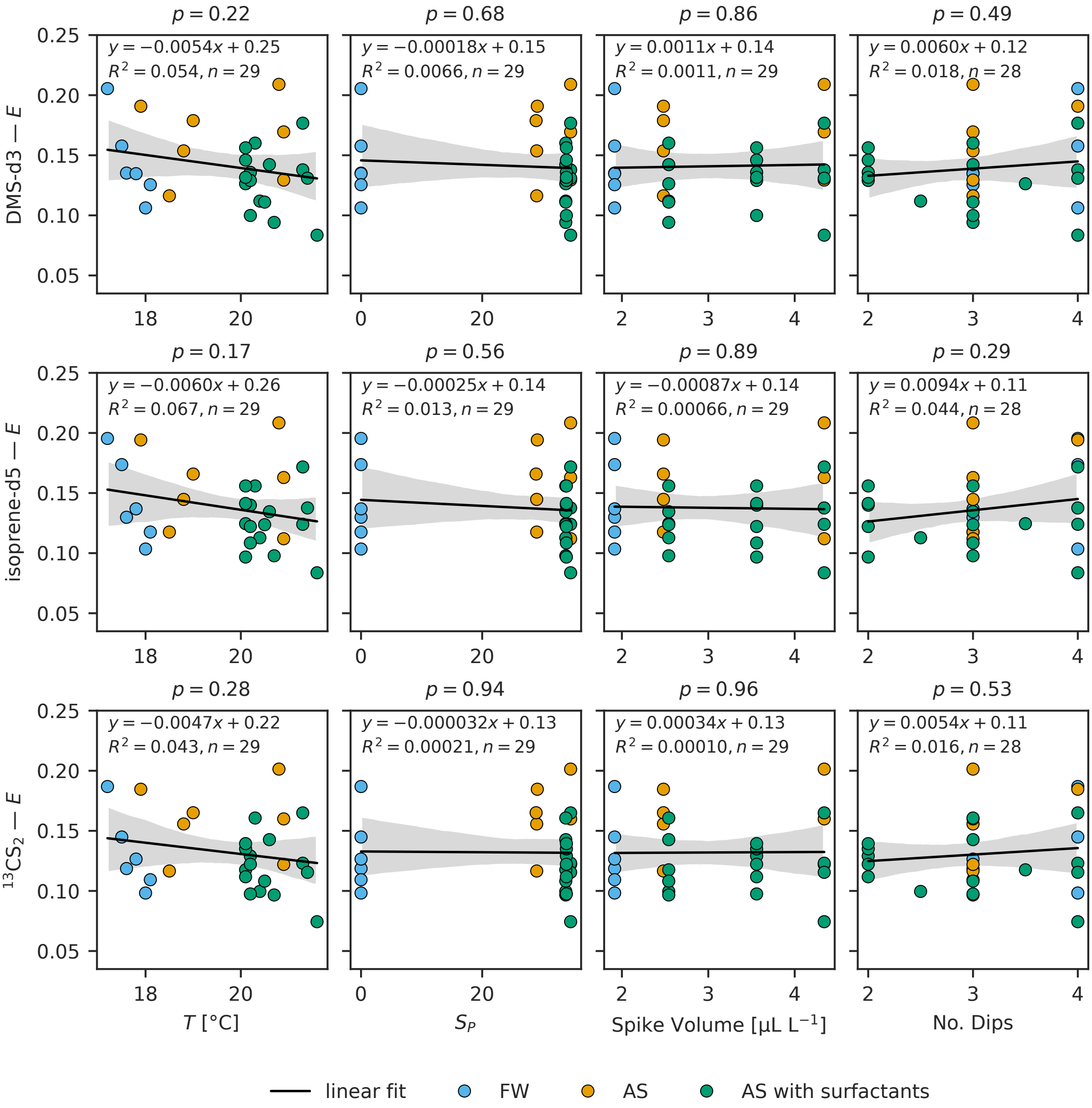

Figure S7. Linear regressions of sampling efficiency (E) for DMS-d3 (top), isoprene-d5 (middle), and $^{13}\mathrm{CS}_2$ (bottom) against water temperature, salinity, spike volume per litre and number of dips in fresh water (FW) and artificial seawater (AS) without and with surfactants treatment. Linear fit, R^2 and number of samples (n) are given in top corner of each subplot. Linear regression of surface activity (SA) is shown in Fig. S8. Null hypothesis was not rejected, as all p-values >0.05.

m, approximated with Eq. (S5).

$$h_{DBL} = a\sqrt{\pi D t} \tag{S5}$$

where h_{DBL} is the thickness of the DBL in m, $a = 3$ is a common coefficient that defines h_{DBL} in relation to $99\,\%$ of C_{ULW}. Finally, the concentration in the DBL in relation to the concentration in the ULW, i.e. the concentration sampled by the glass plate is calculated by Eq. (S6).

$$\frac{C_{DBL}}{C_{ULW}} = \frac{n_{DBL}}{V_{DBL} C_{ULW}} \tag{S6}$$

where C_{DBL} is the concentration in the DBL, C_{ULW} is the concentration in the ULW in $\mathrm{mol\,L^{-1}}$, and $V_{DBL} = A\,h_{DBL}$ is the volume of the water in the DBL in m^3, which equates to 0.79 for both experiments.

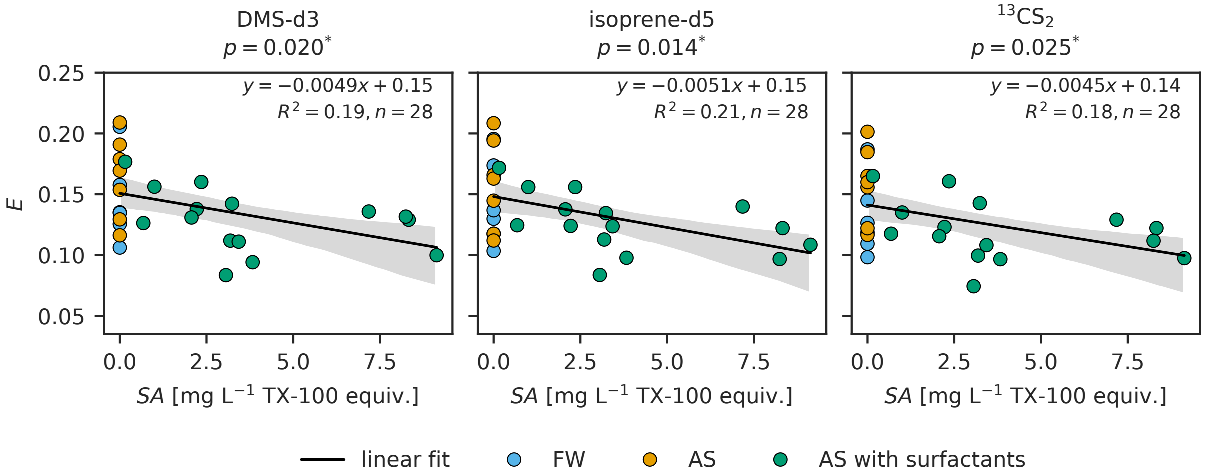

Figure S8. Linear regression of sampling efficiency (E) for DMS-d3 (left), isoprene-d5 (middle), and $^{13}\mathrm{CS}_2$ (right) against surface activity (SA) in SML in fresh water (FW) and artificial seawater (AS) without and with surfactants treatment. Linear fit, R^2 and number of samples (n) are given in top corner of each subplot. Linear regressions of water temperature, salinity, spike volume per litre and number of dips are shown in Fig. S7. * marks where the null hypothesis was rejected, with p-value <0.05.

References

Saltzman, E. S., King, D. B., Holmen, K., and Leck, C.: Experimental Determination of the Diffusion Coefficient of Dimethylsulfide in Water, Journal of Geophysical Research, 98, 16 481–16 486, https://doi.org/10.1029/93JC01858, 1993.

Table S2. Multiple linear regression results for DMS-d3 in fresh water (FW) and artificial seawater (AS), using statsmodels `smf.ols(...).fit(cov_type='HC3')`

```
                               OLS Regression Results                               
====================================================================================
Dep. Variable:     ratio_sml_over_ulw_dmsd3   R-squared:                       0.709
Model:                                  OLS   Adj. R-squared:                  0.626
Method:                       Least Squares   F-statistic:                     5.639
Date:                      Sat, 01 Nov 2025   Prob (F-statistic):            0.00643
Time:                              15:37:10   Log-Likelihood:                 45.086
No. Observations:                        19   AIC:                            -80.17
Df Residuals:                            14   BIC:                            -75.45
Df Model:                                 4                                         
Covariance Type:                        HC3                                         
=========================================================================================================
                                            coef    std err          z      P>|z|      [0.025      0.975]
---------------------------------------------------------------------------------------------------------
Intercept                                 0.1292      0.007     18.107      0.000       0.115       0.143
temperature_water_degc                   -0.0223      0.011     -2.021      0.043      -0.044      -0.001
salinity_psu                              0.0041      0.008      0.513      0.608      -0.012       0.020
cummulative_spike_volume_mikrol_per_l     0.0342      0.012      2.769      0.006       0.010       0.058
dips                                      0.0117      0.009      1.350      0.177      -0.005       0.029
==============================================================================
Omnibus:                        0.354   Durbin-Watson:                   1.951
Prob(Omnibus):                  0.838   Jarque-Bera (JB):                0.074
Skew:                           0.145   Prob(JB):                        0.964
Kurtosis:                       2.903   Cond. No.                         2.58
==============================================================================

Notes:
[1] Standard Errors are heteroscedasticity robust (HC3)
```

Table S3. Multiple linear regression results for isoprene-d5 in fresh water (FW) and artificial seawater (AS), using statsmodels `smf.ols(...).fit(cov_type='HC3')`

```
                                  OLS Regression Results
=========================================================================================
Dep. Variable:     ratio_sml_over_ulw_isoprened5   R-squared:                       0.691
Model:                                       OLS   Adj. R-squared:                  0.602
Method:                            Least Squares   F-statistic:                     6.803
Date:                           Sat, 01 Nov 2025   Prob (F-statistic):            0.00294
Time:                                   15:37:10   Log-Likelihood:                 43.711
No. Observations:                             19   AIC:                            -77.42
Df Residuals:                                 14   BIC:                            -72.70
Df Model:                                      4
Covariance Type:                             HC3
=========================================================================================================
                                            coef    std err          z      P>|z|      [0.025      0.975]
---------------------------------------------------------------------------------------------------------
Intercept                                 0.1267      0.008     16.425      0.000       0.112       0.142
temperature_water_degc                   -0.0169      0.012     -1.455      0.146      -0.040       0.006
salinity_psu                             -0.0069      0.009     -0.741      0.459      -0.025       0.011
cummulative_spike_volume_mikrol_per_l     0.0404      0.014      2.812      0.005       0.012       0.069
dips                                      0.0213      0.009      2.367      0.018       0.004       0.039
==============================================================================
Omnibus:                        3.169   Durbin-Watson:                   1.648
Prob(Omnibus):                  0.205   Jarque-Bera (JB):                1.515
Skew:                          -0.648   Prob(JB):                        0.469
Kurtosis:                       3.486   Cond. No.                         2.58
==============================================================================

Notes:
[1] Standard Errors are heteroscedasticity robust (HC3)
```

Table S4. Multiple linear regression results for $^{13}CS_2$ in fresh water (FW) and artificial seawater (AS), using statsmodels `smf.ols(...).fit(cov_type='HC3')`

```
                               OLS Regression Results
====================================================================================
Dep. Variable:     ratio_sml_over_ulw_c13s2   R-squared:                       0.729
Model:                                  OLS   Adj. R-squared:                  0.652
Method:                       Least Squares   F-statistic:                     6.742
Date:                      Sat, 01 Nov 2025   Prob (F-statistic):            0.00305
Time:                              15:37:10   Log-Likelihood:                 45.959
No. Observations:                        19   AIC:                            -81.92
Df Residuals:                            14   BIC:                            -77.20
Df Model:                                 4
Covariance Type:                        HC3
=========================================================================================================
                                            coef    std err          z      P>|z|      [0.025      0.975]
---------------------------------------------------------------------------------------------------------
Intercept                                 0.1202      0.007     17.774      0.000       0.107       0.133
temperature_water_degc                   -0.0219      0.010     -2.104      0.035      -0.042      -0.001
salinity_psu                              0.0053      0.007      0.758      0.448      -0.008       0.019
cummulative_spike_volume_mikrol_per_l     0.0353      0.012      2.932      0.003       0.012       0.059
dips                                      0.0125      0.008      1.662      0.096      -0.002       0.027
==============================================================================
Omnibus:                        0.054   Durbin-Watson:                   1.864
Prob(Omnibus):                  0.973   Jarque-Bera (JB):                0.147
Skew:                           0.094   Prob(JB):                        0.929
Kurtosis:                       2.612   Cond. No.                         2.58
==============================================================================

Notes:
[1] Standard Errors are heteroscedasticity robust (HC3)
```

Table S5. Multiple linear regression results for DMS-d3 in experiment C including treatments fresh water (FW), artificial seawater (AS) without and with surfactants, using statsmodels `smf.ols(...).fit(cov_type='HC3')`

```
                                OLS Regression Results
====================================================================================
Dep. Variable:     ratio_sml_over_ulw_dmsd3   R-squared:                       0.392
Model:                                  OLS   Adj. R-squared:                  0.247
Method:                       Least Squares   F-statistic:                     2.006
Date:                      Sat, 01 Nov 2025   Prob (F-statistic):              0.119
Time:                              16:06:07   Log-Likelihood:                 62.118
No. Observations:                        27   AIC:                            -112.2
Df Residuals:                            21   BIC:                            -104.5
Df Model:                                 5
Covariance Type:                        HC3
=========================================================================================================
                                            coef    std err          z      P>|z|      [0.025      0.975]
---------------------------------------------------------------------------------------------------------
Intercept                                 0.1393      0.006     23.395      0.000       0.128       0.151
temperature_water_degc                   -0.0324      0.016     -1.995      0.046      -0.064      -0.001
salinity_psu                              0.0152      0.013      1.158      0.247      -0.011       0.041
cummulative_spike_volume_mikrol_per_l     0.0213      0.010      2.184      0.029       0.002       0.040
dips                                     -0.0016      0.007     -0.242      0.809      -0.015       0.011
SA_mg_per_l_tx100_eq_sml                 -0.0138      0.007     -1.960      0.050      -0.028    -3.4e-06
==============================================================================
Omnibus:                        0.493   Durbin-Watson:                   1.896
Prob(Omnibus):                  0.781   Jarque-Bera (JB):                0.067
Skew:                           0.115   Prob(JB):                        0.967
Kurtosis:                       3.081   Cond. No.                         5.21
==============================================================================

Notes:
[1] Standard Errors are heteroscedasticity robust (HC3)
```

Table S6. Multiple linear regression results for isoprene-d5 in experiment C including treatments fresh water (FW), artificial seawater (AS) without and with surfactants, using statsmodels `smf.ols(...).fit(cov_type='HC3')`

```
                                   OLS Regression Results
=========================================================================================
Dep. Variable:     ratio_sml_over_ulw_isoprened5   R-squared:                       0.367
Model:                                       OLS   Adj. R-squared:                  0.216
Method:                            Least Squares   F-statistic:                     1.921
Date:                           Sat, 01 Nov 2025   Prob (F-statistic):              0.133
Time:                                   16:06:07   Log-Likelihood:                 61.383
No. Observations:                             27   AIC:                            -110.8
Df Residuals:                                 21   BIC:                            -103.0
Df Model:                                      5
Covariance Type:                             HC3
=========================================================================================================
                                            coef    std err          z      P>|z|      [0.025      0.975]
---------------------------------------------------------------------------------------------------------
Intercept                                 0.1365      0.006     22.385      0.000       0.125       0.148
temperature_water_degc                   -0.0309      0.016     -1.993      0.046      -0.061      -0.001
salinity_psu                              0.0169      0.013      1.265      0.206      -0.009       0.043
cummulative_spike_volume_mikrol_per_l     0.0167      0.010      1.700      0.089      -0.003       0.036
dips                                      0.0016      0.007      0.231      0.817      -0.012       0.015
SA_mg_per_l_tx100_eq_sml                 -0.0132      0.007     -1.812      0.070      -0.027       0.001
==============================================================================
Omnibus:                        0.008   Durbin-Watson:                   1.978
Prob(Omnibus):                  0.996   Jarque-Bera (JB):                0.186
Skew:                          -0.020   Prob(JB):                        0.911
Kurtosis:                       2.596   Cond. No.                         5.21
==============================================================================

Notes:
[1] Standard Errors are heteroscedasticity robust (HC3)
```

Table S7. Multiple linear regression results for $^{13}CS_2$ in experiment C including treatments fresh water (FW), artificial seawater (AS) without and with surfactants, using statsmodels `smf.ols(...).fit(cov_type='HC3')`

```
                               OLS Regression Results
====================================================================================
Dep. Variable:     ratio_sml_over_ulw_c13s2   R-squared:                       0.377
Model:                                  OLS   Adj. R-squared:                  0.229
Method:                       Least Squares   F-statistic:                     2.203
Date:                      Sat, 01 Nov 2025   Prob (F-statistic):             0.0925
Time:                              16:06:07   Log-Likelihood:                 62.526
No. Observations:                        27   AIC:                            -113.1
Df Residuals:                            21   BIC:                            -105.3
Df Model:                                 5
Covariance Type:                        HC3
=========================================================================================================
                                            coef    std err          z      P>|z|      [0.025      0.975]
---------------------------------------------------------------------------------------------------------
Intercept                                 0.1305      0.006     22.465      0.000       0.119       0.142
temperature_water_degc                   -0.0321      0.015     -2.191      0.028      -0.061      -0.003
salinity_psu                              0.0212      0.012      1.836      0.066      -0.001       0.044
cummulative_spike_volume_mikrol_per_l     0.0159      0.010      1.534      0.125      -0.004       0.036
dips                                     -0.0003      0.007     -0.047      0.963      -0.013       0.013
SA_mg_per_l_tx100_eq_sml                 -0.0137      0.007     -2.045      0.041      -0.027      -0.001
==============================================================================
Omnibus:                        0.822   Durbin-Watson:                   1.945
Prob(Omnibus):                  0.663   Jarque-Bera (JB):                0.514
Skew:                           0.333   Prob(JB):                        0.774
Kurtosis:                       2.882   Cond. No.                         5.21
==============================================================================

Notes:
[1] Standard Errors are heteroscedasticity robust (HC3)
```