

Supplementary information for

The influence of dissolved organic matter on the marine production of carbonyl sulfide (OCS) and carbon disulfide (CS₂) in the Eastern Tropical South Pacific

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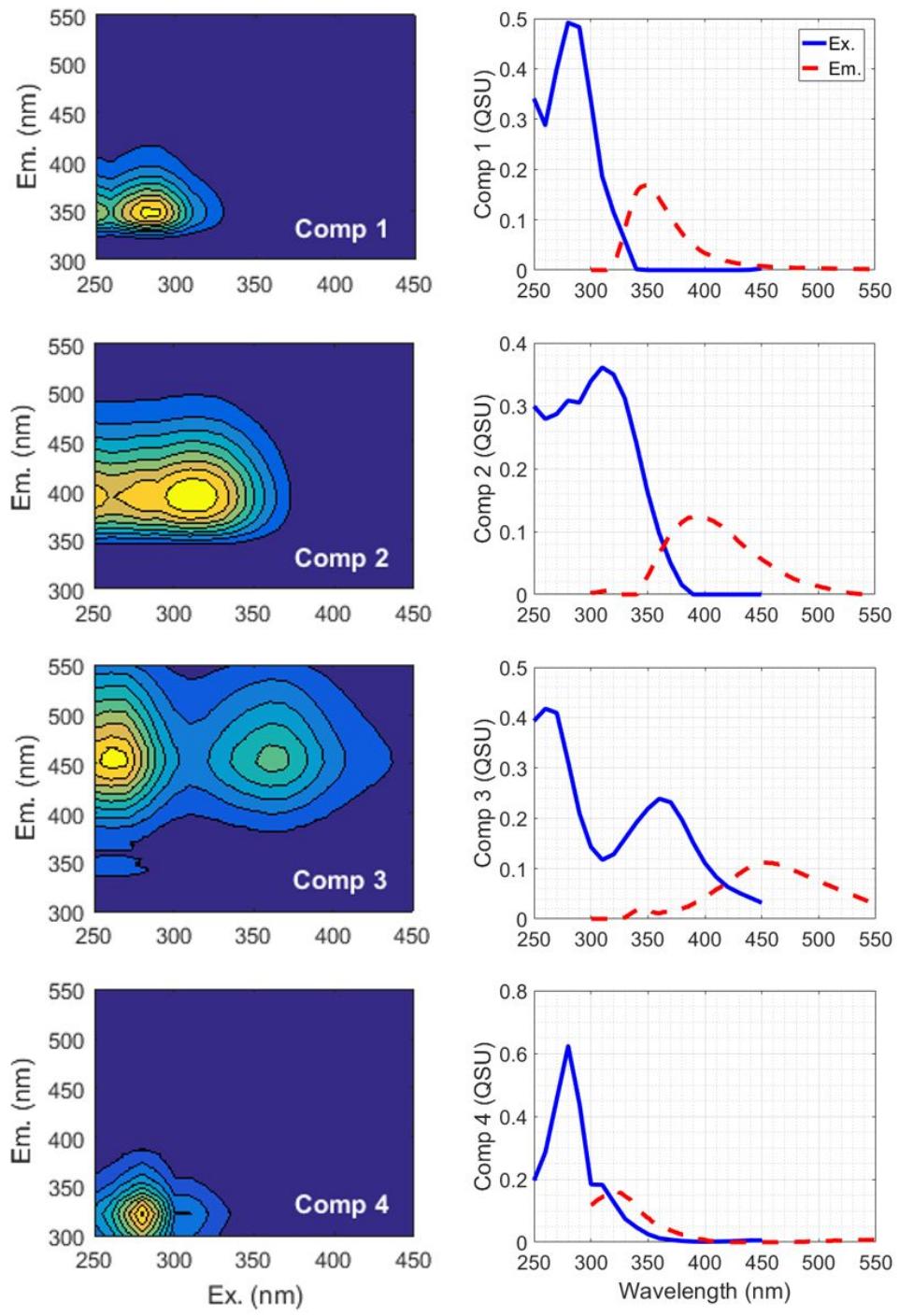
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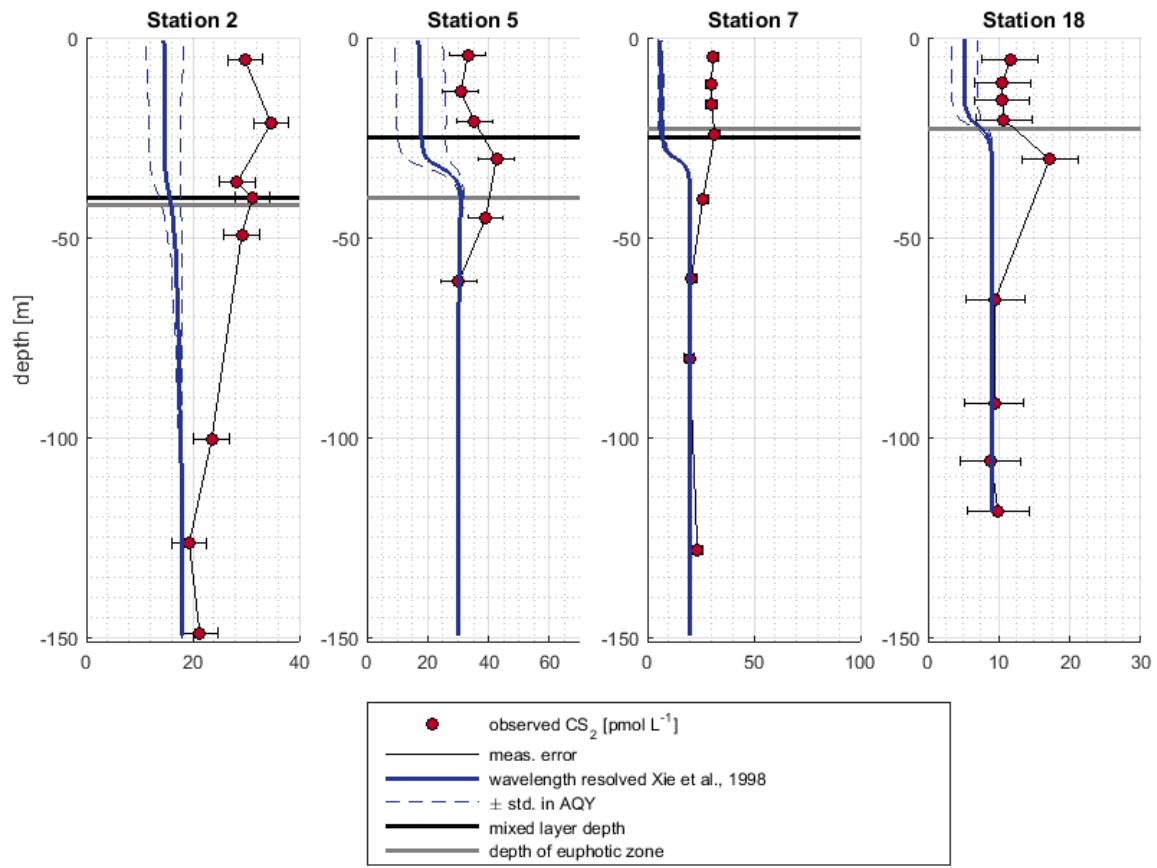
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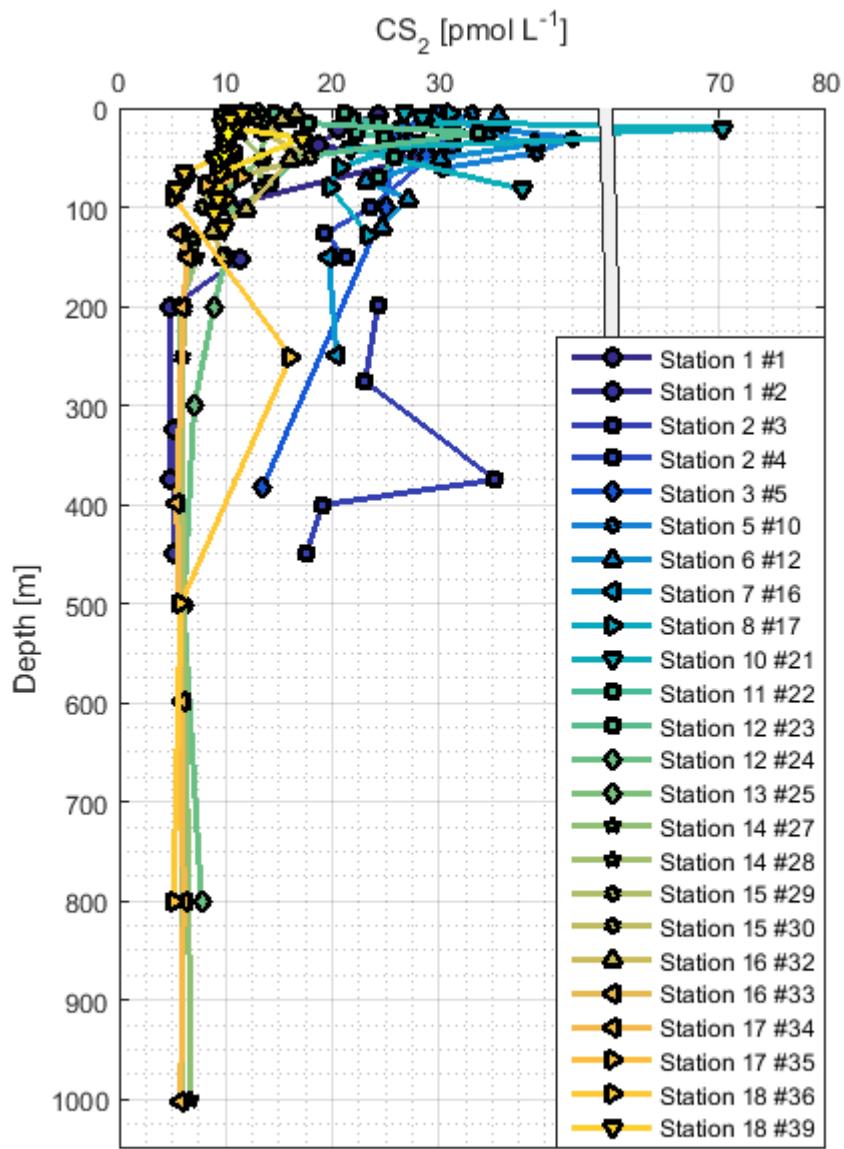
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S-Figure 1: Three-dimensional fluorescence landscapes (left) and the excitation and emission spectra (right) for a four component model derived from PARAFAC analysis for fluorescent dissolved organic matter (FDOM). C1 and C4 fluoresce in the UV range and represent protein-like fractions, whereas C2 and C3 fluoresce in the visible range and represent humic-like fractions of the DOM pool.



S-Figure 2: Profile measurements of CS_2 concentrations and 1D FABM/GOTM model results for the CS_2 model experiments using the apparent quantum yield (AQY) reported by Xie et al. (1998). All concentrations in pmol L $^{-1}$.



S-Figure 3: Concentration depth profiles for discrete measurements of CS_2 for open ocean regions (stations 1-5, blueish colors) and stations closer to the shelf (stations 6-13, green/yellow colors).

S-Table 1: Forcing parameter for the box model and the FABM/GOTM 1D water column model.

Parameter	Box model	FABM/GOTM module
CDOM a_{350}	in-situ measurements, 3-hourly measurements	in-situ measurements from CTD casts at stations, constant for the duration of the simulation
UV radiation	Global radiation from shipboard measurements (10 min. averages), corrected to UV radiation as described in von Hobe et al. (2003) and Lennartz et al. (2017)	4% of global radiation from the host (GOTM), penetration depth and profile shape from in-situ measurements integrated over the wavelengths 300-400nm
Temperature	Continuous in-situ measurements, Seabird MicroCat SBE41	In-situ measurements from CTD, constant for the duration of the simulation
Salinity	Continuous in-situ measurements, Seabird MicroCat SBE41	In-situ measurements from CTD, constant for the duration of the simulation
pH	fixed value 8.1	fixed value 8.1
Air pressure	In-situ measurements	In-situ measurements, daily average, constant for the duration of the simulation
Atmospheric mixing ratio	OCS: sampled onboard, ca. 3-hourly resolution, for quality control: air canister samples analysed at RSMAS (Schauffler et al., 1998; de Gouw et al., 2009) CS ₂ : no measurements available, assumed mixing ratio of 0 ppt	OCS: sampled onboard, for quality control: air canister samples analysed at RSMAS (Schauffler et al., 1998; de Gouw et al., 2009), daily averages CS ₂ : no measurements available, assumed mixing ratio of 0 ppt
Wind speed	measured onboard, corrected to 10 m height, 10 minute averages	In-situ measurements, corrected to 10m height, daily average, constant for the duration of the simulation
Mixed layer depths	obtained from CTD profiles, using the Lorbacher (Lorbacher et al., 2006) criterion, 0-4 times per day	-

S-Table 2: Model forcing for the simulations in GOTM/FABM.

	Station 2		Station 5		Station 7		Station 18	
	OCS	CS ₂	OCS	CS ₂	OCS	CS ₂	OCS	CS ₂
location	0.00° N 85.50°W	0.00° N 85.50°W	10.00°S 81.92°W	10.00°S 81.92°W	9.18° S 79.46° W	9.18° S 79.46° W	15.32 °S 75.27 °W	15.32 °S 75.27 °W
Date of 2015 UTC	7.10. 16h	7.10.2015 23h	11.10. 3h	10.10. 19h	12.10. 9h	12.10. 3h	19.10. 20h	19.10. 18h
length of simulation [days]	5	21	5	21, 6	5	21	5	21
depth of simulation [m]	100	150	150	150	120	150	120	120
SST [°C]	24.3	20.5	20.6	20.6	20.1	20.1	15.6	15.71
average T [°C]	21.1	19.3	17.5	17.6	17.9	17.3	14.7	14.6
average S [-]	34.9	34.9	35.1	35.1	35.1	35.1	35.0	35.0
average a_{350} [m ⁻¹]	0.13	0.13	0.12	0.12	0.14	0.14	0.14	0.14
abs. coef. n	8.8	8.8	6.5	6.5	4.1	4.1	4.5	4.5
Wind speed [m s ⁻¹]	8.1	8.1	8.6	8.6	6.7	6.7	8.8	8.8
rel. hum. [%]	100.0	100.0	77.8	77.8	80.9	80.9	88.0	88.0
air pressure [hPa]	1011.3	1011.3	1011.9	1011.9	1013.9	1013.9	1016.7	1016.7
cloud coverage [-]	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1

References

de Gouw, J. A., Warneke, C., Montzka, S. A., Holloway, J. S., Parrish, D. D., Fehsenfeld, F. C., Atlas, E. L., Weber, R. J., and Flocke, F. M.: Carbonyl sulfide as an inverse tracer for biogenic organic carbon in gas and aerosol phases, Geophysical Research Letters, 36, n/a-n/a, 10.1029/2008gl036910, 2009.

Lennartz, S. T., Marandino, C. A., von Hobe, M., Cortes, P., Quack, B., Simo, R., Booge, D., Pozzer, A., Steinhoff, T., Arevalo-Martinez, D. L., Kloss, C., Bracher, A., Röttgers, R., Atlas, E., and Krüger, K.: Direct oceanic emissions unlikely to account for the missing source of atmospheric carbonyl sulfide, Atmos. Chem. Phys., 17, 385-402, 10.5194/acp-17-385-2017, 2017.

Lorbacher, K., Dommeneget, D., Niiler, P. P., and Köhl, A.: Ocean mixed layer depth: A subsurface proxy of ocean-atmosphere variability, *Journal of Geophysical Research: Oceans*, 111, n/a-n/a, 10.1029/2003jc002157, 2006.

Schauffler, S. M., Atlas, E. L., Flocke, F., Lueb, R. A., Stroud, V., and Travnicek, W.: Measurements of bromine containing organic compounds at the tropical tropopause, *Geophysical Research Letters*, 25, 317-320, 10.1029/98gl00040, 1998.

von Hobe, M., Najjar, R. G., Kettle, A. J., and Andreae, M. O.: Photochemical and physical modeling of carbonyl sulfide in the ocean, *Journal of Geophysical Research*, 108, 10.1029/2000jc000712, 2003.

Xie, H., Moore, R. M., and Miller, W. L.: Photochemical production of carbon disulphide in seawater, *Journal of Geophysical Research: Oceans*, 103, 5635-5644, 10.1029/97jc02885, 1998.