Supplement of

Winter season Southern Ocean distributions of climate-relevant trace gases

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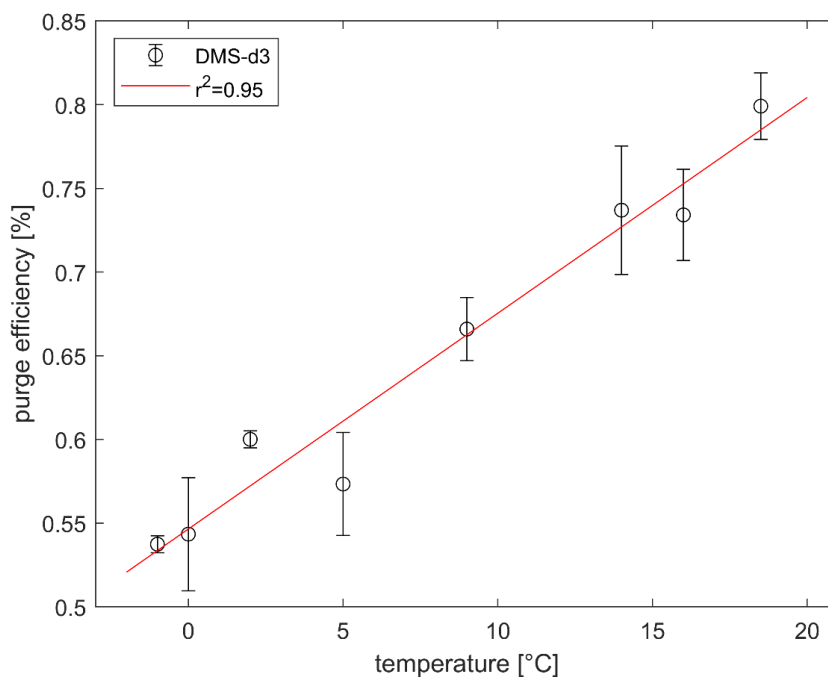
Methods

Analysis

10 The dimethylsulfide (DMS) purge efficiency of the purge and trap system was tested during SCALE, because of the low sea surface temperatures (SSTs) encountered. The same tests were not performed for isoprene, as isoprene has a lower solubility than DMS and is always efficiently purged from the sample, even at low temperatures. The tests were performed by adding the same concentration of deuterated DMS (DMS-d3) standard to the purge vials and purging at different temperatures (Figure S1). The purge efficiency at different temperatures was obtained by dividing the

15 measured response value by the response value of a known 100% purge efficiency. Temperature and purge efficiency are highly positively correlated, where the highest purge efficiency of approximately 80% is found around 20°C. We corrected the results presented in the manuscript using the ambient temperature during the purging to obtain the appropriate efficiency.

     Figure S1. DMS purge efficiency from <0°C to 20°C.

Results and Discussion

Hydrological characteristics

Typically, measurements over the entire mixed layer (or deeper) are used for classifying hydrological regions, but we only had surface measurements available in this study. In order to determine the contrasting regions presented in the text, we use the ratio of field temperature and salinity data and the method of Luis and Lotlikar (2021), which is to calculate the difference in the ratio of temperature and salinity over time. Luis and Lotlikar (2021) presented in situ observations of Southern Ocean temperatures and salinity to determine hydrological regions against which we compared our results. We computed the difference in ratio over 100 min averages, as this was the shortest averaging time that allowed us to distinguish small differences (Figure S2).

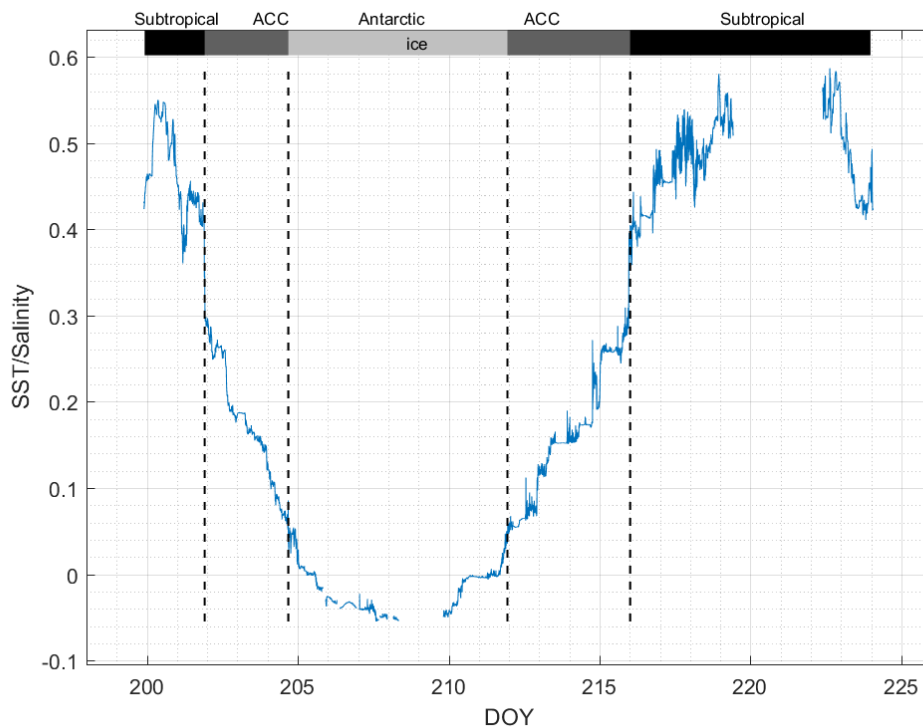



Figure S2. Difference in ratio of temperature (SST) to salinity of surface waters during the cruise. The bars across the top of the figure denote the different hydrographic regions. ACC= Antarctic Circumpolar Current.

Relationships between DMSPt:DMSOt and DMSPt:DMS and SST over the whole cruise

In addition to the regional averages presented in Figure 7 (main text), we computed individual DMSPt:DMSOt vs. SST over the entire SCALE cruise (Figure S3 left). The general pattern matches that presented in Figure 7, with the ratio being highest when the temperature is between 5° and 10°C. We also calculated individual DMSPt:DMS vs. SST over the entire cruise track (Figure S3 right) in order to more concretely highlight the effect of SST on this relationship. A similar pattern emerges – the ratio increases with temperature until around 10°C, then decreases with temperature until about 20°C. Both relationships indicate that there is a switch between the controls on the sulfur compounds between 5-10°C consistent with previous findings (Simó and Vila-Costa, 2006; Zindler et al., 2013). Besides the change of ratio over different SSTs the absolute value of DMSPt:DMSOt is on average up to 5.3 times lower than the DMSPt:DMS, which clearly indicates a direct production of DMSO from DMSP, without the intermediate conversion

of DMSP to DMS, and the subsequent photooxidation to DMSO over the whole range of SST. Iglesias-Rodríguez et al. (2002) indicate that around 9°C (3–15 °C) blooms of coccolithophores occur in high latitudes (Iglesias-Rodríguez et al., 2002). According to Stefels et al. (2007), DMSP production decreases with increasing temperature. In addition, enhanced microbial cleavage of DMSP to DMS occurs at higher temperatures (Stefels et al., 2007; Yoch, 2002). Both
50   changes would lead to a decreasing ratio with temperature.

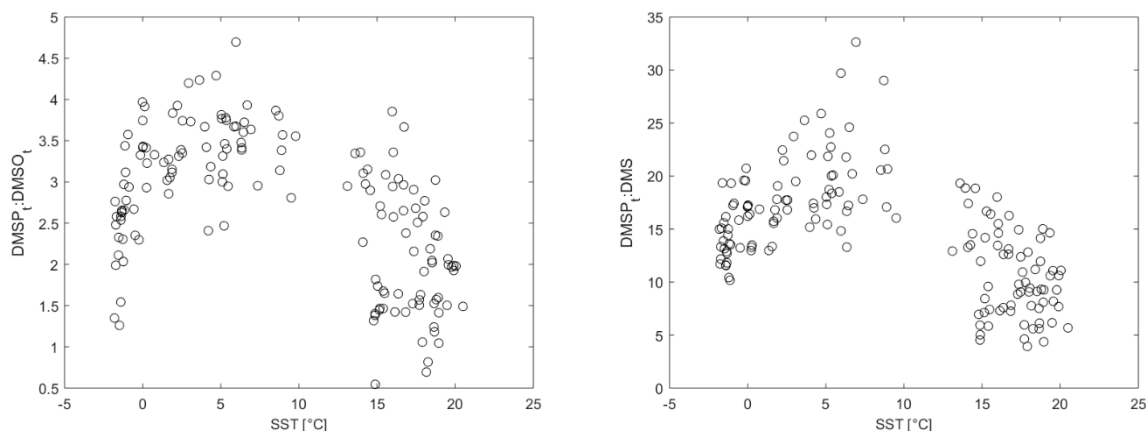



Figure S3. DMSPt:DMSOt (left) and DMSPt:DMS (right) against SST over the entire SCALE cruise.

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Iglesias-Rodríguez, M. D., Brown, C. W., Doney, S. C., Kleypas, J., Kolber, D., Kolber, Z., Hayes, P. K., and Falkowski, P. G.: Representing key phytoplankton functional groups in ocean carbon cycle models: Coccolithophorids, Global Biogeochemical Cycles, 16, 47-41-47-20, https://doi.org/10.1029/2001GB001454, 2002.
Luis, A. J. and Lotlikar, V. R.: Hydrographic characteristics along two XCTD sections between Africa and Antarctica
60   during austral summer 2018, Polar Science, 30, 100705, https://doi.org/10.1016/j.polar.2021.100705, 2021.
Simó, R. and Vila-Costa, M.: Ubiquity of algal dimethylsulfoxide in the surface ocean: Geographic and temporal distribution patterns, Marine chemistry, 100, 136-146, https://doi.org/10.1016/j.marchem.2005.11.006, 2006.
Stefels, J., Steinke, M., Turner, S., Malin, G., and Belviso, S.: Environmental constraints on the production and removal of the climatically active gas dimethylsulphide (DMS) and implications for ecosystem modelling,
65   Biogeochemistry, 83, 245-275, https://doi.org/10.1007/s10533-007-9091-5, 2007.
Yoch, D. C.: Dimethylsulfoniopropionate: Its sources, role in the marine food web, and biological degradation to dimethylsulfide, Applied and Environmental Microbiology, 68, 5804-5815, https://doi.org/10.1128/aem.68.12.5804-5815.2002, 2002.
Zindler, C., Bracher, A., Marandino, C. A., Taylor, B., Torrecilla, E., Kock, A., and Bange, H. W.: Sulphur compounds,
70   methane, and phytoplankton: interactions along a north-south transit in the western Pacific Ocean, Biogeosciences, 10, 3297-3311, https://doi.org/10.5194/bg-10-3297-2013, 2013.