Supplement of

Global analysis of the controls on seawater dimethylsulfide spatial variability

George Manville[1], Thomas G. Bell[2], Jane P. Mulcahy[3], Rafel Simó[4], Martí Galí[4,5], Anoop S. Mahajan[6], Shrivardhan Hulswar[6], Paul R. Halloran[1]

[1]Faculty of Environment, Science and Economy, University of Exeter, Exeter, EX4 4PY, UK
[2]Plymouth Marine Laboratory (PML), Plymouth, PL1 3DH, UK
[3]Met Office, Exeter, EX1 3PB, UK
[4]Institut de Ciències del Mar (ICM-CSIC), Barcelona, 08003, Catalonia, Spain
[5]Barcelona Supercomputing Center (BSC-CNS), Barcelona, 08034, Catalonia, Spain
[6]Indian Institute of Tropical Meteorology (IITM), Ministry of Earth Sciences, Pune, 411008, India

Correspondence to: George Manville (gm441@exeter.ac.uk) and Thomas G. Bell (tbe@pml.ac.uk)

Table S1: Summary of previous VLS studies

Study	Interpolation measure	Characteristic lengthscale	DMS variability lengthscale (range)
Hales & Takahashi, 2004	Absolute error	63% of the asymptotically approached maximum (under)sampling error	–
Tortell, 2005	Correlation coefficient	First zero crossing of autocorrelation function	15 ± 4 km
Nemcek et al., 2008	Mean absolute error. Relative standard error	63% of the asymptotically approached maximum (under)sampling error. Error magnitude compared to DMS concentration (as a %)	7.4 km
Tortell & Long, 2009	Standard error	Semivariogram analysis. Distance beyond which samples become uncorrelated	250 km
Tortell et al., 2011	Root mean squared error	63% of the asymptotically approached maximum (under)sampling error	14.5 ± 3.4 km
Asher et al., 2011	Mean squared error	Change in slope (heuristic)	7.4 ± 2.2 km
Royer et al., 2015	Mean squared error	Change in slope (by eye) after averaging over increasing bin widths (only binning approach)	(15 – 50 km)

Table S2: Summary of mean DMS concentration (nM) and VLS (km), and metadata for each sampling campaign used in this study. Data are sourced from the global surface seawater DMS database (GSSDD, see https://saga.pmel.noaa.gov/dms/ last access: 15 April 2022), Malaspina Expedition in 2010 – split into three subsets (M10 a, b, c, Royer et al., 2015), the four North Atlantic Aerosol and Marine Ecosystem Study campaigns 2015–2018 (NAAMES, Bell et al., 2021), and the Southern oCean SeAsonaL Experiment in 2019 (SCALE, Manville et al. In Prep).

Figure 1 Colour & No.	Data Source (Contribution)	Contributor	Region	Period	Geometric Mean DMS conc. (nM)	Geometric Mean DMS VLS (km)
1	GSSDD (164)	Johnson	Gulf of Maine	2004/07/09 – 2004/08/12	2.09	19.99
2	GSSDD (165)	Johnson	Gulf of Mexico	2006/08/23 – 2006/09/11	2.25	16.72
3	GSSDD (166)	Johnson	E Equatorial Pacific	2006/10/14 – 2006/10/26	1.85	24.19
4	GSSDD (173)	Johnson	Atlantic Ocean	2007/10/09 – 2007/10/12	1.19	24.83
5	GSSDD (174)	Johnson	E Tropical Pacific	2007/10/16 – 2007/11/11	2.30	25.21
6	GSSDD (175)	Johnson	N Atlantic	2008/03/21 – 2008/04/24	1.27	22.57
7	GSSDD (196)	Archer	Southern Ocean	2008/03/03 – 2008/04/07	1.44	14.09
8	GSSDD (233)	Saltzman	N Atlantic	2007/07/17 – 2007/07/24	3.80	29.34
9	GSSDD (243)	Johnson	E Equatorial Pacific	2008/10/20 – 2008/11/22	2.57	23.38
10	GSSDD (244)	Johnson	California coast	2010/05/14 – 2010/06/07	5.10	29.00
11	GSSDD (246)	Bell	N Atlantic	2011/06/30 – 2011/07/14	2.82	4.11
12	GSSDD (247)	Bell	Southern Ocean	2012/02/15 – 2012/03/06	5.13	7.47
13	GSSDD (248)	Herr	NE Pacific	2004/08/12 – 2004/08/19	2.96	18.73
14	GSSDD (249)	Herr	NE Pacific	2007/06/01 – 2007/06/16	2.33	21.94
15	GSSDD (250)	Herr	NE Pacific	2007/08/16 – 2007/08/30	4.28	19.80
16	GSSDD (251)	Herr	NE Pacific	2008/06/01 – 2008/06/15	3.64	12.61
17	GSSDD (252)	Herr	NE Pacific	2008/08/14 – 2008/08/30	5.22	13.58
18	GSSDD (253)	Herr	NE Pacific	2010/07/22 – 2010/08/15	7.39	19.71
19	GSSDD (254)	Herr	NE Pacific	2010/06/01 – 2010/06/04	2.51	24.45
20	GSSDD (256)	Herr	NE Pacific	2014/08/29 – 2014/08/31	3.99	13.24
21	GSSDD (257)	Herr	NE Pacific	2016/07/12 – 2016/07/27	2.50	14.75
22	GSSDD (258)	Herr	NE Pacific	2017/08/12 – 2017/08/27	2.80	16.26
23	GSSDD (259)	Jarnikova	Southern Ocean	2009/01/07 – 2009/01/19	4.49	9.30
24	GSSDD (260)	Jarnikova	Southern Ocean	2005/12/27 – 2006/01/17	5.05	15.76

25	GSSDD (261)	Jarnikova	Southern Ocean	2006/11/03 – 2006/12/11	4.93	13.22
26	GSSDD (262)	Jarnikova	Southern Ocean	2010/11/30 – 2010/12/14	1.40	18.87
27	GSSDD (263)	Jarnikova	Southern Ocean	2013/11/22 – 2013/12/13	7.18	13.39
28	GSSDD (264)	Jarnikova	Labrador Sea	2015/07/13 – 2015/08/18	2.03	13.05
29	GSSDD (265)	Zhang	Southern Ocean, E Indian, W Pacific	2014/02/07 – 2014/04/11	2.17	13.47
30	M10 (a)	Mahajan & Simo	S Atlantic	2010/12/17 – 2011/02/18	1.09	5.93
31	M10 (b)	Mahajan & Simo	S Indian, S Australia coast, Tasman Sea	2011/03/03 – 2011/04/12	1.00	6.67
32	M10 (c)	Mahajan & Simo	Tropical & sub-tropical Pacific	2011/04/19 – 2011/07/12	0.93	1.86
33	NAAMES (1)	Bell	N Atlantic	2015/11/11 – 2015/11/29	1.28	11.93
34	NAAMES (2)	Bell	N Atlantic	2016/05/14 – 2016/06/03	2.02	18.40
35	NAAMES (3)	Bell	N Atlantic	2017/09/06 – 2017/09/23	2.98	20.89
36	NAAMES (4)	Bell	N Atlantic	2018/03/21 – 2018/04/12	3.20	21.94
37	SCALE	Manville	Southern Ocean	2019/10/18 – 2019/11/18	3.28	3.78

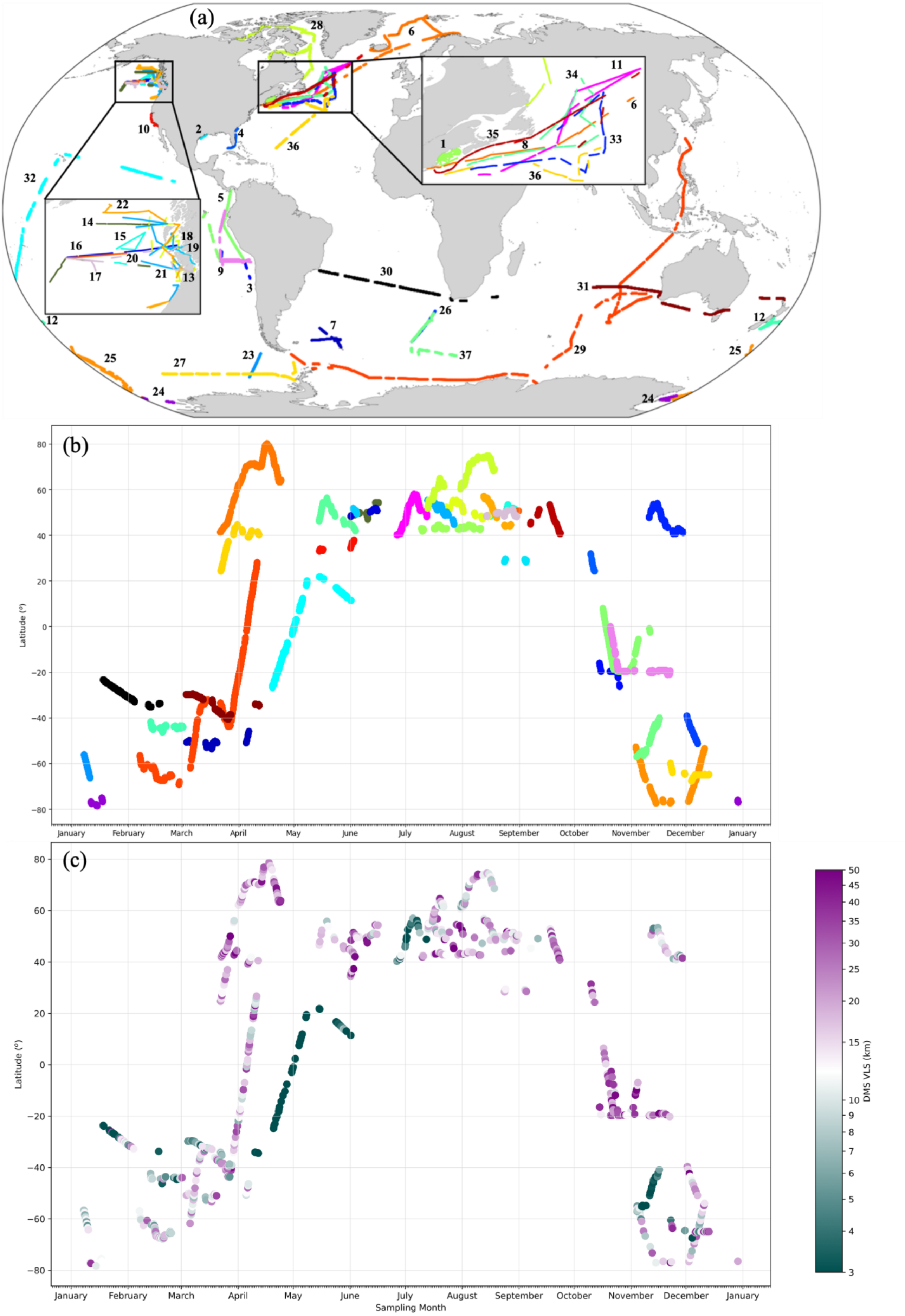


Figure S1: (a) Global extent of the 37 high frequency DMS campaigns included in this analysis (coloured and numbered), (b) spatiotemporal distribution of DMS campaigns, highlighting acute seasonal sampling bias, (c) spatiotemporal distribution of 763 transects coloured by VLS_{DMS} (km, log scale) (see Table S2 for metadata relating to each sampling campaign).

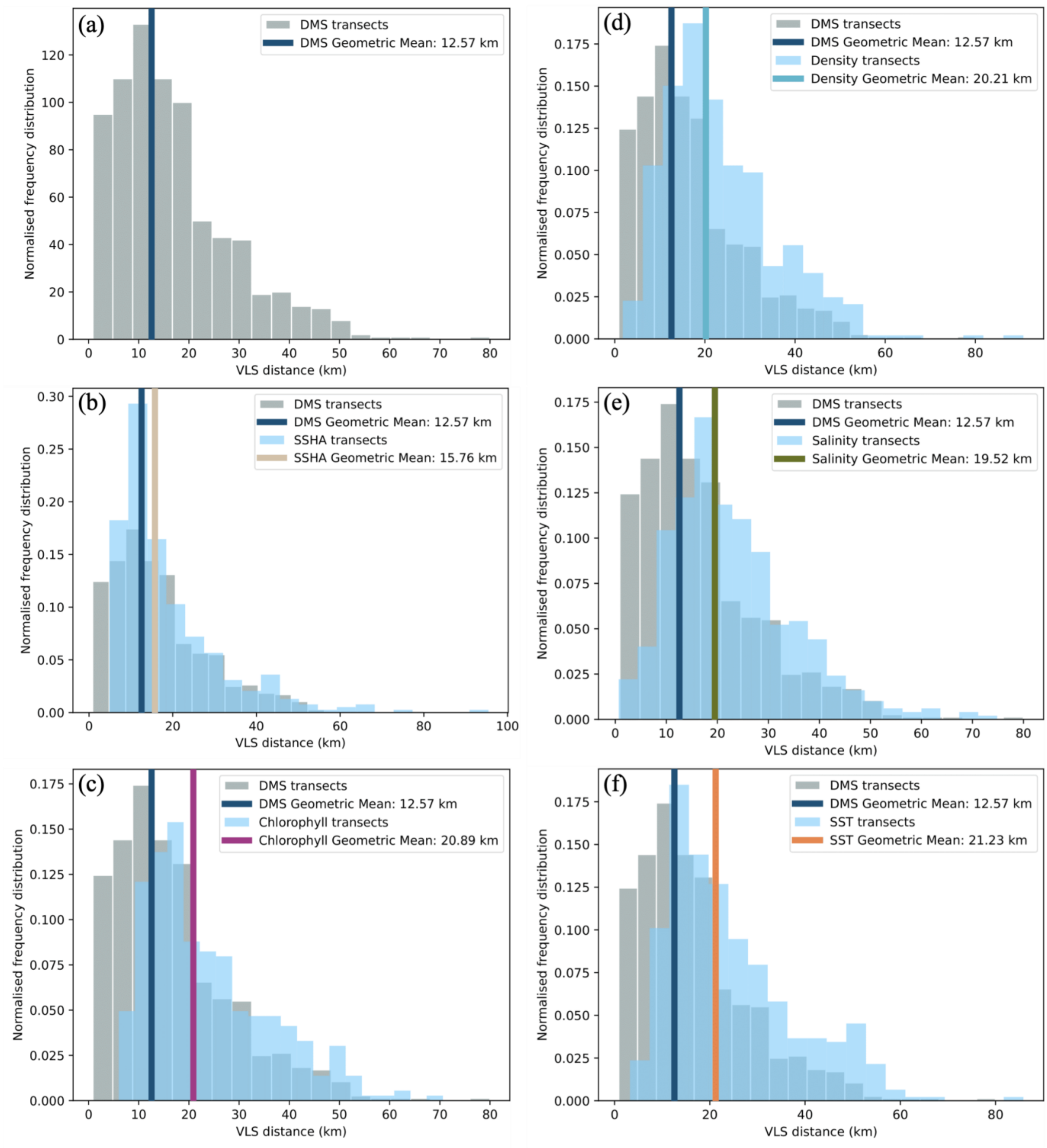
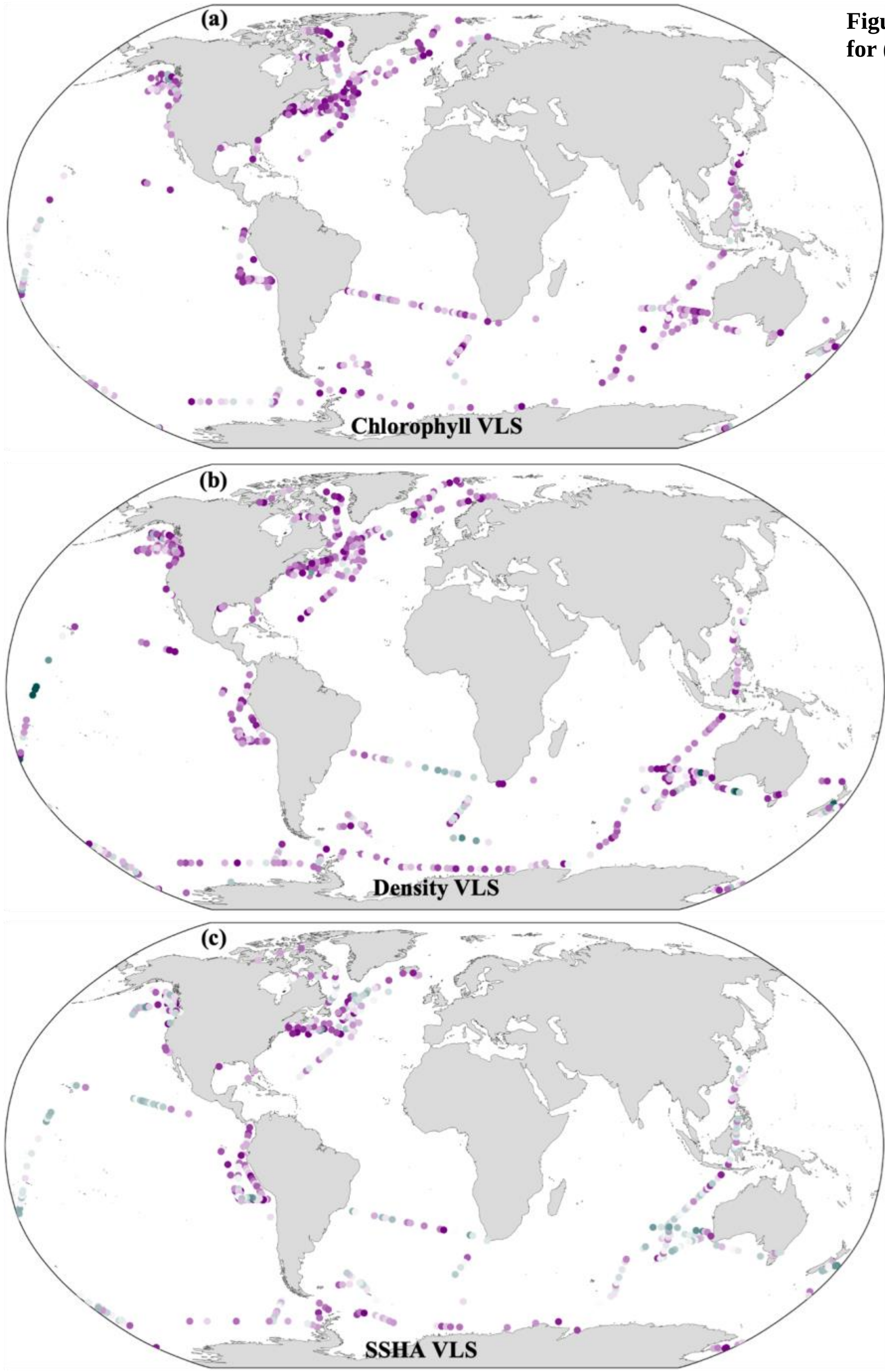
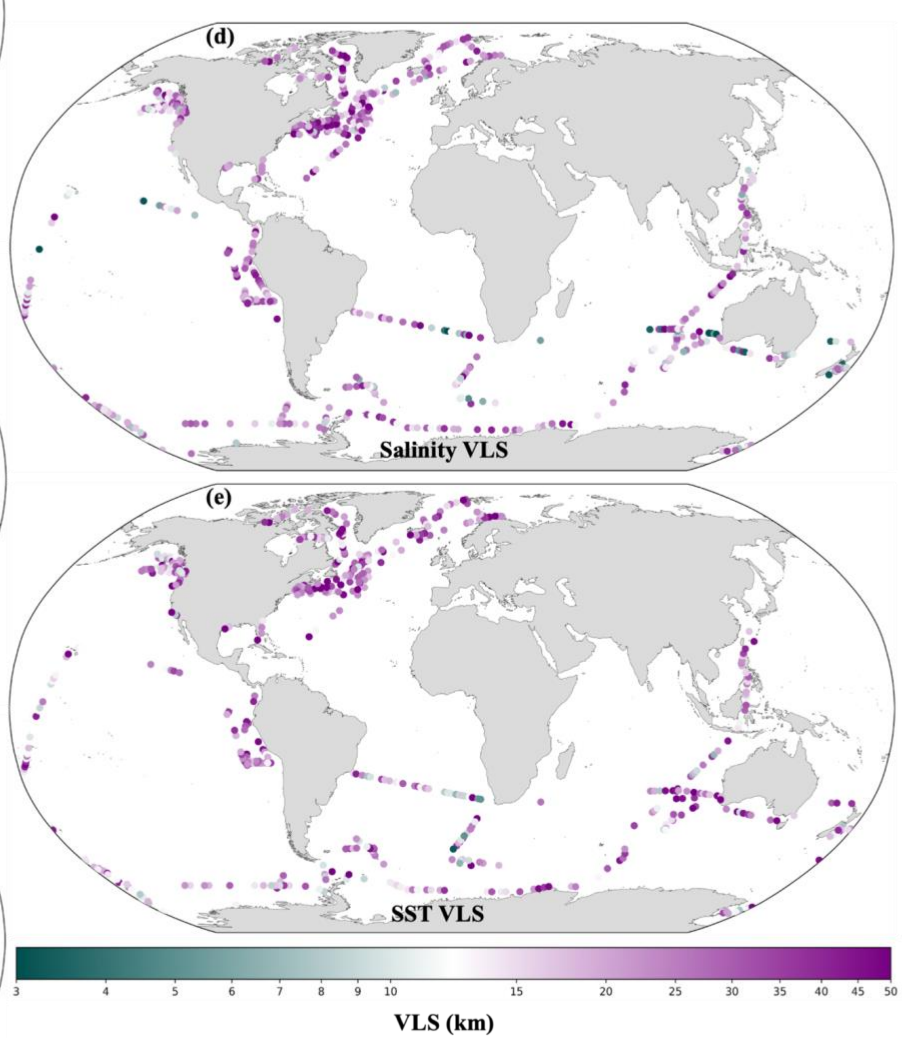


Figure S2: All panes: Frequency distribution of variability lengthscales (VLS, km) for all DMS transects (grey bars), with the global geometric mean VLS$_{DMS}$ (dark blue line). Panes b–f: Frequency distribution of transect VLS for each variable (light blue bars), normalised to the maximum transect frequency of the VLS$_{DMS}$ and superimposed on the VLS$_{DMS}$ frequency distribution. Vertical coloured lines correspond to global geometric mean from all transects for (a) VLS$_{DMS}$ (blue), (b) VLS$_{SSHA}$ (red), (c) VLS$_{Chl}$ (green), (d) VLS$_{density}$ (yellow), (e) VLS$_{salinity}$ (purple), (f) VLS$_{SST}$ (orange).

Figure S3: Global distribution of all viable (763) transects coloured by VLS (km, log scale) for (a) Chl, (b) density, (c) SSHA, (d) salinity, (e) SST.





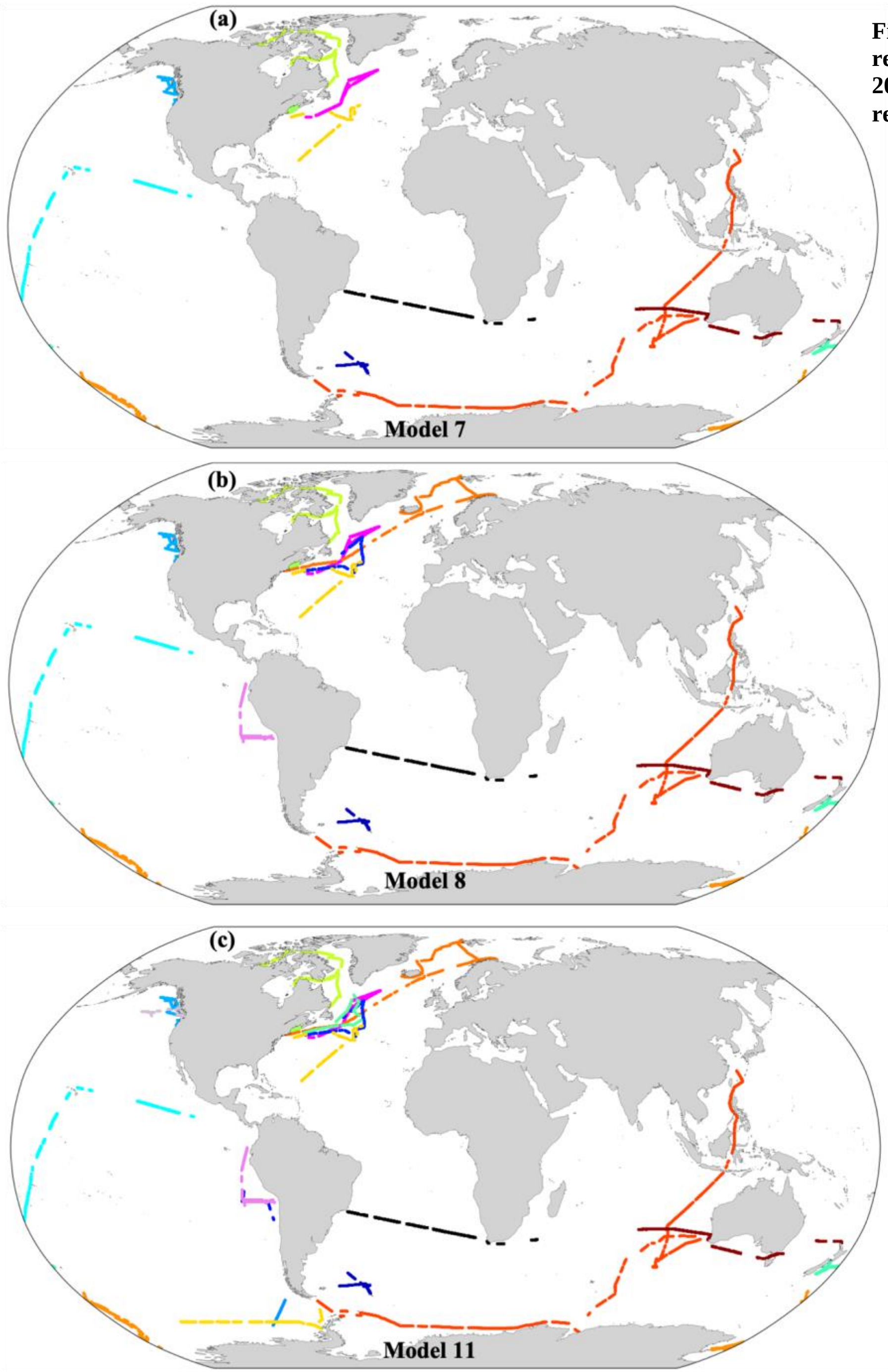


Figure S4: Cruise tracks of the DMS data sampling campaigns included in multiple linear regression (MLR) models (a) Model 7: 12 datasets, (b) Model 8: 15 datasets, (c) Model 11: 20 datasets, (d) Model 10: 25 datasets, (e) Model 9: 26 datasets. See Table S1 for metadata regarding each sampling campaign.

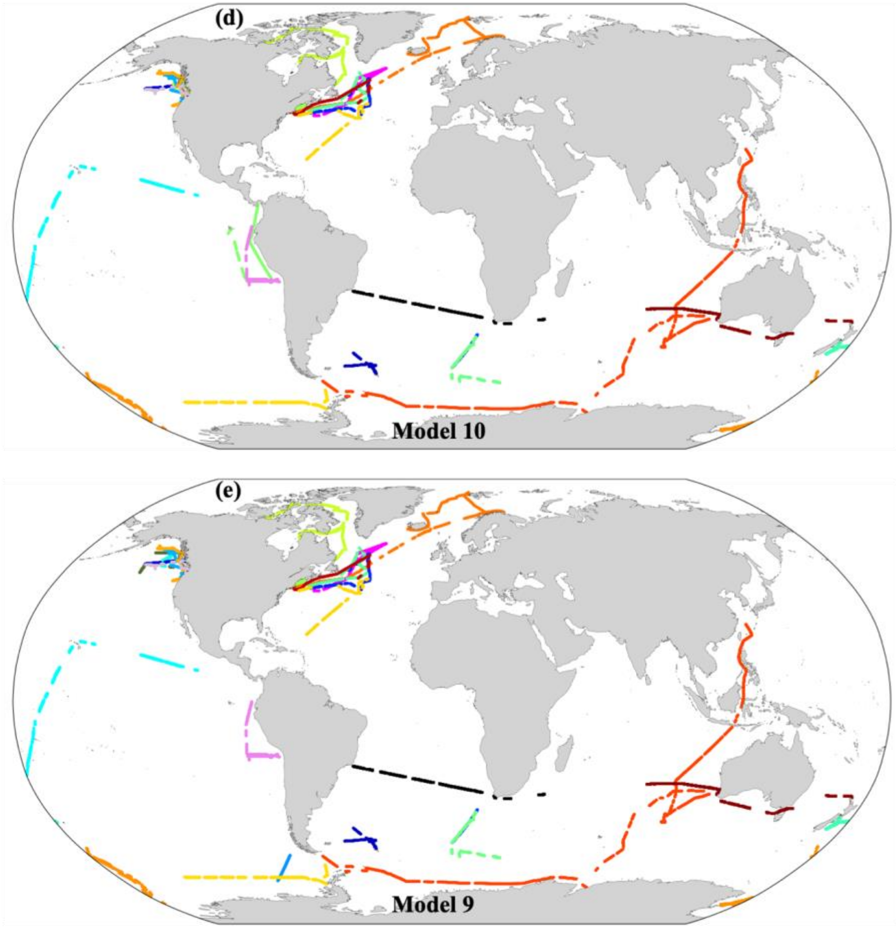


Table S3: Regression results for the prediction of campaign average VLS_{DMS}, equivalent to Table 1 in the main text but using the 'relaxed criterion' approach (see main text Section 3.3.2 for details). Models that are significant (*p < 0.01*) are denoted using *.

Model no.	Input parameters	R^2	Adj. R^2	p	Relative importance (%)	N (no. of campaigns)	No. transects used to calculate campaign averages (of 760)
Linear Regression							
1	VLS_{Chl}	0.2	–	<0.01*	100	35	361
2	VLS_{SSHA}	0.31	–	<0.01*	100	34	387
3	$VLS_{density}$	0.41	–	<0.01*	100	35	486
4	$VLS_{salinity}$	0.25	–	<0.01*	100	35	496
5	VLS_{SST}	0.25	–	<0.01*	100	35	462
6	Latitude (abs.)	0.02	–	0.375	100	35	760
Multiple Linear Regression							
7	VLS_{Chl}	0.61	0.58	<0.01*	21	34	361
	VLS_{SSHA}				37		387
	$VLS_{density}$				42		486
8	VLS_{Chl}	0.46	0.4	<0.01*	26	34	361
	VLS_{SSHA}				54		387
	$VLS_{salinity}$				20		496
9	VLS_{Chl}	0.5	0.47	<0.01*	29	35	361
	$VLS_{density}$				71		486
10	$VLS_{salinity}$	0.44	0.41	<0.01*	49	35	496
	VLS_{SST}				51		462
11	VLS_{Chl}	0.45	0.41	<0.01*	35	34	361
	VLS_{SSHA}				65		387
12	VLS_{Chl}	0.3	0.25	<0.01*	42	35	361
	$VLS_{salinity}$				58		496
13	VLS_{SSHA}	0.37	0.33	<0.01*	65	34	387
	$VLS_{salinity}$				35		496
14	VLS_{Chl}	0.41	0.38	<0.01*	44	35	361
	VLS_{SST}				56		462
15	VLS_{SSHA}	0.42	0.39	<0.01*	60	34	387
	VLS_{SST}				40		462
16	VLS_{SSHA}	0.52	0.5	<0.01*	45	34	387
	$VLS_{density}$				55		486
17	VLS_{Chl}	0.56	0.51	<0.01*	27	35	361
	VLS_{SSHA}				44		387
	VLS_{SST}				29		462

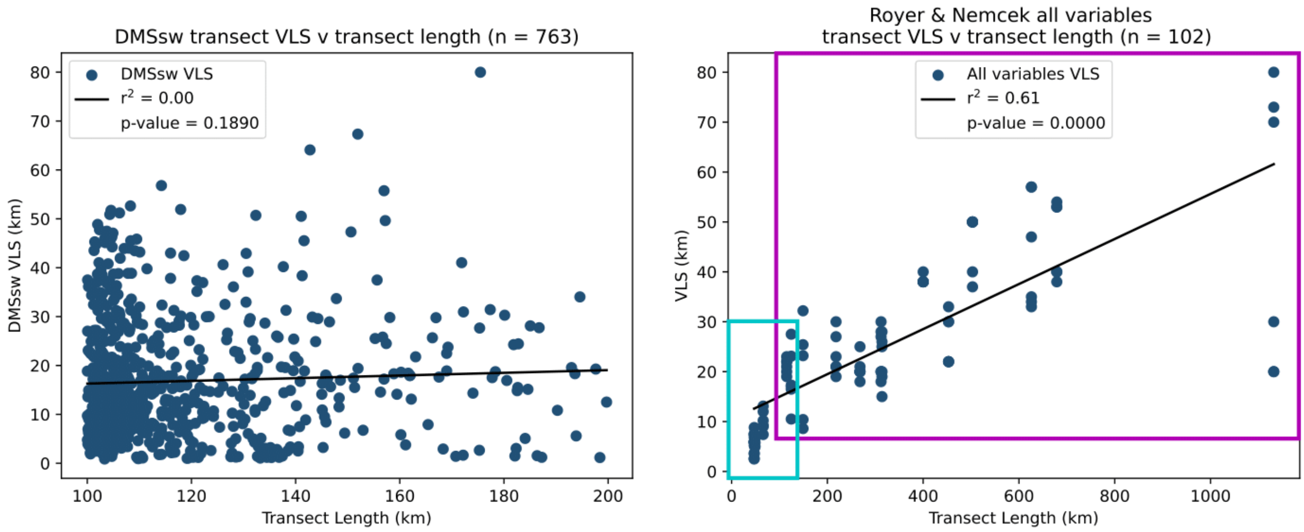


Figure S5: The importance of consistent transect lengths for analysing VLS. (a) VLS_{DMS} in this study is not significantly correlated to transect length for the 763 consistent (100-200 km) transects, (b) VLS of all parameters is dependent on transect length from both Nemcek et al. (2008) (~50-150 km, green box) and Royer et al. (2015) (~100-1100 km, red box).

Table S4 – Regression results for the prediction of campaign average VLS_{DMS}, equivalent to Table 1 in the main text but including regression coefficients. Input variables and coefficients can be applied for the prediction of VLS_{DMS} following Eq. (S1):

$$\boldsymbol{y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3}$$

where $\boldsymbol{\beta}$ corresponds to the coefficient for each input variable $\boldsymbol{x}$, and $\boldsymbol{\beta_0}$ is the constant.

Model no	Input parameters (x_1, x_2, x_3)	R^2	Adj. R^2	p	Coefficients ($\beta_1, \beta_2, \beta_3$)	Constant (β_0)
Linear Regression					β_1	
1	VLS_{Chl}	0.2	–	<0.01*	0.8099	-2.991
2	VLS_{SSHA}	0.31	–	<0.01*	0.642	2.8003
3	$VLS_{density}$	0.41	–	<0.01*	0.6524	1.1319
4	$VLS_{salinity}$	0.25	–	<0.01*	0.7393	0.0703
5	VLS_{SST}	0.25	–	<0.01*	0.6055	1.8129
6	Latitude (abs.)	0.02	–	0.375	-0.0703	19.0409
Multiple Linear Regression					$\beta_1, \beta_2, \beta_3$	
7	VLS_{Chl} VLS_{SSHA} $VLS_{density}$	0.61	0.58	<0.01*	0.3262 0.8791 0.1725	-11.0697
8	VLS_{Chl} VLS_{SSHA} $VLS_{salinity}$	0.46	0.4	<0.01*	0.6863 0.5683 0.0153	-9.5223
9	VLS_{Chl} $VLS_{density}$	0.5	0.47	<0.01*	0.6256 0.3953	-7.178
10	$VLS_{salinity}$ VLS_{SST}	0.44	0.41	<0.01*	0.9182 0.1269	-7.1162
11	VLS_{Chl} VLS_{SSHA}	0.45	0.41	<0.01*	0.2456 0.5247	-0.5942
12	VLS_{Chl} $VLS_{salinity}$	0.3	0.25	<0.01*	0.6606 0.1557	-3.5472
13	VLS_{SSHA} $VLS_{salinity}$	0.37	0.33	<0.01*	0.5444 0.1747	1.3005
14	VLS_{Chl} VLS_{SST}	0.41	0.38	<0.01*	0.6509 0.3517	-7.6643
15	VLS_{SSHA} VLS_{SST}	0.42	0.39	<0.01*	0.5456 0.3233	-2.5339
16	VLS_{SSHA} $VLS_{density}$	0.52	0.5	<0.01*	0.5475 0.2495	-0.6278
17	VLS_{Chl} VLS_{SSHA} VLS_{SST}	0.56	0.51	<0.01*	1.028 -0.7187 -0.2228	7.282

References

Asher, E. C., Merzouk, A., & Tortell, P. D. (2011). Fine-scale spatial and temporal variability of surface water dimethylsufide (DMS) concentrations and sea-air fluxes in the NE Subarctic Pacific. *Marine Chemistry*, *126*(1–4), 63–75. https://doi.org/10.1016/j.marchem.2011.03.009

Bell, T. G., Porter, J. G., Wang, W. L., Lawler, M. J., Boss, E., Behrenfeld, M. J., & Saltzman, E. S. (2021). Predictability of Seawater DMS During the North Atlantic Aerosol and Marine Ecosystem Study (NAAMES). *Frontiers in Marine Science*, *7*, 1200. https://doi.org/10.3389/FMARS.2020.596763/BIBTEX

Hales, B., & Takahashi, T. (2004). High-resolution biogeochemical investigation of the Ross Sea, Antarctica, during the AESOPS (U. S. JGOFS) Program. *Global Biogeochemical Cycles*, *18*(3). https://doi.org/10.1029/2003GB002165

Nemcek, N., Ianson, D., & Tortell, P. D. (2008). A high-resolution survey of DMS, CO2, and O2/Ar distributions in productive coastal waters. *Global Biogeochemical Cycles*, *22*(2). https://doi.org/10.1029/2006GB002879

Royer, S. J., Mahajan, A. S., Galí, M., Saltzman, E., & Simõ, R. (2015). Small-scale variability patterns of DMS and phytoplankton in surface waters of the tropical and subtropical Atlantic, Indian, and Pacific Oceans. *Geophysical Research Letters*, *42*(2), 475–483. https://doi.org/10.1002/2014GL062543

Tortell, P. D. (2005). Small-scale heterogeneity of dissolved gas concentrations in marine continental shelf waters. *Geochemistry, Geophysics, Geosystems*, *6*(11). https://doi.org/10.1029/2005GC000953

Tortell, P. D., Guéguen, C., Long, M. C., Payne, C. D., Lee, P., & DiTullio, G. R. (2011). Spatial variability and temporal dynamics of surface water pCO2, δO2/Ar and dimethylsulfide in the Ross Sea, Antarctica. *Deep-Sea Research Part I: Oceanographic Research Papers*, *58*(3), 241–259. https://doi.org/10.1016/j.dsr.2010.12.006

Tortell, P. D., & Long, M. C. (2009). Spatial and temporal variability of biogenic gases during the Southern Ocean spring bloom. *Geophysical Research Letters*, *36*(1). https://doi.org/10.1029/2008GL035819