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Data collation for climate-cooling gas dimethylsulfide in Antarctic snow, sea ice and underlying seawater

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Dimethylsulfide (DMS) is a climatically active volatile sulfur compound found in Earth's oceans and atmosphere that plays an important role in cloud formation. DMS originates from its precursor dimethylsulfoniopropionate (DMSP), which is produced by several classes of phytoplankton. Concentrations of DMS and DMSP in Antarctic sea ice, snow and underlying seawater are not well documented and there is currently no dataset available to find the existing data. The purpose of this project was to compile historical measurements into a publicly available dataset. A total of 220 samples collected since 1992 were compiled using the Antarctic Sea ice Processes and Climate program template, in accordance with the existing datasets for chlorophyll-a, macronutrients, and dissolved iron. Analyses performed on the completed DMS dataset showed that the spatial and temporal coverages are limited; there are barely any measurements in autumn and winter, nor in the Amundsen or Ross seas. These findings provide a basis for future sampling efforts in the Antarctic region.

Background & Summary

Sea ice plays an important role in the regulation of the Earth system, largely due to its high albedo and the habitat it provides for marine life. Antarctic sea ice is an important habitat for microbial and algal communities both at the ice-water interface and throughout the ice matrix because it retains them near the ocean surface where there is enough sunlight and nutrients for algae to grow[1]. Dimethylsulfoniopropionate (DMSP) is a bi-product of microbial production that is closely associated with the presence of sea-ice algae[2,3]. DMSP acts as an osmolyte (compound that regulates osmotic pressure in cells) for aquatic algae in general, but is also thought to act as a cryoprotectant (antifreeze) for these primary producers, allowing them to withstand the extreme gradients in temperature and salinity experienced in the Antarctic environment[4]. DMSP can remain in sea ice and the water column but can also be converted into dimethylsulfide (DMS) by sea-ice algae or bacteria through enzymatic cleavage[5]. Unlike DMSP, DMS can transfer from the ice or ocean into the atmosphere. In the atmosphere, DMS is oxidised into sulphur-containing aerosols such as sulfuric acid and methanesulfonic acid, which are known as cloud condensation nuclei[1]. Therefore, these sulphur particles can increase cloud formation and scattering properties, which can in turn increase the amount of solar radiation reflected by the Earth. Through this mechanism, DMS emission from Antarctic sea ice is likely to translate into increased albedo over the Antarctic region, thereby counteracting some of the positive climate feedbacks[6].

DMS is abundant in the oceans around the world, and DMS and DMSP concentrations have both been extensively measured in the tropical and temperate oceans; however remote and inaccessible places such as the polar regions have been less well studied, leading to gaps in our knowledge. Only a handful of studies have explored the concentrations of DMS and DMSP in Antarctic sea ice, showing that the recorded concentrations greatly vary both spatially and seasonally[5]. Notably, all these data were publicly unavailable, making it difficult for researchers to further our understanding of the roles DMS and DMSP play in the Earth system.

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Study	Location	Ice type	Season and year	Type of sample	Variable	No. cores/samples
Carnat *et al.*[20,21]	Ross Sea	pack	autumn-winter 2013	ice core	DMSP	4
	Weddell Sea	pack	winter 2017	ice core	DMSP	3
	McMurdo Sound	fast	spring-summer 2011–2012	ice core	DMSP	7
*Damm *et al.*[5]	East Antarctica SIZ	pack	spring 2012	ice core, slush core	DMSP	2
*Gambaro *et al.*[22]	Terra Nova Bay	fast	summer 2000–2001	ice core	DMSP	5
Nomura *et al.*[23]	Lützow-Holm Bay	fast	summer 2006–2007	ice core	DMS + DMSP	6
Nomura *et al.*[24]	Lützow-Holm Bay	fast	summer 2010	under-ice water, slush	DMS	14
Tison *et al.*[2]	Western Weddell Sea	pack	spring-summer 2004	ice core, under ice water, brine	DMS, DMSP	42
*Trevena and Jones[3]	Prydz Bay	pack	summer 1997–1998	ice core	DMSP	2
*Trevena *et al.*[25]	Prydz Bay	pack	spring 1997	ice core	DMSP	7
*Trevena[26]	Prydz Bay	fast	spring 1997	ice core	DMSP	12
*Turner *et al.*[27]	Bellingshausen Sea	pack	spring 1992	ice core	DMSP	3
Wright and Jones[28]	East Antarctica SIZ	pack	spring-summer 1997–1998	ice core	DMSP	62
*Zemmelink *et al.*[29]	Weddell Sea	pack	summer 2004	snow sample	DMS	47
						Total: 216

Table 1. A summary of the studies from which DMS and DMSP data were collected. Studies where GRABIT[7] was used are marked with (*).

This project aimed to collate as much data as possible from these existing studies into one dataset to advance our understanding of the current spatial and temporal distribution of the data as well as inform future research efforts. From eighteen studies identified in a literature search, we were able to access data from twelve of those studies, either directly from the authors or using the MATLAB File Exchange GRABIT[7], totalling 216 samples (Table 1). Data include measurements from both free-floating sea ice (pack ice) and sea ice attached to the Antarctic continent (fast ice)[8]. As well as sea ice and underlying seawater, measurements are included from snow on top of sea ice, slush, formed when water is introduced to the snow[9], and brine that is expelled from the ice matrix during freezing[9].

Table 1 summarises the collated data, demonstrating that there is incomplete representation of all sample types and variables. The dataset contains eleven studies that sampled sea ice and slush, two that include under-ice seawater and only one measurement for snow. There are also significantly more DMSP data than the DMS data; the dataset is made up of 38.43% DMS measurements, 58.80% DMSP measurements, and 2.78% combined measurements. This may be because of the relative difficulty of extracting DMS compared to DMSP from sea ice[10]. This dataset would be more valuable if there were more measurements of DMS added to it as this variable is crucial for biogeochemical model developments.

The vast majority of the data were collected during the Austral spring and summer, when there is increased biological activity (Table 1, Fig. 1). The majority of DMS and DMSP samples were collected in East Antarctica and around McMurdo Station, with some near the west Antarctic Peninsula (Fig. 2). There are only three samples included from the Bellingshausen/Amundsen Sea and four from the Ross Sea. The high representation of East Antarctic sites may be because Australian data were the most easily accessible. The Antarctic Sea ice Processes and Climate (ASPeCt)-Bio dataset[11], which is the collation of chlorophyll-*a* (Chl*a*) in Antarctic sea ice, contains more samples with a wider distribution and shows high Chl*a* concentrations in ice cores in the Weddell, Ross and Amundsen seas. More extensive sampling may show that these high Chl*a* areas are also high in DMS due to the biological activity.

Ideally some of the DMS and DMSP data from this dataset may be compared with other variables such as dissolved iron[12], macronutrients[13], or Chl*a*[11,14] from other data compilations (such as ASPeCt-Fe[12] or ASPeCt-Bio[11,14]). However, some of these studies measured DMS from different cores with different depth ranges to the Chl*a* or iron cores, making direct comparison difficult. A cross-comparison of the ASPeCt datasets could still be a valuable undertaking in the future to investigate possible correlations between biogeochemical variables.

This dataset should provide useful and centralised data for researchers who want to analyse and add to the current understanding of DMS in Antarctica. The dataset can be analysed using any programming language. For a Matlab or Octave user, it can be analysed using a MATLAB ice core analyzer[15], to which we have written the accompanying script, 'DMS Analyzer[16]'. This script allows the user to easily extract data from the dataset and make profile plots such as Fig. 3, which shows an example of a DMSP depth profile, incorporating the snow, ice and water layers, that can be made using this tool.

Methods

Data collation was conducted in the style of Lannuzel *et al.*[12] and Meiners *et al.*[11] as illustrated in Fig. 4. A comprehensive literature search was carried out using keywords to identify as many studies as possible that had documented measurements of DMS and/or DMSP in Antarctic sea ice, snow or underlying seawater. The information of interest included the sample depths and mean concentrations of DMS and DMSP measured in nanomoles per litre (nmol l^{-1}), for the associated depths. Ancillary data such as nutrients, temperature and Chl*a* concentrations were also recorded, as well as descriptive data for the sampling sites, such as date, coordinates, type of ice, snow and ice thickness, core diameter, etc., which provide key information on the history and

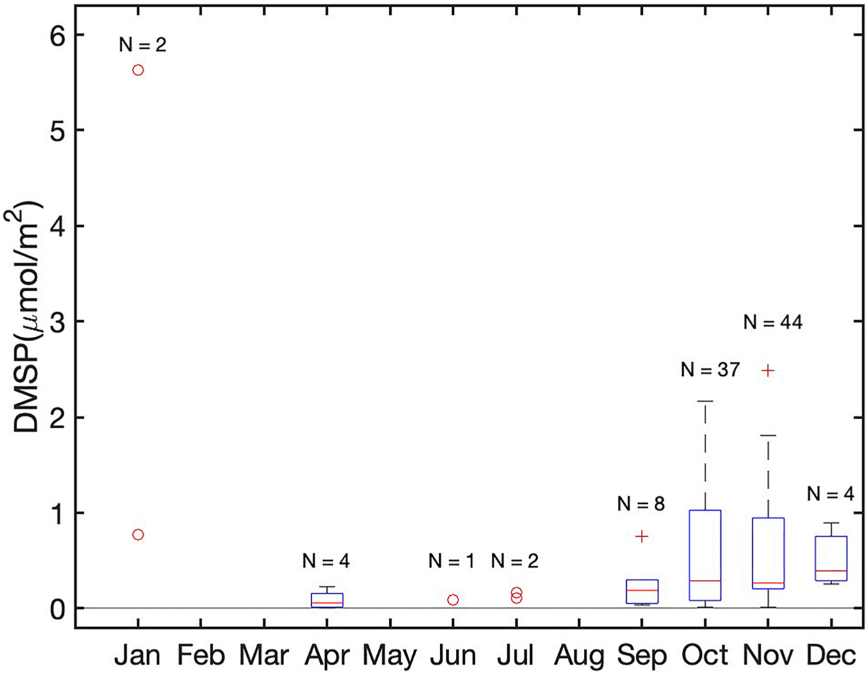

Fig. 1 Temporal analysis of DMSP sea-ice core data in this dataset. The boxplot shows the range of DMSP concentrations for all depth-integrated ice cores against the month in which they were collected. Boxes represent the interquartile range of DMSP concentrations, with lower and upper whiskers showing the nonoutlier minima and maxima, respectively, red lines showing the medians, and the symbol (+) representing the outliers. The thin grey horizontal line marks the DMSP values at 0. Months with insufficient data points are plotted with dots. Sample size for each month is shown as N.

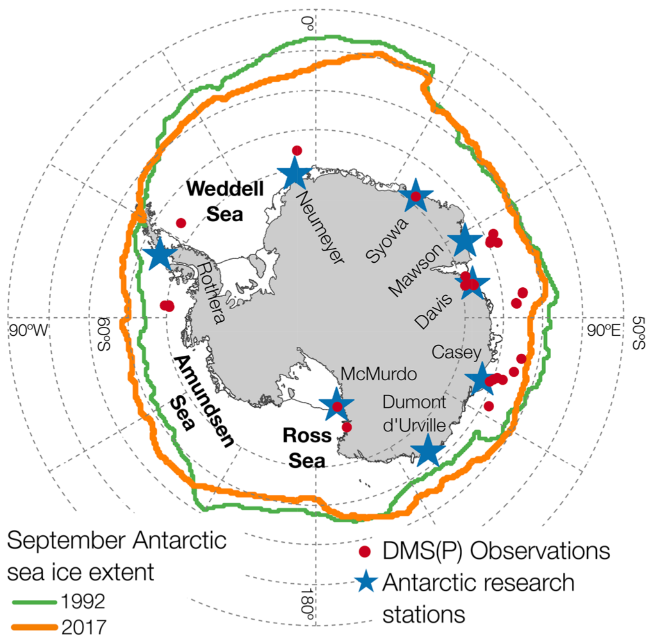

Fig. 2 Sampling sites for DMS and DMSP from all the studies in Table 1. The red dots mark the locations of the samples, and blue stars the Antarctic research stations. September mean sea-ice extents for the years spanning DMS(P) data records, acquired from National Snow and Ice Data Centre[30], are shown for context. Most data were collected in East Antarctica, the Ross Sea or near the Antarctic Peninsula.

properties of the ice for analysis and modelling. These data were sometimes included in the paper, sometimes attached as an appendix to the online publication and occasionally publicly available on one of many online data repositories such as the Australian Ocean Data Network, the Southern Ocean Observing System, the Australian

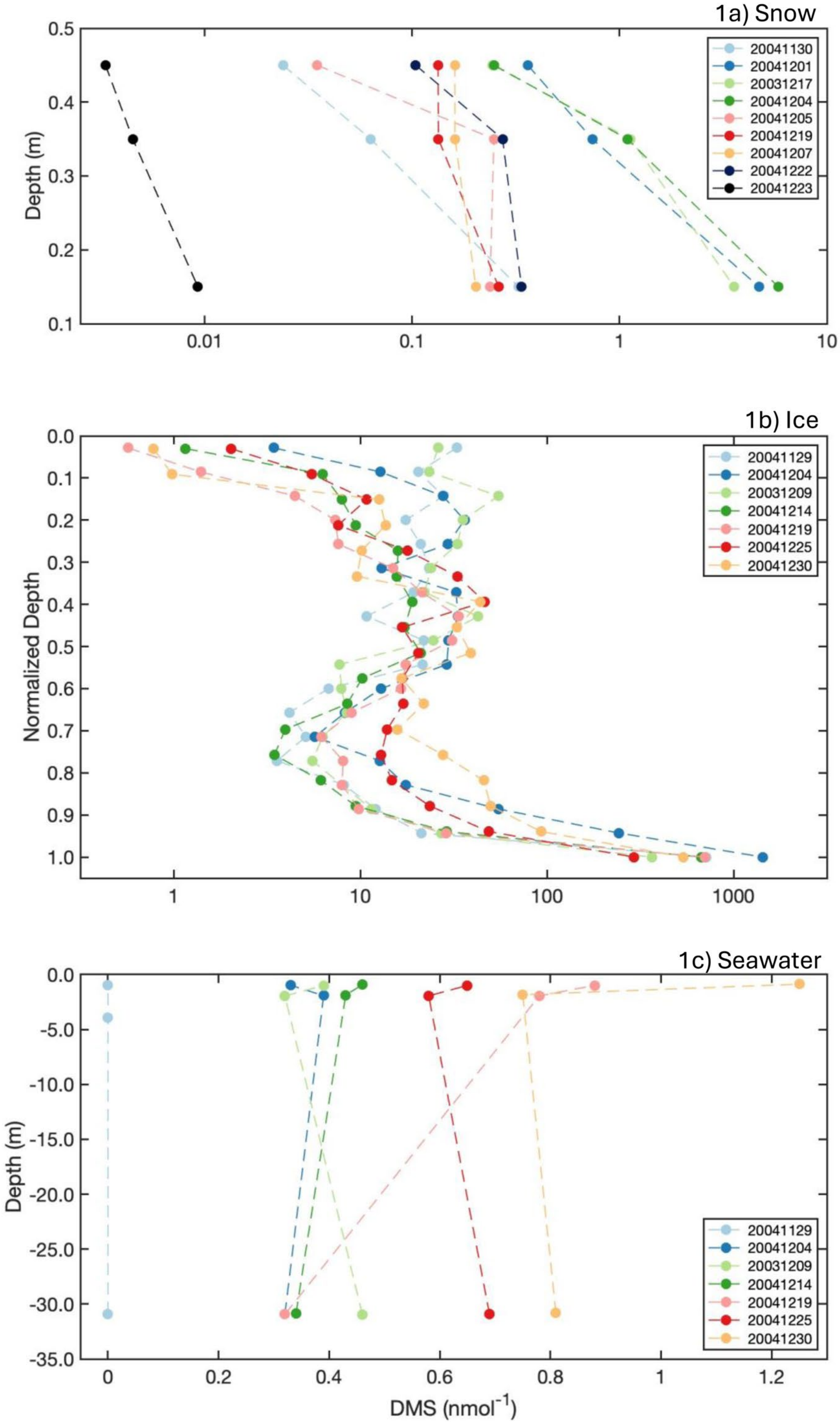

Fig. 3 Example of vertical profiles of (**a**) snow, (**b**) sea ice, and (**c**) under-ice seawater DMS concentrations plotted using the BEPSII DMS Analyzer[16], Using data from Tison *et al.*[2]. Note that for the middle panel, 0 refers to the air/ice interface and 1 refers to the bottom of the sea ice/ocean interface. Cores/samples are color-coded by date collected.

Antarctic Data Centre and the British Oceanographic Data Centre. In cases where the data were not publicly available, the corresponding author was contacted, and we requested they make them available for collation.

Data were also requested through relevant scientific communities such as the Biogeochemical Exchange Processes at the Sea Ice Interfaces (BEPSII), the Cryosphere and Atmospheric Chemistry (CATCH) activity, the Australian Antarctic Partnership Program (AAPP), the Australian Centre for Excellence in Antarctic Science (ACEAS), the Scientific Committee on Antarctic Research (SCAR) and the Australian Research Council Centre

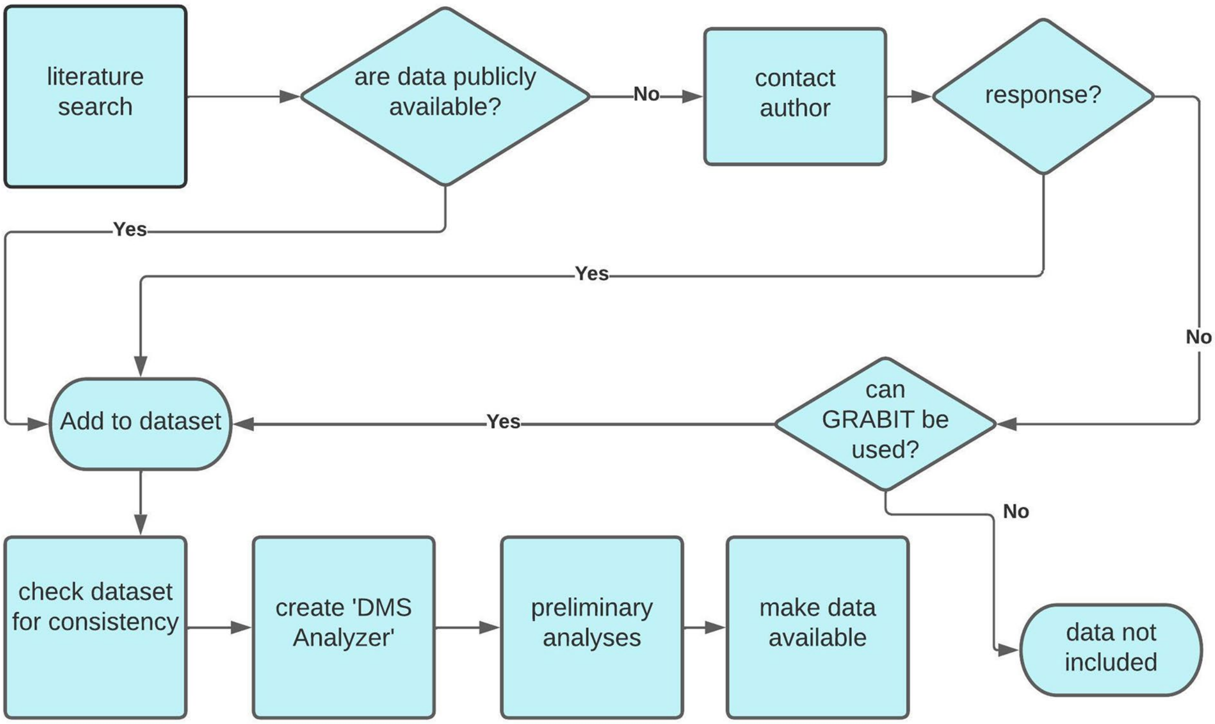

Fig. 4 Workflow diagram depicting the data collation process.

on Excellence for Climate Extremes (CLEX). Where data could not be accessed through any of these means, they were extracted directly from figures using the MATLAB package GRABIT[7]. Note that in studies in which GRABIT was used, figures did not represent the entire dataset, and the GRABIT software is only fit for the best approximation of the data in the figure. Additionally, there was often no way to find exact dates for the sampled stations, or other ancillary data such as ice thickness or ice type. In these cases, samples were labelled to the month they were collected, with the value '00' for the day. The studies where GRABIT was used are specified in Table 1.

Once the data were acquired, they were collated into the ASPeCt dataset template using Microsoft Excel, to which the fields DMS and DMSP had been added, along with depth ranges for each. Samples were classified as being measurements of ice, snow, slush, seawater or brine, with one excel spreadsheet representing one ice core, snow sample or seawater sample as a vertical profile with section depth ranges. These methods curate the existing data into a standardised format and centralise them into one location, allowing easy analysis over the spatial and temporal scales at which they have been collected. The accompanying script, 'DMS Analyzer'[16] was written in MATLAB, and created to be an extension of the package 'BEPSII ice core analyzer'[15], allowing users to construct vertical profiles and easily analyse these curated data.

These methods curate the existing data into a standardised format and centralise them into one location, allowing easy analysis over the spatial and temporal scales at which they have been collected.

Data Records

This dataset is available at the Australian Antarctic data Centre (AADC) (Metadata URL: DMS_DMSP_Antarctica_Snow_Ice_Seawater_DataCollation, https://data.aad.gov.au/metadata/DMS_DMSP_Antarctica_Snow_Ice_Seawater_DataCollation)[17]. The dataset consists of folders for measurements of sea ice, snow, slush, seawater and brine. Each excel file represents one sea-ice core, snow or seawater sample as a vertical profile with section depth ranges. It includes ancillary data such as nutrients, temperature and Chl*a* concentrations if available, as well as descriptive data for the sampling sites, such as date, coordinates, type of ice, snow and ice thickness, core diameter, etc.

Technical Validation

No data were produced by the authors; the dataset solely includes measurements from previously published and peer-reviewed studies. Similar collations have already been successfully carried out for historical sea-ice core data relating to other biogeochemical variables such as Chl*a*[11], iron[12] and macronutrients[13,18]. These were compiled following the protocols of the Antarctic Sea ice Processes and Climate (ASPeCt) sea ice physics (http://aspect.antarctica.gov.au/) and BEPSII (https://sites.google.com/site/bepsiiwg140 /home) programs. Here, we build on these previous efforts, following the same format, with the goal of creating an ASPeCt dataset (e.g., Meiners *et al.*[11]) for DMS and DMSP in Antarctic sea ice, snow and underlying seawater. The dataset consists of Microsoft Excel files following the ASPeCT template, which allows users to easily access the data provided in an identical format. We verify that the collated data are consistent from one another by developing and running the Matlab script 'DMS Analyzer'[16].

Data availability

No custom code was generated to create this dataset itself, but the DMS Analyzer was used to check the consistency of the data being added to the dataset. The MATLAB package 'BEPSII Ice Core Analyzer' can be downloaded using the following link: https://pagesperso.locean-ipsl.upmc.fr/mvlod/. The accompanying script, 'DMS Analyzer' was created to assist users with analyses of these data (e.g., Fig. 3), and can be downloaded from Zenodo.com at https://zenodo.org/records/13831861. Figures were generated in MATLAB version R2022b. The code used to generate Figs. 1, 2[19] is available for download from Zenodo at https://zenodo.org/records/13827062.

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Author contributions

The study was conceptualized by H.H., P.W. and D.L. G.B. carried out the data collation, wrote the DMS Analyzer script, prepared the publication of the data, and wrote the first draft of the manuscript. All authors contributed to and edited the manuscript.

Competing interests

The authors declare no competing interests.

Additional information

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