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New processing methodology to incorporate marine halocarbons and dimethyl sulfide (DMS) emissions from the CAMS-GLOB-OCE dataset in air quality modeling studies

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Abstract

Oceans are the largest source of biogenic emissions to the atmosphere, including aerosol precursors like marine halocarbons and dimethyl sulfide (DMS). During the last decade, the CAMS-GLOB-OCE dataset has developed an analysis of daily emissions of tribromomethane ($CHBr_3$), dibromomethane (CH_2Br_2), iodomethane (CH_3I), and DMS, due to its increasingly recognized role on tropospheric chemistry and climate dynamics. The potential impacts of these compounds on air quality modeling remain, however, largely unexplored. The lack of a reliable and easy methodology to incorporate these marine emissions into air quality models is probably one of the reasons behind this knowledge gap. Therefore, this study describes a methodology to adapt the CAMS-GLOB-OCE dataset to be used as an input of the preprocessor software Sparse Matrix Operator Kernel Emissions (SMOKE). The method involves nine steps to update file attribute properties and to bilinearly interpolate compound emission fields. The procedure was tested using halocarbon and DMS emissions fields available within the CAMS-GLOB-OCE database for the Southern Ocean around Antarctica. We expect that this methodology will allow more studies to include the marine emissions of halocarbons and DMS in air quality studies.

Keywords Marine emissions · SMOKE · NetCDF Command Operator · CAMS-GLOB-OCE · CMAQ

Introduction

Since the 1970s, reactive halogen radicals generated from the action of tribromomethane ($CHBr_3$), dibromomethane (CH_2Br_2), iodomethane (CH_3I), and dimethyl sulfide (DMS) have increasingly been recognized as essential components of tropospheric chemistry (Simpson et al. 2015). In the ocean, these substances are mainly generated via biological and photochemical processes related to the productivity and decay of marine phytoplankton, i.e., microscopic algae (Quack et al. 2007). Once released into the marine atmosphere, they interact with atmospheric oxidants through many photolysis and reaction pathways such as the catalytic destruction of tropospheric O_3, modification of the oxidative capacity via altering the balance of nitrogen oxides (NO_x) and hydrogen oxides (HO_x), the formation of ultrafine particles, the destruction of methane (CH_4), and the oxidation of mercury (Hg) (Saiz-Lopez and von Glasow 2012; Simpson et al. 2015).

The presence of the enzyme bromoperoxidase in the phytoplankton seems to be the main pathway for the $CHBr_3$ (bromoform) formation in the open ocean (Stemmler et al. 2015).

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$CHBr_3$ is considered the main organic bromine species released from the ocean to the atmosphere (Jia et al. 2019). The emissions of bromoform from the ocean are estimated to be around eight times higher than for CH_2Br_2 which is the second largest contributor to the oceanic emissions of halocarbons (Ordóñez et al. 2012). Both halocarbons are also produced from sea ice algae in Artic and Antarctic regions (Abrahamsson et al. 2018). CH_3I is the main iodine species emitted from the ocean to the atmosphere (Saiz-Lopez et al. 2012). Several studies have shown that CH_3I is produced in the ocean by biological and photochemical processes (Tegtmeier et al. 2013).

Annual emissions of marine dimethyl sulfide account for about half of the global sulfur emissions according to available estimates (Lana et al. 2011). Biogenic DMS is the product of bacterial enzymatical conversion of the dimethylsulfoniopropionate (DMSp) produced by phytoplankton (Yang et al. 2014). Biogenic DMS is the primary precursor of non-sea salt sulfates and greatly affects the abundance and composition of marine aerosols in the troposphere. Marine aerosols directly reflect radiation and act as cloud condensation nuclei (CCN), making DMS an important regulator of Earth's global climate system (Mahajan et al. 2015; Choi et al. 2020) (Woodhouse et al. 2013). DMS is also associated with urban aerosol and ozone formation in coastal cities like Los Angeles, USA (Muñiz-Unamunzaga et al. 2018) and Shanghai, China (Li et al. 2020b).

DMS and halocarbons are considered biogenic (i.e., produced by living organisms) very short-lived species (VSL) due to their relatively short lifetimes in the atmosphere (less than 6 months). During the last decade, air quality modeling studies have shown that VSL are an essential component of tropospheric chemistry (Sarwar et al. 2014, 2015; Sherwen et al. 2016; Stone et al. 2018; Badia et al. 2019; Hoffmann et al. 2019; Iglesias-Suarez et al. 2020; Li et al. 2020a), recommending the inclusion of halogenated chemistry and emission inventories in photochemical modeling assessments of coastal air pollution. Similarly, Iglesias et al. (2020) concluded that halogenated chemistry is a crucial component of the troposphere, controlling a significant fraction of present O_3 dynamics and determining its abundance and distribution under current climate change scenarios. Furthermore, marine emissions of halocarbons and DMS are projected to increase in the future due to enhanced air-sea exchange related to warmer surface waters. Despite all these evidences, up to date marine emissions of halocarbons and DMS are mostly neglected in air quality modeling studies. Therefore, we have developed a methodology to use and incorporate the halocarbons and DMS emissions within the Copernicus Atmosphere Monitoring Service (CAMS) database in air quality modeling studies.

CAMS is a well-known and easy to use database that has recently developed a marine emission inventory for $CHBr_3$, CH_2Br_2, CH_3I, and DMS, as part of the CAMS-GLOB-OCE dataset (Granier et al. 2019). The fluxes have been calculated using empirical equations (Nightingale et al. 2000; Lana et al. 2011; Ziska et al. 2013; National Oceanographic Data Center 2017; Granier et al. 2019) and reported seawater concentrations of halocarbons and DMS. The CAMS-GLOB-OCE dataset has an excellent spatiotemporal resolution with daily registries mapped into a $0.5° \times 1.0°$ grid resolution amenable to regional scale studies. The latest release version of CAMS-GLOB-OCE dataset contains the estimates between 2000 and 2019 and is available on the Emissions of Atmospheric Compounds and Compilation of Ancillary Data (ECCAD) website.

The CAMS-GLOB-OCE dataset could be helpful in air quality modeling studies using numerical models. The Community Multiscale Air Quality (CMAQ) (Byun and Schere 2006) is a photochemical model widely used in this context on a regional, hemispherical, and global scale. The recently released version CMAQ5.3.2 (Development 2020) includes halogen species and DMS reactions. Those chemistries were usually avoided in past air quality modeling studies (Hoffmann et al. 2016), but in recent years, many researchers worldwide are interested in the effect of those marine emissions on air quality. In general, more air quality studies including marine emissions of halocarbons and DMS are needed. The CAMS-GLOB-OCE dataset is an excellent tool to overcome the lack of in situ concomitant assessments of those emissions when carrying out an air quality modeling study. One barrier to the more widespread use of this dataset in air quality modeling may be the difficulties of converting the CAMS-GLOB-OCE data into a format usable by air quality models like CMAQ. Another obstacle to a wider use of this dataset could be the lack of information about the preprocessing steps required for input into the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (Baek and Seppanen 2018), which is the processor of the emission inventory data needed to obtain the emissions inventory file required by CMAQ. The files in CAMS-GLOB-OCE data have a format that is not readable as an input into SMOKE. This dataset has the variable and the attribute "time"; meanwhile, SMOKE requires input gridded data without it (Baek and Seppanen 2018). Besides, the CAMS-GLOB-OCE has NetCDF-4 file format and $0.5° \times 0.1°$ as grid cell resolution, and SMOKE only accepts NetCDF classic file format with $0.1 \times 0.1°$ as gridded input data (Pino-Cortés 2021). Unfortunately, up to date no specific methodology has been published detailing the steps needed to convert the files within CAMS-GLOB-OCE dataset into a format usable by SMOKE and CMAQ models, which in turn limits the capacity of the research community to answer pressing questions related to air quality.

The main purpose of this article is to report a usable methodology to transform CAMS-GLOB-OCE data so it can be used by SMOKE and then CMAQ. This methodology will allow air quality studies to include these emissions in areas where in situ concomitant emission inventories are lacking.

Methodology

Preprocessing steps

The methodology was developed following the scheme summarized in Fig. 1. After free user registration, the data files must be requested through the website (https://eccad3.sedoo.fr/). Afterwards, the user will receive two separate emails, the first confirming the files requested and the second with the instructions and link to access and download the data. The downloaded files are then processed to obtain the input format required by SMOKE, as shown in Table 1 and explained as follows.

Step 1: the default downloaded file from the ECCAD website has daily emissions arranged by time in consecutive order. That is why the first step is to extract a single-day data emission by using the command "ncks" while creating an identifying date file for the next steps. For example, if the desired date is 2019, August 1st[st], and the user downloaded daily emissions for the entire year, the statement must be as follows: ncks -O -d time,181 CAMS_OCEAN_FILE_2019.nc August01.nc

Step 2: is to delete the attribute "time" from the created single day using the command "ncwa." This action is crucial because the SMOKE model requires a gridded emission file as an input without "time" attribute or variable

Step 3: is to apply the command "ncks" to transform the file generated in the previous step into a Classic NetCDF file, which is also a required input for SMOKE

Step 4: is to invert the latitude information, starting from 89.95° N and finishing at −89.95° S. This step is also crucial because its omission generates wrong results in the SMOKE output files, showing the opposite hemisphere emissions (see details in Pino-Cortés et al. 2022).

Steps 5 and 6: create the units and name for attribute "lat" (latitude), respectively, using the command "ncatted." Steps 7 and 8: generate a similar modification of the attribute "lon" (longitude).

After step 8, the processed file has the input formats required by SMOKE except the grid resolution. All commands for steps 1–8 are from the NetCDF Command Operator (NCO) software. Otherwise, as mentioned before, the CAMS-GLOB-OCE dataset has cells with 0.5° × 1.0°, and SMOKE only reads gridded input files with 0.1° × 0.1°, which is why a regridding modification step is required. We used the Climate Data Operators (CDO) software (Schulzweida 2020) for the regridding step. For this step (step 9), a file with the resolution and formats required by SMOKE is needed. The file ¨File_Gridd_Origin¨ (see supplementary material) was generated by processing the GFASv1.3 database following the procedures in Pino-Cortés et al. (2022).

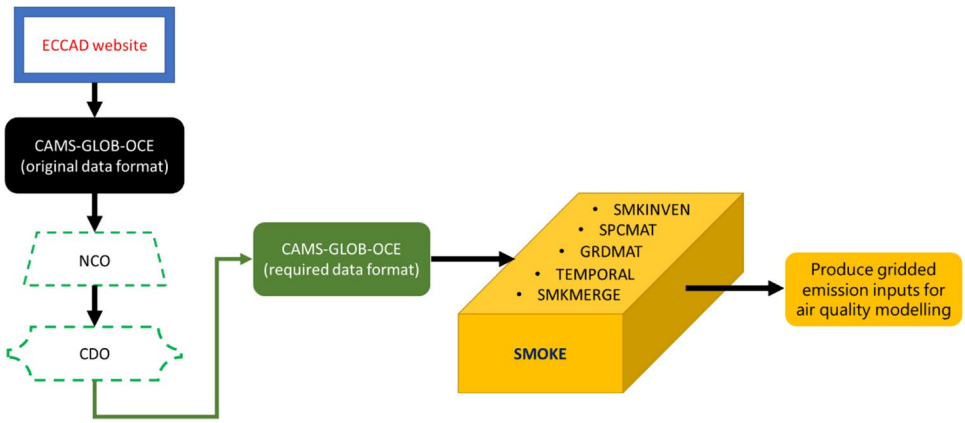

Fig. 1 Procedure scheme using CAMS-GLOB-OCE dataset to obtain emission data readable in SMOKE for air quality modeling

Table 1 Main steps for processing the CAMS-GLOB-OCE dataset to input into SMOKE

Step	Command	Example
1	ncks	ncks -O -d time,"Number related to the day of analysis" CAMS_file File_out
2	ncwa	ncwa -O -a time File_out File_out
3	ncks	ncks -O -3 File_out File_out
4	ncpdq	ncpdq -O -h -a -lat File_out File_out
5	ncatted	ncatted -O -a units,lat,c,c,'degrees_north' File_out File_out
6	ncatted	ncatted -O -a long_name,lat,c,c,'latitude' File_out File_out
7	ncatted	ncatted -O -a units,lon,c,c,'degrees_east' File_out File_out
8	ncatted	ncatted -O -a long_name,lon,c,c,'longitude' File_out File_out
9	remapbil	cdo remapbil, File_Gridd_Origin File_out File_for_SMOKE_Bilinear.nc

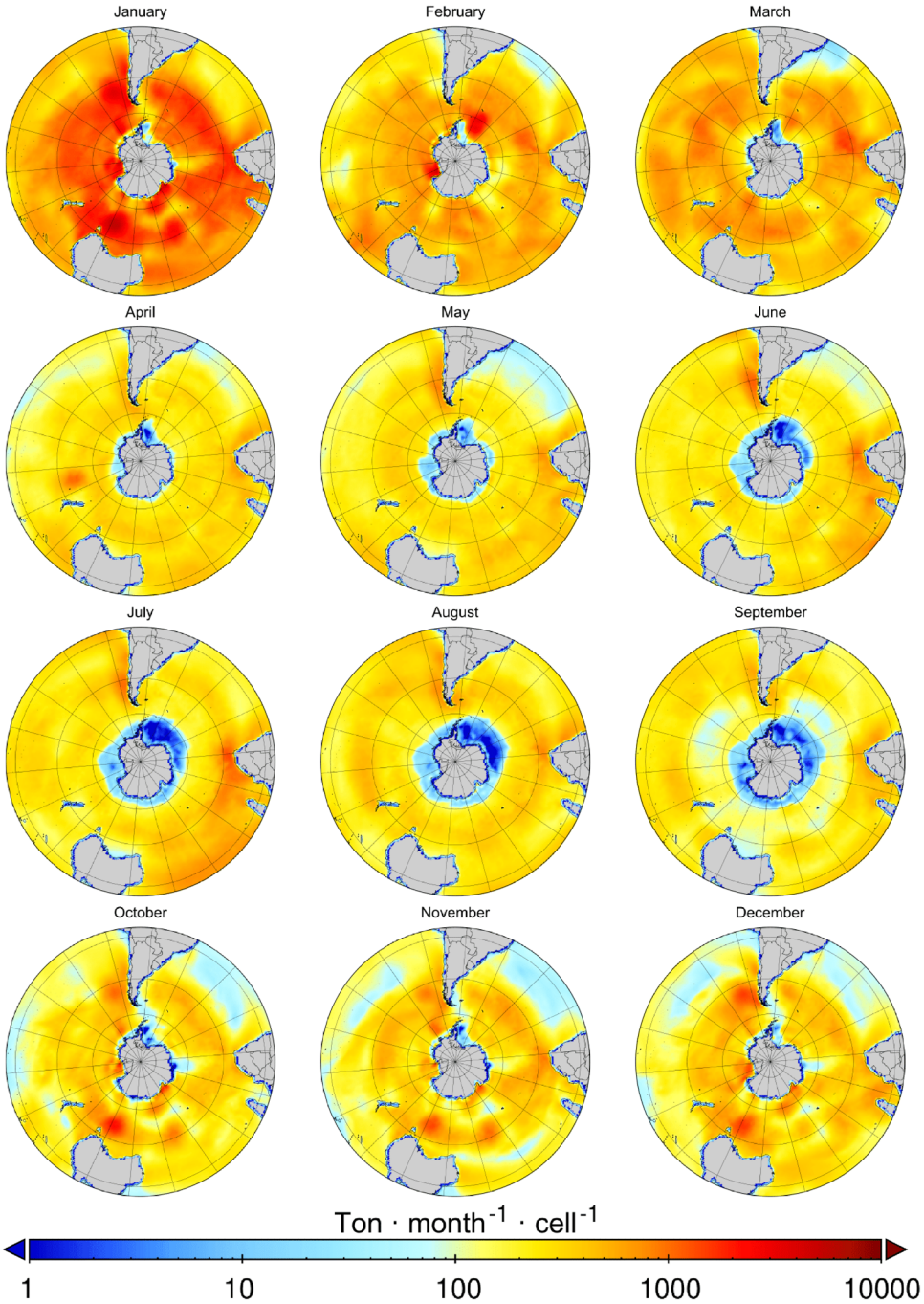

Fig. 2 Monthly DMS emissions for 2019

In this study, we applied a bilinear interpolation during step 9 to look for a smoother transition from the coarse grid to the finer grid, taking a value from a weighted average of the four surrounding points in the coarser grid. This type of regridding is suitable for highly spatially correlated variables at all time-scales, like temperature (NCAR 2014). We assume this property for the marine emissions in the CAMS-GLOB-OCE dataset due to their close correlation with temperature and wind speed (see details in Nightingale et al. 2000; Lana et al. 2011; Ziska et al. 2013; National Oceanographic Data Center 2017; Granier et al. 2019).

Case study: including Southern Hemisphere halocarbons and DMS emissions

The southern hemisphere was studied to identify marine emissions of halocarbons and DMS. The analysis domain was created in Weather Research and Forecasting (WRF) model (Skamarock et al. 2019) with 180 cells per side and 108 km as the horizontal resolution. An hourly run was simulated in WRF and the output file was processed using Meteorology - Chemistry Interface Processor (MCIP), which reduced the domain to 177

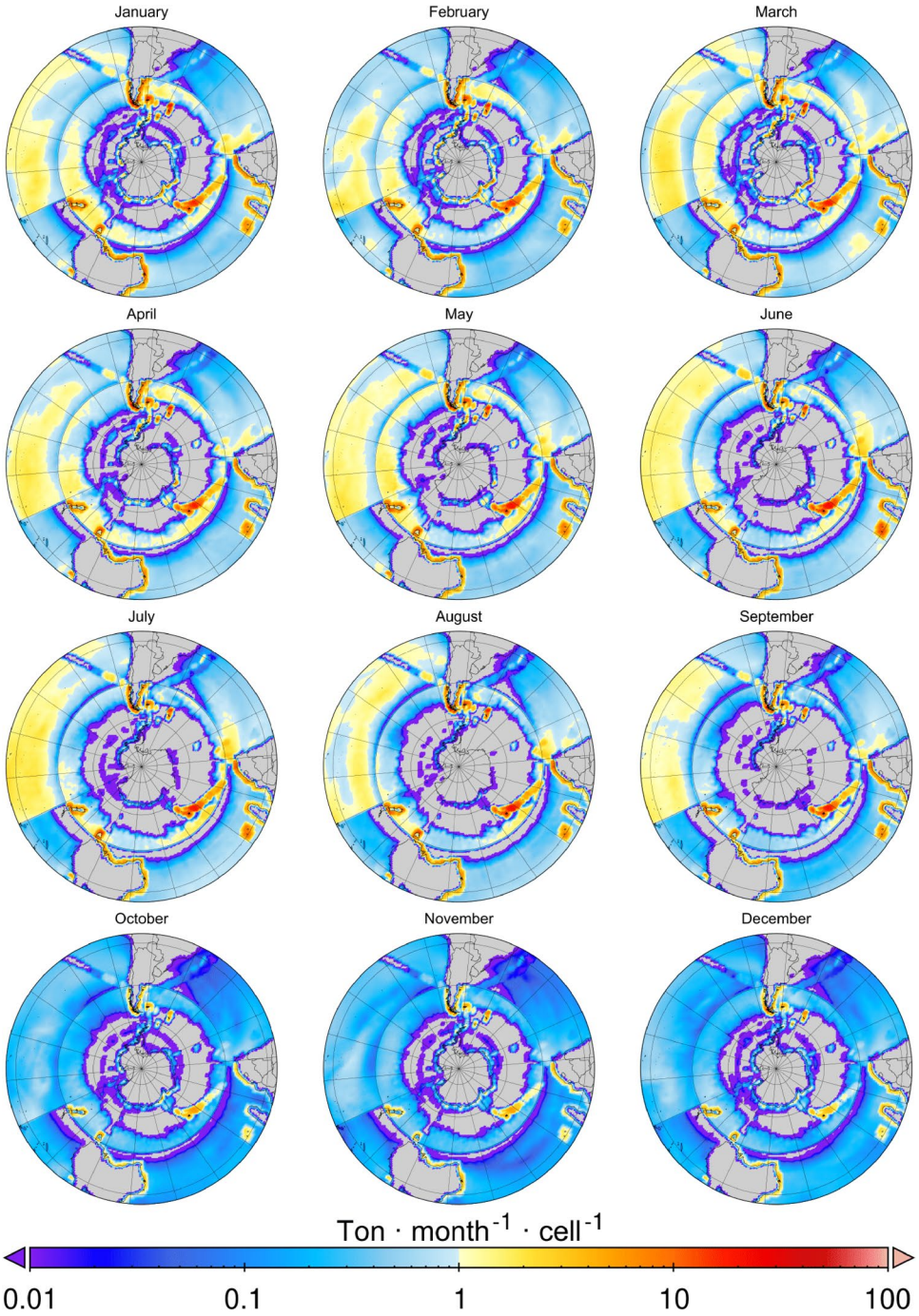

Fig. 3 Monthly $CHBr_3$ emissions for 2019

cells per side but kept the original resolution. The output files from MCIP were METCRO2D, METBDY, GRIDCRO2D, and GRIDDESC, containing the geolocation information required by SMOKE to define the spatial distribution of the emissions. Then, the daily files of CAMS-GLOB-OCE were processed following the methodology above and then simulated in SMOKE as an area source (Pino-Cortés 2021; Pino-Cortés et al. 2022) by using five modules of this model. The data import was realized with SMKINVEN. The module SPCMAT distinguishes the pollutants between compounds inside the particulate matter and gaseous phase. The spatial distribution and hourly profile of the emissions are then processed in GRDMAT and TEMPORAL modules. All the files generated in those modules are then merged using SMKMERGE, which produces a final emission inventory file readable by air quality models.

In this study, we analyzed the year 2019, but the methodology is suitable to any given time period. The CAMS-GLOB-OCE dataset has the same file format for any given year. The users need to download the specific year of analysis and apply the same commands shown in Table 1.

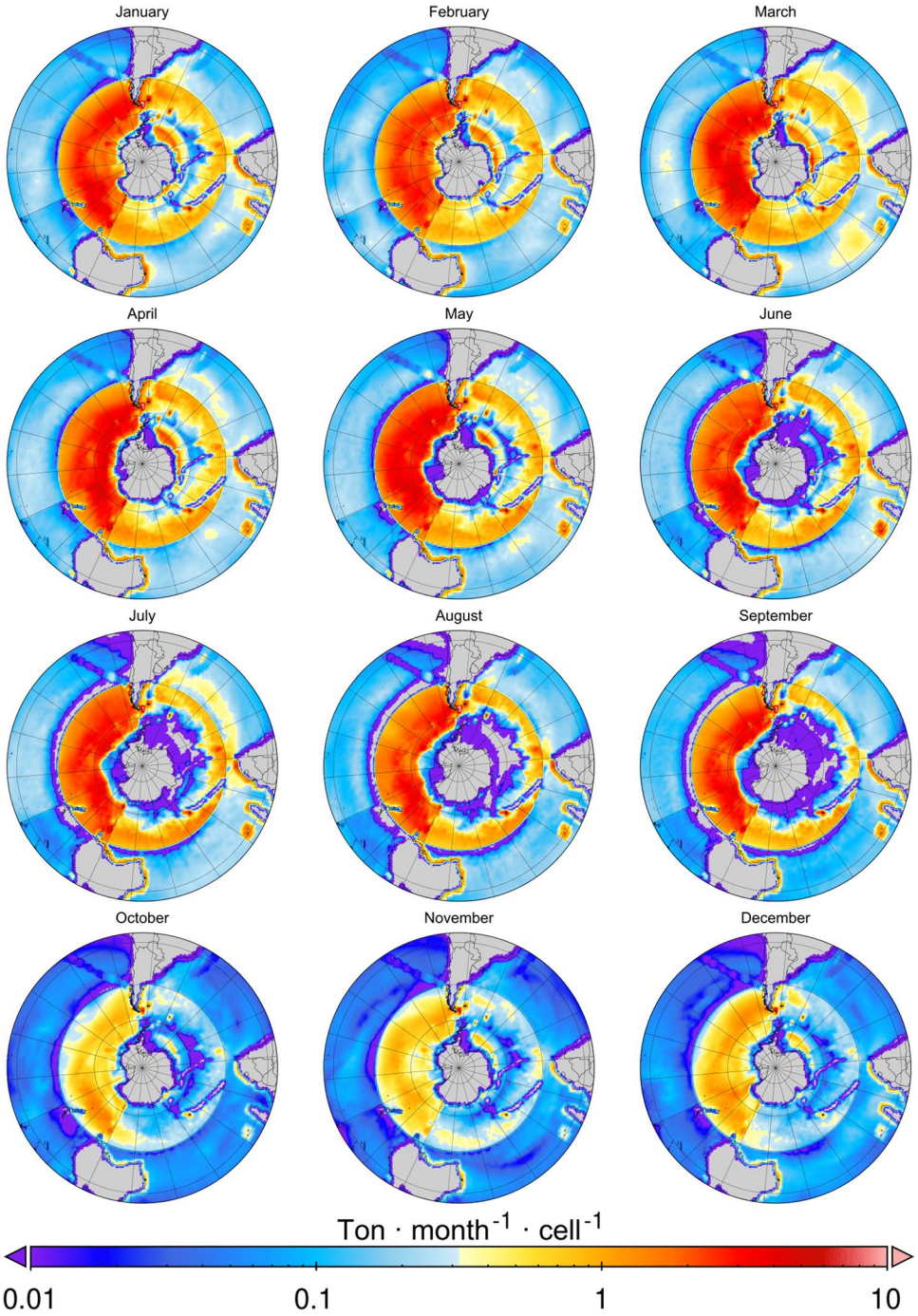

Fig. 4 Monthly CH_2Br_2 emissions for 2019

Results and discussion

The daily files generated in SMOKE were pieced together by months after application of the methodology proposed in this study. It is remarkable to distinguish that every daily file obtained has 24 hourly emissions data, expressed in mol/s. Then, the arranged emissions of DMS, $CHBr_3$, CH_2Br_2, and CH_3I were summed up obtaining the specific monthly emissions for each compound.

Figure 2 shows monthly DMS emission maps for 2019 processed in SMOKE. The highest records occurred during austral summer (January), when there is a peak in phytoplankton productivity as days grow longer, temperatures rise and sea ice retreat towards Antarctica (see Fig. S1). The highest DMS emissions' records of up to (~5000 ton·month^{-1}·cell^{-1}) were detected in Southern Ocean waters south off Australia, in mid-summer, with a clearly defined peak during January (Webb et al. 2019; Bock et al. 2021). Comparable high emissions between 1000 and 2000 ton cell^{-1} per month were predicted in the southeast Pacific Ocean (close to Bellingshausen Sea) and in Cooperation Sea,

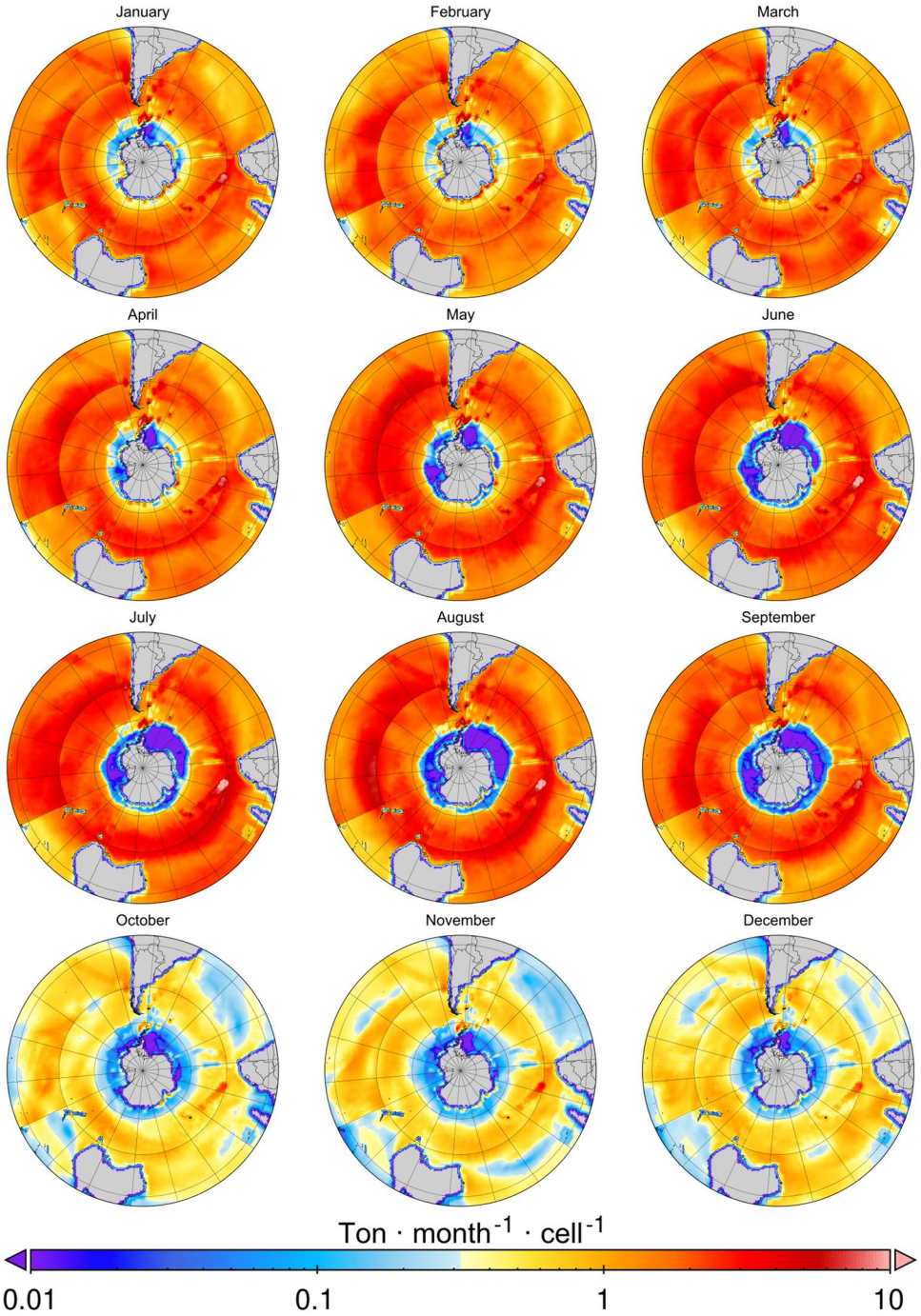

Fig. 5 Monthly CH_3I emissions for 2019

Weddell Sea, and Ross Sea, close to Antarctica. At the latter two locations, the highest emissions peak also continued during February, in agreement with the slightly delayed and longer growing season of phytoplankton in those regions due to the presence of polynyi (von Berg et al. 2020). Meanwhile, the monthly lowest emissions are related to the zone of analysis. Reduced solar radiation and colder temperatures promote reduced DMS emissions in the Southern Ocean during the late fall, coinciding with the maximum sea ice extent in September. There is a first decay during summer following the peak in production in spring-early summer, and then just a decay that maps well to the extent of sea ice. The case of the South Atlantic Ocean off Brazil showed higher emissions of DMS during January and from July to September.

The monthly emissions of halocarbons in 2019 are shown in Figs. 3, 4, and 5. In general, the monthly emissions of $CHBr_3$ showed low variation from January to September in all open waters. However, during the period between October and December, the emissions diminished in this ocean compared to other months. Analyzing the data by zones, the

highest values were observed during June and July in the open Pacific Ocean. Meanwhile, the lowest monthly records were in December in this region, when a large area emitted less than 10 tons/month per grid cell. Otherwise, high emissions were observed near the coastal zones in high latitudes and the circumpolar region. The highest emissions of this halocarbon are mainly related to macro-algae and anthropogenic activities (Boudjellaba et al. 2016; Jia et al. 2019). Meanwhile, lowest emissions are observed in open waters. Special attention should be given to the lower emissions shown in zones of the Atlantic Ocean compared to the Pacific and Indian Oceans. Otherwise, zero emissions were located in the Southern Ocean most of the year. It could be related to non-measured data of the primary input to the CAMS-GLOB-OCE dataset.

Emissions for CH_2Br_2 showed higher levels within the limits of the Southern Ocean during all year of 2019, compared to other regions. This agrees with the results reported by Ziska et al. (2013). The area with the highest emissions (~10 tons per month per cell) is located between the Southern Pacific Ocean and Western Antarctica. Meanwhile, the lower records were located in Eastern Antarctica (minimum during August–September) and in the coast of South America. The emissions of CH_2Br_2 decreased between October and December, showing a similar pattern to the emissions of $CHBr_3$. The ratio $CHBr_3/CH_2BR_2$ is in order with that reported by Ordóñez et al. (2012).

The seasonal pattern for CH_3I is similar to the records obtained for $CHBr_3$. It is remarkable to distinguish that the emissions of the iodine species also depend on biological and anthropogenic activities (Tegtmeier et al. 2013). In the Southern Ocean, the lowest monthly emissions were in September, similar to the records registered for DMS in the same area and applying showing its indirect relation with sea ice extent.

Conclusions

This study presents a methodology to transform the emission files from the CAMS-GLOB-OCE dataset into the input format required by SMOKE. The preprocessing stage required eight steps with NCO commands when the attribute "time" was deleted, the classic NetCDF format was added, the order of the latitude coordinates was inverted, and the names and units of the attributes "longitude" and "latitude" were modified, respectively. Finally, one step of bilinear interpolation with the CDO command was applied to generate an interpolated emissions inventory with the required grid size (0.1° × 0.1°). This methodology was used for the year 2019, but it is suitable for any given time period.

The emission files were then processed in SMOKE covering a Southern Hemisphere domain. The emission files obtained from SMOKE showed the same profile as the climatology data used to create the CAMS-GLOB-OCE dataset. We suggest that future studies in photochemical air quality modeling with CMAQ would benefit by applying the proposed methodology to evaluate and analyze, with more accurate information, the dispersion and chemistry of marine species emissions.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/s11869-022-01301-0.

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Data Availability All data generated or analyzed during this study are included in this published article and its supplementary information files.

Code availability The SMOKE codes can be downloaded at www.cmascenter.org. Maps used in the spatial plots were created using Panoply and it is available at www.giss.nasa.gov/tools/panoply.

Declarations

Ethics approval Not applicable

Consent to participate Not applicable

Consent for publication Not applicable

Competing interests The authors declare no competing interests.

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