CASCADE - The Circum-Arctic Sediment CArbon DatabasE

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Abstract

Biogeochemical cycling in the ~~extensive shelf seas and in the interior basins of the~~ semi-enclosed Arctic Ocean ~~are~~ is strongly influenced by land-ocean transport of carbon and other elements, and is ~~. The Arctic carbon cycle system is also inherently connected with the climate, and thus~~ vulnerable to environmental and climate changes. Sediments of the Arctic Ocean are important ~~an active and integral~~ part ~~in~~ of ~~Arctic~~ biogeochemical cycling in the Arctic, and provide the opportunity to study present and historical input and fate of organic matter (e.g., through permafrost thawing).

Comprehensive sedimentary records are required to ~~Comprehensive sedimentary records are required To~~ to compare differences between the Arctic regions and to study Arctic biogeochemical budgets~~, comprehensive sedimentary records are required~~. To this end, the Circum-Arctic Sediment CArbon DatabasE (CASCADE) was established to curate data primarily on concentrations of organic carbon (OC) and OC isotopes ($\delta^{13}C$, $\Delta^{14}C$), yet also on total N (TN) as well as of terrigenous biomarkers and other sediment geochemical and physical properties. This new database builds on ~~drawn both from~~ the published literature and ~~from~~ earlier unpublished records through an extensive international community collaboration.

This paper describes the establishment, structure and current status of CASCADE. The~~is~~ first public version includes OC concentrations in surface sediments at 4244 oceanographic stations including 2317 with TN concentrations, 1555 with $\delta^{13}C$-OC values, 268 with $\Delta^{14}C$-OC values and 653 records with quantified terrigenous biomarkers (high molecular weight *n*-alkanes, *n*-alkanoic acids and lignin phenols). ~~distributed over the shelves and the central basins of the Arctic Ocean.~~ CASCADE also includes data from 326 sediment cores, retrieved by shallow box- or multi-coring, ~~and~~ deep gravity/piston coring, ~~as well as~~or sea-bottom drilling. The comprehensive dataset reveals ~~several~~ large-scale features of ~~, including clear differences in~~ both OC content and ~~isotope-based diagnostics of~~ OC sources between the shelf sea recipients. This ~~indicates, for instance, the~~offers insight to release of ~~strongly~~ pre-aged terrigenous OC to the East Siberian Arctic shelf and ~~and~~ ~~and~~ younger terrigenous OC to the Kara Sea. Circum-Arctic sediments thereby reveal patterns of terrestrial OC remobilization and ~~and thus~~ provide~~s~~ clues about e.g. ~~land-ocean transport of material released by~~ thawing of permafrost.

CASCADE enables synoptic analysis of OC in Arctic Ocean sediments and facilitates a wide array of future empirical and modelling studies of the Arctic carbon cycle. ~~CASCADE~~ The database is openly and freely available online (https://doi.org/10.17043/cascade; Martens et al., 2020b), is provided in various machine-readable data formats (data tables, GIS shapefile, GIS raster), and also provides ways for contributing data for future CASCADE versions. We ~~CASCADE~~ will ~~be~~ continuously update~~d~~ CASCADE with newly published and contributed data over

the foreseeable future as part of the database management of the Bolin Centre for Climate Research at Stockholm University.

1 Introduction

The Arctic Ocean receives large input of terrestrial organic matter from ~~its large~~ rivers and ~~from~~ coastal erosion, making it ~~both~~ a valuable receptor system for studying both large-scale terrestrial carbon remobilization and marine biogeochemistry. Rising temperatures ~~are~~ cause~~ing~~ multiple changes to the Arctic, including reduced sea-ice cover, accelerated erosion of ice-rich permafrost shorelines and enhanced river runoff, which ~~. These changes~~changes ~~affect~~ the input of terrestrial organic matter to the Arctic Ocean ~~,~~(AMAP, 2017). This affects nutrients and the detrital load, ~~which in turn affects~~ the ocean optical field, marine primary productivity, ocean acidification and many other aspects of biogeochemical cycling ~~in the Arctic Ocean~~ (Stein and Macdonald, 2004; Vonk and Gustafsson, 2013). On land, climate change causes warming and thaw of terrestrial permafrost (Biskaborn et al., 2019), potentially remobilizing parts of its large dormant pool of OC (1300 Pg; Hugelius et al., 2014) into active carbon cycling.~~. By transformation and translocation of previously frozen organic matter,~~ ~~r~~Rising temperatures may thus shift balances in the Arctic carbon cycle by transformation and translocation of previously frozen organic matter, which ~~leading~~ leads to system hysteresis effects and translocated carbon-climate feedback (e.g., Vonk and Gustafsson, 2013). Couplings between the large permafrost-carbon pools and amplified climate warming in the Arctic represent a potential "tipping point" in the climate system (Lenton, 2012). These perturbations may affect both OC sequestration in the biosphere and release of climate-forcing greenhouse gases (e.g., AMAP, 2017; IPCC, 2019) as well as ~~other major effects such as~~ the coupling between permafrost carbon remobilization and ocean acidification across the extensive shelf seas (Semiletov et al., 2016).

Continental shelves cover less than 10% of the global ocean area but account for the largest part of OC accumulation in marine sediments and thereby provide an excellent archive for both terrestrial carbon input and marine productivity (Hedges et al., 1997). ~~The semi-enclosed structure of t~~The Arctic Ocean is semi-enclosed ~~with its~~and dominated[BW1] by its extensive shelves, including the World's largest continental shelf system, the East Siberian Arctic Shelf (ESAS; the Laptev, East Siberian and Russian part of the Chukchi Sea). This~~,~~ further accentuates the particular importance of shelf sediments for ~~the~~ carbon cycling in the Arctic (Stein et al., 2004; Vetrov and Romankevich, 2004). Earlier landmark contributions have provided comprehensive observational perspectives on the distribution of organic matter in marine sediments at the global scale (e.g., Berner, 1982; Romankevich, 1984; Hedges and Keil, 1995). Focusing in greater detail on carbon in the Arctic, the book by Vetrov and Romankevich (2004) "*Carbon Cycle in the Russian Arctic Seas*" and the book edited by Stein and Macdonald (2004) "*The Organic Carbon Cycle in the Arctic Ocean*" provided the first more comprehensive perspectives on the Arctic land-ocean carbon couplings across various regions. Therein, the authors~~ and ~~ synthesized the collected knowledge of carbon sources, transformations and burial in Arctic marginal seas and the central Arctic Ocean. These compilations demonstrated substantial regional variations in carbon cycling between different Arctic shelf seas, while also acknowledging the near lack of observational data for key parameters and regions. S~~ince then, s~~ubstantial progress ~~has been reported in~~was made by individual and region-specific studies since then; with~~. Key progress includes~~ key advances in isotope and organic geochemistry that~~,~~ expand~~ing~~ the variety of biogeochemical proxies to trace both sources and organic matter degradation. S~~S~~table carbon isotopes (δ^{13}C-OC) ~~—~~have been ~~have been~~widely used to distinguish between marine and terrigenous sources in Arctic Ocean sediments (e.g., Naidu et al., 1993; Mueller-Lupp et al., 2000; Semiletov et al., 2005) ~~—~~and have since then been greatly supplemented by an expanded use of natural abundance radiocarbon (Δ^{14}C-OC). This has ~~not only ~~improved source apportionment of OC in bulk sediments across Arctic regions and time scales (e.g., Vonk et al., 2012; Goñi et al., 2013; Martens et al., 2020)~~,~~ and~~ but also~~ in sediment density fractions (Tesi et al., 2016b), suspended particulate organic matter (e.g., Vonk et al., 2010, 2014; Karlsson et al., 2016), and at the molecular level (e.g., Drenzek et al., 2007; Gustafsson et al., 2011; Feng et al., 2013). Extensive studies of a wide set of molecular biomarkers (e.g., Fahl and Stein, 1997; Goñi et al., 2000; Belicka et al., 2004; Yunker et al., 2005; van Dongen et al., 2008; Tesi et al., 2014; Sparkes et al., 2015; Bröder et al., 2016) have provided growing insights in OC distribution and fate, particularly for terrigenous organic matter. ~~In order t~~A~~o effectively a~~ccess to ~~and interpret ~~the~~is~~ ~~rapidly ~~growing number of observational data in a readily-accessible interactive format would be greatly beneficial ~~on organic matter in the Arctic Ocean, it would be greatly beneficial to have all these data organized in a readily-accessible interactive format ~~to ~~facilitate a broad array of ~~wider system assessments and ~~comparisons~~interpretations of organic matter in the Arctic Ocean.

The overarching objective of this effort is to curate and harmonize all available data on OC in Arctic Ocean sediments in an open and freely available database. The Circum-Arctic Sediment CArbon DatabasE (CASCADE) builds on ~~both ~~previously-published and unpublished collections holding information on OC and total N (TN) concentrations, as well as OC isotopes (δ^{13}C-OC, Δ^{14}C-OC) ~~and molecular biomarkers with an initial focus on terrigenous organic matter (i.e., high molecular weight – HMW *n*-alkanes, *n*-alkanoic acids, lignin phenols) ~~in sediments of all continental shelves and the deep central basins of the Arctic Ocean. Furthermore, CASCADE contains molecular data with an initial focus on terrestrial biomarkers (i.e., high molecular weight - HMW *n*-alkanes, *n*-alkanoic acids, lignin phenols) to facilitate studies of terrestrial OC remobilization. The backbone of CASCADE are large data collections, including i) OC concentrations, δ^{13}C/Δ^{14}C-isotope data and biomarkers from the informal two-decades long Swedish-Russian collaboration network the International Siberian Shelf Study (ISSS; Semiletov and Gustafsson, 2009) (e.g., Guo et al., 2004; Semiletov et al., 2005; van Dongen et al., 2008; Vonk et al., 2012; Tesi et al., 2016a; Bröder et al., 2018; Martens et al., 2019, 2020; Muschitiello et al., 2020); ii) OC concentrations from the Arctic portion of the "Carbon Database" of the Shirshov Institute of Oceanology, Russian Academy of Sciences (Romankevich, 1984; Vetrov and Romankevich, 2004); iii) previously-published databases and online collections (e.g., Pangaea.de) with many contributions from German-Russian partnerships and cruises involving the Alfred-Wegener-Institute, Germany (e.g., Stein et al., 1994; Mueller-Lupp et al., 2000; Stein and Macdonald, 2004; Xiao et al., 2015); iv) US and Canadian based research (e.g., Naidu et al., 1993, 2000; Goñi et al., 2000, 2013; Grebmeier et al., 2006); and v) data from various other contributors that are acknowledged in the database. ~~Furthermore, CASCADE~~The initial version also includes previously unpublished data, with some ~~also~~ generated here in the upstart of CASCADE~~CASCADE effort~~, to fill gaps for particularly data-lean regions such as the Barents and Kara Seas, the Canadian Arctic Archipelago, and the Chukchi Sea.

The aim of the CASCADE effort is to provide a foundation for future studies. These may~~,~~ include~~ing~~ large-scale assessments of the carbon cycle, such as characteristics of OC input, and its distribution and fate in the Arctic Ocean. This paper describes the creation and the structure of CASCADE, including a discussion of data availability and quality.

2 Data collection and methods

2.1 The physical compartments: Arctic shelf seas and interior Arctic Ocean basins

The CASCADE includes OC data from the entire Arctic Ocean with special focus on the seven Arctic continental shelf seas (Fig. 1; Table 1). Accordingly, a distinction is made among the c~~C~~entral Arctic Ocean and the following marginal seas: Beaufort Sea, Chukchi Sea, East Siberian Sea, Laptev Sea, Kara Sea, Barents Sea (incl. White Sea), and the Canadian Arctic Archipelago (we exclude data from Baffin Bay, Foxe Basin and Hudson Bay, as they are outside the Circum-Arctic scope of the database). For defining the limits of these Arctic shelf seas, Jakobsson (2002) is followed, which distinguishes the Arctic Ocean constituent seas using hypsometric criteria. Therein, ~~,~~ ~~defining~~ *shelf* is defined as the seaward extension of the continental margin until the increase in steepness at the shelf break (Jakobsson, 2002). ~~CASCADE d~~Data for the central Arctic Ocean~~, which~~ was treated as one individual unit that~~,~~ covers all area beyond the shelf break and includes the continental slope, rise, deep basins and mid-ocean ridges.

2.2 Georeferencing and sampling

The coordinate system used for CASCADE is WGS1984 and coordinates are kept in machine-readable decimal degrees (Latitude in °N, Longitudes in the -180° to 180° format) to harmonize the data across all GIS applications. ~~The spatial references also include information about the sediment depth interval that the reported data represent (Table 1). In addition to the geographical coordinates, CASCADE lists the bathymetric water depth of the sampling point as reported in the primary literature.~~ The collection of data from oceanographic stations is the main part of CASCADE and is organized ~~The core part of CASCADE is~~ in a table format that contains columns for the station number (‘STATION’) and~~,~~ geographical coordinates (‘LAT’; ‘LON’). The spatial references also include~~,~~ information about the sediment depth interval that reported data represent ~~the name of the expedition and/or ship (‘EXPEDITION’), the year when the sample was taken (‘YEAR’) and the sediment depth interval~~ (‘UPPERDEPTH’; ‘LOWERDEPTH’), where the upper depth is equal to 0 cm in the case of surface sediments. In addition, the table contains a column for water depth (‘WATERDEPTH’)~~, all~~ as reported by the data source. ~~For samples where the sampling year was unknown, the year of the earliest published record was used instead.~~ In cases where the water depth was not reported, the water depth was estimated using the latest version (v4) of the bathymetric map of IBCAO (Jakobsson et al., 2020) corresponding to the position of the oceanographic station and reported in a separate column (‘IBCAODEPTH’). Furthermore, the name of the expedition and/or ship (‘EXPEDITION’) and the year when the sample was taken (‘YEAR’) are reported. For samples where the sampling year was unknown, users may use the year of publication instead.

2.3 Surface sediments and sediment cores

The first stage of the CASCADE development focused on maximizing spatial coverage for surface sediments of the seven Circum-Arctic shelf sea systems and the central Arctic Ocean. Here, ~~S~~surface sediments are ~~here~~ defined as those collected from the water-sediment interface to a depth of maximum 5 cm. Data for surface sediments are provided in a table (‘CASCADEsurfsed~~_v1.0~~’) as .txt and .xlsx files~~, as~~ and ~~well~~ ~~as~~ in a ready-to-use GIS shapefile format. This database also includes deeper sediments from sediment cores, which represent longer time-scales and add a third dimension to the geographical referencing. ~~In CASCADE~~Types of sediment cores are distinguished in CASCADE such that different biogeochemical processes, acting on~~by~~ three depositional time scales, may be addressed. The three time scales are~~ using the following criteria~~:

1. Centennial scale cores (core scale 1) in upper sediments of the Arctic Ocean, e.g., multi corer, Gemini corer, box corer, van Veen grab sampler, other short gravity corers up to 1 m length;
2. Millennial scale cores (core scale 2) of shelf sediments roughly covering the depositional time frame from the late Holocene to the last glacial/interglacial transition, by e.g., piston corer, long gravity corer, kasten corer;
3. Glacial cycles scale cores (core scale 3) from the continental slopes or the deeper Arctic Ocean basins covering periods from earlier than the Last Glacial Maximum, including e.g. drill coring on the Circum-Arctic shelves or deep-sea piston cores.

Downcore data are stored in three separate data tables ('CASCADEcorescale1~~_v1.0~~'; 'CASCADEcorescale2~~_v1.0~~'; 'CASCADEcorescale3~~_v1.0~~') in addition to the surface sediment files, including a column for the sampling depth of core subsamples in cm below the sediment surface ('COREDEPTH').

2.4 Database parameters

CASCADE contains information~~, where available, ~~about the concentration,~~ as well as~~ isotopic and molecular composition of OC in marine Arctic sediments. In addition to i) OC concentrations (column 'OC'), the database includes ii) concentrations of TN ('TN') and iii) the gravimetric ratio of OC/TN ('OC/TN'), which may provide additional information about the organic matter source (e.g., Goñi et al., 2005; van Dongen et al., 2008). Furthermore, CASCADE contains data of iv) $\delta^{13}C$-OC ('d13C') as a parameter to distinguish between marine and terrestrial sources (e.g., Fry and Sherr, 1989), and v) $\Delta^{14}C$-OC ('D14C') to assess the presence of aged organic matter released from e.g., permafrost deposits (e.g., Gustafsson et al., 2011; Vonk et al., 2012) or from petrogenic sources such as sedimentary rocks (e.g., Yunker et al., 2005; Goñi et al., 2013) in marine sediments. More details about the CASCADE parameters and their units are provided in Table 2.

Data of terrigenous biomarkers ~~To~~ may facilitate further investigations of terrigenous OC input~~, CASCADE also includes data of terrigenous biomarkers~~ (Table 2). The~~is~~ first version of CASCADE compiles total concentrations of *n*-alkanes with high molecular weight (HMW) and C_{21}-C_{31} carbon atoms ($\sum C_{21}$-C_{31}; column 'HMWALK'), as well as the often separately-reported more specific *n*-alkanes $\sum C_{27}+C_{29}+C_{31}$ ('HMWALK_SPEC'). CASCADE also contains the sum of the HMW *n*-alkanoic acids $\sum C_{20}$-C_{30} ('HMWACID'). Both compound classes stem mostly from terrigenous compartments as they derive from epicuticular leaf waxes of land plants with a typical pattern of dominating odd-numbered homologues for HMW *n*-alkanes and even-numbered homologues for HMW *n*-alkanoic acids (Eglinton and Hamilton, 1967). Furthermore, ~~CASCADE~~ the database holds concentrations of lignin phenols (∑syringyl, vanillyl, cinnamyl; 'LIGNIN'), which are products from the break-up of the lignin biopolymer, a compound only produced by vascular plants (Hedges and Mann, 1979). These three compound classes are frequently used as tracers of the sources and fate of terrestrial organic matter sequestered in Arctic Ocean sediments (Fahl and Stein, 1997; Goñi et al., 2000; Tesi et al., 2014; Bröder et al., 2016). It is recognized that there are more parameters that could be included and CASCADE can add further extensions in future versions.

2.5 Reference to the original publication

~~To maintain a high level of transparency, e~~Each data source added to CASCADE is fully cited (in the formatting style of Earth Systems Science Data; ESSD) to maintain a high level of transparency. When applicable, citations also ~~including~~ include a digital object identifier (doi) that is linked to ~~its~~ the reference in the primary literature next to each parameter column. Accordingly, the CASCADE data sheet distinguishes between a common reference for OC, TN and OC/TN data ('CN_CITATION') as ~~it is~~they are ~~they are~~ often combined in one measurement, and separate references for OC isotopes ('d13C_CITATION'; 'D14C_CITATION') and concentrations of biomarkers ('BM_CITATION'). This facilitates to register multiple measurements based on the same or split sediment sample material for individual oceanographic stations. A full list of references is separately provided on the CASCADE website and in the Supplementary Information of this paper.

2.6 Data source and quality

A part of CASCADE builds on previous separate and partly inaccessible databases of OC parameters that key partners of the CASCADE consortium and others have collected over the years. This includes data from the informal Swedish-Russian led collaboration network called the International Siberian Shelf Study (ISSS; Semiletov and Gustafsson, 2009) and the "Carbon" database of the Shirshov Institute of Oceanology. This basis for CASCADE was strengthened by an extensive survey of the peer-reviewed literature and data mining in the grey literature of scientific cruise reports. ~~All data are fully cited in a separate column (Table 2). We applied a number~~To facilitate ~~of~~ quality assurance criteria ~~and~~ by the end users the database also ~~also~~ records metadata (e.g., sampling technique in the field, sample storage) and quality data when available. The quality assurance ~~criteria~~[BW2] information for data ~~to be included~~ in CASCADE are:

- Data need to be (geo-)referenceable and located in the target region (i.e. the Arctic Ocean).
- Information about the analysis method is provided by the data source.
- For OC concentrations, values were generated by elemental analyzer (EA) or Rock Eval pyrolysis and reported as weight-% OC. Total N concentrations and OC/TN ratios are based on EA only.
- ~~All~~ For δ^{13}C-OC data stored in CASCADE are based on isotope ratio mass spectrometry (IRMS), often coupled to an EA and calibrated against the PDB/V-PDB analytical standards.
- For Δ^{14}C-OC the measurements of ^{14}C data are based on ~~accelerator~~ mass spectrometry ~~(AMS)~~ with ^{14}C data reported as Δ^{14}C, fraction modern (F_m) or conventional ^{14}C age in the original publication. We also kept records of the ^{14}C/AMS lab code of the sample if given.
- Terrigenous biomarker analysis was carried out by solvent extraction (for HMW *n*-alkanes and *n*-alkanoic acids) or by alkaline CuO oxidation of the lignin biopolymer (for lignin phenols) of the sediments, followed by wet chemistry purification and quantification using gas chromatography analysis with either flame ionization or mass spectrometry detection.

In addition to the above-mentioned ~~criteria~~information, the aim was to also include information about carbonate removal by acid treatment prior to the measurement of OC, δ^{13}C-OC and Δ^{14}C-OC. However, details about applied procedures were missing in most cases and it is therefore assumed that the carbonate fraction was removed from total carbon prior to OC, δ^{13}C-OC and Δ^{14}C-OC measurements. All meta information (sampling, storage, analysis) to each CASCADE entry is included in a respective column in the data spreadsheet (Table 2).

2.7 New gap filling analyses

2.7.1 Bulk OC and carbon isotopes

Gap filling was performed in surface sediments of regions with particularly poor data density~~to complement data obtained from literature, cruise reports and in other ways described above, in regions of particularly poor data density~~. These efforts thus focused on areas north of western Siberia (Barents and Kara Sea region) and in the Canadian Arctic Archipelago, using archived sample material that was provided by CASCADE collaborators. For OC, TN and δ^{13}C-OC analysis, about 10 mg each of a total of 153 freeze-dried sediment samples were weighed in silver capsules and acidified drop-wise with 3 M HCl in order to remove carbonates. The measurement was carried out using a Carlo Erba NC2500 elemental analyzer coupled to an isotope-ratio mass spectrometer (Finnigan DeltaV Advantage) in the Department of Geological Sciences, Stockholm University, with ±3% precision for OC analysis and ±0.15‰ precision for δ^{13}C-OC isotopic measurements.

Furthermore, a subset of 95 samples was selected for gap-filling bulk-level Δ^{14}C-OC analysis at the Tandem Laboratory, Department of Physics, Uppsala University. A sample amount corresponding to 1 mg OC was weighed in tin capsules and acidified with 3 M HCl to remove carbonates. Samples with low OC concentrations (<0.5 %) were placed in small beakers and exposed to acid fumes in a desiccator for 24 h to remove carbonates and combusted to CO_2 in evacuated quartz tubes prior to graphitization at the ^{14}C/AMS laboratory. An additional set of 30 gap-filling samples was analyzed for Δ^{14}C at the ^{14}C ~~AMS~~ laboratory of ETH Zurich after acid fumigation. The measurements at Uppsala University had a precision of on average ±1.9% while the precision at ETH Zurich was on average ±1.1% (based on ^{14}C counting statistics).
In CASCADE, all new data points are labelled by citing the database (‘Martens et al., 2021. CASCADE - The Circum-Arctic Sediment CArbon DatabasE. Bolin Centre for Climate Research, Stockholm University, Sweden. doi:10.17043/cascade, 2021.’) in the respective reference columns.

2.7.2 Analysis of lignin phenols

Gap-filling analysis was also performed for lignin phenols as molecular biomarkers for terrestrial organic matter using a set of 64 samples from data-lean regions. To extract lignin phenols from marine sediments we applied an alkaline CuO oxidation protocol using a microwave-based method as originally presented by Goñi and

Montgomery (2000) and followed the same laboratory routine as described in greater detail elsewhere (Tesi et al., 2014; Martens et al., 2019).

2.8 Data conversion and harmonization

Recalculations of literature data (e.g., for unit conversions) were in some cases necessary to harmonize the data to the standard units as defined in Table 2.

- In CASCADE the concentration of OC is reported in percent (%) of the dry weight; values previously published as mg OC per g dry weight were divided by a factor of 10.
- CASCADE uses $\Delta^{14}C$ with age correction (equation 1) to report the activity of radiocarbon according to convention (Stuiver and Polach, 1977; Stenström et al., 2011). For radiocarbon values that were reported as conventional ^{14}C ages we used equation 2 to calculate the age-corrected $\Delta^{14}C$.

$$\Delta^{14}\mathrm{C} = (F_m \cdot e^{\lambda_c(1950-Y_C)} - 1) \cdot 1000‰ \qquad (1)$$

$$\Delta^{14}\mathrm{C} = (e^{-\lambda_L \cdot T_{14C-years}} \cdot e^{\lambda_C(1950-Y_C)} - 1) \cdot 1000‰ \qquad (2)$$

Where F_m is the fraction modern, λ_C the decay constant of the Cambridge half-life of ^{14}C ($T_{1/2-C}$ = 5730; λ_C = 1/8267), Y_C the year of sample collection, λ_L the decay constant of the Libby half-life of ^{14}C ($T_{1/2-L}$ = 5568; λ_C = 1/8033 and $T_{14C\text{-years}}$ the conventional ^{14}C age (Stuiver and Polach, 1977).

- All biomarker concentrations of HMW *n*-alkanes and *n*-alkanoic acids are reported as µg per g OC while lignin phenols are reported as mg per g OC. Biomarker concentrations that in the original publication were reported as normalized to dry sediment weight were for CASCADE normalized to the OC concentration of the sample.

2.9 Data interpolation

CASCADE provides interpolated ~~GIS raster~~ files (GEOtiff, ASCII; coordinate system WGS 1984 Arctic Polar Stereographic) for OC content, $\delta^{13}C$-OC and for $\Delta^{14}C$-OC in surface sediments across the Arctic Ocean. OC data was mapped in ArcGIS 10.6 and interpolated to a resolution of 5x5 km per grid cell using the Empirical Bayesian Kriging function (EBK; Gribov and Krivoruchko, 2020) in the commercially-available ArcGIS 10.8 software package (ESRI). Kriging builds on the assumption that two points located in proximity are more similar than two points further distant and creates a gridded surface of predicted values using an empirical semivariogram model.

As an advancement to Kriging, EBK repeatedly simulates semivariogram models in subsets of up to 200 data points and thus not only improves the prediction but also optimizes interpolation across areas with strongly varying data availability in the Arctic Ocean (e.g., shelf seas vs. central basins).

3 Results and Discussion

3.1 Data set inventory

~~For s~~Surface sediments show by far the largest data availability. ~~,~~The dataset of OC concentrations in CASCADE includes 4244 different locations across the Arctic Ocean (Fig. 2), ~~for which the OC concentration is known,~~ while the concentration of TN and ~~, including~~ the OC/TN ratio are ~~, is~~ known for 2317 locations (Table 1). For carbon isotopes, the number of individual δ^{13}C-OC values is 1555 and for Δ^{14}C-OC it is 268. CASCADE also holds concentrations of terrigenous biomarkers at 131-213 locations per compound group~~,~~. Most of the biomarker data is~~of which most are~~ for HMW *n*-alkanes, with either concentrations of HMW *n*-alkanes ($\sum C_{21}$-C_{31}; 213 stations) or ~~of *n*-alkane~~ chain lengths more specific for higher plants ($\sum C_{27}$, C_{29}, C_{31}; 164). Fewer data are available for concentrations of HMW *n*-alkanoic acids ($\sum C_{20}$-C_{30}; 131) and the concentrations of lignin phenols (145).

In addition to surface sediments, a total number of 326 sediment cores (79 centennial, 229 millennial, and 18 glacial cycle scale cores) ~~across the Arctic Ocean~~ is included in the~~is~~ first version of CASCADE. Combined, these hold another 1055~~3~~2 observations of OC concentrations, 4769 concentrations of TN and 2122 δ^{13}C-OC ratios in core samples from across the Arctic Ocean.

3.2 Spatial distribution of data

The data coverage for surface sediments is highly variable among the shelf seas, yet improved by the extensive gap-filling analysis (Table 1). The largest number of OC concentrations is in the Barents Sea (1092; Table 1). Despite the large total number of available Arctic sediment OC concentrations, there are only 236 samples analyzed for δ^{13}C-OC and 33 with Δ^{14}C-OC in the Barents Sea, and of these most are located in the Norwegian (western) sector of the Barents Sea. For the eastern Siberian Arctic and the North American sector of the Arctic Ocean, observations of OC concentrations are lower but the availability of δ^{13}C-OC data is higher (Table 1, Fig 2b, c). Accordingly, the Kara, Laptev, East Siberian and Chukchi Seas each support more than 200 δ^{13}C-OC observations.

The number of Δ^{14}C-OC observations is generally lower but reveals highest coverage in near-coastal areas, with 28 values in the Kara Sea, 42 values in the Laptev and 71 values in the East Siberian Sea. Data availability in the Chukchi Sea for Δ^{14}C-OC is lower (n=12), stressing the need for future analysis. The lowest availability of data is in the Canadian Arctic Archipelago. ~~where the g~~Gap-filling analysis of OC~~, as part of this study~~ here~~,~~ increased the number of OC concentrations from 21 to 54, with a similar ~~ly low~~ number ~~of~~ for carbon isotopes (51 of δ^{13}C-OC; 22 of Δ^{14}C-OC) distributed over its vast area of 1,171,000 km^2. The largest individual regime area is covered by the interior basins of the c~~C~~entral Arctic Ocean, which holds 529 observations of OC concentrations, 130 of δ^{13}C-OC and 27 of Δ^{14}C-OC values.

3.3 Assessment of data quality

Based on the quality assurance data available, ~~Most sources of data used to populate~~ CASCADE provide~~d~~s detailed information about the techniques involved in analyzing OC concentrations, isotopes and biomarkers~~, or cited references or cruise reports that contained this information~~. The development of CASCADE included the collection of meta information about sampling, storage and analysis, as described in section 2.6. This information is included and detailed in CASCADE. The quality assurance information shows that 86% of the reported OC concentrations were analyzed using EA and only a minority was analyzed by Rock Eval pyrolysis. For δ^{13}C-OC, in 66% of the cases IRMS coupled to EA was ~~given~~ reported as the method of analysis. Regarding sample storage, information was given in about 59% of all data sources that the samples were kept frozen between sampling and analysis, while for <1% of the cases it was documented that the samples were stored refrigerated; this means that for 40% of the samples, there was no information provided about sample storage. For 78% of the Δ^{14}C-OC values, the laboratory ^{14}C/AMS label was documented and thus also added to the CASCADE sheet.

3.4 Circum-Arctic carbon features

Visualization of CASCADE data directly reveals several large-scale features of OC in Arctic Ocean sediments. These include clear differences in both OC concentration and source-diagnostic isotope composition among the shelf seas. For instance, interpolated OC concentrations (Fig. 2) indicate that high sedimentary OC content is found both in regions of high terrestrial input (e.g., Kara Sea, Laptev Sea, East Siberian Sea and Beaufort Sea) and in regions of high nutrient availability and marine primary productivity (Barents Sea and Chukchi Sea). The combination of $\delta^{13}C$ and $\Delta^{14}C$ isotope values delineate large-scale differences in OC sources. Values of $\delta^{13}C$-OC close to marine OC (-21‰; Fry and Sherr, 1989) and $\Delta^{14}C$ reflecting contemporary carbon are consistent with high marine primary productivity in the Barents Sea and Chukchi Sea. ~~By contrast, t~~The Kara Sea~~,~~ receives~~ing~~ input from major West Siberian catchments (Ob and Yenisey rivers), with sediment OC that~~,~~ appears~~s~~ to reflect OC from contemporary terrestrial sources (~-27‰; Fry and Sherr, 1989). By contrast,~~, while~~ the terrigenous OC fraction in the Laptev and East Siberian Seas is much older with a presumably substantial contribution from remobilization of thawing permafrost or other old deposits via erosional or fluvial processes (Fig. 1; Fig. 2). These and other features can now be investigated through CASCADE at greater quantitative detail over large intra- and inter-system scales.

4 Vision and future development

The CASCADE is the largest and most comprehensive open-access database of OC parameters for Arctic Ocean sediments. It is a resource that can facilitate a wide range of investigations on OC cycling in the high northern latitudes.~~,~~ ~~which, f~~For instance, CASCADE may help ~~address~~ research ~~questions~~ on sources of organic matter, marine primary production, OC degradation, OC transport both in the offshore direction and vertically from the sea surface to the sediment; and all this both in the contemporary and the historical perspectives. CASCADE provides opportunities to expand our still limited understanding of how sensitive terrestrial permafrost in different circum-Arctic regions is towards remobilization in both~~,~~ ~~in~~ the current and over earlier periods of rapid climate change. Future versions of CASCADE may also expand on parameters by adding more compound classes of terrestrial biomarkers, marine biomarkers, environmental contaminants (e.g., Hg and organic legacy and emerging substances) and others to investigate biogeochemical distribution and fate of these in the Arctic Ocean.

5 Data availability

CASCADE will be hosted and actively updated and extended by a database management at the Bolin Centre for Climate Research at Stockholm University. CASCADE is accessible at the Bolin Centre data repository (https://doi.org/10.17043/cascade; Martens et al., 2020b). When using the CASCADE, this paper and the database should be cited. The website also includes contact details, which can be used to submit new data for incorporation into future versions of CASCADE – a community effort and resource.

Author contributions

The CASCADE database was conceptualized and planned by a team led by ÖG, IS and ER. JM, NB, BW and ÖG developed the technical framework of the CASCADE. JM executed the development of the CASCADE, populated the database with published and unpublished data from the literature and internal records, coordinated gap-filling analyses and created maps. JM drafted and coordinated the manuscript in close collaboration with ÖG and BW. All authors contributed to the realization of the CASCADE database and participated in the editing of the manuscript.

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Competing interests

The authors declare that they have no conflict of interest.

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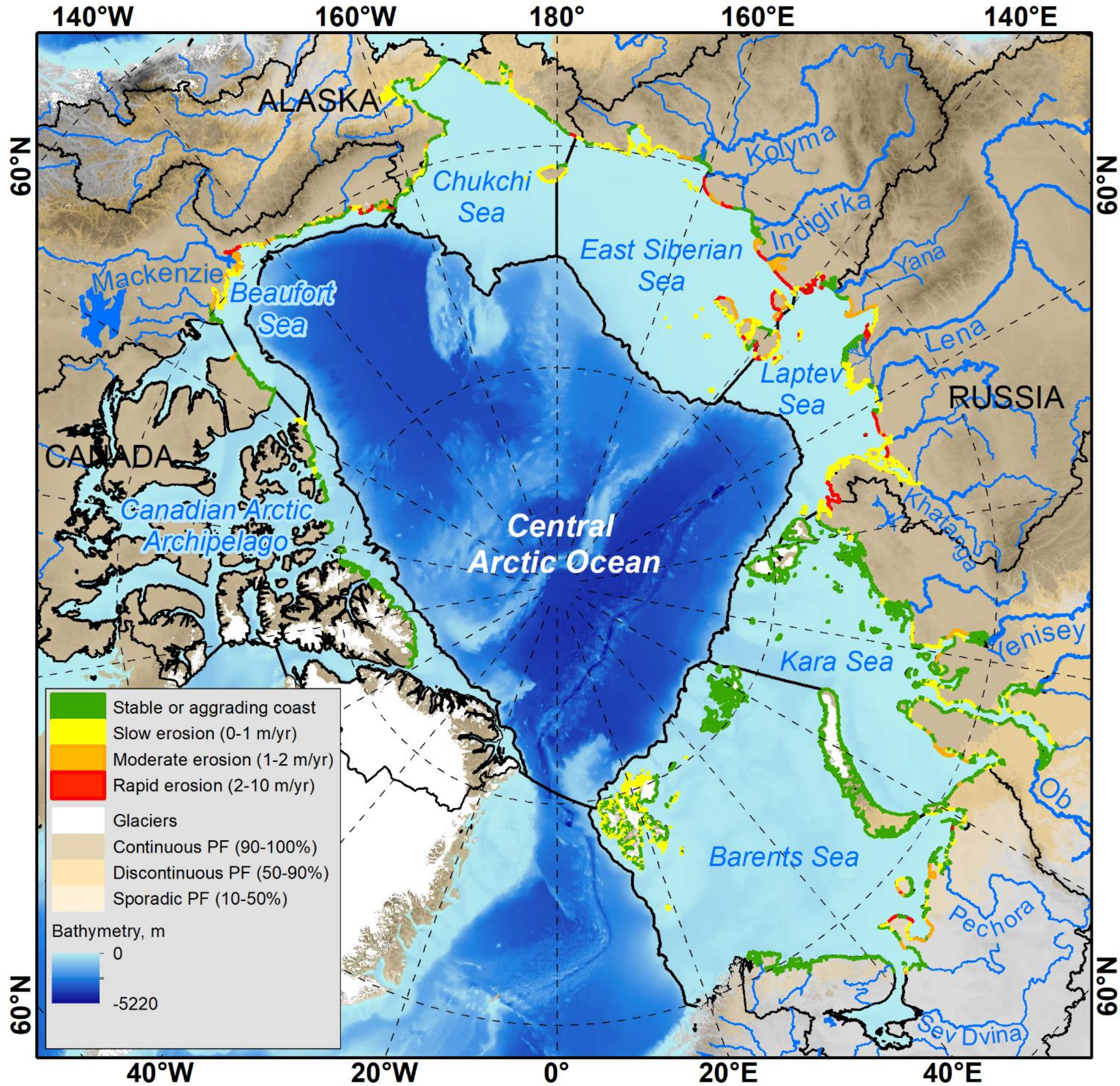

Figure 1: Overview map of the Arctic Ocean compartments defined and used in CASCADE, with the permafrost distribution based on numerical modelling (Obu et al., 2019), rates of coastal erosion (Lantuit et al., 2012); and the latest IBCAO v4 bathymetry (Jakobsson et al., 2020). Black lines delineate the extent of the Arctic Ocean shelf seas and each respective watershed on land.

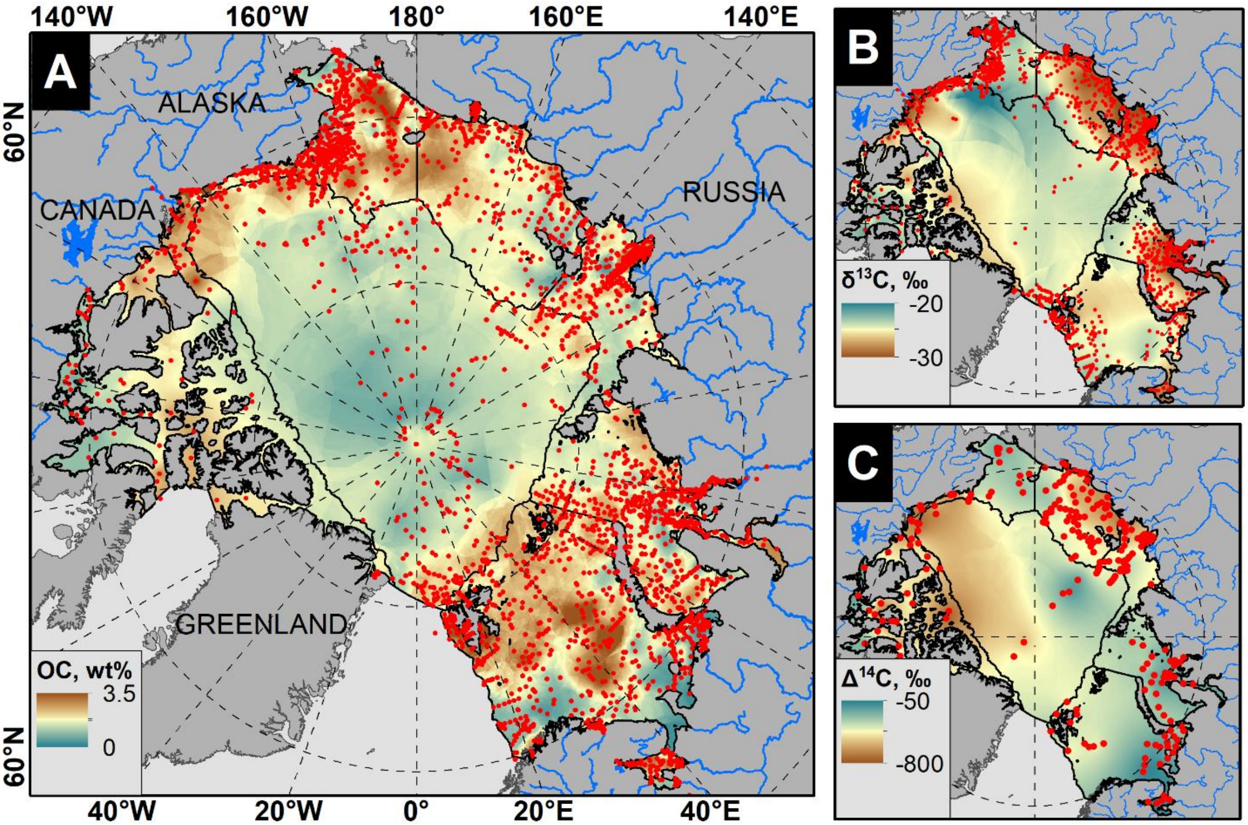

Figure 2: CASCADE data location for OC concentrations (panel A), carbon isotopes $\delta^{13}C$ (panel B) and $\Delta^{14}C$ (panel C) marked as red dots, with interpolated fields as indicated by the inserted color scale and as described in the main text.

Table 1: CASCADE data availability per circum-Arctic shelf sea and for the interior basin

Shelf area		Area 10^3 km^2	OC *n*	TN	$\delta^{13}C$ *n*	New $\delta^{13}C$ *n*	$\Delta^{14}C$ *n*	New $\Delta^{14}C$ *n*	Alk1[1] *n*	Alk2[2] *n*	Acid[3] *n*	Lignin[4] *n*	New lignin *n*
1.	Barents Sea[5]	1626	1092	353	236	48	33	33	0	13	0	0	0
2.	Kara Sea	942	637	201	262	22	29	22	2	90	2	0	0
3.	Laptev Sea	505	312	110	214	8	42	14	33	46	31	36	19
4.	East Siberian Sea	1000	259	217	187	17	71	16	28	13	10	68	40
5.	Chukchi Sea	639	1084	950	256	9	12	10	67	14	58	3	0
6.	Beaufort Sea	183	247	122	219	5	32	3	5	1	2	11	0
7.	Canadian Arctic Archipelago[6]	1171	92	87	55	29	22	19	0	0	0	9	0
8.	Central Arctic Ocean[7]	4500	529	282	130	15	27	10	29	36	28	18	5
	Total	10566	4252	2322	1559	153	268	127	164	213	131	145	64

1. Alk1: HMW *n*-alkanes ΣC_{21}-C_{31}
2. Alk2: HMW *n*-alkanes $C_{27}+C_{29}+C_{31}$
3. Acid: HMW *n*-alkanoic acids ΣC_{20}-C_{30}
4. Lignin: lignin phenols syringyl, vanillyl and cinnamyl
5. incl. White sea and shelf northwest of Svalbard
6. incl. shelf northeast of Greenland
7. incl. continental slope, rise and abyssal plain

Table 2: Parameter description and name of the respective columns in the CASCADE data sheet

Parameters	Description	Column name
CASCADE entry ID	Serial number	ID
Georeference and sampling information		
Sample code	Expedition station ID	STATION
Latitude	Decimal latitude according to WGS1984	LAT
Longitude	Decimal longitude according to WGS1984	LON
Upper sample depth (cm)	Sample depth (for surface sediments only)	UPPERDEPTH
Lower sample depth (cm)	Sample depth (for surface sediments only)	LOWERDEPTH
Median sample depth (cm)	Median sample depth (for core samples only)	COREDEPTH
Water depth (m b.s.l.)	Water depth of sampling according to shipboard measurement	WATERDEPTH
Water depth based on IBCAO (m b.s.l.)	Water depth according to IBCAOv4	IBCAODEPTH
Expedition or vessel name	Vessel name, expedition name, cruise number	EXPEDITION
Sampling year	Year when the sample was taken as reported in literature	YEAR
Carbon and Nitrogen (CN) data		
OC (%)	Total OC concentration of the bulk sediment; carbonate removal assumed	OC
TN (%)	Total N concentration of the bulk sediment	TN
OC/TN	OC/TN ratio (gravimetric); published values or calculated	OC_TN
Carbon isotopes		
δ^{13}C (‰ VPDB)	δ^{13}C-OC; carbonate removal assumed	d13C
Δ^{14}C (‰)	Δ^{14}C-OC corrected for age; carbonate removal assumed	D14C
Biomarkers		
n-alkanes $C_{21\text{-}31}$ (µg g^{-1} OC)	OC-normalized concentration of HMW *n*-alkanes	HMWALK
n-alkanes $C_{27,29,31}$ (µg g^{-1} OC)	OC-normalized concentration of specific HMW *n*-alkanes	HMWALK_SPEC
n-alkanoic acids $C_{20\text{-}30}$ (µg g^{-1} OC)	OC-normalized concentration of HMW *n*-alkanoic acids	HMWACID
lignin phenols (mg g^{-1} OC)	OC-normalized concentration of syringyl, vanillyl, cinnamyl	LIGNIN
Quality parameter and meta information		
Sediment sampler	Method of sediment sampling	SAMPLER
Sample storage	0 unknown, 1 frozen, 2 refrigerated, 3 dried onboard	STORAGE
CN measurement	Description of the method of analysis of the OC and TN data	CN_METHOD
δ^{13}C measurement	Description of the method of analysis of δ^{13}C-OC	d13C_METHOD

~~^{14}C measurement~~	~~Description of the method of analysis of ^{14}C-OC~~	~~D14C_METHOD~~
AMS/^{14}C label	Laboratory number of the Δ^{14}C measurement	D14C_LABEL
Citation of the data source		
Citation of CN data	Full citation in ESSD style incl. info about publication format	CN_CITATION
Citation of δ^{13}C data	Authors, title, journal, volume, pages, doi, year	d13C_CITATION
Citation of Δ^{14}C data	Full citation in ESSD style incl. info about publication format	D14C_CITATION
Citation of biomarker data	Full citation in ESSD style incl. info about publication format	BM_CITATION