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Bridging the gaps between particulate backscattering measurements and modeled particulate organic carbon in the ocean

Martí Galí[1], Marcus Falls[1], Hervé Claustre[2], Olivier Aumont[3], Raffaele Bernardello[1]

[1]Barcelona Supercomputing Center (BSC)
5 [2]CNRS and Sorbonne Université, Laboratoire d'Océanographie de Villefranche, LOV, 06230 Villefranche-sur-7Mer, France
[3]Sorbonne Université (CNRS/IRD/MNHN), LOCEAN-IPSL, Paris, France

Correspondence to: Martí Galí (marti.gali.tapias@gmail.com)

Abstract. Oceanic particulate organic carbon (POC) is a relatively small (~4 Pg C) but dynamic component of the global carbon cycle with fast mean turnover rates compared to other oceanic, continental and atmospheric carbon stocks.
10 Biogeochemical models historically focused on reproducing the sinking flux of POC driven by large fast-sinking particles (bPOC). However, suspended and slow-sinking particles (sPOC) typically represent 80–90% of the POC stock, and can make important seasonal contributions to vertical fluxes through the mesopelagic layer (200–1000 m). Recent developments in the parameterization of POC reactivity in the PISCES model (PISCESv2_RC) have greatly improved its ability to capture sPOC dynamics. Here we evaluated this model by matching 3D and 1D simulations with BGC-Argo and satellite
15 observations in globally representative ocean biomes, building on a refined scheme for converting particulate backscattering profiles measured by BGC-Argo floats to POC. We show that PISCES captures the major features of sPOC and bPOC as seen by BGC-Argo floats across a range of spatiotemporal scales, from highly resolved profile time series to biome-aggregated climatological profiles. Our results also illustrate how the comparison between the model and observations is hampered by (1) the uncertainties in empirical POC estimation, (2) the imperfect correspondence between modelled and
20 observed variables, and (3) the bias between modelled and observed physics. Despite these limitations, we identified characteristic patterns of model-observations misfits in the mesopelagic layer of subpolar and subtropical gyres. These misfits likely result from both suboptimal model parameters and model equations themselves, pointing to the need to improve the model representation of processes with a critical influence on POC dynamics, such as sinking, remineralization, (dis)aggregation and zooplankton activity. Beyond model evaluation results, our analysis identified inconsistencies between
25 current estimates of POC from satellite and BGC-Argo data, as well as POC partitioning into phytoplankton, heterotrophs and detritus deduced from in situ bio-optical data. Our approach can help constrain POC stocks, and ultimately budgets, in the epipelagic and mesopelagic ocean.

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1 Introduction

The biological carbon pump (BCP) is the ensemble of processes that transfer the organic matter produced by plankton in the sunlit ocean surface to deeper layers (Volk and Hoffert, 1985). This vertical flux plays a central role in the Earth's climate, as it influences the oceans' capacity to absorb and ultimately store atmospheric CO_2 over centennial or millennial time scales (Kwon et al., 2009). The BCP is also central to biogeochemical functioning of the ocean, as it determines the quality and quantity of organic matter available to the ocean interior (Arístegui et al., 2009; Hernández-León et al., 2020) and the seafloor. Organic matter respiration in the ocean interior influences the distribution of oxygen, inorganic carbon and remineralized nutrients (Duteil et al., 2012; Oschlies et al., 2018; Weber et al., 2016), and their return pathways to the surface. Sinking particles are also efficient trace metal scavengers (Hayes et al., 2015). In consequence, the BCP is intimately linked to, and feeds back on, upper ocean productivity.

Over the last decades, BCP research has placed emphasis on understanding the ecological and physical factors that control export efficiency (the fraction of net primary production exported below the euphotic layer) and transfer efficiency (Teff; the fraction of export production that reaches a given depth below the euphotic layer), both of which vary widely across ocean biomes and along the seasonal cycle (Buesseler and Boyd, 2009; Buesseler et al., 2020). Therefore, biogeochemical models have been built, and their parameters tuned, to be able to reproduce sparse observations of export production and vertical carbon flux attenuation (Guidi et al., 2015; Henson et al., 2011; Laws et al., 2000), sometimes reaching apparently contradictory results (Marsay et al., 2015). In comparison, the models' ability to represent marine particle concentrations has received less attention (Lam et al., 2011).

Marine particles are mainly composed of living microbial plankton cells, living metazoans and detritus ("marine snow" aggregates, fecal pellets, zooplankton feeding structures), whose size ranges from <1 μm to several mm (Stemmann and Boss, 2012). Indeed, these particles also feature wide variations in shape, density, chemical composition and reactivity towards microbial degradation (Kharbush et al., 2020). Building on the overall increase in gravitational sinking speed with particle size (Cael and White, 2020; Stemmann et al., 2004a), particle populations are usually partitioned into a few functional size classes: big particles, typically defined as larger than 50 or 100 μm, which sink at several tens or hundreds of m d^{-1}; and small particles, including suspended and slow-sinking (<10 m d^{-1}) particles. In this study, the particulate organic carbon (POC) is divided into small POC (sPOC) and big POC (bPOC), with a nominal cutoff at 100 μm (Table 1; section 2.2.2).

60   The traditional BCP paradigm posits that bPOC controls the vertical carbon flux (Sarmiento and Gruber, 2006). However, a
wider paradigm has emerged during the last decade, shifting our attention to carbon export processes other than gravitational
sinking. These processes were collectively termed "particle injection pumps", and include both the "active flux" mediated by
the vertical migration of metazoans and the physical "particle injection pumps" resulting from oceanic convection and water-
mass subduction at various scales (Boyd et al., 2019). In parallel, the role of dissolved organic carbon in vertical carbon

65   export has been widely recognized (Jiao et al., 2010; Legendre et al., 2015).

One aspect that has recently received considerable attention is the role of suspended and slow-sinking particles. Owing to
their longer residence time, small particles represent the majority of the POC stock (Aumont et al., 2017; Baker et al., 2017)
and may support a proportional fraction of the respiration (Baltar et al., 2010a, 2010b; Belcher et al., 2016; Iversen and

70   Ploug, 2010). Small POC can drive vertical POC fluxes across the mesopelagic layer during episodes of convection (Bishop
et al., 1986; Dall'Olmo and Mork, 2014; Lacour et al., 2019) or subduction (Llort et al., 2018; Omand et al., 2015;
Resplandy et al., 2019), potentially making large contributions to POC export (Alonso-Gonzalez et al., 2010; Henson et al.,
2015). Sources of sPOC to the mesopelagic layer and below it are not limited to gravitational sinking or detrainment from
the surface, because sPOC can be produced through the fragmentation of sinking bPOC, caused by physical disaggregation,

75   bacterial solubilization and zooplankton activity (Briggs et al., 2020; Goldthwait et al., 2004; Mayor et al., 2020; Stemmann
et al., 2004b), and also through bacterial chemosynthesis (Arístegui et al., 2009). Altogether, these findings illustrate how
our limited knowledge of POC characteristics and cycling hampers mechanistic understanding of the BCP and mesopelagic
carbon budgets (Burd et al., 2010; Giering et al., 2014; Steinberg et al., 2008).

80   Biogeochemical models designed to capture only gravitational POC sinking fail to represent POC stocks in the ocean
interior. Aumont et al. (2017) recently showed that the Pelagic Interactions Scheme for Carbon and Ecosystem Studies
model (PISCESv2; Aumont et al., 2015) underestimated POC by one order-of-magnitude or more below the epipelagic
layer. This pitfall is likely common to any state-of-the-art model with similar structure (Laufkötter et al., 2016; Séférian et
al., 2020). Aumont's work also showed that the implementation of a variable reactivity scheme for POC improved

85   dramatically the fit to observed deep-ocean POC concentrations, without harming vertical POC flux estimation. This
parameterization treats detrital particles, both small and big, as a mixture of particles distributed along a reactivity continuum
(RC). The most labile fractions are rapidly consumed below the productive illuminated surface layer, such that vertically
exported POC becomes progressively more refractory. This results in enhanced preservation of sPOC in the model and a
much more realistic fraction of sPOC with respect to total POC (tPOC) in the ocean interior.

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Despite this breakthrough in the representation of POC fractions in PISCESv2_RC (hereafter "PISCES"), the new
parameterization was evaluated using only sparse in-situ measurements. During the last decade, the launching of the
biogeochemical Argo (BGC-Argo) program of robotic observations has revolutionized the study of particles in the ocean

interior (Claustre et al., 2020). BGC-Argo floats provide vertical profiles of temperature, salinity, bio-optics and chemical

95 variables between 0–1000 m every 1 to 10 days in near-real time, and are thus especially well suited to study particles in the mesopelagic layer, where the strongest POC gradient occurs. The rapidly growing fleet of BGC-Argo floats equipped with bio-optical sensors enables comparison between models and observations at global scales with enhanced spatiotemporal resolution. Unfortunately, BGC-Argo floats measure only a bio-optical proxy of POC, the particulate backscattering coefficient (usually at 700 nm, b_{bp700}) and empirical conversion factors are needed to estimate POC from b_{bp700} (Cetinić et al.,

100 2012; Stramski et al., 2008).

In this study we compare sPOC and bPOC concentrations estimated from BGC-Argo floats to their PISCES-simulated counterparts, as well as satellite-retrieved surface POC. The comparison is enabled by a novel empirical algorithm to convert b_{bp700} to POC. Observations and simulations are matched in 3D (biome-wide climatological scale) and 1D (at defined

105 locations over an annual cycle). These complementary strategies allow us to evaluate the skill of PISCES at simulating POC stocks and fractions, and indirectly the drivers of POC export and mesopelagic POC budgets, in globally representative biomes.

2 Methods

2.1 Definition of vertical and horizontal domains

110 Studies of the BCP usually decompose the ocean into vertical domains: a surface layer where autotrophic activities dominate, and one or several ocean interior layers where heterotrophic processes dominate. Functional definitions based on light penetration, peak export production, vertical mixing or long-term carbon sequestration are usually the most appropriate ones for process studies (Buesseler and Boyd, 2009; Buesseler et al., 2020; Guidi et al., 2015; Palevsky and Doney, 2018). Because this paper is mainly descriptive and combines observations and simulations, we will refer to layers defined by fixed

115 depths: epipelagic (0–200 m), mesopelagic (200–1000 m) and bathypelagic (1000–4000 m).

Over the horizontal dimensions, our comparisons between observations and model results rely on the ocean biomes defined by Fay and McKinley (2014). These authors subdivided each ocean basin (Atlantic, Pacific, Indian, and Southern Ocean) into different biomes on the basis of observed variables, namely: sea surface temperature, spring/summer chlorophyll *a*

120 concentrations (Chla), ice fraction, and maximum mixed layer depth (MLD), all on a 1°×1° grid. This division resulted in 17 regions ascribed to one of the following five biomes: the ice biome, the subpolar seasonally stratified biome, the subtropical seasonally stratified biome, the subtropical permanently stratified biome, and the equatorial biome. The analyses reported herein focus on the following four biomes (Fig. 1): the seasonally stratified North Atlantic subpolar gyre (NASPG); the permanently stratified Atlantic and Pacific subtropical gyres, which were grouped together (STG); the seasonally stratified

125 Southern Ocean (Subantarctic); and the Mediterranean Sea, which was added here owing to the abundance of BGC-Argo

data, and represents a seasonally stratified subtropical biome. Fay and McKinley's definition allows biome boundaries to change from one year to another. Here we analysed only data from the core of each biome, defined as the grid cells that never changed classification during the 1998–2010 satellite observation periods.

2.2 BGC-Argo observations

130   The global dataset acquired by the array of BGC-Argo floats was downloaded on 14 January 2020 from the Global Data Assembly Center hosted by Ifremer (ftp://ftp.ifremer.fr/ifremer/argo/dac/) (Argo, 2000). We selected floats equipped with at least a Chla fluorometer and a sensor for optical backscattering at 700 nm (b_{bp700}), in addition to the conductivity-temperature-depth (CTD) probe. The downloaded measurements had undergone the standard processing, which includes the application of calibration equations to raw sensor output and the performance of near-real-time quality control to both CTD

135   (Wong et al., 2021) and Chla measurements (Schmechtig et al., 2018). Since no specific quality control procedure has been established yet for b_{bp700} profiles, the latter were only flagged according to the general criteria (Schmechtig et al., 2016). Thus, we used all b_{bp700} measurements with quality control flag ≤ 3 (equivalent results were obtained with flag ≤ 2). Two different processing pipelines were applied to different subsets of the BGC-Argo data, as described below.

2.2.1 Global gridded climatologies (3D approach)

140   The global dataset acquired between 2010 and 2019 was used to produce global gridded monthly and seasonal climatologies for b_{bp700} and Chla. The measurements were binned onto the ORCA2_L31 grid used for NEMO-PISCES simulations (see 2.4.1), which has an horizontal resolution of about 2° that increases to 0.5° in the meridional direction in the equatorial domain, and 30 oceanic vertical levels between the surface and the ocean bottom. The thickness of the vertical bins increases progressively from 10 m at the surface to 339 m in the 22nd bin (870–1209 m), the deepest one containing BGC-Argo data.

145   In each grid element, the average, median, range and data counts were computed. Profiles from the CSIRO and INCOIS data assembly centers were not used because, at the time of download, they had not taken into consideration the new calibration files provided by the manufacturer. A total of 72460 profiles were used to calculate the global gridded climatologies.

2.2.2 Profile time series for individual floats sampling at higher resolution (1D approach)

A subset of the floats, deployed mostly by the projects NAOS, remOcean and Bio-Argo France (model NKE PROVOR

150   CTS-4), were programmed to sample at higher temporal and vertical resolution than the Argo defaults (10 days and 10 m). These floats made vertical profiles between 1,000 m and the surface every 2, 5 or 10 days with a vertical resolution of 10 m between 1,000 and 250 (or 350) m, 1 m between 250 (or 350) and 10 m, and 0.2 m between 10 m and the sea surface. We processed this dataset with a dedicated pipeline to extract additional information on POC size fractions and their dynamics. Along each vertical profile we computed depth, conservative temperature, absolute salinity, σ_θ and spiciness (Flament, 2002)

155   from the calibrated pressure, temperature and salinity using the R package *oce* (Kelley, 2011). The MLD was calculated as the shallowest depth where σ_θ exceeded the surface reference value by 0.03 kg m^{-3}. The surface reference corresponded to

the σ_θ at 5 m after applying a 5-point running mean to the top 10 m of the profile. Eleven additional MLD criteria were also calculated to assess the robustness of the approach (Fig. S1). Following Briggs et al. (2011, 2020), each b_{bp700} vertical profile was smoothed with sequential 11-point running-minimum and running-maximum filters to separate the baseline from the

160 spikes. The baseline signal corresponds to the bulk population of small particles, whose diameter is smaller than 100 µm and mostly between 0.5 and 30 µm (Dall'Olmo et al., 2009; Organelli et al., 2018). Each spike reflects the passage of a particle (organism or aggregate) larger than about 100 µm in front of the sensor window. Unlike Briggs et al. (2020), we did not subtract from the baseline profile the 850–900 m signal, which in that study was attributed to a background of small refractory particles with constant concentration. The baseline and spike signals were converted to sPOC and bPOC,

165 respectively, as described in the next section. All measurements were subsequently averaged into 18 vertical bins of progressively increasing thickness, such that the deepest bins contained at least 10 measurements. Finally, each profile was interpolated onto the L75 vertical grid commonly used in NEMO simulations. This grid has 46 bins between the surface (0–1 m) and the deepest layer considered here (901–996 m). The profile time series was temporally binned into 5-day periods.

170 For the comparison to PISCES 1D simulations, BGC-Argo time series were cut into one-year periods (shifted by 6 months in the Southern hemisphere), which we will call coherent annual time series (CATS) hereafter. The CATS fulfilled the following conditions: (1) sampling dates spanned at least between days of year 25 and 340; (2) the float remained in the same region and did not cross major oceanic fronts according to the vertical-temporal evolution of temperature, salinity, σ_θ and spiciness; (3) bottom depth was > 1000 m for all profiles (bathymetry obtained from the 15 arc-second GEBCO 2019

175 product; https://www.gebco.net/data_and_products/gridded_bathymetry_data/gebco_2019/gebco_2019_info.html); and (iv) the Chla and b_{bp700} sensors were stable according to both the vertical profiles and the continuous measurements acquired during drift at 1000 m between profiles. A total of 50 CATS from 28 different floats were selected, with 10–16 CATS in each biome, 32 (18) in the Northern (Southern) hemisphere (Table S1).

2.3 Conversion of b_{bp700} to POC

180 To convert the profiles of the backscattering coefficient at 700 nm (b_{bp700}) to POC we developed an empirical algorithm, whose behaviour is summarized in Fig. 2, building on previous studies (Bol et al., 2018; Evers-King et al., 2017). The variability of POC/b_{bp700} enclosed in this algorithm results from processes that alter the size distribution, dominant shapes, and chemical composition of the particle assemblage, and ultimately its bulk optical properties, as discussed in section 4.2. Further details are provided in the Appendix. The algorithm estimates the POC/b_{bp700} ratio along the vertical profile between

185 0 and 1000 m, and proceeds in two steps. First, the POC/b_{bp700} ratio is calculated by prescribing a POC/b_{bp700} ratio in the surface layer ($z_{surf,biome}$) and an exponential decrease with depth in the underlying water column, which converges asymptotically towards a constant deep value (c):

$$POC/b_{bp,700}(z) = c + a_{biome}*exp(-b*(z-z_{surf,biome})*0.001), \quad z > z_{surf,biome} \tag{1}$$

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The a_{biome} coefficient is biome-specific, whereas the asymptote at depth is fixed at c = 1000 mmol C m^{-3} m. The $z_{surf,biome}$ corresponds to the 5% quantile of the climatological MLD in summer in a given biome. The POC/$b_{bp,700}$ ratios at $z_{surf,biome}$, corresponding to a_{biome} + c in Eq. 1, are taken from the literature and range between 2600 and 4900 mmol C m^{-3} m (Fig. 2; Table A1). Second, the POC/$b_{bp,700}$ profile derived from Eq. 1 is modified by extrapolating a constant POC/$b_{bp,700}$ value,

195   taken from a reference depth, z_{ref}, to the sea surface. In each vertical profile, z_{ref} is defined as the deepest of $z_{surf,biome}$ and the MLD:

$$POC/b_{bp700}(z) = POC/b_{bp700}(z_{ref}), \quad z \leq z_{ref}; \qquad z_{ref} = \max(z_{surf,biome}, MLD) \tag{2}$$

200   The exponential decrease prescribed by Eq. 1 is similar to that proposed by Bol et al. 2018, except for the inclusion of the constant term c that prevents the ratio from becoming 0 at depth. The slope of the exponential decrease (b = -6.57) is constant in all biomes and based on our fit to the Cetinić et al. (2012) dataset, using the same depth bins as Bol et al. (2018), but additionally forcing the curve towards c at 1000 m.

205   The uncertainty of regional b_{bp700}-POC conversion factors in the epipelagic is typically <10% according to the standard error of the POC vs. b_{bp700} linear regression slopes (Table A1). The few available measurements in the mesopelagic suggest a POC/b_{bp700} uncertainty lower than a factor of two. Through this study, we will assume that model/observation ratios larger/smaller than 2/0.5 can safely be regarded as model over/underestimates, which possibly is a conservative criterion for the epipelagic layer.

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The conversion of b_{bp700} to POC was done using different MLD data for the global climatologies and the CATS. For the global climatologies we used the Monthly Isopycnal & Mixed-layer Ocean Climatology (MIMOC) of Schmidtko et al. (2013), downloaded from https://www.pmel.noaa.gov/mimoc/, which was reprojected onto the ORCA2 horizontal grid. Although MIMOC is based on an algorithm that evaluates several MLD criteria, it has been shown to be globally consistent

215   with the MLD based on a 0.03 kg m^{-3} σ_θ threshold (Holte and Talley, 2009; Sallée et al., 2021). For the float time series, we used the MLD defined by a 0.03 kg m^{-3} threshold computed for each individual profile.

2.4 Ocean color satellite data

Satellite observations for the 1997–2019 period were downloaded from GlobColour (https://www.globcolour.info), a merged multisensor dataset, on 2 March 2020. Monthly sea-surface POC fields based on the algorithm of Stramski et al. (2008) were

220   used to compute monthly climatologies that were subsequently reprojected onto the ORCA2 grid.

2.5 PISCES simulations and matching with observations

Simulations were run using the ocean biogeochemistry model PISCESv2 (Aumont et al., 2015) with the RC parameterization for detrital POC (Aumont et al., 2017). The configuration of PISCES used here has 24 tracers: two classes of phytoplankton ("nanophytoplankton" and diatoms), detrital particles (small and big), and zooplankton (micro- and mesozooplankton), plus
225   18 additional tracers that comprise dissolved inorganic macronutrients and iron, inorganic carbon chemistry variables, dissolved organic carbon (DOC), and different particulate stocks of iron and silica. Phytoplankton growth depends on light, inorganic nitrogen, phosphorus and iron, with an additional silicate requirement for diatoms. Microzooplankton and mesozooplankton consume the two classes of phytoplankton and detrital particles with different preferences, and mesozooplankton also predate on microzooplankton. Detrital particles are produced through the mortality of phytoplankton
230   and zooplankton (which are routed to small and big particles in different proportions), zooplankton sloppy feeding, and DOC coagulation. Production of large detritus also results from enhanced diatom mortality upon bloom collapse, aggregation of small detritus, and zooplankton mortality and fecal pellet production (the latter two derived from a closure term that accounts for unresolved higher trophic levels). Small and big detrital particles are nominally smaller/larger than 100 μm and sink, respectively, at 2 and 50 m d^{-1}. Both small and big detritus are remineralized by implicit bacterial activity, and consumed by
235   flux-feeding mesozooplankton. Remineralization follows first-order kinetics with an initial specific rate "k" of 0.035 d^{-1} (at 0°C) for freshly produced detritus in the upper mixed layer. This "k" decreases with depth as an emergent result of the RC parameterization. The flux feeding rate depends on the particles' sinking flux, and thus attenuates the flux of large particles more strongly. Additionally, a small fraction of the large detritus intercepted by flux feeders is fragmented into small detritus. Phytoplankton growth rates and remineralization rates increase with temperature with a Q_{10} of 1.9, whereas
240   zooplankton growth rates have a Q_{10} of 2.14.

To evaluate PISCES simulations against in situ POC measurements or their proxies, the correspondence between PISCES tracers (*in italics*) and observed POC fractions has to be established. In this study we assumed that sPOC corresponds to the sum of PISCES-simulated nanophytoplankton (*PHY*), diatoms (*PHY2*), small detrital particles (*POC*) and microzooplankton
245   (*ZOO*), whereas bPOC corresponds to the sum of PISCES-simulated big detrital particles (*GOC*) and mesozooplankton (*ZOO2*) (Table 1). Total POC (tPOC) corresponds to the sum of those six PISCES tracers or, what is the same, sPOC + bPOC. Heterotrophic prokaryotes (*BACT*) are not a prognostic tracer in PISCES, and are not explicitly included in our analysis. The correspondence between observed and simulated POC fractions, explicit and implicit, is discussed in section 4.3.

250   **2.5.1 PISCES 3D simulations vs. biome-aggregated observations**

For the global-scale comparison between PISCES outputs and observations from BGC-Argo and satellites, we used the simulation presented by Aumont et al. (2017), which was forced by pre-computed dynamical fields from a pre-industrial run

of the ocean circulation model NEMO. Global monthly climatological fields of the PISCES tracers were used to compute seasonal climatologies of modeled sPOC, bPOC and tPOC. To enable direct comparison to the BGC-Argo observations,

255   model output was resampled at locations where BGC-Argo profiles were available over the 2010–2019 period. Prior to comparison with modeled fields, BGC-Argo observations were further screened to remove "outliers" in each biome and season. Outliers were defined as grid cells where the mean b_{bp700} in the upper 50 m was above the 95% percentile or greater than 0.008 m^{-1} (Briggs et al., 2020). The same resampling was applied to satellite-retrieved POC.

2.5.2 PISCES 1D simulations vs. BGC-Argo coherent annual time series (CATS)

260   A more detailed comparison was undertaken by matching each of the CATS from individual BGC-Argo floats with a PISCES water-column ("PISCES 1D") simulation. The match was based on the coherence between the seasonal cycle of MLD observed by the float and the turbulent layer simulated by NEMO. The pre-computed dynamical fields used to evaluate the match-ups were obtained from an ocean-only historical simulation (NEMO v3.6) at 1-degree resolution with 75 vertical levels (ORCA1_L75 grid) forced with the JRA-55 atmospheric reanalysis that covered the 1958–2018 period

265   (Tsujino et al., 2020) following the OMIP2 protocol (Griffies et al., 2016). The float-observed MLD and the NEMO-simulated turbocline depth (defined by turbulent diffusivity $> 5 \cdot 10^{-4}$ m^2 s^{-1}) were compared over the entire annual cycle in all the model grid cells that had been visited by the float on a given year. The best model grid cell was selected on the basis of model-observations correlation, root-mean-square error, and time lag in the onset date of summer stratification. An example of the metrics used to match NEMO dynamical fields and BGC-Argo MLD is provided in Fig. S1-S4.

270

PISCES 1D offline simulations were forced using the dynamical fields from the selected model grid cells. The same annual forcing, corresponding to the year of the BGC-Argo observations, was repeated over 5 simulation years. After 4 years of spin-up, the output from year 5 at 5-days resolution was used for the comparison to the BGC-Argo CATS. Initial conditions (climatological fields of inorganic nutrients and carbon chemistry variables) and boundary conditions (atmospheric

275   deposition) were the same used for PISCES 3D (Aumont et al., 2015, 2017). Nutrient fields were restored towards the mean annual profile below 300 m. This procedure avoided drift in nutrient stocks by replenishing the upper ocean with the same amount of nutrients each year, resulting in regular seasonal cycles after one year and identical cycles from year 4 onwards.

3 Results

3.1 Climatological POC fields

280   This section describes the comparison among tPOC fields estimated from BGC-Argo and satellite observations and PISCES simulations across four ocean biomes. Fig. 3 compares monthly climatologies at the sea surface (0–20 m), Fig. 4 compares seasonal climatologies between 0–1000 m, and Fig. 5 displays skill metrics (Pearson's correlation, model/observations ratio and bias) for the vertical profiles shown in Fig. 4, as well as for the 1D simulations matched to BGC-Argo CATS.

3.1.1 Seasonally stratified subpolar biomes

285   In the subpolar biomes, near-surface tPOC ranged between ~1 mmol m^{-3} in the winter months and around 5 (Subantarctic) or 10 (NASPG) mmol m^{-3} in early summer. In these biomes, PISCES-simulated tPOC was within the 2.5–97.5% bounds of BGC-Argo observations for the majority of months (Fig. 3). During the apex of the bloom (months 5–7), however, median PISCES estimates exceeded those obtained from BGC-Argo (by ~80%) and satellites (by ~15%). In the Subantarctic, this pattern extended through the fall. Satellite tPOC was in poor agreement with both PISCES and BGC-Argo tPOC outside the

290   apex of the bloom, as discussed in section 4.1.

PISCES reproduced the vertical decrease of tPOC concentration down to 1000 m (Fig. 4) with generally good skill (Fig. 5), but some misfits were observed. In the North Atlantic subpolar gyre (NASPG), PISCES underestimated tPOC through the epipelagic and the upper mesopelagic during the winter by ~40% (Fig. 4) as a result of too vigorous convection in the

295   NEMO dynamical fields that kept phytoplankton under insufficient light exposure. In the Subantarctic biome, simulated tPOC exceeded BGC-Argo estimates in the upper portion of the mesopelagic layer in spring, and the overestimation pattern propagated downwards through the summer and fall. A similar but smaller overestimation pattern was observed in the NASPG in summer and fall.

3.1.2 Permanently and seasonally stratified subtropical biomes

300   In the oligotrophic biomes, monthly median surface tPOC displayed low seasonal amplitude. Total POC concentrations estimated from BGC-Argo data typically oscillated around 2 mmol m^{-3}, with a maximum/minimum ratio of around 1.6 in the Mediterranean and 1.3 in the Atlantic and Pacific subtropical gyres (STG). In the STG, satellite and BGC-Argo tPOC were in good agreement, which could be expected because b_{bp700}-POC conversion factors and satellite POC are based on the same study (Stramski et al., 2008). On the contrary, PISCES tPOC exceeded BGC-Argo tPOC by around twofold in the STG. In

305   the Mediterranean, satellite tPOC exceeded BGC-Argo tPOC by ~80%, pointing to the differences in the respective POC estimation algorithms. PISCES tPOC was nearly fourfold higher than BGC-Argo tPOC at the surface in the Mediterranean, an overestimation that results from unrealistic physics in that basin caused by the coarse (2°) model grid (see 3.3 and 4.3). Vertical tPOC profiles evidenced the shortcomings of PISCES simulations in the oligotrophic gyres. Compared to BGC-Argo profiles, PISCES simulations produced too-sharp deep POC maxima and underestimated tPOC in the waters above and

310   below (Fig. 4). Overall, these patterns prompted us to examine in greater detail the seasonal cycles of POC in different biomes.

3.2 Coherent annual time series of sPOC and bPOC: case studies

In this section we describe two CATS from BGC-Argo floats and their PISCES 1D counterparts (section 3.2.1). The floats, identified by their World Meteorological Organization (WMO) number, are the 6901486 in the NASPG (year 2015) and the

6901660 in the South Pacific STG (year 2017). The float 6901486 represents the most productive conditions of our dataset, with annual median (maximum) Chla of 0.60 (10.7) mg m^{-3} and tPOC of 5.5 (16.7) mmol m^{-3} in the near-surface layer (0–20 m). By contrast, float 6901660 represents the most oligotrophic waters, with annual median (maximum) Chla of 0.011 (0.036) mg m^{-3} and tPOC of 1.8 (2.5) mmol m^{-3} in the near-surface layer. In Fig. S5–S10 we provide additional examples of the CATS-PISCES 1D match-ups in the four biomes and in two subregions within the NASPG.

3.2.1 Labrador Sea (North Atlantic subpolar gyre)

Float 6901486 was deployed in June 2013 close to the Reykjanes Ridge in the Irminger Sea, NW Atlantic subpolar gyre. After drifting SW carried by the East Greenland Current, the float was trapped in the Labrador Sea cyclonic circulation between 2014 and July 2017, when it stopped communication after completing 344 profiles (cycles). During its multi-year sampling in the Labrador Sea (56-60°N latitude and 48–54°W longitude), over a bottom depth of around 3500 m, the float showed stable physical and bio-optical records at 1000 m, broken only by winter convection events, and recurring annual patterns of spring-summer phytoplankton blooming and vertical carbon export as depicted by Chla and POC profiles. Here we describe the year 2015 (Fig. 6), characterized by deep convection during February and March, when the MLD generally exceeded 1000 m (Fig. S1). Epipelagic tPOC increased rapidly upon water-column re-stratification in mid-April and peaked in mid-May. A secondary bloom peaked in late June after a transient MLD deepening caused by stormy weather. Epipelagic tPOC decreased progressively thereafter until a small bloom was observed in October linked to pycnocline erosion. This bloom terminated rapidly and epipelagic tPOC reached the baseline level in late December. The sPOC fraction dominated epipelagic tPOC all year round, and highest bPOC fractions of nearly 20% were recorded at the apex of the spring-summer blooms. Distinct vertical particle export events were observed in May and June, matching the surface phytoplankton blooms, and August, when nutrient limitation likely triggered bloom collapse. These export pulses produced synchronous increases in sPOC and bPOC through the mesopelagic layer, though with different magnitudes. After reaching relative minima in October, mesopelagic sPOC and tPOC increased again in November, but they showed different vertical patterns.

The matching PISCES 1D simulation captured with good skill the patterns of sPOC and bPOC in the epipelagic and, to a lesser extent, the mesopelagic layer (Fig. 6). Excellent correlation (r = 0.92) and bias (-0.5%) between BGC-Argo and PISCES were found for vertically integrated epipelagic tPOC (Fig. 6i). A delayed start of the bloom was observed in the simulation, which can be partly attributed to a delay of around one week in the onset of permanent stratification in the model. It is also plausible that modelled phytoplankton reacted too weakly to the cessation of deep convection, which was captured by alternative MLD metrics in BGC-Argo profiles (Fig. 6a and b). Despite the general good agreement between observed and simulated sPOC, the model produced a conspicuous plume of sPOC that sank from the surface spring bloom into the mesopelagic layer, at the prescribed constant rate of 2 m d^{-1}, which was not found in the observations. In the core of this plume, PISCES POC exceeded BGC-Argo sPOC by more than twofold. A similar model-observations mismatch was observed in all the northern and southern subpolar CATS as well as in some CATS in the Mediterranean (Figures S5-S8 and

S10). On average, simulated bPOC exceeded BGC-Argo bPOC by 36% and 96% in the epi- and mesopelagic layers, respectively. The largest overestimation was observed during the midsummer export event. On the other hand, bPOC
350 underestimation was found during the May bloom between 0–400 m.

PISCES qualitatively reproduced the late summer peak of mesopelagic bPOC, which was observed in all the subpolar North Atlantic CATS. On the contrary, it failed to reproduce both the decrease of sPOC and bPOC in fall between 600-800m and the bPOC increase below 800 m. The latter occurred in 6 out of 11 CATS in the NASPG, all located in the Labrador Sea.
355 The apparent decoupling of deep mesopelagic bPOC from the overlying water column may be related to the insufficient temporal resolution of BGC-Argo profiling during that period compared to bPOC sinking speed, or reflect bPOC export events from surface waters areas not located vertically over the float (Siegel and Deuser, 1997).

3.2.2 South Pacific subtropical gyre

Float 6901660 was deployed in March 2015 in the western South Pacific STG, and drifted westwards until it deflected SW
360 while approaching Tahiti. As of March 2021, the float was still active and had completed 244 cycles with stable continuous records at the 1000 m drift depth. Between July 2017 and June 2018 (18-21°S latitude and 148-157°E longitude), the period selected for the CATS analysis, the BGC-Argo profiles portrayed a stably stratified water column typical of the core of the subtropical gyres (Fig. 7). Vertical mixing events that reached a depth of around 100 m were observed in July, August and October. However, their effect on surface sPOC was hardly noticeable, indicating that turbulent entrainment of nutrients was
365 too weak to stimulate new production significantly. A deep Chla maximum was present all year round between 150 and 200 m as identified by the maximum Chla gradient. This Chla maximum did not translate into a deep POC maximum. The fraction bPOC/tPOC was consistently around 6% in the epipelagic and 12% in the mesopelagic according to the vertically integrated stocks. The vertical-temporal distribution of bPOC was patchy in the lower mesopelagic (500–1000 m), perhaps reflecting the difficulty to detect rare aggregates from b_{bp700} spikes.
370

The epipelagic tPOC stock (driven by sPOC) simulated by PISCES matched well the observations, with a high temporal correlation coefficient (r = 0.69; Fig. 7i) despite the low seasonal variability in this tropical setting. The low mean bias of epipelagic sPOC (9%) resulted from mutually compensating biases, as PISCES overestimated sPOC between the base of the mixed layer and the deep Chla maximum, and underestimated sPOC below it. In the mesopelagic layer, vertically integrated
375 PISCES sPOC was on average 45% lower than BGC-Argo sPOC, and showed low negative temporal correlation to the observations. Regarding bPOC, the simulated stock was nearly twice as large as BGC-Argo estimates in the epipelagic, with the largest overestimation seen in the deep Chla maximum. In the mesopelagic, PISCES bPOC exceeded BGC-Argo estimates by 25% on average. Despite model-observations discrepancies in terms of bPOC concentration, PISCES simulations supported the increase in the bPOC/tPOC fraction between the epipelagic and the mesopelagic layers.

3.3 Coherent annual time series of sPOC and bPOC: generalized approach

Although each of the 50 CATS included in this study has unique features, some of the misfit patterns between PISCES and BGC-Argo data described in the previous section are common to the majority of CATS in a given biome or, more broadly, in subpolar vs. subtropical biomes. In this section we generalize the quantitative comparison between the 50 BGC-Argo CATS and their PISCES 1D counterparts across the four biomes. We consider separately the epipelagic and mesopelagic domains, focusing on mean annual sPOC and bPOC standing stocks (Fig. 8), the sPOC/tPOC fraction (Fig. 9), and the mesopelagic Teff of sPOC and bPOC (Fig. 10).

Epipelagic sPOC stocks ranged between 193–425 mmol C m^{-2} and 282–537 mmol C m^{-2}, respectively, according to BGC-Argo observations and PISCES 1D simulations. Although the ranges of the different biomes overlapped, smaller stocks were usually found in the more oligotrophic (STG and Mediterranean) biomes. The agreement between simulated and observed epipelagic sPOC was better in the STG and NASPG biomes, whereas simulated epipelagic sPOC exceeded observations by around 50% in the Mediterranean and Subantarctic biomes. Still, a significantly positive correlation between simulated and observed stocks (r = 0.45, p = 9·10^{-4}) was found overall.

In the mesopelagic domain, observed and simulated sPOC stocks ranged between 145–283 mmol C m^{-2} and 105–308 mmol C m^{-2}, respectively, and the correlation between simulated and observed mesopelagic sPOC stocks was not significant (r = -0.08, p = 0.55). PISCES sPOC was similar to or slightly higher than BGC-Argo sPOC in the subpolar biomes, but up to two-fold lower in the STG and Mediterranean biomes (as already shown in Fig. 4 and 7).

Epipelagic bPOC stocks were smaller and showed wider inter-biome variability than sPOC stocks, with around twofold higher bPOC in subpolar biomes. The positive correlation between simulated and observed bPOC was highly significant (r = 0.78, p = 2·10^{-11}). Yet, PISCES bPOC (range 19–83 mmol C m^{-2}) typically exceeded BGC-Argo bPOC (range 27–119 mmol C m^{-2}) by around 50%, and up to threefold for some CATS. A lower but still highly significant correlation was found in the mesopelagic (r = 0.64, p = 5·10^{-7}), where PISCES bPOC was usually within a factor of 1.5 of observations, except for the NASPG biome where it exceeded BGC-Argo bPOC by around twofold.

The sPOC/tPOC fraction showed low variability in the epipelagic layer (Fig. 9), with a median (range) of 89% (84–94%) and 85% (75–91%) for BGC-Argo and PISCES, respectively. The simulated sPOC/tPOC fraction was within ±10% of BGC-Argo estimates for all biomes except the NASPG, where PISCES tended to underestimate the observed percentage of sPOC. A significant positive correlation (r = 0.56, p = 2·10^{-5}) was found between simulations and observations in the epipelagic layer. The sPOC/tPOC fraction was lower in the mesopelagic layer according to both BGC-Argo (75–90%) and PISCES (66–85%) estimates. In this case, CATS from the Subantarctic biome showed excellent model-observations agreement,

whereas PISCES was 20% lower than BGC-Argo estimates in the other three biomes. No significant correlation was found between the simulated and observed sPOC/tPOC fraction in the mesopelagic.

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Transfer efficiency (Teff; Fig. 10) was computed as the ratio between the sPOC or bPOC concentrations in the depth bins centered at 697 m (range 662–734 m) and 200 m (range 190–210 m). The shallowest bin corresponds to the bottom of the epipelagic layer, and the 500 m interval was chosen following previous studies (Lam et al., 2011; Dall'Olmo and Mork, 2014). Different depth ranges between 180 and 800 m gave similar Teff patterns. Analysis of Teff yielded some important

420 insights:

1. Small and big POC showed similar Teff, both in the observations (medians of 0.39–0.41) and in the model (medians of 0.27–0.29). Similar patterns were found when each biome was considered separately.

2. BGC-Argo Teff usually exceeded PISCES Teff and spanned a wider range. The best agreement was generally found in the STG and the Subantarctic biomes, and the poorest agreement occurred in the Mediterranean where

425 BGC-Argo Teff was typically twice the modelled Teff.

3. Distinct patterns were found for four CATS in the Labrador Sea (NASPG) characterized by high epipelagic tPOC (>440 mmol C m^{-2}). In this subset, PISCES and BGC-Argo Teff were in good agreement for sPOC (median 0.40 for both) whereas, for bPOC, PISCES Teff (0.36–0.45) doubled BGC-Argo Teff (0.12–0.28), which had some of the lowest values of the dataset. These CATS showed a bPOC minimum at 600–800 m in fall, which PISCES could not

430 reproduce (section 3.2.1).

4. PISCES and BGC-Argo Teff showed a weak positive correlation for sPOC (r = 0.26, p = 0.07), with some improvement when the Labrador Sea "outliers" were removed (r = 0.34, p = 0.02). A negative correlation between simulations and observations was found in the case of bPOC Teff (r = -0.29, p = 0.04), which became non-significant without the Labrador Sea "outliers" (r = 0.04, p = 0.81).

435

Our observational estimates are sensitive to the choice of b_{bp700}-POC conversion factors. These factors are especially uncertain in the mesopelagic due to data scarcity, which prompted us to use a constant global value for "c" in Eq 1. (Fig. 2); c = 1000 mmol C m^{-2} is the asymptotic POC-b_{bp700} conversion factor below 1000 m, taken from Cetinić et al. (2012). To address this uncertainty, we conducted sensitivity tests where c was halved or doubled. The resulting range of 500–2000

440 mmol C m^{-2} is probably generous, as our indirect estimates based on the study of Bishop et al. (1999) suggest a plausible range of 815–1630 mmol C m^{-2} (Appendix A). As expected, changing c had little effect on epipelagic POC, a larger effect on mesopelagic POC and Teff, and no effect on the sPOC/tPOC fraction (because the same conversion factor is used to estimate sPOC and bPOC). Halving c resulted in steeper POC profiles, which brought mesopelagic sPOC closer to the 1:1 line in the STG and Mediterranean, at the expense of increasing the sPOC bias in the subpolar biomes and that of bPOC everywhere

445 (Fig. S11). Doubling c caused a less steep vertical decrease of BGC-Argo POC, which overall worsened the model-observations agreement in the mesopelagic (Fig. S12) for sPOC stocks, bPOC stocks (except in the NASPG) and Teff.

4. Discussion

4.1 Towards a globally consistent picture of POC fields in observations and models

Global quantification of POC stocks through the water column has been elusive until recently. On the one hand, direct
450   chemical measurements (Lam et al., 2011) and indirect bio-optical observations from ships (Bishop et al., 1999; Gardner et
al., 2006) were sparse, and the ocean interior was severely undersampled compared to the euphotic layer. On the other hand,
biogeochemical models were unable to capture even the order-of-magnitude POC concentration in the meso- and
bathypelagic layers (Aumont et al., 2017). Our joint analysis of PISCES simulations, satellite observations and over 70,000
BGC-Argo vertical profiles reveals a globally consistent picture across the epi- and mesopelagic layers (Fig. 3-10). PISCES-
455   simulated tPOC concentration is on average within a factor of 1.56 (1.42) of BGC-Argo estimates for the median (mean)
seasonal biome profiles shown in Fig. 4 (Mediterranean excluded). Aumont et al. (2017) reported a similar reliability index
of 1.6 for the comparison between PISCES and in situ chemically determined POC profiles. Thus, our evaluation lends
further confidence to the POC reactivity continuum parameterization implemented in PISCES, which represents both sPOC
and bPOC as a mixture of fractions with different lability (Aumont et al., 2017), in globally representative biomes.

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PISCES simulates a global tPOC stock of 4 Pg C, shared in a proportion of 39% (1.6 Pg C), 25% (1 Pg C) and 36% (1.4 Pg
C) between the epi-, meso- and bathypelagic layers (Table 2). The PISCES-derived estimate for the epipelagic layer, 1.6 Pg
C, lies well within the range of previous estimates based on satellite observations. Gardner et al. (2006) estimated the global
POC stock within the first attenuation depth using a compilation of in-situ POC and c_p measurements leveraged by ocean
465   color satellite data. They obtained a global stock of 0.43 Pg C, and invoked some scaling arguments to estimate that the total
POC stock down to middle-mesopelagic "background levels" would range 1–2 Pg C. Stramska (2009) obtained a global
epipelagic POC stock of 1.8–2.3 Pg C using the algorithm of Stramski et al. (2008). Our analysis of the match-ups between
BGC-Argo and satellite observations indicates that the latter algorithm overestimates POC at high latitudes outside of the
summer season (Fig. 3). Potential explanations are the satellite algorithm being calibrated mostly against samples from lower
470   latitudes (50°N–30°S), or its sensitivity to the differential atmospheric attenuation of the blue and green wavelengths at low
solar elevation (i.e. at high latitudes in winter). Recently, Evers-King et al. (2017) calculated the global mixed-layer POC
stock using several satellite algorithms (including that of Stramski et al., 2008) and indicated that 0.77–1.3 Pg C was a
plausible range. Our PISCES-based estimate for the mixed-layer POC stock, using the same MLD climatology (Schmidtko
et al., 2013), is 0.58 Pg C. In this case, the lower PISCES-derived estimate may arise from the combination of POC
475   overestimation by some satellite algorithms, discussed above, with PISCES' tendency to underestimate mixed-layer POC in
oligotrophic areas. This negative bias in PISCES is compensated by POC overestimation in deep Chla maxima below the
MLD (Fig. 4 and 7), resulting in good agreement between BGC Argo and PISCES over the entire epipelagic layer in the
STG biome (Fig. 8 and S13). Given the limited coverage of in situ seawater sampling and satellite observations in some

regions and seasons (Evers-King et al., 2017), further intercomparison between those observations, BGC-Argo data and

480   models is needed to better constrain epipelagic POC stocks.

POC in the lower mesopelagic and below has been traditionally treated as a "background" signal (Bellacicco et al., 2019; Gardner et al., 2006; Loisel and Morel, 1998). This approach is convenient for studies that focus solely on upper-ocean processes because POC concentration decreases exponentially with depth. Yet, our global estimates and several previous

485   studies highlight the need to turn our attention to the large POC stocks (>2 Pg C) that reside in the mesopelagic and below it, whose dynamics are still poorly understood. In line with previous studies (Dall'Olmo and Mork, 2014; Poteau et al., 2017), we showed that mesopelagic POC exhibits clear seasonal cycles in productive regions (Fig. 6, S5–S7 and S10), owing to their connection with the upper-ocean through numerous biological and physical processes (Boyd et al., 2019; Briggs et al., 2020). Despite being less reactive on average than upper-ocean POC, meso- and bathypelagic organic particles are microbial

490   hotspots that host key biogeochemical functions, from enzymatic decomposition of macromolecules (Arnosti et al., 2012; Baltar et al., 2010a, 2010b) to aerobic and anaerobic respiration (e.g., Karthäuser et al., 2021) and chemosynthesis (Arístegui et al., 2009; Pachiadaki et al., 2017). Moreover, mesopelagic particles are consumed by upper trophic levels that sustain fisheries (Bode et al., 2021; Woodstock et al., 2021).

495   In situ bio-optical measurements are poised to play a key role in monitoring marine POC stocks in layers that cannot be accessed by remote sensing. For example, Sauzède et al. (2020) illustrated the power of merging BGC-Argo and satellite observations to obtain a dynamic 3D view of particle backscattering. Using a data-driven machine learning approach, they were able to predict the profiles of $\log_{10}b_{bp700}$ measured by two BGC-Argo floats in the NASPG and STG biomes (R^2 of around 0.85 and MAPD of around 12%) from the sole knowledge of physical properties of the water column and surface

500   ocean color (remote sensing reflectance). Their approach was recently extended to provide POC estimates (Sauzède et al., 2021), which can be of great utility for constraining biogeochemical models. Here we took an entirely different approach, based on converting b_{bp700} to POC with a simple empirical algorithm (Fig. 2) and then comparing it to the outputs of the PISCES model. Our PISCES-based estimates obtained a median $R^2 = 0.86$ and MAPD = 38% for 5-day depth-binned $\log_{10}$POC for 28 globally distributed floats. This good skill is remarkable because neither the empirical POC estimates nor

505   PISCES were tuned to maximize their mutual agreement. Still, our study shows that the comparison of bio-optics-derived POC measurements and PISCES is affected by different types of uncertainty that we analyze in the four sections below.

4.2 Bio-optical underpinnings of POC fields based on BGC-Argo observations

Accurate interconversion between bio-optical variables and concentrations is key for constraining ocean particle dynamics and their model representation (Bishop et al., 2004; Gardner et al., 2006). The variability in b_{bp700}-POC conversion factors is

510   shaped by several concurrent processes that alter particle abundance, size distribution, shape, composition, and ultimately

optical properties. Below we discuss the processes that appear to drive, to first order, the variability of the POC/b_{bp700} ratios embodied in Eq. 1 and 2 (Fig. 2; Appendix A), and the main strengths and weaknesses of our scheme.

Changes in the trophic status appear as the primary driver POC/b_{bp700} variability in the epipelagic layer (Cetinić et al., 2012;

515   Figure A1). Productive waters host greater absolute and relative abundance of diatoms (Uitz et al., 2006) (see also Table 2), which have lower POC per cell volume (Menden-Deuer and Lessard, 2000) and are covered with silica frustules that may scatter light more efficiently than naked cells (Twardowski et al., 2001), altogether resulting in lower POC content per unit b_{bp700} (Cetinić et al., 2012; Oubelkheir et al., 2005). The proportions of different autotrophic and heterotrophic organisms and detritus are also likely to vary with upper ocean productivity (see 4.3). If the mass-specific backscattering coefficients of

520   these components were better known, their systematic variation patterns could be used to develop a continuous formulation for POC/b_{bp700}, rather than the regionalized conversion factors used here. However, POC/b_{bp700} is influenced by other seawater constituents whose occurrence is less predictable. Foremost, biogenic calcite (e.g. from coccolithophores) and desert dust (Claustre, 2002; Loisel et al., 2011), both of which enhance b_{bp700}. In our data set, we detected a CATS (float WMO 6901647, year 2016) that was strongly affected by coccolith backscattering in the Iceland Basin, an area known for its

525   massive coccolithophore blooms (Moore et al., 2012). This CATS was an obvious outlier in our model-observations scatterplots (Fig. S13), likely because coccolith-enhanced b_{bp700} resulted in spuriously high observed tPOC, and was therefore removed from the analysis.

The decrease in POC/b_{bp700} along the vertical axis (Fig. 2) reflects the increase in the particles' index of refraction, hence the

530   backscattering ratio (Cetinić et al., 2012; Nencioli et al., 2010). This change is likely caused by the remineralization of organic materials (Martin et al., 1987) that leaves a higher mineral fraction (Honjo et al., 2008; Lam et al., 2011), and the increase in the structural complexity of aggregates with depth (Organelli et al., 2018). According to our sensitivity analysis (Fig. S11 and S12), the prescribed exponential decrease of POC/b_{bp700} towards a constant POC/b_{bp700} (c = 1000 mmol C m^{-2}) at depths >1000 m provides a good compromise globally, given the limited knowledge of mesopelagic

535   POC/b_{bp700} and its variability across regions. However, the comparison between simulated and observed mesopelagic sPOC (and thus tPOC) is more favorable in subpolar than in subtropical biomes. In the latter, better model-observations agreement was found when POC/b_{bp700} was halved (c = 500 mmol C m^{-2}). A lower c would also bring the simulated Teff for sPOC and bPOC closer to BGC-Argo estimates. It is tempting to hypothesize that lower latitudes have lower mesopelagic POC/b_{bp700} owing to the greater proportion of calcite (Francois et al., 2002; Honjo et al., 2008; Lam et al., 2011, 2015). These

540   hypotheses need further verification.

Finally, the decrease of surface POC/b_{bp700} with deeper vertical mixing imposed by Eq. 2 reflects the dilution of surface particle assemblages by entrainment of deeper waters (Lacour et al., 2019) with lower POC/b_{bp700} (Bol et al., 2018). Modulation of POC/b_{bp700} by vertical mixing improves the agreement between PISCES and BGC-Argo data in regions with

545 wide seasonal MLD amplitude such as the NASPG. Note also that if POC/b_{bp700} in the mixed layer was constant, it would have to decrease abruptly below the mixed layer to meet the low POC/b_{bp700} in the mesopelagic. On the other hand, the behavior prescribed by Eq. 2 may not be appropriate for situations when vertical mixing cannot erode the seasonal thermocline or pycnocline, because in such cases it will entrain water from the deep Chla maximum, and not mesopelagic water, to the upper mixed layer.

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Our POC-b_{bp700} conversion algorithm omits several aspects that may have caused further uncertainty. Foremost, it assumes that sPOC and bPOC have the same POC/b_{bp700} ratio, which largely corresponds to that of the more abundant sPOC (Fig. 6–8). In addition, the in-situ data used to parameterize Eq. 1 and 2 are not free of uncertainty (Cetinić et al., 2012; Lam et al., 2011; Morán et al., 1999; Organelli et al., 2018; Strubinger Sandoval et al., 2021). While the development of more

555 sophisticated POC-b_{bp700} interconversion schemes is desirable, the POC-b_{bp700} conversion scheme used here provides POC estimates that are generally consistent with PISCES (Fig. 8) and with previous assessments (Aumont et al., 2017). Moreover, this scheme allowed us to identify potential shortcomings of satellite-based assessments (Evers-King et al., 2017; Stramski et al., 2008). Indeed, bio-optical estimates of POC, and more generally BCP studies, would greatly benefit from the measurement of mass-specific bio-optical properties of various seawater constituents across different ocean basins and

560 depths.

4.3 Correspondence between observed and simulated POC fractions

An additional source of uncertainty in our analysis is the imperfect match between the PISCES tracers and the observable POC fractions (Table 1). A positive aspect of our evaluation is the reasonable agreement between the simulated sPOC/tPOC fraction and the BGC-Argo estimates based on the b_{bp700} spike signal (Fig. 9). Our estimates converge to a global median

565 value of 85%, with 95% of the data between 69–92%, fully within the range of size-fractionated chemical POC determination (Aumont et al., 2017 and references therein). Our sPOC/tPOC estimates can also be compared to the suspended POC estimated with the marine snow catcher during spring in subpolar epipelagic and upper mesopelagic waters (Baker et al., 2017). The slow-sinking POC measured by the marine snow catcher should not be included in this comparison because it sinks at around 18 m d^{-1}, a range more typical of particles > 100 μm (Giering et al., 2016). The median 94% of

570 suspended (non-sinking) POC reported by Baker et al. is higher than the 86% (81%) sPOC/tPOC estimated here from BGC-Argo (PISCES) in the subpolar biome, suggesting further comparison between different approaches is needed. The tendency of sPOC/tPOC to decrease between the epipelagic and the mesopelagic, found in both PISCES and BGC-Argo data (Fig. 9, Table 2), was also reported in previous studies (Aumont et al., 2017 and references therein; Organelli et al., 2020), lending further confidence to our estimates. On the other hand, the simulated partitioning of sPOC and bPOC into different living

575 and detrital compartments is probably less realistic, as discussed in greater detail below.

A problematic aspect in the current representation of sPOC in PISCES is the partitioning between phytoplankton and non-phytoplanktonic (detrital + heterotrophic) POC in the upper ocean. This partitioning is far from being well established, neither from bio-optical observations nor from direct determination. Starting with bio-optical approaches, Oubelkheir et al.

580 (2005) found that detritus accounted for around 60% of POC across a wide range in ocean productivity, and 70–85% of POC was assigned to detritus + heterotrophs. These percentages accord well with those found by Claustre et al. (1999) in the tropical Pacific (their Table 1; see also Organelli et al., 2020). By contrast, Bellacicco et al. (2020) suggested that the non-phytoplanktonic b_{bp700} fraction varies widely, between <10% in the productive NASPG to >80% in subtropical gyres. Given the similar refractive indexes of living cells and organic detritus, hence similar POC/b_{bp700}, the latter and former estimates are

585 hardly compatible when compared in POC units. Estimates based on direct POC stock determinations across wide productivity gradients are also conflicting. Gasol et al. (1997) found a general increase in the autotrophic/heterotrophic ratio with productivity, with ratios as low as 0.1 at low autotrophic biomass. By contrast, Graff et al. (2015) found that phytoplankton accounted for between 15–85% of POC, with decreasing phytoplankton contributions at lower POC or Chla concentration (their figures 4 and 7), leaving no room for heterotrophs and detritus. Indeed, the two latter studies agree in the

590 wide scatter in large-scale POC partitioning patterns, may further confound in situ bio-optical estimates. The low fraction of detrital POC in PISCES near the sea surface, 15–31% (Fig. 4; Table 2) is at odds with most observations, and suggests too slow transfer of planktonic biomass to detritus and/or too fast detrital POC removal, especially in oligotrophic waters.

PISCES bias may also arise from inappropriate representation of some POC reservoirs, such as heterotrophic prokaryotes

595 (bacteria and archaea, *BACT* in PISCES), which have long been recognized as important contributors to the suspended POC (Morel and Ahn, 1990; Gasol et al., 1997). However, *BACT* are not explicitly modelled in PISCES as prognostic tracers, meaning they are not interacting fully with other tracers. Instead, they are diagnosed in the productive surface layer from zooplankton biomass, based on an old model version that had interactive *BACT*. Below this layer, *BACT* biomass is propagated downwards with a power function based on Arístegui et al. (2009), which resembles a Martin curve (Martin et

600 al., 1987) and is therefore very sensitive to the reference depth (Z_0) (Buesseler et al., 2020). We find two main arguments against the inclusion of PISCES-estimated *BACT* in our POC estimates with the current model configuration. First, the empirical *BACT* estimation in PISCES has not been validated, to our knowledge, and may introduce noise in the comparisons. Second, PISCES-simulated POC already includes heterotrophic prokaryotes, because their biomass was not removed from the in situ POC measurements used to adjust the POC parameters in PISCESv2 (Aumont et al., 2017). In

605 consequence, adding *BACT* to sPOC causes overestimation of mesopelagic POC (Fig. S14–S16) and can produce unrealistic temporal patterns (Fig. S15). Nevertheless, we believe that inclusion of prognostic bacteria would enable more realistic simulation of POC stocks, with the potential side effect of improving the simulation of element fluxes in PISCES.

The comparison between simulated and observed bPOC is a novel contribution of our study. The method of Briggs et al.

610 (2011, 2020), originally developed to study intense POC export events, was here extended to estimate sPOC and bPOC

separately over the full annual cycle through the epi- and mesopelagic domains. Our analysis shows that, despite the mismatch in terms of concentration, the bPOC derived from the spikes of high-resolution bio-optical profiles is strongly correlated to the PISCES-simulated bPOC (r = 0.78, r^2 = 0.61) along a wide trophic gradient (Fig. 8). This result is encouraging and supports the more widespread deployment of instruments that perform high-resolution bio-optical sampling

615 to shed light on the spatiotemporal dynamics of large aggregates and particles (Briggs et al., 2020; Lampitt et al., 1993; Stemmann et al., 2008). On the other hand, it is unclear to what extent the bPOC inferred from the b_{bp700} spike signal is capturing mesozooplankton biomass, in addition to aggregates. Exclusion of PISCES mesozooplankton (*ZOO2*) from the comparison increases model-observations mismatch, with BGC-Argo bPOC exceeding PISCES estimates by around twofold, although the correlation remains nearly unchanged (r = 0.76, p < 10^{-10}). Imaging devices mounted on BGC-Argo

620 floats may provide more accurate quantification of bPOC, allowing for the separation of detrital bPOC (Trudnowska et al., 2021) from mesozooplankton and micronekton (Haëntjens et al., 2020).

4.4 Importance of realistic physics and model evaluation across scales

In Fig. 5, PISCES simulations and BGC-Argo observations are compared using an array of skill metrics computed on the seasonal vertical profiles of tPOC between 0–1000 m. Starting with the 3D seasonal climatology, we observed that the

625 correlation between the median (aggregated) profiles was generally better than the correlation between the spatially collocated (non-aggregated) profiles within a given biome and season (Fig. 5a), whereas no differences were found in terms of dispersion metrics (Fig. 5b and c). The difference in correlation was larger in subpolar biomes, suggesting that the model-observations spatial mismatch was magnified in regions with more energetic ocean dynamics and sharper physical and biogeochemical gradients, whose real-world location may not be well reproduced by the ocean circulation model used to

630 force PISCES. For PISCES 1D simulations, their correlation coefficients with their CATS counterparts was usually in the high range of the correlation coefficients obtained by the biome-median PISCES 3D profiles. In terms of dispersion metrics, the ensemble of PISCES 1D simulations showed wider dispersion, but the best 1D simulations clearly outperformed the 3D simulation in a given region and season. The better skill of 1D simulations was more evident during spring, a season characterized by the onset of stable stratification after deep winter vertical mixing in middle and high latitudes. The greatest

635 difference between 3D and 1D simulations was found in the Mediterranean, highlighting the more realistic vertical mixing and upper ocean productivity in the 1D simulations.

Our cross-scale evaluation indicates how crucial it is to evaluate model physics before extracting conclusions on biogeochemical model performance (Doney et al., 2004; Kriest et al., 2020; Löptien and Dietze, 2019). In our 1D CATS

640 approach, the skill of PISCES simulations was maximized by carefully matching observed and modelled vertical mixing (Fig. S1–S4), which is a key driver of upper ocean ecosystems. This approach has a subjective component, and may also suffer from the idealized assumption that BGC-Argo profiles reflect mostly vertical-scale processes, disregarding horizontal advection (Alonso-González et al., 2009). Yet, the similar misfit patterns encountered for different CATS within a given

biome support the robustness of the 1D matching approach (compare Fig. 6 versus S6, and Fig. 7 versus S9). To further

645   evaluate this issue, we matched different neighboring NEMO grid cells to the same in situ CATS. Again, this exercise indicated that our main conclusions are not sensitive to the choices made for 1D model-observations matching (compare Fig. 6 and Fig. S5). Indeed, alternative matching approaches can be devised, each of which with advantages and pitfalls, for example: (1) sampling the outputs of biogeochemical models at the locations visited by BGC-Argo floats, which may require high resolution models; (2) deploying virtual BGC-Argo floats (van Sebille et al., 2018) and comparing them statistically to

650   observations; or (3) forcing 1D biogeochemical simulations with observed physical fields, e.g. vertical mixing (Llort et al., 2015) or light (Terzić et al., 2019). As a general rule, the good skill of the best PISCES 1D simulations (Fig. 5) indicates that our CATS approach can be used to tease apart model-observations misfits caused by model physics from those caused by the parametric uncertainty and the structure of the biogeochemical model, opening up new avenues for parameter optimization (Falls et al., *submitted*) and model development.

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Our cross-scale evaluation is also informative as to the spatiotemporal scales that can be addressed with a given model setup. This matter was recently tackled by Bisson et al. (2019) using the export production model of Siegel et al. (2014), which is forced by satellite-derived primary production. In particular, they showed that this diagnostic model could be optimized to reproduce global climatological patterns, but exhibited poor skill when faced with non-climatological datasets, which reflect

660   local snapshots of ecosystem functioning. Model evaluation at climatological scales provides an incomplete picture, especially in productive regions where much POC export can take place during intense but short-lived events (Briggs et al., 2020). Such events are smoothed out when climatologies are computed, and their coherence with the physical forcing is lost. Our work shows that a prognostic model like PISCES can afford both event-scale and climatological scale predictions. This capability is important to test our process-level understanding, which underpins climate change projections.

665   **4.5 Joint use of BGC-Argo and models for process-level understanding**

Properly representing POC stocks is crucial for constraining epi- and mesopelagic carbon budgets and, ultimately, estimating the strength of the BCP and predicting its future evolution. The mismatch patterns between simulated and observed POC profiles (Fig. 4, 6 and 7) indicate different types of model shortcomings in subpolar and subtropical latitudes. The poorest agreement between PISCES and BGC-Argo data is found when their respective estimates of mesopelagic Teff are compared

670   (Fig. 10), which should prompt further research on this key descriptor of the BCP, both in terms of POC fluxes (Buesseler et al., 2020) and stocks (Lam et al., 2011; this study), and their relationship with the structure and productivity of the upper ocean ecosystem.

In the subpolar biomes, we find discrepancies between the patterns of sPOC and bPOC vertical export triggered by the

675   intense surface phytoplankton blooms typical of these waters (Fig. 6, S5–S7 and S10). The observed rapid sPOC increase at depth cannot be explained by the sPOC gravitational sinking, and fragmentation of rapidly sinking bPOC has to be invoked

(Briggs et al., 2020). This fragmentation is most likely caused by zooplankton feeding (Mayor et al., 2020; Stemmann et al., 2004a, 2004b; Stukel et al., 2019) and swimming (Goldthwait et al., 2004), combined with bacterial hydrolysis of aggregate-binding polymers (Arnosti et al., 2012; Baltar et al., 2010a). In relative terms, mesopelagic sPOC increases less strongly than

680   bPOC during blooms (Fig. 6i), which is consistent with sPOC being a byproduct of the transformation of less-abundant bPOC. Fragmentation processes may supply fresher sPOC to the mesopelagic, enhancing the coexistence of suspended particles with variable freshness (Alonso-Gonzalez et al., 2010; Aumont et al., 2017) and overall contributing to POC remineralization (Giering et al., 2014; Mayor et al., 2020).

685   In the subtropical gyres and the most oligotrophic Mediterranean waters, PISCES underestimates tPOC between 0–1000 m except for the deep Chla maximum, where it overestimates tPOC. The prominent deep POC maximum simulated by PISCES is generally not found in observations from the STG biome (Fig. 7 and S9), where deep Chla maxima generally reflect phytoplankton photoacclimation, not enhanced phytoplankton biomass (Cornec et al., 2021). Thus, PISCES possibly overestimates the productivity of deep Chla maxima globally, indirectly causing stronger nutrient limitation at the surface.

690   Between the deep Chla maximum and 200 m, POC pools decrease more steeply in PISCES than in BGC-Argo observations. Between 200 and 700 m, by contrast, simulated sPOC and bPOC Teff are only 10% lower than observations, well within observation uncertainty. Thus, the mesopelagic sPOC deficit simulated by PISCES in the STG originates mostly through the insufficient vertical POC export at 200 m depth. The Mediterranean represents a different case, whereby the large disagreement between PISCES and BGC-Argo Teff may result from either poorly constrained POC/b_{bp700}, simulated POC

695   dynamics, or both. Thus, this region may provide a good testbed for studying the role of the mineral fraction in the BCP, including the controversial ballast hypothesis (Francois et al., 2002; Klaas and Archer, 2002; Passow, 2004).

In summary, the mismatch with observations suggests the need to improve the representation of sPOC–bPOC interconversion in PISCES. The size distribution of POC along the vertical axis is a key variable for constraining POC

700   budgets, because it reflects the interplay between gravitational sinking, remineralization, trophic transfer and 3D dynamics including horizontal POC advection (Alonso-González et al., 2009; Boyd et al., 2019). In many instances (Fig. 9), our analysis suggests that better model performance in the mesopelagic may be achieved by increasing the net transfer of bPOC to sPOC and the Teff of both fractions, which may require further balancing the interplay between various mechanisms of POC export and flux attenuation. The vertical model-observations mismatch patterns observed here emphasize that POC

705   budgets have to be computed with the highest vertical resolution affordable, or otherwise an apparent POC budget balance may result from compensating imbalances in different horizons (Giering et al., 2014; Marsay et al., 2015). The detailed level of information available from BGC-Argo floats may prove to be extremely valuable to help improve the POC schemes embedded in models such as PISCES.

5. Conclusions and outlook

710   In this study we compared globally distributed POC observations between 0–1000 m made by BGC-Argo floats to the predictions made by the PISCES model (PISCESv2). A subset of BGC-Argo floats profiling at high vertical resolution enabled us to analyze small and big POC separately. The comparisons rely on a proposed new scheme for converting a bio-optical measurement (b_{bp700}) to POC. Although PISCES recreates with good skill the main features observed in subpolar and subtropical biomes, the comparison is still hampered by: (1) spatial and temporal variability in POC/b_{bp700} conversion

715   factors, (2) mismatches in observed and simulated physics, and (3) imperfect correspondence between observed and simulated POC fractions. Evaluation of these uncertainties allowed us to detect limitations of the biogeochemical model parameterizations, which may arise from both suboptimal model parameters and model structure. Therefore, the descriptive work and model-data matching strategies presented here pave the way towards the use of BGC-Argo observations for data assimilation and model parameter optimization (Falls et al., *submitted*) and, ultimately, model development.

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Widespread use of BGC-Argo data for understanding POC budgets and the BCP can complement classical model constraints based on vertical POC fluxes and ocean-interior nutrient remineralization. Merging of BGC-Argo and satellite data streams through data-driven approaches —which allow for great flexibility—, and mechanistic models —which provide process-level understanding—, can soon provide us with a high-resolution 4D view of the oceanic carbon cycle. Further work is

725   granted to investigate POC dynamics through combination of PISCES2 and autonomous observations.

Below we list several research priorities, whose implementation would advance the study of the biological carbon pump through the synergies between BGC-Argo observations and modelling.

- Observations:

730   o   High-resolution bio-optical profiles are indispensable for process-level understanding. Combination of low- and high-resolution sampling in separate or individual floats (e.g. burst sampling) may provide a good compromise between float lifetime and observation capabilities.

      o   More in situ collocated measurements of chemical and bio-optical variables are needed to constrain b_{bp700}-POC conversion factors, especially in meso- and bathypelagic waters.

735   o   Inclusion of new sensors (e.g. Claustre et al. (2020) and extension of measurements into the bathypelagic (Deep-Argo; e.g. Roemmich et al., 2019) hold high potential for advancing BCP research.

      o   Further developments in BGC-Argo data processing are needed, with the final goal of supplying a wide public with user-friendly data products in near real time.

- Models:

740   o   Evaluating model skill at resolving POC stocks, in addition to fluxes, is key to ensure that models reproduce observed fluxes for the right reasons.

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- o Evaluation against globally consistent datasets is critical to avoid model overtuning towards small, sparse datasets, such as vertical POC fluxes.

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- o Continuous development of schemes representing particle dynamics across the entire size spectrum is needed to constrain ecologically, climatically and economically relevant element fluxes.
- o Extension of prognostic modelling of bio-optical properties (Dutkiewicz et al., 2019) into the meso- and bathypelagic layers would enable direct matching with measurements made from autonomous platforms, facilitating their assimilation by models.

- • Joint planning of field observation and modelling projects, from their very conception and through their entire

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development, is key to fully exploit the capabilities of each approach.

Appendix A: Calculation of POC/b_{bp700} ratios and related optical considerations

POC/b_{bp700} ratios at the sea surface were obtained from the slope of the linear regression between POC and b_{bp700} (Table A1). Our approach essentially follows the literature compilation made by Cetinić et al. (2012). The linear regressions generally yielded small and non-significant y intercepts for sea-surface data. Therefore, we assumed the slopes were equal to the POC/b_{bp700} ratio. When the b_{bp} measurements were made at another wavelength, we converted them to b_{bp700} assuming an exponent $\eta = 0.41$ (Cetinić et al., 2012), according to the equation:

$$b_{bp}(\lambda_1) = b_{bp}(\lambda_0) * (\lambda_1/\lambda_0)^{\eta} \qquad (A1)$$

For measurements taken at 555 nm, which was the wavelength used in two studies (Table A1), this resulted in 10% lower b_{bp700} compared to b_{bp555}, thus higher POC/b_{bp700} ratios.

The dataset of Cetinić et al. (2012) was the only one showing a significant negative intercept of the POC vs. b_{bp700} linear regression. Unlike the other datasets, where the POC vs. b_{bp700} relationship reflected mostly sea-surface variability in a given biome, this was the only dataset that included data collected between the sea surface and 600 m. Bol et al. (2018) reprocessed this dataset by computing the linear regression between POC and b_{bp700} in different depth bins, forcing the intercept through zero. The slope of the POC vs. b_{bp700} regressions, and therefore the POC/b_{bp700} ratio, decreased by more than twofold between the surface and the 600 m bins. These results suggest that the POC vs. b_{bp700} relationship may be better modelled with nonlinear equations, as done for surface data in some previous studies (Balch et al., 2010; Johnson et al., 2017; Stramski et al., 1999). However, one must keep in mind that the ecosystem processes that define POC/b_{bp700} ratios in the surface layer may be different from those occurring in the mesopelagic (see Discussion, 4.2).

The conversion between POC and particulate beam attenuation at 660 nm, c_p, in the surface ocean has been analyzed on more occasions than its b_{bp700} counterpart. The backscattering ratio, b_{bp}/b_p, relates particulate backscattering to the total particulate scattering, and is directly related to the refractive index of the particle assemblage (Babin et al., 2003; Dall'Olmo et al., 2009; Loisel et al., 2011; Organelli et al., 2018; Stramski and Kiefer, 1991; Stramski et al., 1999; Twardowski et al., 2001; Ulloa et al., 1994). Light absorption by particles is negligible in the 650-700 nm spectral region, such that total beam attenuation c_p is a good approximation of the scattering coefficient b_p. Thus, once the known absorption and scattering coefficients of seawater are removed, b_{bp}/c_p is a good approximation of the backscattering ratio, and can be used to compare the relationships between POC vs. c_p and POC vs. b_{bp700}.

The observed POC/b_{bp700} variability in the surface layer across biomes reflected in our POC estimation algorithm is analogous to that found for the relationship between POC/c_p by Cetinić et al. (2012), as shown in Figure A1, although fewer POC-b_{bp700} datasets are available. The POC content per unit b_{bp700} decreases with the maximum b_{bp700} of each dataset, which may be related to the structure and species composition of upper-ocean ecosystems (see Discussion, 4.3). Given that the

805 backscattering coefficient is sensitive mostly to particles smaller than 30 µm (Organelli et al., 2018), it is also plausible that the portion of POC that contributes to backscattering varies across sites, further enhancing POC/b_{bp700} variability.

The number of studies that tackled POC vs. bio-optical conversion in the mesopelagic layer is much smaller than those that focused on the epipelagic layer. Besides Cetinić et al. (2012) in the subpolar North Atlantic, we are only aware of the study

810 of Bishop et al. (1999) in the northeast Subarctic Pacific. The latter study found a POC vs. c_p slope of 16.3±0.49 mmol C m^{-2} (= mmol C m^{-3} / m^{-1}) over the 0–1000 m depth range (the positive regression y-intercept in that study corresponds to absorption by seawater). This slope lies in the low range of the compilation shown in Fig. A1a (196±5.9 mg C m^{-2} in mass units). A close-up into the lower measurement range (Fig. 5 of Bishop et al., 1999) shows that the slope was not clearly distinct for POC concentration < 0.5 mmol m^{-3}, typical of the mesopelagic layer. If we assume that the backscattering ratio

815 was likely between 1 and 2% in the mesopelagic, then we obtain a POC/b_{bp700} ratio of 815-1630. This range is compatible with the POC/b_{bp700} of ~1000 mmol C m^{-2} found at 600 m by Bol. et al. 2018, which we used as the asymptotic deep POC/b_{bp700} ratio in Eq. 1. Note that the linear relationship between c_p and POC is compatible with the nonlinear relationship between POC and b_{bp700} along the vertical profile if the backscattering ratio also increases with depth, as found by Cetinić et al. (2012). The latter study found an increase in the backscattering ratio (b_{bp700}/c_{p653}) from around 1.2% at the surface to

820 around 1.5% in the upper mesopelagic. The b_{bp700}/c_{p653} ratio was more variable in deeper layers and values > 2% were not rare (see also Nencioli et al., 2010; Organelli et al., 2018; Twardowski et al., 2001).

Beyond the natural variability, the interconversion between POC and bio-optical proxies is also confounded by methodological, most of which were not fully addressed in the studies compiled here. Measurement of POC in the lower

825 mesopelagic (below 500 m) requires filtration of large sample volumes in the m^3 range (Bishop et al., 1999), otherwise POC concentration rapidly approaches the detection limit with procedures and filtration volumes used for the epipelagic and the upper mesopelagic (Cetinić et al., 2012; Strubinger-Sandoval et al., 2021).

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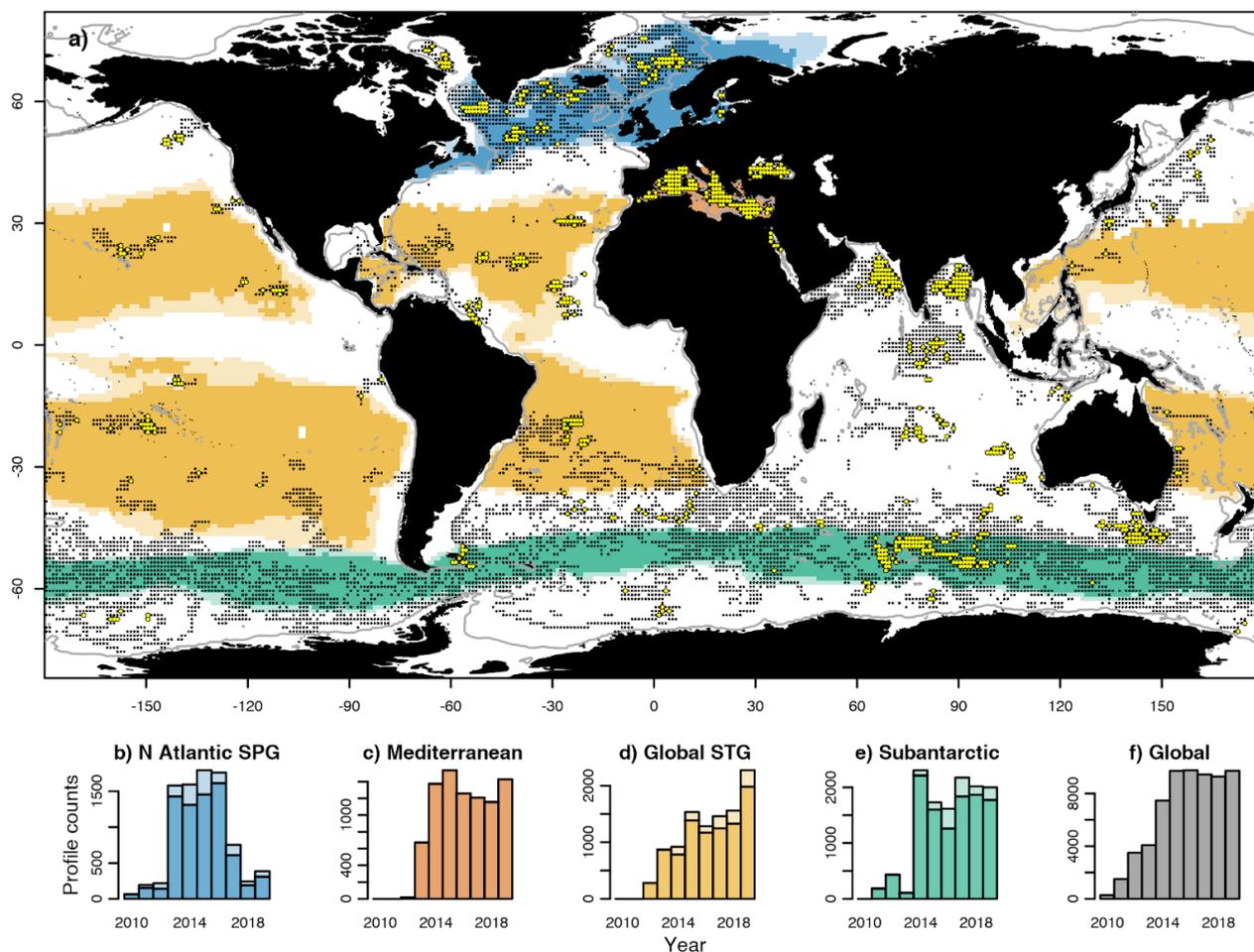
Figures

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Figure 1. Global distribution and abundance of BGC-Argo profiles between 2010 and 2019. Grid cells (1°x1°) with at least 1 profile of the backscattering coefficient at 700 nm (b_{bp700}) are marked with black dots, and those with at least 20 profiles are marked with yellow-filled circles. The gray contours indicate the 1000 m isobath. Color shading indicates ocean biomes (see text), whose names are indicated on top of the bottom histograms. For each biome, light color indicates its average extent over 13 years of satellite observations (1998-2010), whereas the darker color indicates the "core" grid cells that never changed biome classification during the same period. Bottom panels (b-f) show the number of BGC-Argo bbp700 profiles per year in the four selected biomes and in the global ocean.

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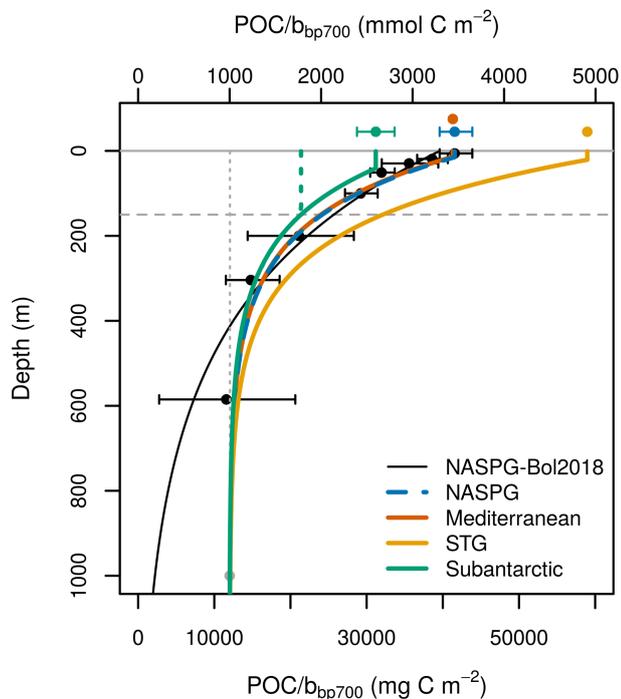
Figure 2. Empirical model used to convert the backscattering coefficient at 700 nm (bbp700) to particulate organic carbon (POC). Black dots and error bars show the dataset of Cetinić et al. (2012) as binned by Bol et al. (2018). The black curve shows the exponential fit of Bol et al. (2018) to the Cetinić dataset. The blue curve shows our fit to the same dataset (NASPG: North Atlantic Subpolar Gyre), forced to converge to a nonzero minimum value at depth. The remaining curves show similar functions with the same exponential slope (b = -6.57) as the NASPG fit, but with different surface values derived from the following studies: Loisel et al. (2001) for the Mediterranean Sea; Stramski et al. (2008) for the ensemble of subtropical and tropical areas excluding equatorial upwellings (STG); and Johnson et al. (2017) for the Southern Ocean (Subantarctic). The depth of the homogeneous surface layer, $z_{surf,biome}$ in Eq. 1 and 2, corresponds to the 5% quantile of the climatological MLD in summer in a given biome: 15 m in the NASPG, 14 m in the MED, 21 m in the STG and 41 m in the SO. The dotted green line, shown for the SO case only, illustrates the behavior of the algorithm for a mixed layer depth of 150 m.
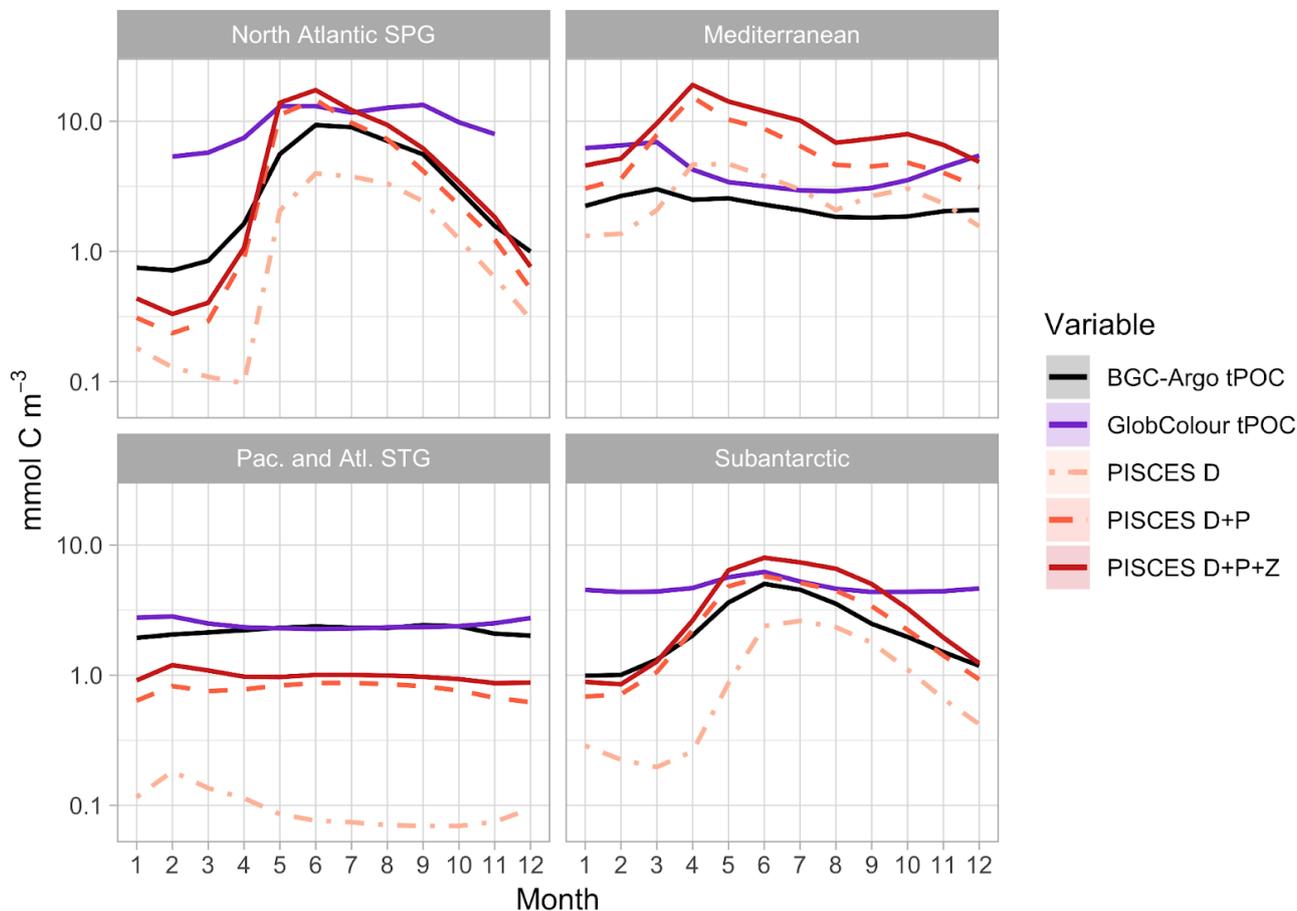
Figure 3. Monthly sea-surface particulate organic carbon (POC) concentration. Shown are POC estimates based on BGC-Argo (derived from the backscattering coefficient at 700 nm, bbp700), satellite (GlobColour) and PISCES. PISCES tPOC results from the addition of the detritus (D), phytoplankton (P) and zooplankton (Z) tracers (Table 1), which are shown here as cumulative sums.

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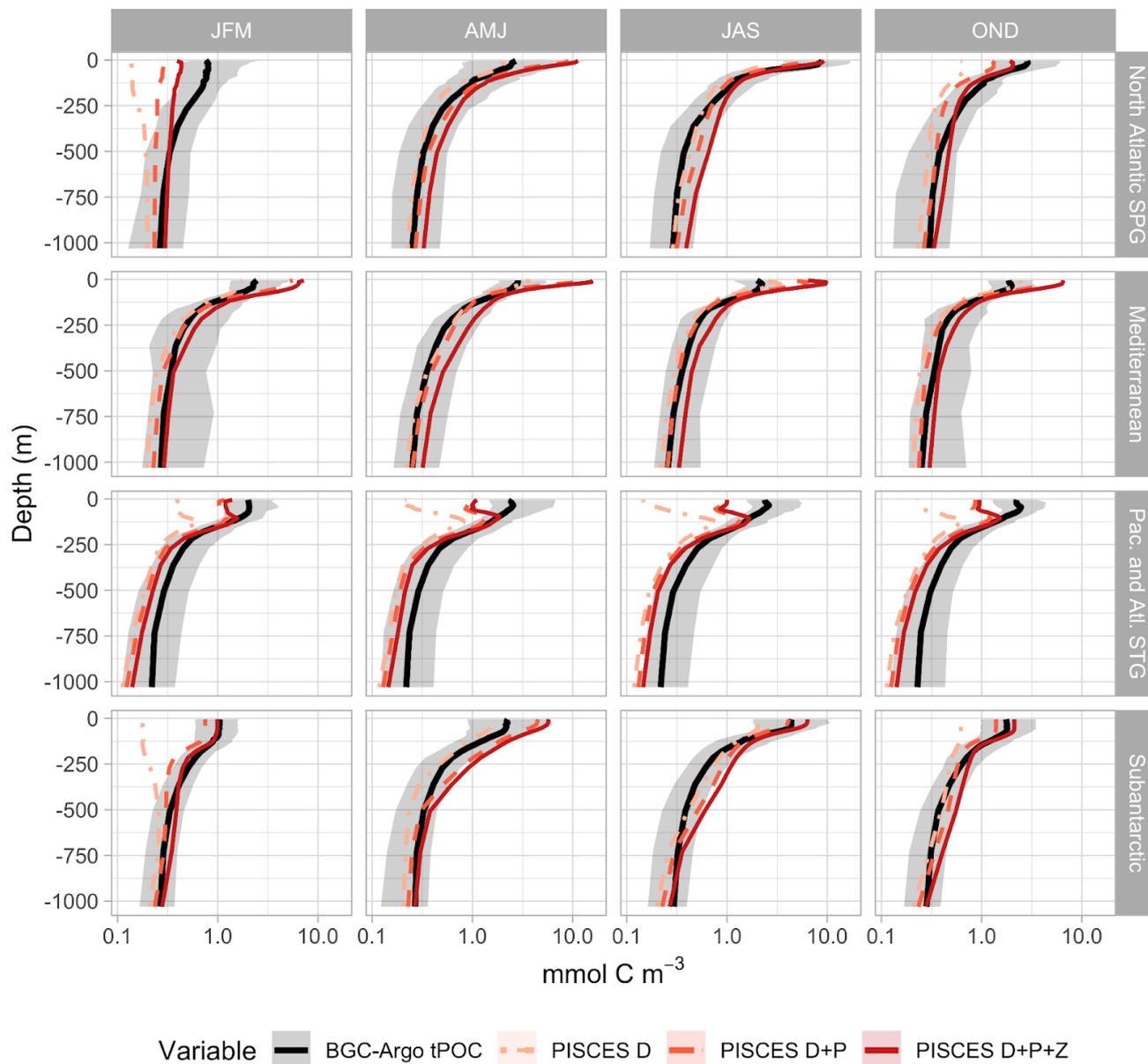
Figure 4. Seasonal 0–1000 m particulate organic carbon (POC) profiles. BGC-Argo observations (based on the backscattering coefficient at 700 nm, bbp700) are represented with the median and the 0.025–0.975 quantiles within each biome. PISCES tPOC results from the addition of the detritus (D), phytoplankton (P) and zooplankton (Z) tracers (Table 1), which are shown here as cumulative sums.
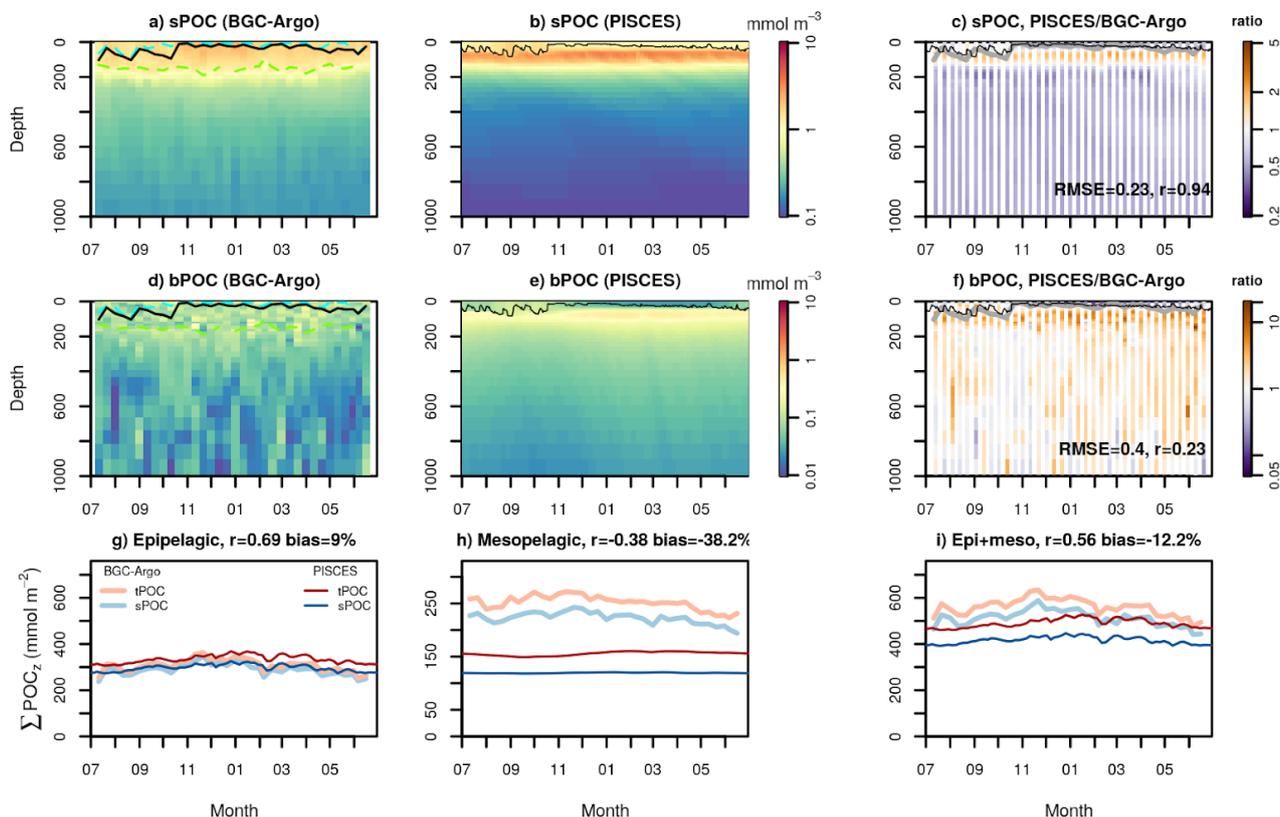
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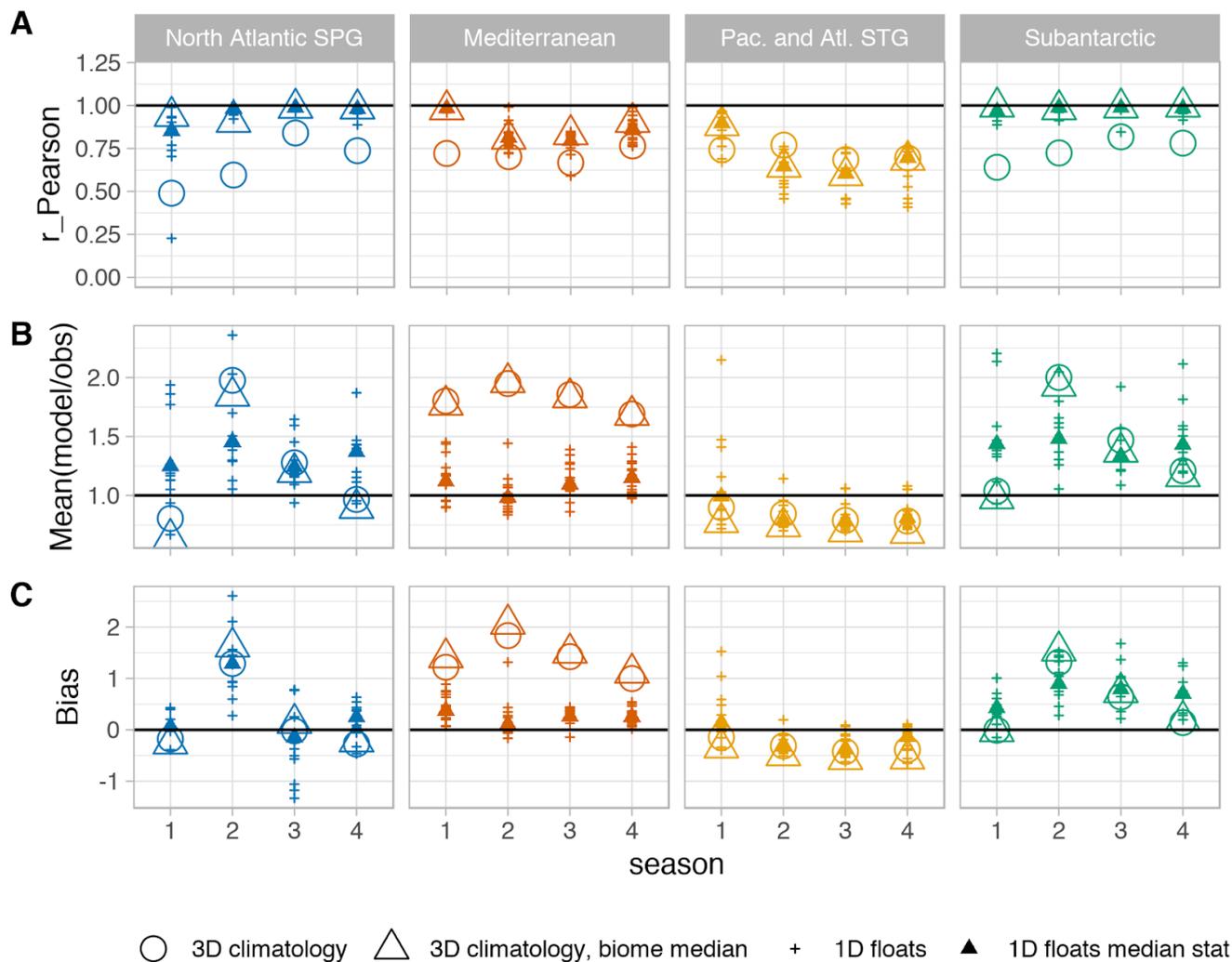
Figure 5. Summary of skill metrics for the comparison between PISCES and BGC-Argo particulate organic carbon (POC) profiles in different biomes and seasons. Pearson's correlation coefficient, mean model/data quotient, and mean bias (mmol m^{-3}) are computed in linear space (untransformed data). Horizontal black lines show the benchmark values for each statistic. Symbols represent different types of simulations and data aggregation levels. In the case of the PISCES 3D climatological simulation, the statistics are computed at two spatial aggregation levels: using all the grid cells with matching BGC-Argo profiles in a given biome (circles); and after averaging all the documented grid cells within the biome (empty triangles), as displayed in Fig. 4. In the case of the PISCES 1D simulations, statistics are computed for each individual CATS separately (small crosses), and the biome-season median is also shown (small filled triangles).
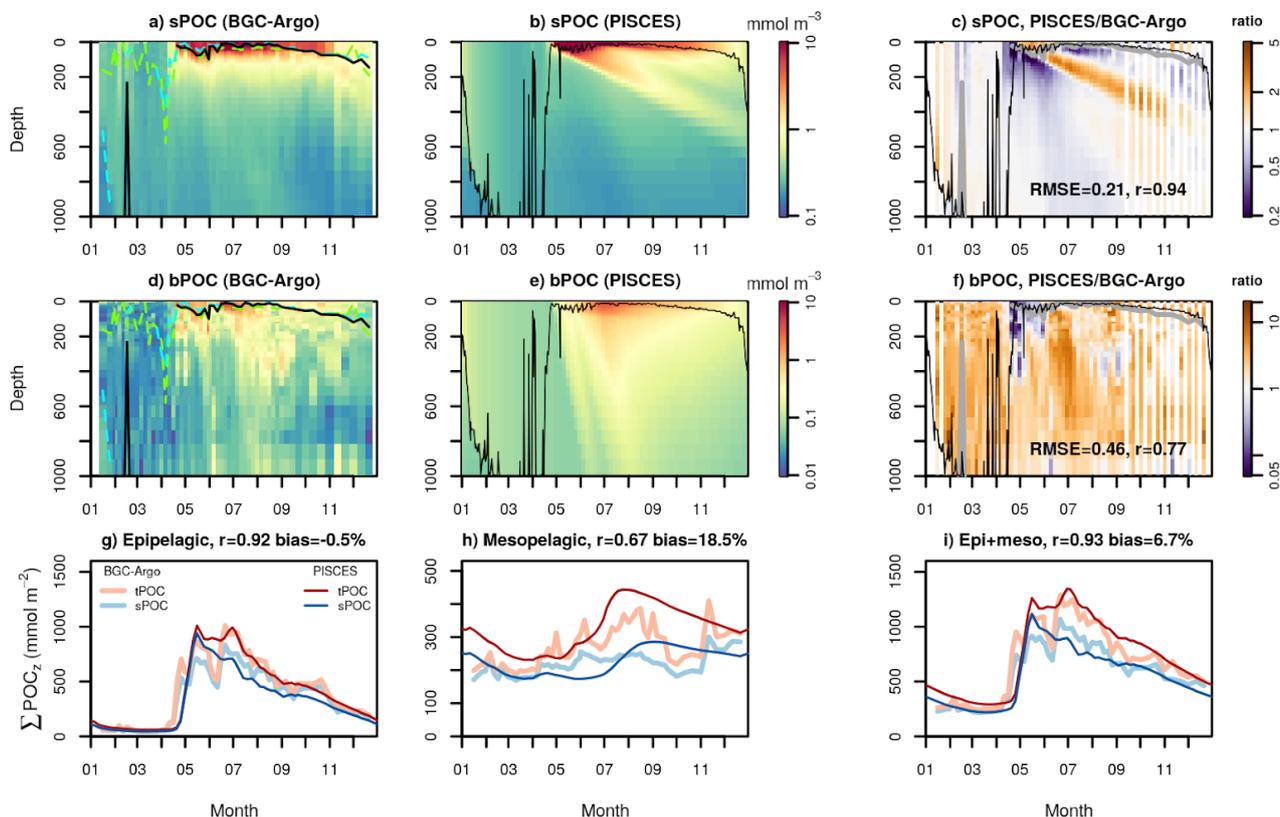
Figure 6. Temporal evolution of small POC (sPOC) and big POC (bPOC) concentrations in the North Atlantic subpolar gyre (NASPG). Panels a and d show observations from the BGC-Argo float WMO 6901486, which drifted in the Labrador Sea during the year 2015. Panels b and e show the corresponding PISCES 1D simulation. Panels c and f show the ratio between the model and the observations and the corresponding correlation coefficient and RMSE in $\log_{10}$ scale. Solid lines depict the observed MLD (a, d) and the simulated turbocline depth (b, e). In panels c and f, the observed MLD is shown in gray to avoid confusion. In panels a and d, dashed lines show the depths of the maximum chlorophyll fluorescence gradient (green) and an alternative MLD estimated with a 0.005 density threshold to capture weak stratification. The bottom panels show the vertically integrated sPOC and bPOC stocks in different layers: 0–200 m or epipelagic (g), 200–1000 m or mesopelagic (g) and 0–1000 m (i). On top of panels g–i we show the correlation and bias between BGC-Argo and PISCES total POC (tPOC).

Figure 7. Temporal evolution of small and big POC concentrations (sPOC and bPOC, respectively) in the South Pacific subtropical gyre (STG). Panels a and d show observations from the BGC-Argo float WMO 6901660, which drifted westwards near Tahiti, during the year 2016. Panels b and e show the corresponding PISCES 1D simulation. Panels c and f show the ratio between the model and the observations and the corresponding correlation coefficient and RMSE in $\log_{10}$ scale. Solid lines depict the observed MLD (a, d) and the simulated turbocline depth (b, e). In panels c and f, the observed MLD is shown in gray to avoid confusion. In panels a and d, dashed lines show the depths of the maximum chlorophyll fluorescence gradient (green) and an alternative MLD estimated with a 0.005 density threshold to capture weak stratification. The bottom panels show the vertically integrated sPOC and bPOC stocks in different layers: 0–200 m or epipelagic (g), 200–1000 m or mesopelagic (g) and 0–1000 m (i). On top of panels g–i we show the correlation and bias between BGC-Argo and PISCES total POC (tPOC).
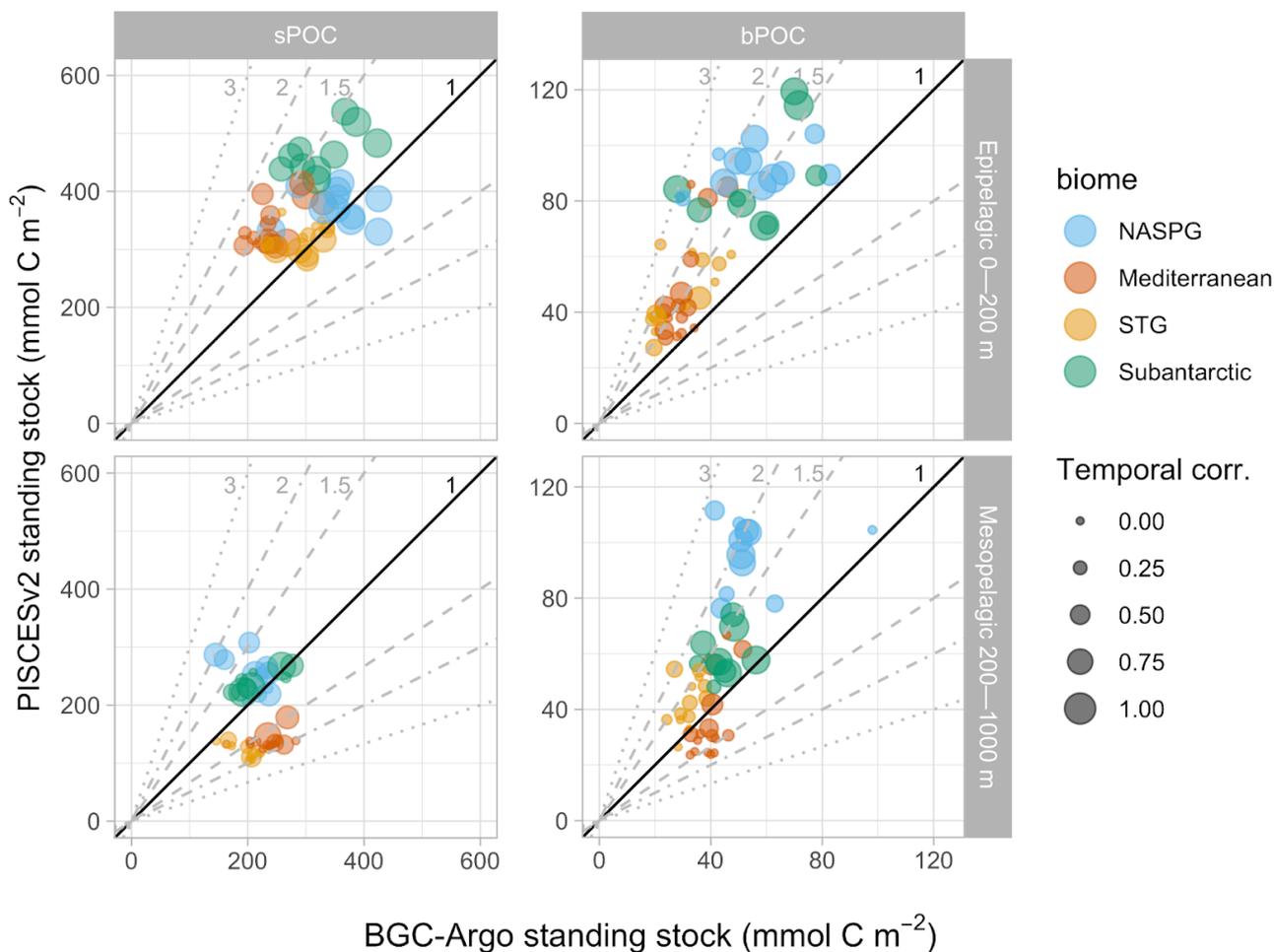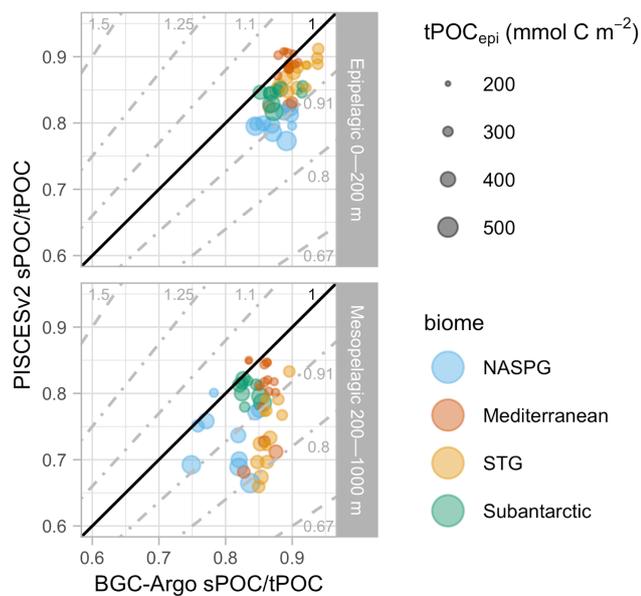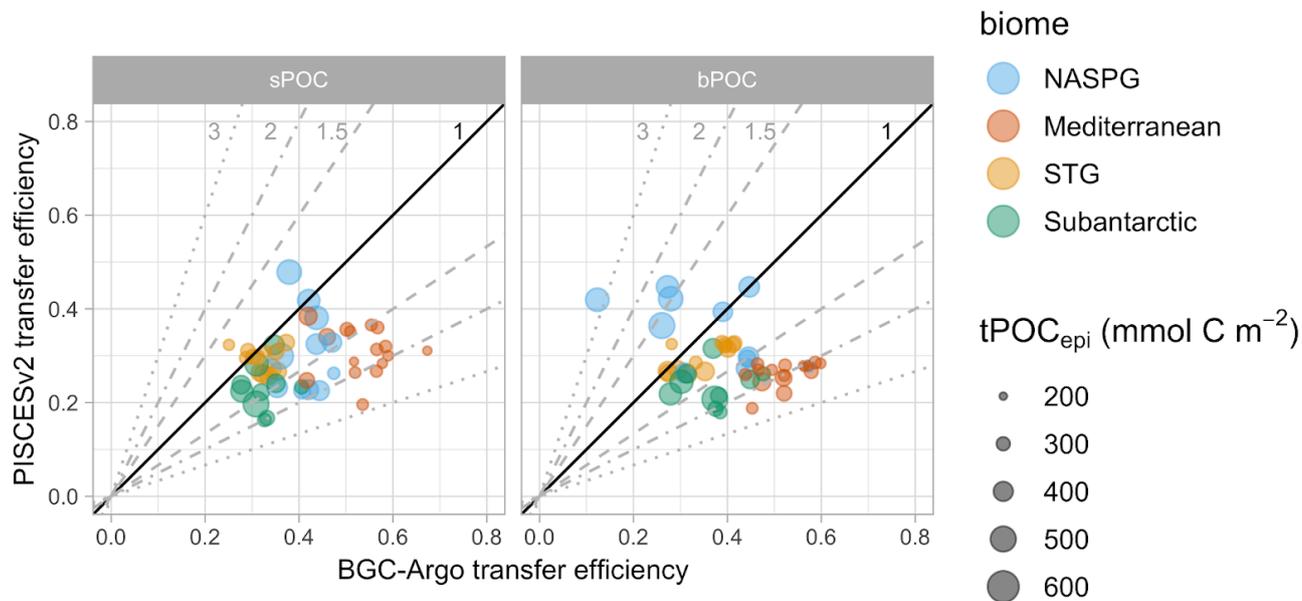
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Figure 8. Mean annual POC stocks. BGC-Argo versus PISCES scatterplots are shown for small POC (sPOC) and big POC (bPOC) in the epi- and mesopelagic layers. Reference lines indicate a range of model:data ratios, from 1:1 (perfect correspondence) to a factor of 3 or its inverse. Biomes are distinguished with different colors, and the size of the circles is proportional to the correlation between BGC-Argo and PISCES stocks (as shown in the bottom panels of Figures 6 and 7).

Figure 9. Mean annual sPOC/tPOC fractions. BGC-Argo versus PISCES scatterplots are shown for small POC (sPOC) and big POC (bPOC) in the epi- and mesopelagic layers. Reference lines indicate a range of model:data ratios, from 1:1 (perfect correspondence) to a factor of 1.5 or its inverse. Biomes are distinguished with different colors, and the size of the circles is proportional to the annual mean tPOC stock in the epipelagic layer, an indicator of productivity.

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Figure 10. Mean annual POC transfer efficiency between 200 and 700 m. BGC-Argo versus PISCES scatterplots are shown for small POC (sPOC) and big POC (bPOC). Reference lines indicate a range of model:data ratios, from 1:1 (perfect correspondence) to a factor of 3 or its inverse. Biomes are distinguished with different colors, and the size of the circles is proportional to the annual mean tPOC stock in the epipelagic layer, an indicator of productivity.

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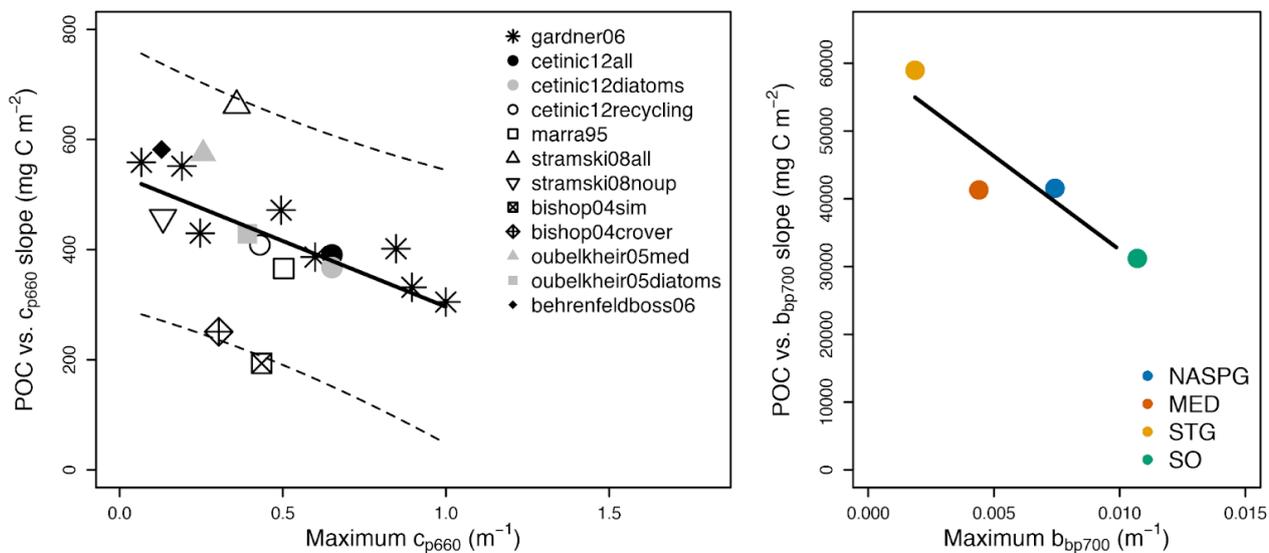
Figure A1. Coherent patterns in the conversion factors between POC and bio-optical variables. The left panel reproduces figure 8
from Cetinić et al. (2012), which shows the relationship between the POC versus c_p slope and the maximum c_p in a given dataset.
The right panel shows the analogous relationship for b_{bp700}, as used in our study. Linear fits are only illustrative.

Tables

Table 1. Match between BGC-Argo observations, PISCES tracers (Aumont et al., 2017), real-world particulate organic carbon pools, and particle size ranges[a].

POC fraction	BGC-Argo observation	PISCES tracer (carbon currency)	Closest real-world correspondence
sPOC	b_{bp700} vertical profiles, despiked signal. Most sensitive to 0.5–30 μm particles (Dall'Olmo et al., 2009; Organelli et al., 2018) Calibrated as POC with Eq. 1 and 2	PHY: "Nanophytoplankton", includes calcifiers (default fraction 30%). Nominally 1–10 μm.	Picocyanobacteria and non-diatom phytoeukaryotes, generally 0.5–20 μm.
		PHY2: Silicifying microphytoplankton. Nominally 10–50 μm.	Diatoms, between 1.5-μm cells (Vaulot et al., 2008) and mm–scale chains. Mean ESD[b] generally < 50 μm in seawater (Snoeijs et al., 2002; Ciotti et al., 2002; Bricaud et al., 2004).
		POC: detrital particulate organic carbon. Nominally < 100 μm. In practice, it includes heterotrophic prokaryotes' biomass with current parameter values (see 4.3).	Detrital particles between ~0.2[c] μm and 100 μm. In practice, measurements may include particle-attached and free-living organisms, viruses, colloids and adsorbed DOC.
		ZOO: Microzooplankton. Nominally 10–200 μm.	Microzooplankton. Mostly ciliates and flagellates with size similar to their prey, down to around 2 μm (Calbet 2008)
		Heterotrophic prokaryotes (BACT): currently not a prognostic tracer in PISCES. Not considered *explicitly* in this study (see 4.3).	Free-living heterotrophic prokaryotes (bacteria and archaea), < 1 μm.
bPOC	b_{bp700} vertical profiles, spike signal. Particle size between ~100 μm (b_{bp700} spike of $2.3 \cdot 10^{-5}$ m^{-1}) and ~2 mm (b_{bp700} spike of $8 \cdot 10^{-3}$ m^{-1}) (Briggs et al., 2020) Calibrated as POC with Eq. 1 and 2	GOC: detrital particulate organic carbon. Nominally > 100 μm	Detrital particles > 100 μm (aggregates, fecal pellets). Includes attached microbes.
		ZOO2: Mesozooplankton. Includes flux feeders[d]. Nominally 0.2–2 mm.	Mesozooplankton[d]

[a] See Stemmann and Boss (2012) for typical seawater particle size spectra.
[b] Equivalent spherical diameter
[c] Particles in the 0.2–0.8 μm size range and DOC are retained with variable efficiency by the filters commonly used to determine POC (Cetinić et al., 2012; Graff et al., 2015; Lee et al., 1995; Morán et al., 1999; Strubinger Sandoval et al., 2021).

[d] PISCES mesozooplankton represents mostly copepods in the euphotic layer and flux feeders below it. The fraction of flux feeders is diagnosed in PISCES from the proportion between flux feeding rates and total mesozooplankton ingestion rates. By construction, flux feeding becomes the dominant mode of mesozooplankton feeding below the euphotic layer under productive surface waters in PISCES. In reality, a wide variety of feeding strategies and organisms are found in the mesopelagic (Ikenoue et al., 2019; Kiørboe, 2011; Mayor et al., 2020; Stukel et al., 2019).

Table 2. Global and regional POC stocks, concentrations and fractions in different layers as simulated by PISCESv2.

Variable	Depth range (m)	Open-ocean biomes					Global[d]
		Ice	SPSS[a]	STSS[b]	STPS[c]	Equatorial	
Area (%)		6.5	14.3	12.0	46.0	9.2	100
tPOC (Tg C)	0–200	73	281	263	263	154	1590
	200–1000	57	221	173	397	90	1006
	1000–5000	80	274	237	633	144	1438
tPOC (mmol C m^{-3})	0–200	1.18	2.22	2.57	1.66	1.99	1.85
	200–1000	0.29	0.48	0.44	0.25	0.29	0.33
	1000–5000	0.14	0.18	0.17	0.10	0.13	0.13
sPOC[e] (%)	0–200	72	81	79	89	84	81
	200–1000	75	75	70	79	71	75
	1000–5000	81	80	77	79	75	79
Phyto[f] (%)	0–20	45	45	41	58	49	50
Diatoms[g] (%)	0–20	28	21	14	3	4	14
Detritus[h] (%)	0–20	15	25	31	26	31	24
	0–200	36	43	48	44	50	42
	200–1000	62	67	70	78	78	70

[a] Subpolar seasonally stratified

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[b] Subtropical seasonally stratified
[c] Subtropical permanently stratified
5 [d] Larger than the sum of biomes because the latter do not include coastal areas.
[e] sPOC / tPOC.
[f] ($PHY + PHY2$) / tPOC.
[g] $PHY2$ / tPOC.
[h] PISCES detritus ($POC+GOC$) divided by tPOC. Heterotrophic prokaryotes are *de facto* included.

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Table A1. Compilation of studies that analyzed the relationship between POC and b_{bp700} in the euphotic layer of the oceans.

Location	Reference	N	Depth range	Slope (mg C m^{-2} m)	Intercept	Comments
North Atlantic Subpolar Gyre	Cetinić et al., 2012	321	0-600	35422 ± 1754	- 14.4 ± 5.8	Downcast
		321	0-600	43317 ± 2092	- 18.4 ± 5.8	Upcast
	Bol et al., 2018	n.a. [a]	0-10	41550	forced through 0	Subset of Cetinić et al., 2012 at the surface
Mediterranean	Loisel et al., 2001	N/A	N/A	41305	1.43	Original measurements at 555 nm
Subtropical and tropical Pacific and Atlantic (upwellings excluded)	Stramski et al., 2008	54	4-8	58968	2.75	Original measurements at 555 nm
Subantarctic	Johnson et al., 2017	67	0-100	31200 ± 2470	3.0 ± 6.8	

[a] n.a. = not available