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1 Water mass analysis along 22 °N in the subtropical North Atlantic
2 for the JC150 cruise (GEOTRACES, GApr08)

3
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26 **Abstract**

27 This study presents a water mass analysis along the JC150 section in the subtropical North Atlantic,
28 based on hydrographic and nutrient data, by combining an extended optimum multiparameter
29 analysis (eOMPA) with a Lagrangian particle tracking experiment (LPTE). This combination,
30 which was proposed for the first time, aided in better constraining the eOMPA end-member choice
31 and providing information about their trajectories. It also enabled tracing the water mass origins
32 in surface layers, which cannot be achieved with an eOMPA. The surface layers were occupied by
33 a shallow type of Eastern South Atlantic Central Water (ESACW) with traces of the Amazon
34 plume in the west. Western North Atlantic Central Water dominates from 100–500 m, while the
35 13 °C-ESACW contribution occurs marginally deeper (500–900 m). At approximately 700 m,
36 Antarctic Intermediate Water (AAIW) dominates the west of the Mid-Atlantic Ridge (MAR),
37 while Mediterranean Water dominates the east with a small but non-negligible contribution down
38 to 3500 m. Below AAIW, Upper Circumpolar Deep Water is observed throughout the section
39 (900–1250 m). Labrador Sea Water (LSW) is found centered at 1500 m, where the LPTE
40 highlights an eastern LSW route from the eastern North Atlantic to the eastern subtropical Atlantic,
41 which was not previously reported. North East Atlantic Deep Water (encompassing a contribution
42 of Iceland-Scotland Overflow Water) is centered at ~2500 m, while North West Atlantic Bottom
43 Water (NWABW, encompassing a contribution of Denmark Strait Overflow Water) is principally
44 localized in the west of the MAR in the range of 3500–5000 m. NWABW is also present in
45 significant proportions (> 25 %) in the east of the MAR, suggesting a crossing of the MAR possibly
46 through the Kane fracture zone. This feature has not been investigated so far. Finally, Antarctic
47 Bottom Water is present in deep waters throughout the section, mainly in the west of the MAR.

48 Source waters have been characterized from GEOTRACES sections, which enables estimations of
49 trace elements and isotope transport within water masses in the subtropical North Atlantic.

50

51 **1 Introduction**

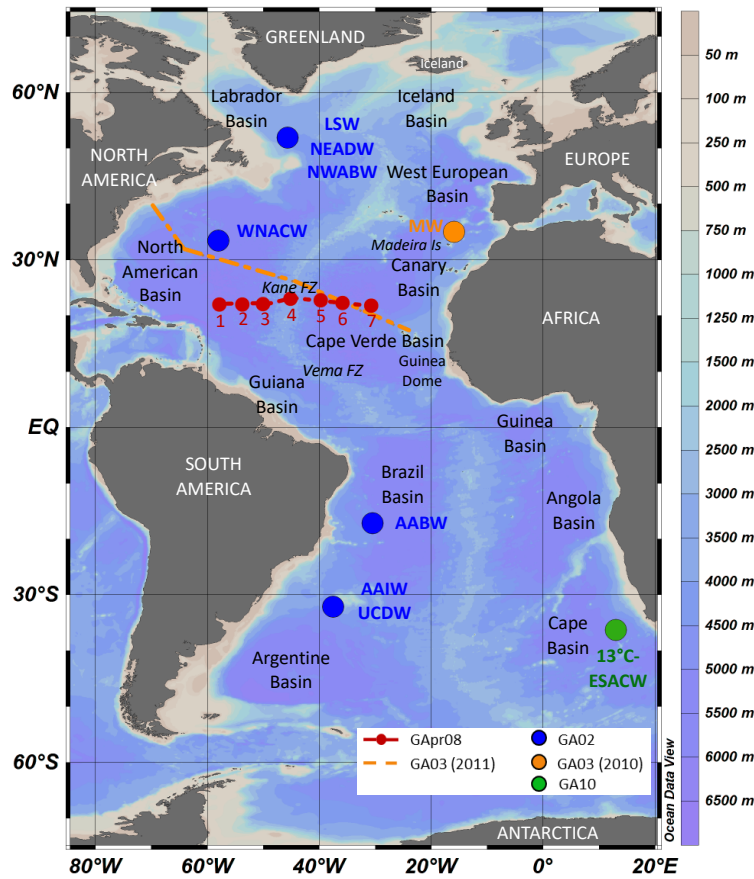
52 Oceanic water masses store and transport considerable amounts of energy, water and
53 chemical elements in the earth's surface. These water masses impact the atmosphere through
54 interactions at the air/sea interface. Water mass analysis, which consist in studying the formation,
55 spreading, and mixing of water masses, is therefore essential to understand the role of oceans in
56 climate processes. The methods used for water mass analysis have evolved from classical
57 descriptions of oceanic circulation based on hydrographic properties to the determination of water
58 mass formation regions, transport pathways, and mixing length scales from numerical models and
59 novel tracer data (Tomczak, 1999). An example of such development is the introduction of the
60 optimum multiparameter analysis (OMPA, Tomczak, 1981). This method enables estimating the
61 contributions of different water masses defined in specific locations (end-members) to a measured
62 ocean section based on a range of hydrographic parameters. This method demonstrates a
63 significant amount of improvement compared to previous methods and has been widely used
64 (Álvarez et al., 2014; García-Ibáñez et al., 2018; Jenkins et al., 2015; Pardo et al., 2012; Peters et
65 al., 2018). However, the results of OMPA are strongly dependent on the choice of water mass end-
66 members that possibly impact the ocean section, and OMPA cannot provide any information
67 related to surface layers. Moreover, a water mass analysis conducted only with OMPA does not
68 provide direct information on the water mass pathways between their formation region and the
69 measured section. Therefore, the water mass analysis proposed in this study combines, for the first
70 time to the best of our knowledge, an extended OMPA with a Lagrangian particle tracking

71 experiment (LPTE) to better constrain the end-members and provide information on water mass
72 pathways. LPTEs are widely used in recent times to investigate several aspects of ocean sciences,
73 such as oceanic circulation (eg. Spence et al., 2014) or biogeochemistry (eg. Cetina-Heredia et al.,
74 2016).

75 The present water mass analysis was conducted for the JC150 “Zinc, Iron and Phosphorus co-
76 Limitation” GEOTRACES process study (GApr08). This cruise departed Point-à-Pitre,
77 Guadeloupe on June 27, 2017 and arrived at Santa Cruz, Tenerife on August 12, 2017. The transect
78 is located at the southern end of the North Atlantic Subtropical gyre (Fig. 1) on both sides of the
79 Mid-Atlantic Ridge (MAR, ~ 22 °N, ~ 58–31 °W). The JC150 section was specifically studied to
80 understand how a low phosphate environment could lead to zinc-phosphorus and iron-phosphorus
81 co-limitation on nitrogen fixation (Browning et al., 2017; Mahaffey et al., 2014; Moore et al.,
82 2009; Snow et al., 2015; Wu et al., 2000). In this context, the trace metals iron, zinc and aluminum,
83 were measured. The aim of the present water mass analysis is two-fold. Firstly, it aims to provide
84 a detailed understanding of the contribution and distributions of the water masses that exist along
85 the zonal section as well as new constraints in water mass circulation in the subtropical North
86 Atlantic that might be of general interest. Secondly, it aims to provide the tools to efficiently
87 combine this hydrodynamic knowledge with the biogeochemical knowledge from the
88 GEOTRACES program. To achieve this objective, all the OMPA end-members were chosen from
89 GEOTRACES cruises with available zinc, iron, and aluminum concentrations. This enables the
90 estimation of transport and mixing of these elements. Such a choice is a first to the best of our
91 knowledge, and it is now possible thanks to the great extent of the GEOTRACES program.

92 This study presents the hydrographic properties measured during JC150, including potential
93 temperature, salinity, and the concentration of oxygen and nutrients (θ , S, O₂, NO₃⁻, PO₄³⁻, and

94 Si(OH)_4 along with a water mass analysis based on an OMPA and a LPTE.



95
96 **Fig. 1.** Map of the JC150 cruise (red dots); locations where the end-members are defined (blue
97 dots - GA02, orange dot - 2010 GA03, and green dot - GA10), and track of the 2011 GA03 cruise
98 (orange dashed line). Refer to Table. 1 for water mass acronyms.

99

100 2 Materials and Methods

101 2.1 Hydrography and nutrients

102 The samples for nutrients, oxygen, and salinity analyses were collected using 24, 10 L trace metal
103 clean Teflon-coated OTE (ocean test equipment) bottles with external springs, mounted on a

104 titanium rosette and deployed on a Kevlar-coated conducting wire. A SeaBird 911plus CTD
105 recorded the temperature, conductivity, and pressure at 24 Hz with an accuracy of $\pm 0,001$ °C, \pm
106 $0,0003$ S/m, and $\pm 0,015$ %, respectively. An SBE43 oxygen sensor measured the dissolved oxygen
107 concentration. Standard SeaBird processing routines were used to extract the raw data. The effect
108 of thermal inertia on the conductivity was removed, and a correction was applied for deep oxygen
109 hysteresis (https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/jc150.pdf).

110 After rosette recovery, the OTE bottles were transferred into a class 1000 clean air shipboard
111 laboratory for sampling. The samples for dissolved oxygen and salinity analyses were collected to
112 calibrate the CTD sensors. For the measurements of dissolved oxygen, triplicate samples from 12
113 depths were fixed immediately and analyzed within 48 h of collection. The samples were analyzed
114 with an automated titrator (Metrohm titrando Titrator). A platinum electrode was used for the
115 potentiometric analysis of Winkler titration. The salinity samples were collected at 6 depths on
116 each cast and analyzed using Guildline's Autosal 8400B. The salinity and oxygen sensors were
117 then calibrated using bottle derived salinity and bottle derived oxygen, which resulted in linear
118 regressions for salinity (calibrated salinity = CTD salinity * 1.0012 - 0.0439) and oxygen
119 (calibrated oxygen ($\mu\text{mol kg}^{-1}$) = CTD oxygen * 0.9768 + 5.3398). The salinity and oxygen data
120 used in this study were the sensor calibrated data obtained with an accuracy of 0,0001 for salinity
121 and $0,5 \mu\text{mol kg}^{-1}$ for oxygen. With measurements of calibrated oxygen, salinity, and potential
122 temperature, we calculated the apparent oxygen utilization (AOU) ($\text{AOU} (\mu\text{mol kg}^{-1}) = \text{saturated}$
123 $\text{oxygen} (\mu\text{mol kg}^{-1}) - \text{calibrated oxygen} (\mu\text{mol kg}^{-1})$). For the AOU calculation, we employed a
124 script, which is originally part of the oceanography toolbox v1.4 compiled by R. Pawlowicz and
125 now available on the MBARI website ([https://www.mbari.org/products/research-software/matlab-](https://www.mbari.org/products/research-software/matlab-scripts-oceanographic-calculations/)
126 [scripts-oceanographic-calculations/](https://www.mbari.org/products/research-software/matlab-scripts-oceanographic-calculations/)).

127 The samples for nutrient analyses were collected unfiltered into acid-cleaned 60 mL HDPE
128 Nalgene bottles from each OTE bottle. Immediately after collection, they were analyzed through
129 colorimetric procedures (Woodward and Rees, 2001) using clean handling GO-SHIP protocols
130 (Hydes et al., 2010). The micromolar nutrient concentrations were measured using a segmented
131 flow colorimetric auto-analyzer: the PML 5-channel (nitrate, nitrite, phosphate, silicic acid, and
132 ammonium) Bran and Luebbe AAIH system. The instrument was calibrated with nutrient stock
133 standards, and the accuracy was determined using Certified Nutrient Reference Materials (batches
134 CA and BU) obtained from KANSO Technos, Japan. The nano-molar nitrate, nitrite, and
135 phosphate concentrations were analyzed through the segmented flow colorimetric technique that
136 improved the analytical detection limits by using a two-meter liquid waveguide as the analytical
137 flow cell. The same colorimetric method as for the micromolar system was used for analyzing
138 nitrate and nitrite, while the method described in (Zhang & Chi, 2002) was used for analyzing
139 phosphate. The nutrient data presented in this study were measured with an uncertainty of 2%.

140

141 2.2 An extended optimum multiparameter analysis (eOMPA)

142 An eOMPA was used to resolve the water mass structure along the JC150 section (Mackas et al.,
143 1987; Poole & Tomczak, 1999; Tomczak, 1981; Tomczak & Large, 1989). This analysis assumes
144 that the waters sampled along a section result from the mixing of several well-defined water
145 masses, called the source water types or end-members. The degree of mixing and the contribution
146 of each end-member is solved using an optimization procedure. Mathematically, an OMPA is an
147 optimal solution to a linear system of mixing equations with the contribution of end-members as
148 variables and the conservative hydrographic properties as the parameters of the system. This model
149 optimizes, for each data point (sample), the end-member parameter contributions to reproduce the

150 observational data. The OMPA is performed as an overdetermined system using non-negative least
151 square optimization.

152 In OMPA, the hydrographic properties are used as parameters in the equation system. In this study,
153 the available parameters are as follows: potential temperature (θ), salinity (S), concentration of
154 dissolved oxygen (O_2), phosphate (PO_4^{3-}), nitrate (NO_3^-), and silicic acid ($Si(OH)_4$), and mass
155 conservation (the sum of all contributions must be equal to unity). A classical OMPA resolves the
156 system assuming that all those parameters are conservative, i.e., they have no sources or sinks in
157 the ocean interior. This assumption was not acceptable for O_2 , NO_3^- , and PO_4^{3-} in our case, as the
158 end-members were defined at the Atlantic basin-wide scale and thus highly susceptible to organic
159 matter remineralization. To consider these biogeochemical processes, we realized an eOMPA for
160 this study. Most eOMPA studies use the quasi-conservative N^* and P^* parameters (García-Ibáñez
161 et al., 2018; Jenkins et al., 2015). We preferred to adopt the parameters PO and NO defined in
162 Broecker (1974) using the following equations, because unlike P^* and N^* , PO and NO do not
163 require any assumption about initial gas equilibrium at the air/sea interface. Other recent studies
164 have also made this choice (Álvarez et al., 2014; Peters et al., 2018).

$$165 \quad PO = [O_2] + R_{O_2/P} * [PO_4^{3-}], \quad (1)$$

$$166 \quad NO = [O_2] + R_{O_2/N} * [NO_3^-], \quad (2)$$

167 where $R_{O_2/P}$ and $R_{O_2/N}$ are Redfield ratios that estimate the number of O_2 moles consumed for one
168 mole of PO_4^{3-} and NO_3^- released during the process of organic matter remineralization,
169 respectively (Anderson & Sarmiento, 1994). In this manner, and under the assumption that the
170 Redfield ratios $R_{O_2/P}$ and $R_{O_2/N}$ are accurate, remineralization has no impact on PO and NO.
171 However, it is important to note that the Redfield ratios are spatiotemporally variable and have

172 been revised since their original definition. Therefore, we qualified PO and NO as quasi-
173 conservative. In this study, we defined $R_{O_2/P} = 155$ and $R_{O_2/N} = 9.69$, in the range of Anderson
174 (1995), and similar to the values used by Peters et al. (2018).

175 These definitions combine the three non-conservative parameters O_2 , PO_4^{3-} , and NO_3^- into two
176 quasi-conservative parameters PO and NO. Transforming three parameters into two reduces the
177 rank of the mixing equation system by one and thereby the number of end-members that can be
178 considered.

179 The conservative character of the $Si(OH)_4$ parameter is also questionable. At depth, the biogenic
180 particulate matter degradation releases $Si(OH)_4$. Unlike PO_4^{3-} and NO_3^- , the $Si(OH)_4$ parameter
181 cannot be corrected using the Redfield ratio, as it is not linked to organic matter remineralization,
182 but to biogenic opal dissolution. In the Atlantic, the magnitude of the $Si(OH)_4$ excess from opal
183 dissolution has been estimated to represent only 5% of the difference between the $Si(OH)_4$
184 concentrations of the northern and southern end-members. Therefore, the opal dissolution effect
185 on water mass properties is insignificant compared to the effect of water mass mixing at the basin
186 scale (Broecker et al., 1991). Thus, the $Si(OH)_4$ concentration was considered as a conservative
187 parameter in this study.

188 The parameters considered to resolve the eOMPA in this work were as follows: θ , S, PO, NO,
189 $Si(OH)_4$, and mass conservation. This led to the following system of mixing equations applied at
190 each sample point with (n) end-members:

$$191 \quad X_1\theta_1 + X_2\theta_2 + \dots + X_n\theta_n = \theta_{\text{sample}} + \varepsilon_\theta, \quad (3)$$

$$192 \quad X_1S_1 + X_2S_2 + \dots + X_nS_n = S_{\text{sample}} + \varepsilon_S, \quad (4)$$

$$193 \quad X_1PO_1 + X_2PO_2 + \dots + X_nPO_n = PO_{\text{sample}} + \varepsilon_{PO}, \quad (5)$$

194 $X_1\text{NO}_1 + X_2\text{NO}_2 + \dots + X_n\text{NO}_n = \text{NO}_{\text{sample}} + \varepsilon_{\text{NO}},$ (6)

195 $X_1 \text{Si(OH)}_{4,1} + X_2 \text{Si(OH)}_{4,2} + \dots + X_n \text{Si(OH)}_{4,n} = \text{Si(OH)}_{4,\text{sample}} + \varepsilon_{\text{Si(OH)}_4},$ (7)

196 $X_1 + X_2 + \dots + X_n = 1 + \varepsilon_x,$ (8)

197 $X_i \geq 0,$ (9)

198

199 where the variables $X_1 - X_n$ ($n = \text{each end-member}$) denote the contribution of the end-members,
 200 and $\varepsilon_\theta, \varepsilon_S, \varepsilon_{\text{PO}}, \varepsilon_{\text{NO}}, \varepsilon_{\text{Si(OH)}_4}$, and ε_x are the residuals, i.e., the difference between the calculated and
 201 observed values. The eOMPA was performed using the OMPA V2.0 MATLAB package
 202 developed by Johannes Karstensen and Matthias Tomczak (<https://omp.geomar.de>).

203

204 As the OMPA should be performed as an overdetermined system, the number of end-members
 205 must be strictly lower than that of available parameters. A total of six parameters were considered
 206 in this study; however, over five end-members probably contributed to the water masses found
 207 along the JC150 section. To solve this problem, we first tried to increase the number of parameters
 208 used. However, no other conservative (or quasi-conservative) tracer was available in the JC150
 209 cruise. We considered adding the potential vorticity as a quasi-conservative tracer. However, the
 210 profiles were observed to be excessively noisy, and despite many filtration attempts, we could not
 211 deduce an approach to obtain benefits from the use of this parameter in the eOMPA calculation.
 212 Therefore, we did not include this parameter. Another way to include over five end-members is to
 213 divide the water column into several layers, because some end-members impact only certain depth
 214 layers. The zonal section was therefore divided into three density layers with the following
 215 isopycnals: $26.50 \text{ kg m}^{-3} - 27.30 \text{ kg m}^{-3}$ (thermocline layer), $27.30 \text{ kg m}^{-3} - 27.75 \text{ kg m}^{-3}$
 216 (intermediate layer) and $> 27.75 \text{ kg m}^{-3}$ (deep layer). These density layers broadly corresponded

217 to depths of 300–700 m (thermocline layer), 700–1500 m (intermediate layer), and 1500 m to
218 seafloor (deep layer). An eOMPA was then applied independently to each of these layers. Waters
219 above ~300 m were excluded from the eOMPA for two reasons: firstly, the hydrographic
220 parameters, including θ and S were non-conservative in the mixed layer (mean annual maximum
221 ~120 m at 22°N, <http://mixedlayer.ucsd.edu>, Holte et al., 2017); secondly, these waters were
222 warmer and saltier than any well-defined end-member in the literature (Fig. 2). To precisely define
223 the boundaries between the density layers (thermocline, intermediate, and deep layers), the
224 samples located close to the layer boundaries were executed in both the overlying and underlying
225 eOMPAs (both thermocline and intermediate eOMPAs and both intermediate and deep eOMPAs).
226 The boundaries of the density layers were chosen where the smallest residuals were obtained. This
227 procedure was performed, similar to those reported by Kim et al. (2013) and Peters et al. (2018).
228 With the availability of six parameters, five end-members can be considered in each layer. We
229 carefully selected them through an in-depth literature review, comparison of the JC150
230 hydrographic section properties with those of the end-member candidates, and interpretation of the
231 LPTE results (see section 3.2). In this study, the end-member characteristics were all selected from
232 GEOTRACES cruises in the core of the water masses and with intervals of variations established
233 by comparison with nearby data areas (refer to Table. 1). These intervals are specific to each of
234 the properties of each end-members and reflect the natural variability of end-member
235 characteristics (temporal, spatial). Perturbation analyses are presented below.

236

237 The eOMPA parameters were weighted according to their signal to noise ratios (measurement
238 accuracy compared to the range of variation among end-members) and conservative character
239 (conservative or quasi-conservative). In most studies, this led to assigning higher weights to θ , S ,

240 and mass conservation than NO_3^- , PO_4^{3-} (or NO, PO), and $\text{Si}(\text{OH})_4$. The mass conservation usually
241 receives the same weighting as the parameter with the highest weight (Poole & Tomczak, 1999;
242 Tomczak & Large, 1989).

243 In this work, different weightings were tested, starting from a uniform value for all parameters to
244 16 times higher weighting for θ , S, and mass conservation than PO, NO, and $\text{Si}(\text{OH})_4$. The
245 minimum residuals were obtained for the following weightings: 24 for θ , 24 for S, 2 for PO, 2 for
246 NO, 2 for $\text{Si}(\text{OH})_4$, and 24 for mass conservation. To compare the residuals of different parameters
247 (for instance, θ and S), we expressed these residuals as percentages of the parameter ranges over
248 the entire layer (Fig. S4).

249 To validate the reliability and robustness of the eOMPA results obtained in this study, a series of
250 perturbation tests (Monte Carlo analysis) were realized. These tests allowed to estimate the extent
251 to which the eOMPA results could be affected by the variability of 1) the end-member
252 characteristics, 2) JC150 data (including the Redfield ratio used to calculate NO and PO), and 3)
253 the chosen weights. For each test, 100 runs were performed in each eOMPA layer. For each run,
254 perturbations were applied to targeted parameters (end-members, JC150 data, or weights) using
255 normal probability density functions with standard deviations scaled to the uncertainty (or
256 variability) attributed to each parameter. For the first test, uncertainties were the end-member
257 property definition intervals, which reflected the possible variation in the end-member
258 characteristics (reported in Table. 1). For the second test, the JC150 data uncertainties were used,
259 i.e., the sensor uncertainties (0,001 for θ , 0,0001 for S, and $0,5 \mu\text{mol Kg}^{-1}$ for O_2) and the nutrient
260 measurement uncertainties (2% for PO_4^{3-} , NO_3^- , and $\text{Si}(\text{OH})_4$). For this test, the Redfield ratios
261 used to define NO and PO were also modified within a 10% range (155 ± 15 for $\text{R}_{\text{O}_2/\text{P}}$, $9,69 \pm$

262 1 for $R_{O_2/N}$), which was consistent with reported Redfield ratio variability (Anderson, 1995;
 263 Anderson & Sarmiento, 1994). For the third test, the weights were modified within the range of
 264 24 +/- 5 for θ and S and 2 +/- 0,7 for PO, NO, and Si(OH)₄. 1000 perturbations were also performed
 265 for the first two tests, and the results obtained (not shown here) were very similar to those obtained
 266 with 100 perturbations.

Acronym	Name	θ (°C)	S	O ₂ ($\mu\text{mol Kg}^{-1}$)	[PO ₄ ³⁻] ($\mu\text{mol Kg}^{-1}$)	[NO ₃] ($\mu\text{mol Kg}^{-1}$)	Si ($\mu\text{mol Kg}^{-1}$)	'PO' ($\mu\text{mol Kg}^{-1}$)	'NO' ($\mu\text{mol Kg}^{-1}$)	Data sources	eOMPA layer
WNACW	West North Atlantic Central Water	17.94 ± 0.1	36.545 ± 0.02	202.30 ± 11	0.13 ± 0.04	3.10 ± 1.2	1.40 ± 0.6	222 ± 16	232 ± 16	GA02 station 18, 22/05/2010, 33.433°N, 58.05°W, 251m	T
ESACW	East South Atlantic Central Water	12.20 ± 0.2	35.117 ± 0.15	205.20 ± 1	0.80 ± 0.04	11.89 ± 2	5.01 ± 1	330 ± 3	320 ± 28	GA10 station 3, 29/12/2011, 36.348°S, 13.140°E, 497m	T&I
MW	Mediterranean Water	10.13 ± 0.4	35.920 ± 0.1	178.10 ± 8	1.06 ± 0.01	16.67 ± 0.2	10.43 ± 0.5	342 ± 3	340 ± 3	GA03 station 3, 19/10/2010, 35.201°N, 16°W, 986m	T&I&D
AAIW	Antartic Intermediate Water	3.89 ± 0.3	34.290 ± 0.05	218.30 ± 10	2.05 ± 0.12	30.29 ± 1.5	28.08 ± 8	536 ± 8	512 ± 6	GA02 station 9, 14/03/2011, 32.089°S, 37.459°W, 1001m	T&I
UCDW	Upper Circumpolar Deep Water	2.84 ± 0.03	34.576 ± 0.08	186.90 ± 5	2.18 ± 0.05	31.93 ± 0.7	54.78 ± 1.7	525 ± 16	496 ± 10	GA02 station 9, 14/03/2011, 32.089°S, 37.459°W, 1501m	T&I
LSW	Labrador Sea Water	3.76 ± 0.15	34.896 ± 0.04	272.30 ± 6	1.09 ± 0.05	16.70 ± 0.3	9.40 ± 0.8	441 ± 3	434 ± 64	GA02 station 9, 09/05/2010, 51.821°N, 45.732°W, 996m	I&D
NEADW	North East Atlantic Deep Water	2.66 ± 0.09	34.917 ± 0.003	273.20 ± 5	1.08 ± 0.02	16.40 ± 0.2	14.00 ± 1.9	441 ± 2	432 ± 3	GA02 station 9, 09/05/2010, 51.821°N, 45.732°W, 2512m	D
NWABW	North West Atlantic Bottom Water	1.63 ± 0.02	34.896 ± 0.09	290.50 ± 0.2	0.98 ± 0.01	14.70 ± 0.1	11.20 ± 0.1	442 ± 0.6	433 ± 0.8	GA02 station 9, 09/05/2010, 51.821°N, 45.732°W, 4041m	D
AABW	Antartic Bottom Water	0.04 ± 0.06	34.680 ± 0.01	217.40 ± 1.9	2.26 ± 0.07	32.72 ± 0.7	122.80 ± 4.5	568 ± 9	534 ± 4	GA02 station 13, 20/03/2011, 17.017°S, 30.599°W, 4889m	D

267

268 **Table. 1.** End-member definitions (values ± uncertainties) from GEOTRACES cruises (refer to
 269 the GA03 special issue, Boyle et al., 2015; GA02 papers, Middag et al., 2015; and Rijkenberg et
 270 al., 2014). Each end-member is included into one or more of the three extended optimum
 271 multiparameter analysis (eOMPA) layers - T: Thermocline, I: Intermediate, and D: Deep. To
 272 facilitate the future use of this eOMPA for biogeochemical studies, trace elements and some
 273 isotope data are available for each end-member on the GEOTRACES Intermediate Data Product
 274 2017 (IDP 2017 v2, Schlitzer et al., 2018).

275 2.3 LPTE

276 To improve the proposed water mass analysis, LPTEs were conducted to complement the eOMPA
 277 (i) to aid in identifying the origin of the water masses sampled along JC150 (and thereby contribute

278 to the eOMPA end-member choices) and (ii) to provide information about water mass trajectories
279 between their formation areas and the JC150 section, which cannot be achieved by a sole OMPA.
280 The LPTE experiments were conducted in the velocity field of an eddy-resolving Ocean General
281 Circulation Model. Through the seeding of numerous ‘virtual’ particles around a point and time of
282 interest (i.e., latitude, longitude, depth, and time), the LPTE can track the particles’ location
283 through reverse time by updating the particles’ position after each time step of the model. This
284 method enables us to identify the particles’ origin over timescales from tens to hundreds of years
285 and reconstruct the trajectories of these particles from the position of origin to the point of interest.
286 As the particles deployed are all marginally offset in space and time relative to the exact sampling
287 position, they generate an ensemble of backward trajectories and origins that can assist in
288 identifying likely water masses constituting the sampled seawater. The model and experiments
289 used in this study are described below.

290 The velocity fields of the Operational Mercator global ocean analysis and forecast system
291 (<http://marine.copernicus.eu>) were used in this study. This system uses the Ocean General
292 Circulation Model from the Nucleus for European Modelling of the Ocean (NEMO) framework
293 (Madec & the NEMO team, 2008) with a horizontal resolution of $1/12^\circ$ and 50 vertical layers. The
294 thickness of each vertical layer increases with depth from 1 m at the surface to 450 m at the bottom
295 (5500 m depth). Partial steps were used for the bottom grid cell of the water column to better
296 represent the bottom topography within the model. The model topography was generated with the
297 bathymetric databases ETOPO2 (Amante & Eakins, 2009) and GEBCO8 (Becker et al., 2009) for
298 open ocean and continental shelves, respectively. For further details on the model product and the
299 validity of its velocity fields, the reader can refer to Lellouche et al. (2018a) and Lellouche et al.

300 (2018b). The velocity fields are available as daily and monthly mean values from 26 December
301 2006 to present.

302

303 The Lagrangian experiments were conducted for each sample obtained from the seven stations
304 (total of 302 samples) occupied during the 40-day JC150 cruise (Fig. 1) using the Lagrangian
305 particle tracking tool ARIANE (Blanke & Raynaud, 1997).

306 As currents are faster in the upper ocean (defined here as the top 800 m), and capturing their
307 behavior requires a finer time resolution, different experimental configurations were defined for
308 each sample based on its sampling depth. Firstly, for depths shallower than 800 m, we employed
309 daily mean velocity fields to track the deployed particles, whereas for depths deeper than 800 m,
310 we used monthly mean values. Secondly, the particles were advected backward in time for varied
311 periods depending on the depth: up to 10 years for the upper ocean samples and up to 300 years
312 for the deep ocean ones.

313 In all cases, an ensemble of particles (or particle clouds) was uniformly distributed around the
314 sampling location and repeatedly deployed across a period that was centered on the sampling time.
315 This ensemble was organized as a vertical cylinder, made of equally spaced disks of particles
316 spaced at $1/12^\circ$ resolution radially.

317 The height of the cylinder, number of disks inside each cylinder, and the number of repeated
318 releases around the sampling time varied between the samples taken within the upper or deep
319 ocean. For example, for the upper ocean, we used a cylinder with a height of 10 m and radius of
320 $1/4^\circ$ and 12-hourly release of particles within a five-day window (nine releases). More details about

321 this experimental setup are provided in S1, while several examples of particle trajectory ensembles
322 for different depths and advection times are shown in Figure S2.

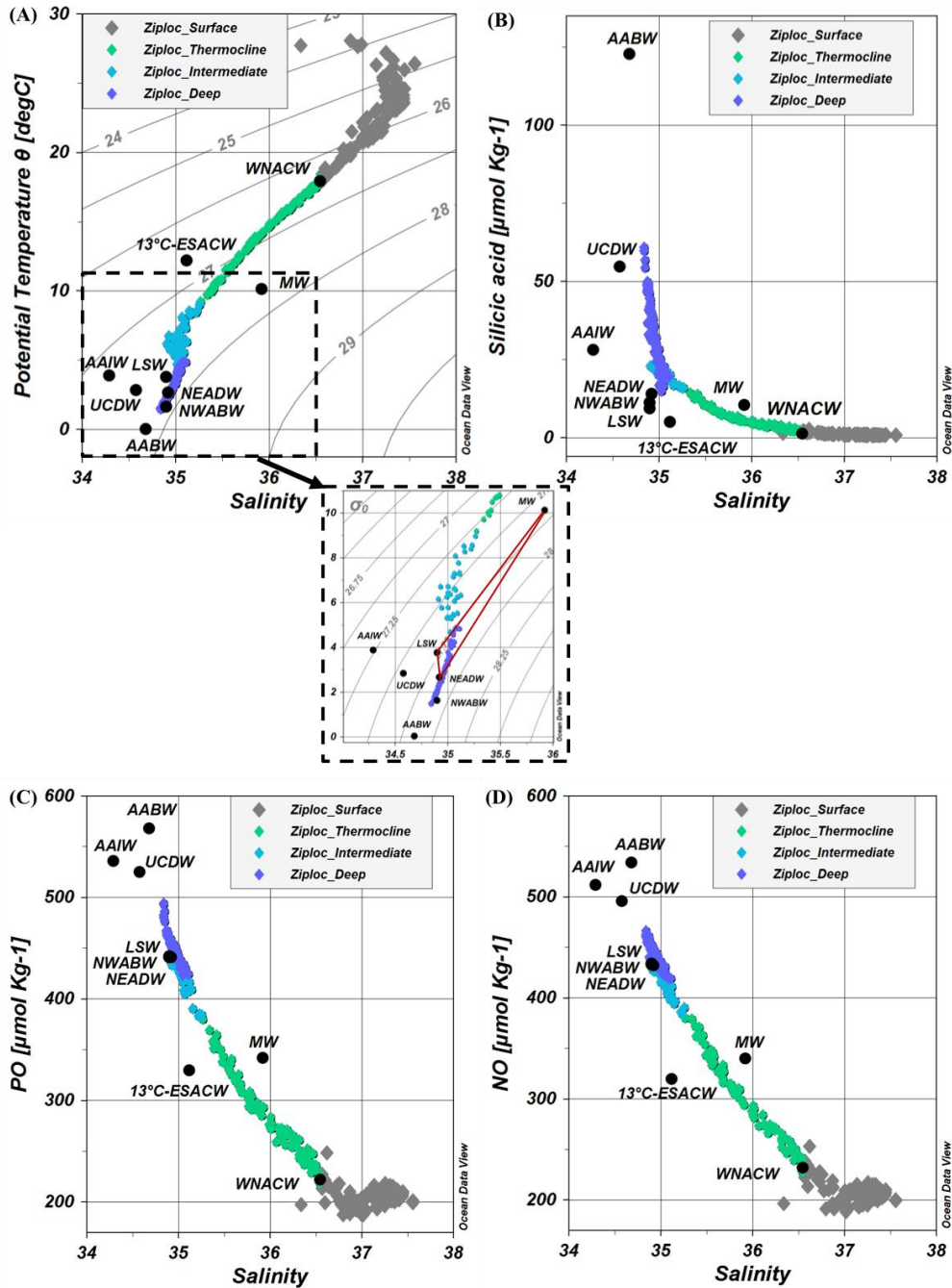
323

324 **3 Water mass analysis: results and discussion**

325 The hydrographic properties measured during JC150, θ , S, AOU, and concentrations of O_2 , PO_4^{3-}
326 , NO_3^- , and $Si(OH)_4$, are presented in this study for the first time. They are shown as
327 property/property plots in Figure 2, and as section in Figure 3.

328 The discussion is organized in three parts. Firstly, the surface waters shallower than 200–300 m
329 (where an eOMPA cannot be performed, because water properties are constantly changing due to
330 ocean-atmosphere exchange) are discussed using satellite data and LPTE results. Secondly, the
331 end-member choice for the three eOMPA layers is extensively discussed using a thorough
332 literature review, meticulous comparison of the JC150 hydrographic section properties with those
333 of the end-member candidates, and the LPTE results. Finally, the results of the eOMPA are
334 presented (end-members contributions) and discussed.

335 The LPTE results are presented in Figure 4. It is beyond the scope of this study to present the
336 LPTE results across all stations and depths. Therefore, for discussion, we selected results at
337 specific depths and from stations 1 and 7, representing the westernmost and easternmost stations,
338 respectively. Finally, the results from the eOMPA are presented in Figure 5.



339

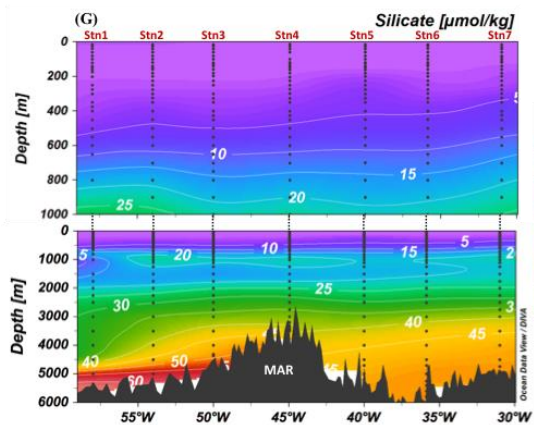
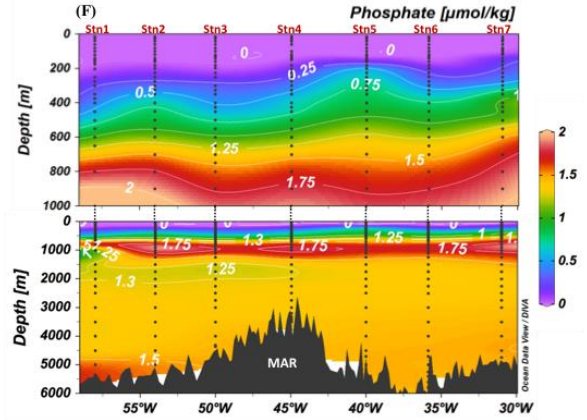
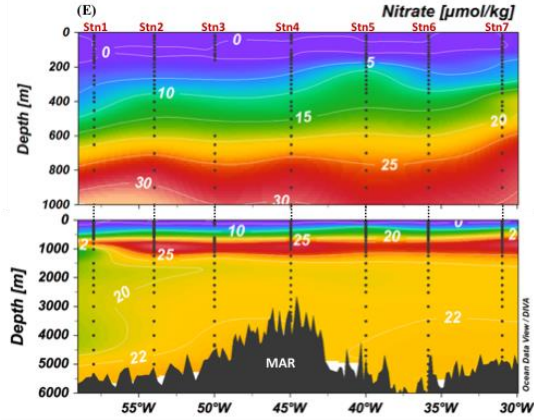
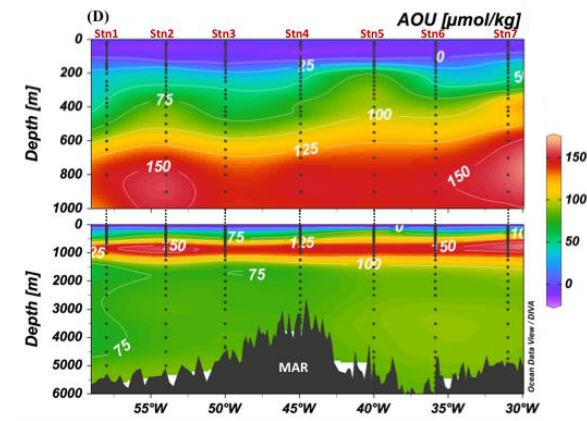
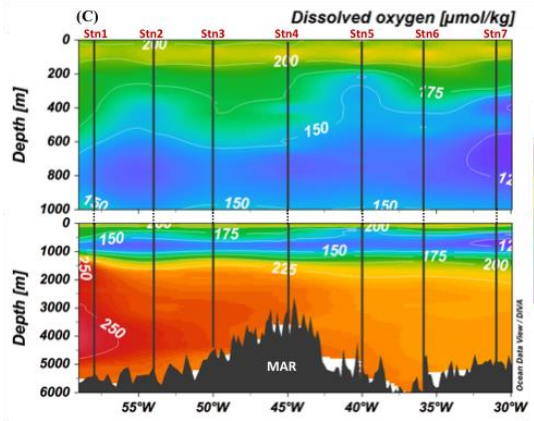
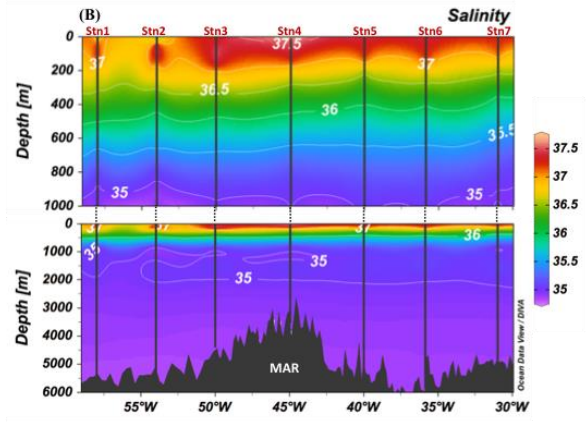
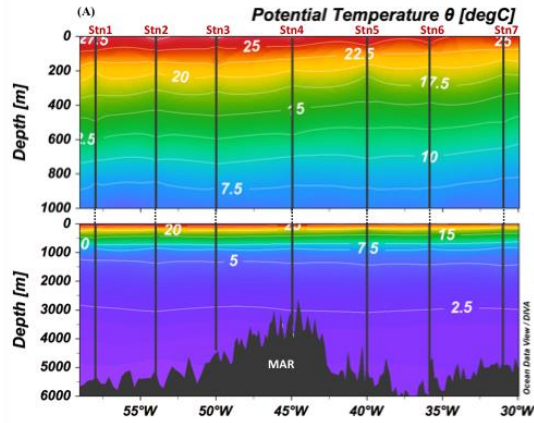
340 Fig. 2. Potential temperature versus salinity with isopycnals (gray lines) and a zoom on water

341 colder than 10 °C, in which the red triangle highlights the impact of Mediterranean Water (MW)

342 in the deep layer (A), silicic acid versus salinity (B), PO versus salinity (C), and NO versus salinity

343 (D) for the JC150 data (color diamonds) and GEOTRACES end-members (black diamonds). PO

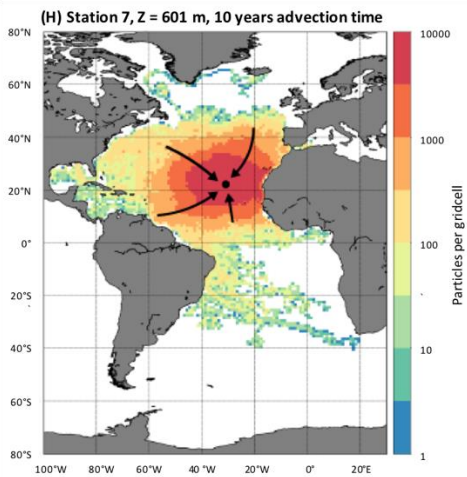
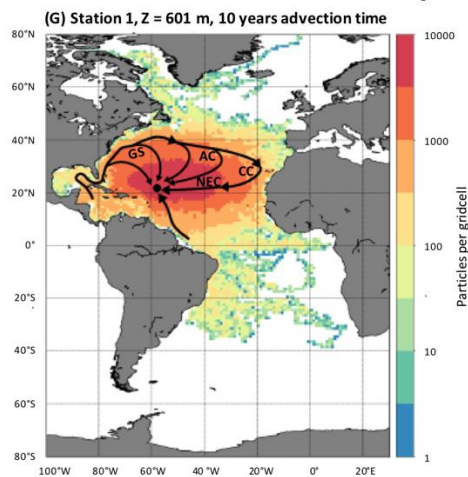
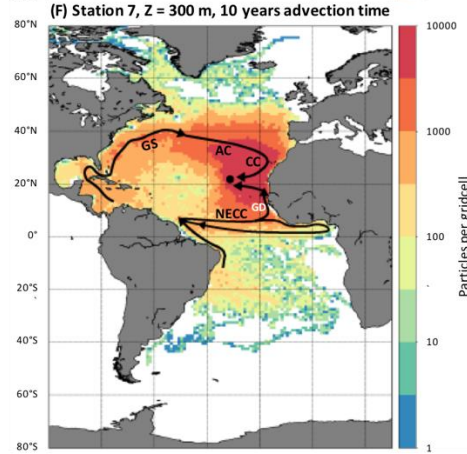
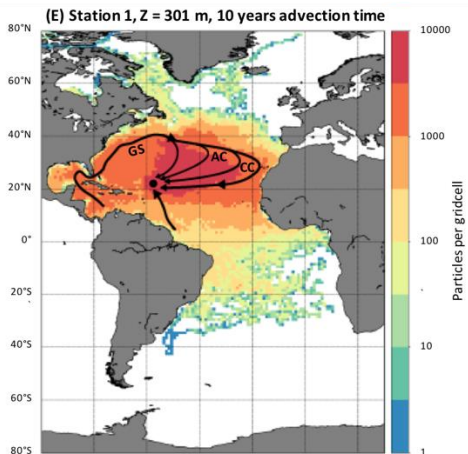
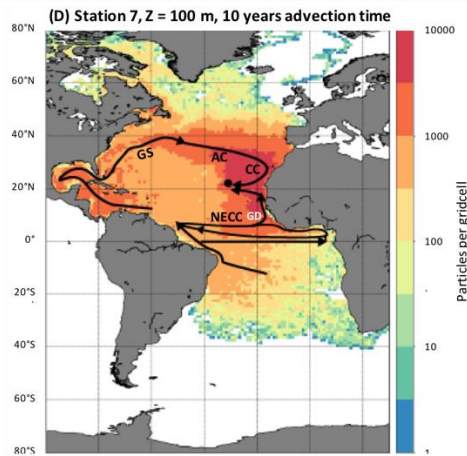
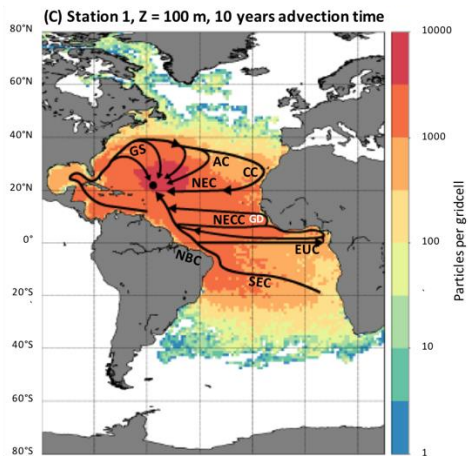
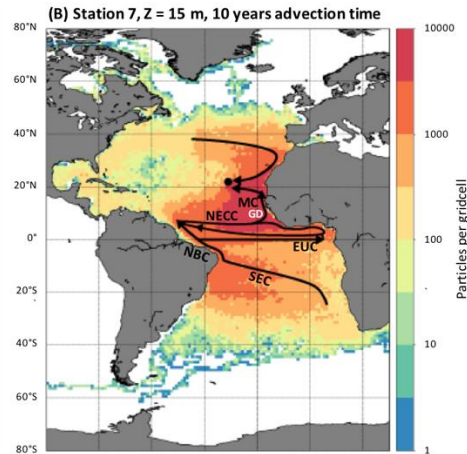
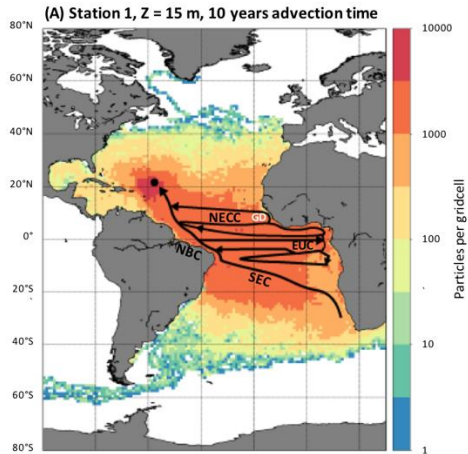
344 and NO definitions are provided in section 2.2.

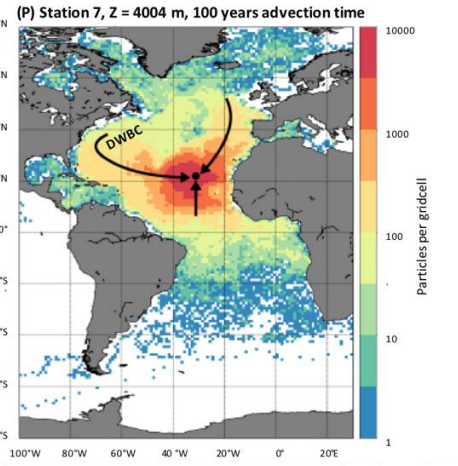
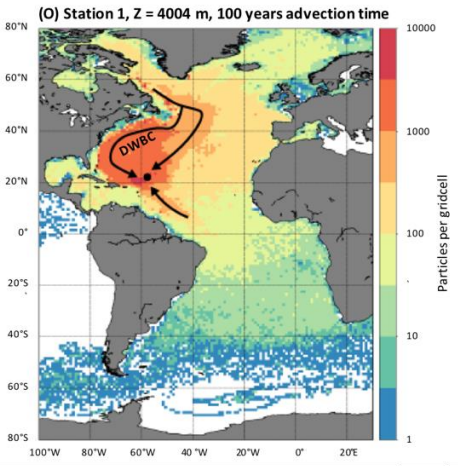
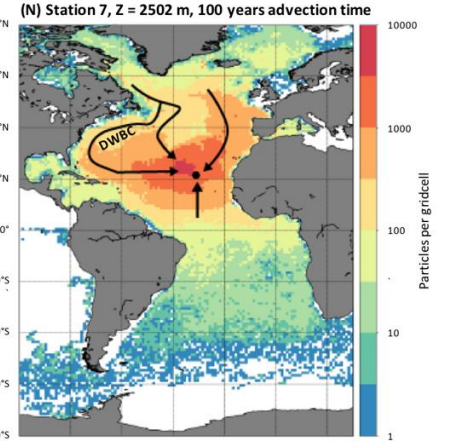
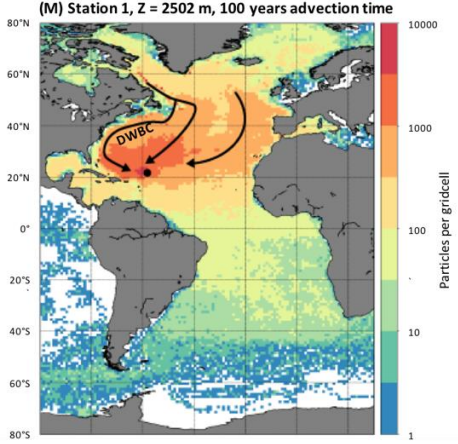
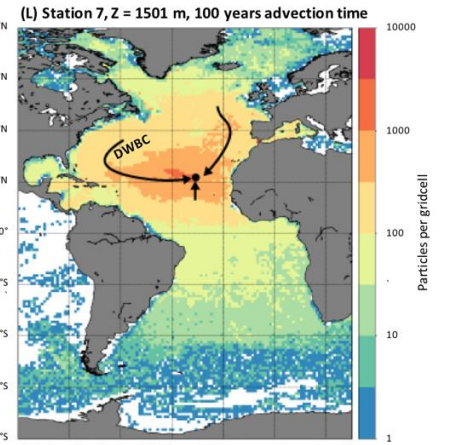
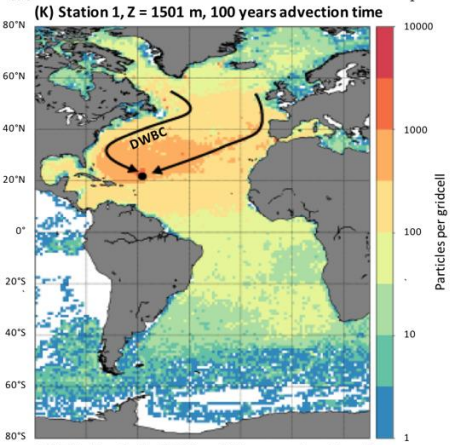
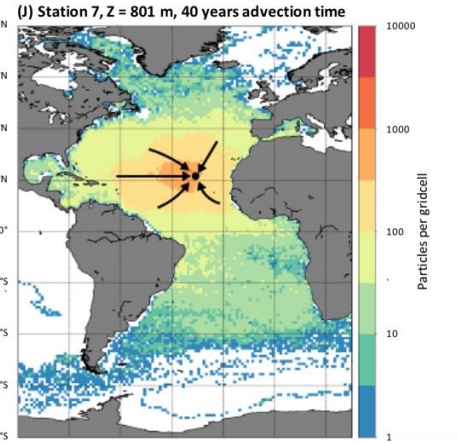
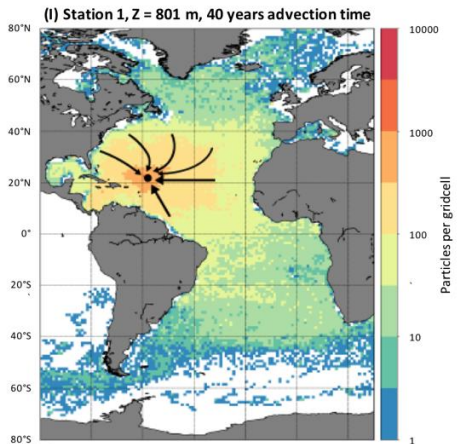


346 Fig. 3. Observed section of potential temperature (A), salinity (B), dissolved oxygen (C), apparent
347 oxygen utilization (AOU, D), and concentrations of nitrate (E), phosphate (F), and silicic acid (G)
348 from the JC150 cruise. The upper figures show zooms on the upper 1000 m, while the lower figures
349 show the full depth range. Data points are represented by black dots.

350

351





354 **Fig. 4.** Particle counts per $2^\circ \times 2^\circ$ grid cells computed by the Lagrangian particle tracking
355 experiment (LPTE), indicating particle origins and particles' most-used pathways to attain the
356 sampling locations. Results are presented for two JC150 stations (westernmost station 1, 22°N ,
357 58°W , left panels and easternmost station 7, 22°N , 31°W , right panels) and different depths.
358 Particles are advected backward in time with an advection time varying with depth. Arrows
359 highlight the main particle paths obtained from the LPTE results and literature general knowledge.
360 The following currents and location are presented in the figures: Gulf Stream (GS), Azores Current
361 (AC), Canary Current (CC), North Equatorial Current (NEC), South Equatorial Current (SEC),
362 North Brazil Current (NBC), Equatorial Undercurrent (EUC), North Equatorial Countercurrent
363 (NECC), Mauritania Current (MC), Deep Western Boundary Current (DWBC) and Guinea Dome
364 (GD). Refer to Fig. S2 for corresponding raw trajectories.

365

366 3.1 Surface waters

367 At the western edge of the section, a near surface tongue of low salinity water (36.3–37) is
368 observed shallower than 27 m at stations 1 and 2 (Fig. 3b). Using a surface satellite salinity map
369 (SMOS, July 2017, Fig. S3), this feature can clearly be attributed to Amazon River plume. This is
370 supported by the LPTE results that show the particle trajectories from near the Amazon River
371 mouth reaching the west of the zonal section (at depths of 15 m and 100 m, as shown in Figs. 4a
372 and 4c, respectively). This feature is constrained to the very surface and does not impact the
373 eOMPA results discussed below.

374 Two well-defined central water masses dominate the tropical Atlantic thermocline layer: the North
375 Atlantic Central Water (NACW) and the South Atlantic Central Water (SACW). The sampled

376 section extends along 22 °N, 58–31 °W, while the transition from NACW into SACW occurs at
377 approximately 15 °N at the Cape Verde Frontal Zone (Fieux, 2010; Tomczak & Godfrey, 1994).
378 Therefore, the impact of NACW and SACW on the sampled waters was investigated.

379

380 SACW encompasses two main water masses, including the Western SACW (WSACW) and the
381 Eastern SACW (ESACW) (Poole & Tomczak, 1999). WSACW is formed in the confluence zone
382 of Brazil and Malvinas Currents (Fieux, 2010) and recirculates within the southern subtropical
383 gyre. Therefore, it is mostly restricted to the western South Atlantic Ocean (Fieux, 2010; Tomczak
384 & Godfrey, 1994). In contrast, ESACW mainly comprises Indian Central Water transferred into
385 the Atlantic Ocean through Agulhas Current rings and is known to cross the Atlantic basin several
386 times during its northwards transit (Fieux, 2010; Tomczak & Godfrey, 1994; Tsuchiya, 1986). Our
387 LPTE trajectories are in good agreement with the current understanding of the ESACW northward
388 transit (Figs. 4a–4d): ESACW is transported northwestwards from the Cape Basin to the equator
389 through the southern branch of the South Equatorial Current and North Brazil Current. Here, the
390 trajectories show a portion of ESACW continuing northward toward the western stations (Figs. 4a
391 and 4c), while a portion retroflects eastward toward the Guinea Dome within components of the
392 equatorial current system (Figs. 4a–4d).

393 In addition to what has been previously described, the LPTE suggested that this shallow ESACW
394 reached the JC150 zonal section from the Guinea Dome by two trajectories: a portion flows
395 northwards within the Mauritania Current to the easternmost stations (Figs. 4b and 4d), while
396 another portion crosses the Atlantic basin westward once more and then flows northward to join
397 the westernmost stations (Figs. 4a and 4c).

398 NACW also comprises several waters masses. More than half of its volume comprises subtropical
399 mode water (Tomczak & Godfrey, 1994). The principal North Atlantic's subtropical mode water
400 is the Western NACW (WNACW, Talley et al., 2011), also called '18 °C water'. WNACW is
401 formed in the Sargasso Sea and identified by a permanent thermostat between 300 and 500 m at
402 approximately 17–18 °C (Fieux, 2010; Tomczak & Godfrey, 1994).

403 Between 100 and 300 m, the LPTE analysis shows waters following the North Atlantic
404 anticyclonic subtropical gyre circulation, i.e., waters originate from the Gulf of Mexico and the
405 Caribbean Sea, flow through the Sargasso Sea and the Gulf Stream and then the Azores and Canary
406 currents, and finally the North Equatorial Current flowing westward redistributes these waters
407 from the eastern to the western JC150 stations. In addition, the LPTE trajectories show a direct
408 transfer from the Gulf Stream to the sampled stations (Figs. 4c–4f). These trajectories correspond
409 very well to the circulation pattern of WNACW. This suggests that this 100 to 300 m depth layer,
410 below the layer mainly occupied by ESACW, is dominated by WNACW.

411

412 In summary, above ~300 m, the salinity data from JC150, SMOS, and LPTE show an Amazon
413 influence in the west of the section, which is restricted to the near-surface. The LPTE results
414 highlight the dominant influence of a shallow variety of ESACW in the upper 100 m and an
415 increasing WNACW impact below 100 m.

416

417 3.2 Analysis of end-members for thermocline, intermediate, and deep eOMPA layers

418 This section discusses the end-member choice for the thermocline (main thermocline from 300–
419 700 m), intermediate (700–1500 m) and deep eOMPA layers (1500 m to seafloor).

420 All end-members of the present eOMPA were selected from GEOTRACES cruises, where
421 numerous parameters, including trace elements and isotopes, are available to facilitate further use
422 of this eOMPA results (these locations are not necessarily in the water mass formation regions).

423

424 3.2.1 Thermocline waters

425 The two central waters discussed above (ESACW and WNACW) are also present below 300 m.
426 WNACW is the only water mass that can account for the warm, salty, and low PO and NO
427 concentration waters found in the thermocline layer (Fig. 2). In addition to supporting the presence
428 of WNACW in surface waters (section 3.1), the LPTE analysis supports the large contribution of
429 WNACW to the thermocline layer (Figs. 4e–4h) with particles following the anticyclonic North
430 Atlantic Subtropical gyre circulation between 300–600 m (refer to WNACW circulation details in
431 section 3.1). Although the surface gyre circulation pattern appears weaker by 800 m (Figs. 4i and
432 4j), WNACW is ultimately an important end-member to be included in the thermocline layer. We
433 used θ , S, concentrations of O_2 , PO_4^{3-} , NO_3^- , and $Si(OH)_4$ data from the GEOTRACES GA02
434 cruise station 18 at ~250 m to define WNACW (Fig. 1). These end-member hydrographic and
435 nutrient values are in agreement with those reported in literature (Hinrichsen & Tomczak, 1993;
436 Talley et al., 2011, cf. Table.1 for detailed properties). As stated earlier (section 3.1), WNACW is
437 the main type of NACW. Other types of NACW, such as the Madeira Mode Water or the East
438 NACW, exist (Harvey, 1982; Talley et al., 2011; Tomczak & Godfrey, 1994). However, the
439 Madeira Mode Water presents a formation rate and volume, which are much lower than those of
440 WNACW. The East NACW is considered in this study as partly included in the Mediterranean
441 Water (MW) definition (refer below, Carracedo et al., 2016; Talley et al., 2011). Therefore,

442 Madeira Mode Water and East NACW were not included as an end-member in the present
443 eOMPA.

444 A type of ESACW, namely the 13 °C-ESACW, is an important contributor to the thermocline of
445 the Atlantic Ocean (Tomczak & Godfrey, 1994; Tsuchiya, 1986). 13 °C-ESACW is needed to
446 account for the warm, low salinity, and low PO, NO, and Si(OH)₄ waters in the thermocline layer,
447 as well as the warm, low salinity, and low PO and NO waters in the intermediate layer (Fig. 2).
448 Even though the LPTE results do not show a dominance of ESACW trajectories below 300 m
449 along the JC150 zonal section (WNACW dominates at 300–800 m), they still show a non-
450 negligible influence from south Atlantic origin waters to depths of 800 m (Figs. 4i and 4j) and
451 1000 m (data not shown). Therefore, 13 °C-ESACW was chosen as an end-member to be
452 considered in both thermocline and intermediate layers. We used θ , S, concentrations of O₂, PO₄³⁻
453 , NO₃⁻, and Si(OH)₄ data from the GEOTRACES GA10 cruise station 3 at ~500 m to define 13
454 °C-ESACW (Fig. 1). These end-member hydrographic and nutrient values are in agreement with
455 those reported in literature (Poole & Tomczak, 1999, refer to Table. 1 for detailed properties).

456 As stated earlier (section 3.1), the other major SACW, which is WSACW, is restricted to the
457 southwest Atlantic (south of 30 °S, Fieux, 2010; Tomczak & Godfrey, 1994). This restriction was
458 underlined by a previous OMPA study, in which almost no contribution of WSACW was observed
459 at 22 °N (Poole & Tomczak, 1999). The LPTE results support these conclusions, as they show no
460 significant particles originating from the West South Atlantic, south of 30 °S, at the thermocline
461 depths (Figs. 4e–4h). Therefore, WSACW was not included in the thermocline eOMPA. Note that
462 the Guinea Dome Water was not explicitly included as an end-member in the present eOMPA;
463 however, it was implicitly included, as it could be considered as ESACW significantly modified
464 by the remineralization processes (Stramma & Schott, 1999).

465

466

467 3.2.2 Intermediate waters

468 At intermediate depths (~700–1500 m), the hydrographic atlases clearly show a high salinity layer,
469 which is attributed to the MW (World Ocean Atlas 2018, Fieux, 2010). MW is formed by the
470 mixing of the Mediterranean Outflow water, entering the Atlantic through the Gibraltar Strait, with
471 the subsurface and intermediate waters of the northeast Atlantic (Baringer, 1997; Carracedo et al.,
472 2016). MW extends northward to the Iceland-Scotland Ridge and westward to the Gulf Stream
473 (core at ~1000 m, Fieux, 2010), thereby presenting an important contribution to intermediate
474 depths across the North Atlantic. However, high salinity MW is not visible along the JC150 section
475 (Fig. 3b). This is because, at ~20 °N, the MW salinity maximum is located at the same depth as
476 low salinity Antarctic Intermediate Water (AAIW), where mixing reduces the salinity (Fieux,
477 2010; Talley et al., 2011). AAIW is the densest and less salty of the subantarctic mode water.
478 Formed along the subantarctic and mostly in the southeast Pacific, AAIW enters into the Atlantic
479 Ocean mainly via the Drake Passage and the Malvinas Current (Pacific type of AAIW) and
480 expands northward (Fieux, 2010 and references therein; Talley, 1996; Tomczak & Godfrey, 1994).
481 This northward expansion of low salinity AAIW is traced as far as 20 °N between 800–1000 m
482 (Fieux, 2010; Hinrichsen & Tomczak, 1993; Talley et al., 2011). This observation possibly
483 explains the lower salinity (< 35) centered at ~1000 m, mainly observed in the west of the MAR
484 during the JC150 cruise (Fig. 3b). Nevertheless, the θ -S diagram (Fig. 2a) shows that MW is the
485 only intermediate water mass that can explain the cold and saline waters in the thermocline layer
486 and the saltiest waters in both intermediate and deep layers (as previously suggested by Reid,
487 1979).

488 Furthermore, a strong O₂ minimum (O₂ < 150 μmol kg⁻¹), which is coincident with a layer of high
489 AOU (AOU > 125 μmol kg⁻¹), is visible across the entire JC150 zonal section centered at ~800 m
490 (Figs. 3c and 3d). This O₂ minimum is also nearly coincident with a layer of maximum NO₃⁻ and
491 PO₄³⁻ concentrations centered at ~900 m (> 25 μmol kg⁻¹ and > 1.5 μmol kg⁻¹, respectively, Figs.
492 3e and 3f, respectively) and relatively high Si(OH)₄ concentration (> 20 μmol kg⁻¹, ~1000 m, Fig.
493 3g). All these properties reflect the remineralization processes known to characterize the Upper
494 Circumpolar Deep Water (UCDW) originating from the Southern Ocean and flowing northward
495 into the Atlantic just below AAIW (Broecker et al., 1985). In the tropics, AAIW joins vertically
496 with UCDW (Talley et al., 2011; Tsuchiya et al., 1994). The resulting AAIW/UCDW complex,
497 traceable by high nutrients rather than low salinity, moves northward into the Gulf Stream system
498 and North Atlantic Current as far as 60 °N just south of Iceland (Talley et al., 2011; Tsuchiya,
499 1989; Tsuchiya et al., 1994). This is consistent with the low O₂, high NO₃⁻, PO₄³⁻, and Si(OH)₄
500 layers described above along the JC150 section. In addition, inclusion of AAIW and UCDW are
501 necessary to explain the coldest and highest PO and NO values in both thermocline and
502 intermediate layers (Fig. 2). UCDW is also specifically needed to explain the highest Si(OH)₄
503 values of the intermediate layer.

504 Although, the LPTE results did not aid us in clearly confirming (nor reject) the contributions of
505 MW, AAIW, and UCDW along the JC150 section, the above discussion is sufficient to conclude
506 that MW was an essential end-member to include in the three eOMPA layers, while AAIW and
507 UCDW were essential end-members in the thermocline and intermediate layers. We used θ, S,
508 concentrations of O₂, PO₄³⁻, NO₃⁻, and Si(OH)₄ data from GEOTRACES GA03 cruise station 3 at
509 ~1000 m to define MW and GEOTRACES GA02 cruise station 9 at ~1000 m to define AAIW and
510 those at ~1500 m to define UCDW (Fig. 1). These end-member properties were in agreement with

511 those reported in literature (Talley et al., 2011; Tsuchiya et al., 1994, refer to Table. 1 for detailed
512 properties).

513 3.2.3 Deep and bottom waters

514 In the west of the section, high O_2 , and relatively low NO_3^- and PO_4^{3-} waters are observed from
515 ~1500–4500 m (Figs. 3c, 3e, and 3f). This feature progressively decreases eastwards, but is still
516 visible east of the MAR. It is well established that these distributions are associated with low
517 nutrients and recently ventilated waters from the North Atlantic, mainly leading to the formation
518 of North Atlantic Deep Water: Labrador Sea Water (LSW), North East Atlantic Deep Water
519 (NEADW), and North West Atlantic Bottom Water (NWABW) (Swift, 1984; Talley et al., 2011).
520 LSW is formed in the Labrador Sea by winter convection leading to a homogenous water mass
521 from the surface to a depth of 1500–2000 m depending on the winter severity (Fieux, 2010; Lazier
522 et al., 2002). From the Labrador Sea, LSW is transported in three main directions, including
523 northward in the Irminger Sea, eastward crossing the MAR, and southward within the Deep
524 Western Boundary Current (DWBC, Fieux, 2010; Talley & McCartney, 1982). At 1500 m, the
525 LPTE results show two main flows that transport LSW to the JC150 section (Figs. 4k and 4l): west
526 of the MAR from the Labrador basin within the DWBC, and east of the MAR from the Iceland
527 basin. The first path within the DWBC has been well documented (Fieux, 2010; Talley et al., 2011;
528 Talley & McCartney, 1982). The presence of LSW in the eastern North Atlantic (the eastern
529 subpolar gyre, Iceland Basin, and the Rockall Trough) has also been well documented (Talley et
530 al., 2011). However, we could not find previous works presenting an evidence of the second LSW
531 pathway, east of the MAR and below 40 °N, from the eastern North Atlantic to the eastern tropical
532 Atlantic.

533

534 Below the LSW layer, NEADW is formed by the mixing of dense Iceland-Scotland Overflow
535 Water (ISOW) with southern origin Lower Deep Water (modified Antarctic Bottom Water),
536 entrained LSW, and subpolar mode water (Lacan & Jeandel, 2005; McCartney, 1992; Read, 2001).
537 NEADW flows in the recirculation cells in the western and eastern parts of the Subpolar North
538 Atlantic Gyre, which are connected to each other through the Charlie-Gibbs Fracture Zone (van
539 Aken, 2007; Fieux, 2010; McCartney & Talley, 1984; Read, 2001; Swift, 1984; Talley et al.,
540 2011). This water mass is known to be transported southward within the DWBC and east of the
541 MAR (Fieux, 2010). The LPTE results (at 2500 m, Figs. 4m and 4n) confirm both pathways.

542 NWABW is the densest water found near the bottom of the northwest Atlantic (Swift, 1984). It
543 originates from the dense, cold, and ventilated Denmark Strait Overflow Water (DSOW) which,
544 descending over the East Greenland continental slope to the bottom of the North Atlantic Subpolar
545 gyre, mixes with Irminger water, LSW, and ISOW (Fieux, 2010). Contrary to LSW and NEADW,
546 NWABW is too deep to cross the MAR and is therefore restricted to the western basin of the North
547 Atlantic Subpolar Gyre. From there, NWABW flows equatorward within the DWBC along the
548 western margin of the North Atlantic (Fieux, 2010). At 3000 m (data not shown) and 4000 m (Figs.
549 4o and 4p), the LPTE results confirm the NWABW transport from the Labrador Sea in the DWBC.

550 The above discussion confirms that LSW, NEADW, and NWABW, which are the main
551 contributors along with the MW to the North Atlantic Deep Water, should be considered as end-
552 members for the JC150 section. The contribution of LSW is specifically required to explain the
553 cold and slightly saline waters of the intermediate layer as well as the warm and low salinity waters
554 of the deep layer (Fig. 2). Therefore, LSW was included in both intermediate and deep layers.

555 LSW, NEADW, and NWABW are needed to explain the Si(OH)_4 , PO, and NO values at low
556 salinity of the deep layer (Figs. 2b–2d). Therefore, NEADW and NWABW were included in the

557 deep layer. We used θ , S, concentrations of O_2 , PO_4^{3-} , NO_3^- , and $Si(OH)_4$ data from the
558 GEOTRACES GA02 cruise station 9 at ~1000 m to define LSW, ~2500 m to define NEADW, and
559 ~4000 m to define NWABW (Fig. 1). These chosen end-member properties are in agreement with
560 those reported in literature (van Aken, 2007, refer to Table. 1 for detailed properties; Fieux, 2010).
561 A marked increase in the $Si(OH)_4$ concentration is observed in the range of 2500 m to the bottom,
562 which attains a maximum value ($> 60 \mu mol kg^{-1}$) in the west of the MAR. This feature reflects the
563 influence of Antarctic Bottom Water (AABW) originating from the Weddell Sea with a $Si(OH)_4$
564 maximum that can be traced to the North Atlantic (Word Ocean Atlas 2018). Its characteristics
565 and northward expansion are influenced by its mixing with overlying water masses and the
566 complex topography (van Aken, 2007; McCartney, 1992; Talley et al., 2011). AABW is the only
567 water mass that can explain the coldest waters as well as the highest $Si(OH)_4$, NO, and PO waters
568 of the deep layer (Fig. 2). The presence of this water mass in the deep layer is indisputable and
569 was therefore included. We used θ , S, concentrations of O_2 , PO_4^{3-} , NO_3^- , and $Si(OH)_4$ data from
570 the GEOTRACES GA02 cruise station 13 at ~4900 m to define AABW (Fig. 1). These chosen
571 end-member properties are in agreement with those reported in literature (van Aken, 2007;
572 McCartney, 1992; Talley et al., 2011).

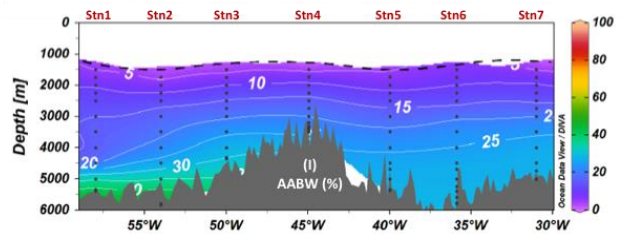
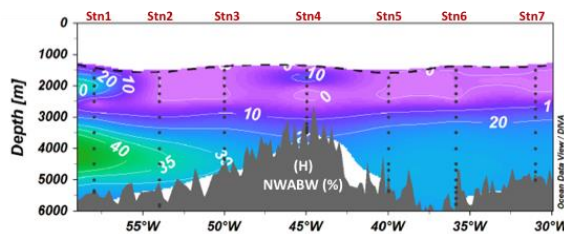
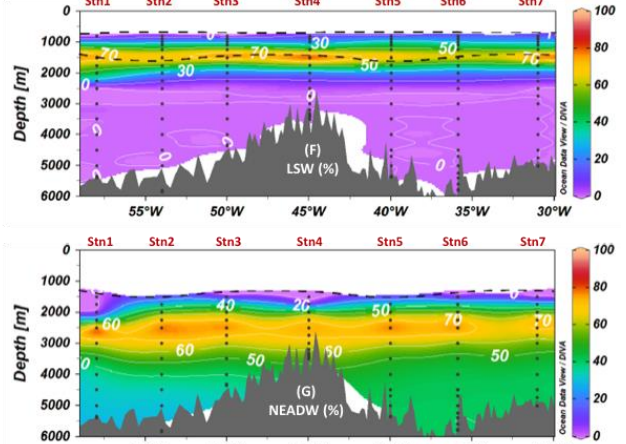
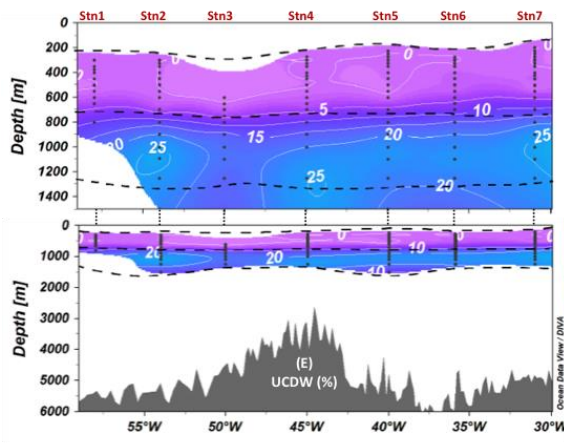
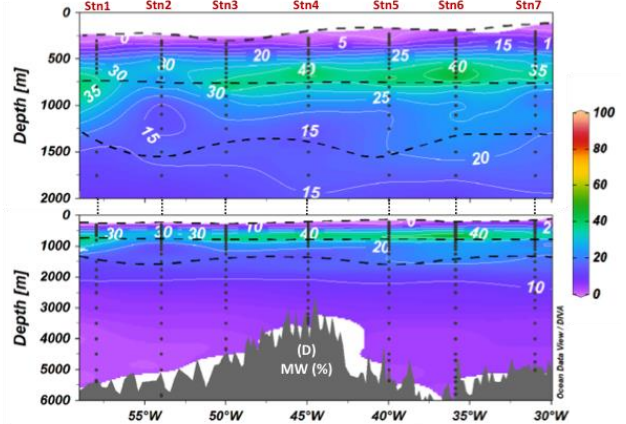
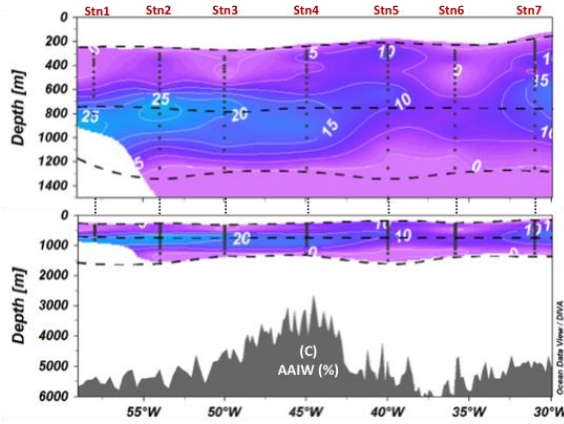
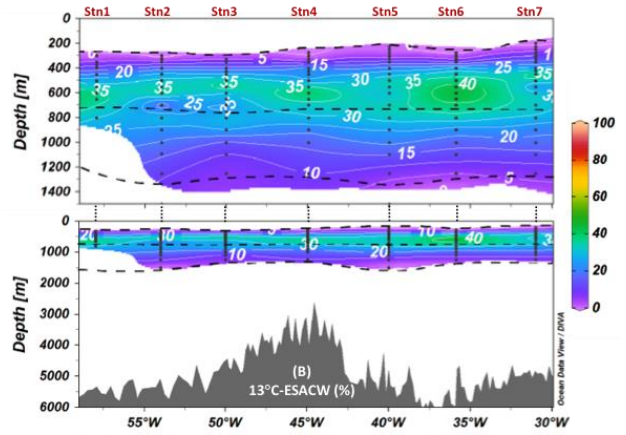
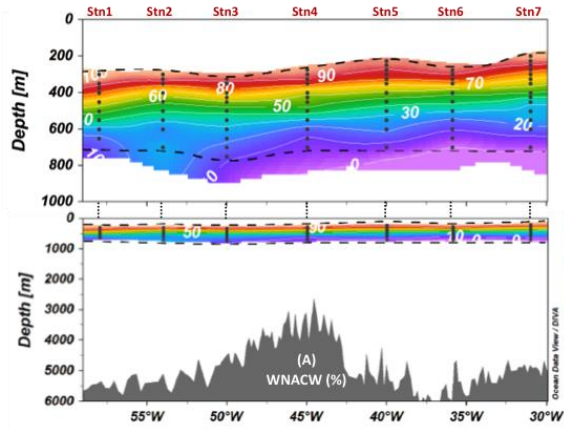
573 In summary, the eOMPA thermocline layer includes WNACW, 13 °C-ESACW, AAIW, UCDW,
574 and MW. The eOMPA intermediate layer includes 13 °C-ESACW, AAIW, UCDW, MW, and
575 LSW. The eOMPA deep layer includes MW, LSW, NEADW, NWABW, and AABW. These end-
576 member properties are summarized in Table. 1.

577

578 3.3 eOMPA

579 The eOMPA MATLAB routine was executed with the section data, end-members, weightings, and
580 the Redfield ratios determined earlier. The results from the eOMPA are presented in Figure 5 as
581 sections of end-member contributions. These results are discussed in detail in this section.

582



584 **Fig. 5.** Contributions (%) of the different end-members to the JC150 section according to the
585 extended optimum multiparameter analysis (eOMPA) of West North Atlantic Central Water
586 (WNACW) (A), 13°C- East South Atlantic Central Water (ESACW) (B), Antarctic Intermediate
587 Water (AAIW) (C), Mediterranean Water (MW) (D), Upper Circumpolar Deep Water (UCDW)
588 (E), Labrador Sea Water (LSW) (F), North East Atlantic Deep Water (NEADW) (G), North West
589 Atlantic Bottom Water (NWABW) (H), and Antarctic Bottom Water (AABW) (I). Sampling
590 points and eOMPA layer boundaries are represented by black dots and horizontal black dashed
591 lines, respectively.

592 3.3.1 Residuals and perturbation tests

593 The validity of the eOMPA results is discussed in this section. Firstly, to verify that the eOMPA
594 reproduces the observed values well, the residuals were closely observed. This aided in
595 determining whether the end-members were accurately selected. Secondly, to evaluate whether the
596 eOMPA results were robust, we discuss the results of the perturbation analysis. This aids in
597 quantifying the sensitivity of the results to our initial choices.

598 The residuals are presented as sections in Figure S4. The residual values are similar for the three
599 eOMPA layers and their average values are as follows: ~0% for θ , < 1% for S, < 7% for PO, < 9%
600 for NO, < 5% for Si, and ~0% for mass conservation. These average values include one outlier at
601 1500 m (over 199 samples, station 5). Except for this sample, that does not change the features of
602 the results, the low residue values indicate that the eOMPA well reproduces the observed values.
603 This a posteriori validates the initial choices about the end-members and Redfield ratios.

604 The results of the three perturbation tests (end-member characteristics, JC150 section data, and
605 parameters weights) enable us to assign an uncertainty/variability (two standard deviation) to each

606 water mass contribution (the section mean values of these uncertainties are reported in Table. S5
607 and presented on sections in Figs. S6, S7, and S8). Overall, the perturbation of both the end-
608 members' properties and the JC150 data result in uncertainties/variabilities of approximately 8%
609 each on average on the water mass percentage results (mean standard deviation over the three
610 eOMPA layers, 2 SD, %). The perturbation of the weights attributed to the eOMPA properties
611 only perturbs the water mass percentage results up to 2% (mean standard deviation over the three
612 eOMPA layers, 2SD, %). Overall, these perturbation analyses show that the main results of the
613 OMPA are robust, i.e., the water mass spatial distribution and their main characteristics (such as
614 dominant water masses) remain unchanged.

615 3.3.2 Thermocline waters

616 WNACW strongly dominates the thermocline layer (Fig. 5a) with a contribution exceeding 90%
617 at ~300 m. This contribution quickly decreases with depth and declines to 50% between 400–500
618 m and under 10% at the depth of ~700 m. The presence of WNACW extends marginally deeper
619 in the west of the section (~100 m deeper than in the east), which is consistent with a stronger
620 WNACW penetration closer to its formation area in the Sargasso Sea (Fieux, 2010; Tomczak &
621 Godfrey, 1994). The dominance of WNACW in this layer was expected based on the two previous
622 basin scale eOMPA studies conducted in the Atlantic Ocean thermocline (Poole & Tomczak,
623 1999) and along the GA03 2011 GEOTRACES section (Jenkins et al., 2015) located close to the
624 JC150 section (refer to Fig. 1). Both studies obtained large NACW contributions at depths above
625 600/800 m and the latitude of JC150. The dominance of WNACW in the thermocline layer is also
626 consistent with the LPTE results, indicating that the density of particles coming from the North
627 Atlantic Subtropical Gyre is dominant in the range of 300–600 m (Figs. 4e–4h).

628 Below the WNACW, a core of 13 °C-ESACW is found across the section with contributions higher
629 than ~30 % in the range of 500–800 m, which attains the maximum at ~600 m depth (35%, Fig.
630 5b). This result remarkably agrees with a previous eOMPA that estimates a contribution of ~25%
631 at 22 °N:25 °W in the range 400–800 m (Poole & Tomczak, 1999). Below 850 m, the 13 °C-
632 ESACW contribution decreases with depth to under 10 % at ~1250 m. No previous eOMPA study
633 included 13 °C-ESACW as an end-member deeper than 800 m in the Atlantic. However, no other
634 water mass could explain the warm, low salinity, and low PO and NO waters observed in the
635 intermediate layer of the JC150 section (Fig. 3).

636 3.3.3 Intermediate waters

637 AAIW is present at depths of 550–1100 m, thereby contributing to both thermocline and
638 intermediate layers. Its contribution is higher west of the MAR, where it attains a maximum at
639 ~700 m (> 30%) (Fig. 5c). UCDW is present over a similar depth range of 700–1500 m just below
640 the AAIW and attains a maximum (> 25 %) at ~1000 m depth. The presence of AAIW and, just
641 below, UCDW in the subtropical Atlantic is consistent with what was reported in previous
642 hydrodynamic studies (Talley et al., 2011; Tsuchiya, 1989; Tsuchiya et al., 1994). This is also
643 supported by two other OMPA studies reporting an AAIW contribution at ~750–900 m
644 immediately above UCDW (Álvarez et al., 2014; Jenkins et al., 2015).

645 The MW contribution exceeds 25% in the depth range of 500–1000 m across the section with a
646 maximum contribution (> 40 %) centered at ~700 m depth (Fig. 5d). The MW contribution is
647 higher and deeper in the east of the MAR (> 20 % at 1500 m) than in the west of the MAR (> 20
648 % at ~1000 m), suggesting a westward expansion of this water mass, which is consistent with the
649 MW propagation in the North Atlantic (Fieux, 2010). The MW contribution results are also

650 comparable with the GA03 OMPA study (Jenkins et al., 2015), according to which the MW
651 contribution extended westward across the MAR at approximately 500–1000 m depth. However,
652 our MW contributions are larger than those reported in other OMPA analyses (Bashmachnikov et
653 al., 2015; Louarn & Morin, 2011). This might be explained by the fact that our MW end-member
654 was defined further away from the Strait of Gibraltar and included a contribution of subsurface
655 and intermediate waters of the Northeast Atlantic (refer to section 3.2.2). The MW maximum
656 contribution is in the same depth range as that of AAIW; however, MW is more pronounced in the
657 east, whereas AAIW is more pronounced in the west. This is consistent with the mixing of MW
658 with AAIW at approximately 20 °N (Fieux, 2010; Talley et al., 2011). In the deep eOMPA layer,
659 the MW contribution is under 10% deeper than 2300 m and under 5% deeper than 3500 m. This is
660 consistent with the GA03 OMPA study that reported an MW contribution of ~10% in the range of
661 2000–3600 m (Jenkins et al., 2015). Though this contribution in our deep layer eOMPA is low, it
662 is not zero. It is absolutely necessary to account for the deep layer saltiest waters (refer to the red
663 triangle in Fig. 2a), which is in agreement with initial findings of Reid et al. (1979).

664 3.3.4 Deep waters

665 LSW is included in both intermediate and deep eOMPA layers. This water mass is present across
666 the section and exceeds a contribution of over 20% in the depth range of 900–2000 m. Its
667 contribution exceeds 50% in the depth range of 1250–1750 m and attains a maximum (> 70 %) at
668 ~1500 m depth (Fig. 5f). This is consistent with the GA01 (Subpolar Gyre) eOMPA study, that
669 found LSW centered at 1500 m in the Iceland and west European Basins (García-Ibáñez et al.,
670 2018). It is also consistent with the GA03 OMPA study that found the Upper LSW centered at
671 1500 m across the MAR (Jenkins et al., 2015).

672 The NEADW contribution exceeds 30% from ~2000 m to the bottom across the section (Fig. 5g).
673 Its maximum (>70 %) is attained at ~2500 m. The NEADW contribution is under 40% at a depth
674 of over 4000 m and in the west of the MAR, while the contribution in the east of the MAR is over
675 40% down to the bottom. This is consistent with the LPTE results and previous studies that suggest
676 that the NEADW contribution is achieved not only from the DWBC, but also directly from the
677 eastern part of the Subpolar North Atlantic Gyre east of the MAR (van Aken, 2007; Fieux, 2010;
678 McCartney, 1992; Read, 2001; Talley et al., 2011).

679 Below the NEADW, NWABW appears from 3000 m (> 10 %) to the bottom and attains its
680 maximum (> 45 %) at approximately 4000–4500 m at the section's western end (Fig. 5h). This
681 maximum seems to expand eastward to the MAR. East of the MAR, the NWABW contribution
682 exceeds 25% from 4000 m to the bottom. Four data points located shallower than 2500 m present
683 an unrealistic high NWABW contribution of over 19% and are clear outliers (Station 1 1750 m,
684 2000 m, and 2251 m and Station 4 1750 m), as a previous work has reported that this water mass
685 is absent at such shallow depths (García-Ibáñez et al., 2018). The lack of continuity between the
686 calculated NWABW core (observed here at 4000–4500 m) and these points is also an argument
687 for excluding these four data points. These four outliers should correspond to a predominance of
688 LSW and NEADW. LSW, NEADW, and NWABW have very close properties (almost
689 undistinguishable in terms of S, PO, NO, and Si(OH)₄ and temperature differences in the order of
690 1 °C, refer to Fig. 2). These similitudes explain that the deep eOMPA did not accurately distinguish
691 the three end-members for these four outliers. However, for the other 84 data points of the deep
692 layer (88 data points in total), the eOMPA appropriately distinguished between LSW, NEADW,
693 and NWABW and provided results, which are consistent with the literature (notably LSW above
694 NEADW above NWABW, Lacan & Jeandel, 2005; Swift, 1984). The maximum NWABW

695 contribution in the west is consistent with what was reported in previous studies on NWABW
696 flowing equatorward from the Labrador basin with DWBC along the western margin of the North
697 Atlantic (Fieux, 2010). However, the significant NWABW contribution east of the MAR (up to ~
698 20%) is unexpected or at least unreported so far. This water mass, which is formed in the Labrador
699 and Irminger Basins, is too dense to cross the MAR through the Charlie-Gibbs Fracture Zone and
700 was therefore never observed east of the MAR in the North Atlantic Subpolar Gyre. Flowing
701 southward from there, the first passage sufficiently deep for the NWABW to cross the MAR is the
702 Kane fracture zone, which is localized at 24 °N (just north of the JC150 section at 22 °N, Fig. 1)
703 with a sill depth of ~4350 m (Morozov et al., 2017). The next passage that is sufficiently deep is
704 the Vema Fracture Zone with a sill depth of ~5000 m; however, it is located much further south
705 (10–11 °N, Kastens et al., 1998). Therefore, our results suggest that NWABW enters the eastern
706 Atlantic through the Kane fracture zone. This eastern trajectory is confirmed by the LPTE results,
707 which indicates particles originating directly from the eastern part of the Subpolar North Atlantic
708 Gyre east of the MAR at 4000 m (Fig. 4p). We could not find any previous study describing this
709 aspect.

710 Note that our results about the localization of NEADW above NWABW contradicts with those of
711 the GA03 OMPA, which found DSOW (that significantly contributes to the formation of
712 NWABW) lying above ISOW (that significantly contributes to the formation of NEADW)
713 (Jenkins et al., 2015). Our results confirm that NWABW (including DSOW) lies below NEADW
714 (including ISOW) in the subtropical North Atlantic. In addition, our results are consistent in terms
715 of the densities of NWABW and DSOW being higher than those of NEADW and ISOW,
716 respectively. It is generally consistent with the current understanding of deep water mass dynamics
717 in the North Atlantic as well (Fieux, 2010; Lacan & Jeandel, 2005; Middag et al., 2015; Swift,

718 1984).

719 Deeper than 3000 m, the AABW contribution exceeds 15% across the section. West of the MAR,
720 AABW attains its maximum contribution (> 35%) from 5000 m to the bottom. East of the MAR,
721 the AABW contribution stays relatively high (> 20%) at a depth of over 3500 m. This AABW
722 contribution to bottom waters of the section and across the MAR is consistent with the findings
723 reported in previous studies, which describe AABW as the densest water in the majority of the
724 Atlantic, moving northward from its formation zone and crossing the MAR at 11 °N through the
725 Vema fracture zone (van Aken, 2007; McCartney, 1992; Talley et al., 2011). This AABW
726 contribution is also consistent with the GA03 OMPA study, in which a contribution of AABW is
727 observed across the MAR in the deepest parts of both the western and eastern basins (Jenkins et
728 al., 2015).

729

730 **4 Conclusions**

731 Based on i) the hydrographic data (θ , S, concentrations of O_2 , NO_3^- , PO_4^{3-} , and $Si(OH)_4$), ii) an
732 eOMPA, and iii) an LPTE conducted in an eddy-resolving ocean circulation model, a water mass
733 analysis has been presented for the 2017 JC150 GEOTRACES process study (GApr08) in the
734 subtropical North Atlantic along 22 °N.

735 This is the first time to the best of our knowledge that a water mass analysis combined an eOMPA
736 with an LPTE. This approach demonstrated several advantages:

737 - In addition to a thorough literature review and a meticulous analysis of the hydrographic data,
738 the LPTE helped select the eOMPA end-members. This is important, because the eOMPA results
739 are very sensitive to end-member choice. This meticulous end-member's choice enabled the

740 eOMPA to reproduce the observations (small residuals) and provide results, which were in good
741 agreement with the current knowledge (notably other Atlantic OMPA studies).

742 - LPTE provided information about water mass trajectories between their formation areas and the
743 studied location, which could not be achieved with a sole eOMPA.

744 - Finally, LPTE was effective in tracing water mass origins in surface layers, where an eOMPA
745 could not be performed due to the non-conservative hydrographic parameters.

746 The following conclusions were drawn from our study. The upper 100 m is occupied by a shallow
747 type of ESACW with impacts of the Amazon River plume in the west of the section. The WNACW
748 contribution dominates the upper part of the transect (mainly between 100–500 m) with a
749 contribution exceeding 90% at approximately 300 m. The 13 °C-ESACW contribution appears
750 marginally deeper with a contribution exceeding 40% at approximately 600 m depth. The AAIW
751 presents a maximum contribution of over 30% in the west of the MAR at ~700 m. At
752 approximately the same depth, MW, whose high salinity signal is lost because of mixing with
753 AAIW, attains its maximum contribution of over 40% in the east of the MAR. We found that
754 MW's contribution, although in small quantities (in the order of 5%), is required down to 3500 m.
755 Just below AAIW, the UCDW maximum contribution of over 25% is observed at ~1000 m depth.
756 The LSW contribution is present in the depth of 900–2000 m with a maximum of over 70% at
757 ~1500 m depth all across the section. Unpredictably, at this depth, we found through the LPTE
758 that the LSW present in the eastern North Atlantic flows southward to the eastern subtropical
759 Atlantic. We could not find previous works presenting this evidence below 40 °N. Below LSW,
760 the NEADW contribution, which includes the ISOW contribution, exceeds 70% at approximately
761 2500 m all across the section. Below NEADW, the NWABW maximum contribution of over 45%
762 is attained at ~4500 m west of the MAR. The NWABW contribution is also found in the east of

763 the MAR in significant proportions ($> 25\%$). Crossing of the MAR by this water mass has not
764 been investigated so far. As this water is too dense to cross the MAR in the Subpolar Gyre (through
765 the Charlie-Gibbs Fracture Zone), we suggest that it crosses the MAR through the Kane fracture
766 zone (sill depth of 4350 m) at $\sim 24^\circ\text{N}$. The occurrence of NWABW (including DSOW) below
767 NEADW (including ISOW) is consistent with the current knowledge about these water masses
768 and notably their densities. This contradicts a recent OMPA result obtained in a nearby area, where
769 ISOW was found below DSOW (GA03, Jenkins et al., 2015). The deeper water mass contributing
770 to our section is AABW with a maximum contribution of over 35% deeper than 5000 m in the
771 west of the MAR.

772 These results will be useful to interpret the biogeochemical datasets from the subtropical North
773 Atlantic, notably those with respect to trace elements and isotope distributions (which can be
774 facilitated by the end-member choices at GEOTRACES stations).

775

776 **Author contributions**

777 CM was the chief scientist of the cruise. CM, MCL, NJW, and EMSW participated in the sampling
778 on board. They participated in the temperature, salinity, dissolved oxygen, and nutrient
779 concentration data production along with JH. SvG produced the Lagrangian particle tracking
780 experiment under the supervision of YD with the contribution of LA and FL. LA and FL produced
781 the optimum multiparameter analysis and conducted the interpretation work. LA drafted the
782 manuscript under the supervision of FL with contributions from SvG, NJW, and all other authors.

783

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