Paleoceanography and Paleoclimatology

Supporting Information for

Deep North Atlantic Last Glacial Maximum Salinity Reconstruction

Kira Homola[1], Arthur J. Spivack[1], Richard W. Murray[2], Robert Pockalny[1],

Steven D'Hondt[1], Rebecca Robinson[1]

Contents

Introduction

This supplement includes the details behind the modeling and mass balance calculations that are

unique to this analysis.

All data used in this study is available in the EarthChem Library at doi:10.26022/IEDA/111472 .

[1]University of Rhode Island Graduate School of Oceanography
[2]Woods Hole Oceanographic Institution

Diffusion Model

We use a centered-difference iteration to forward model the diffusion of *[Cl⁻]* over time *t* and depth *z* in subseafloor porewater.

Each term that varies in depth or time is denoted by (*t,z*).

Modeled porewater chloride is optimized by minimizing the sum of the squared differences between measured and modeled *[Cl](0,z)*. Uncertainty is based on the sum of the squared differences between the measured *[Cl](0,z)* ± 1 standard deviation and the modeled *[Cl](0,z)*. These upper and lower error boundaries to the model fit are differenced to determined the uncertainty in *[Cl](0,z)*.

Domain:

t = Time in seconds: 0 (today) to 100 ka, with a timestep (*Δt*) of 5 x 10^7 seconds.

z = Depth below seafloor in meters: 0 (seafloor) to 100 mbsf, with a depth resolution (*Δz*) of 0.5 m.

[Cl](t,z) = porewater chloride concentration for a time t and depth z at the site under evaluation

Initial Conditions (IC): [Cl] of today's bottom water, synonymous with porewater *[Cl](0,0)*. The initial condition provides a starting point for the model and is adjusted to tune the shape of the modeled *[Cl](0,z)* deeper than the porewater chloride maximum. We begin the model 100,000 years ago to ensure the IC does not affect the modeled porewater chloride maximum.

Boundary Conditions (BC): The *[Cl](t,0)*, the bottom water chloride concentration over time is determined by scaling Miller et al.'s global sea level height compilation to represent chloride concentration. We adjust the boundary condition's amplitude *[Cl](t,0)*, until the model fits the measured data. The model is run multiple times to produce a family of modern porewater [Cl] profiles that can be compared to measured data.

Adjustable parameters:

IC: Set to modern bottom water [Cl] measured at the site being modeled adjusted by $0 - 5\%$ to best encompass the measured data below the porewater [Cl] LGM maximum. Separate model runs are performed to account for uncertainty in the measured porewater *[Cl](0,0)*; *[Cl](0,0)* is set to its measured value and that value ± its uncertainty: three unique ICs.

BC: We normalize Miller et al.'s sea level height compilation and scale it to represent *[Cl](t,0)*. The model is site specific, while this dataset is a global compilation. The maximum sea level height change in Miller's compilation occurs at 21.93 ka, with nearest measured values at 19.03 and 30.04 ka. To allow the possibility of a site specific salinity maximum that may differ in timing within the $19 - 26$ ka LGM, we run a second and third BC determined by adjusting the timing of Miller et al.'s peak from 21.93 ka to 19.03 and 25.43 ka, respectively. Each of these three boundary conditions, unique only in the timing of their maximums, is replicated with a different scale factor until the modeled *[Cl](0,z)* profiles encompasses the measured data. Five scale factors are used for each of the three differently timed boundary conditions for a total of 15 unique boundary conditions.

Diffusion Coefficient: Separate model runs are performed to three unique *D(z)*'s: the

diffusion coefficient for chloride in seawater at 35 g/kg and 0 °C, ± the reported

uncertainty of this coefficient (5 %). *D(z)* is calculated from the seawater Cl– diffusion

coefficient (9.60×10^{-10} m^2/s at 0 °C and 35 g/kg)(Li and Gregory 1974); the slope of *D(z)*

as a function of temperature (0.438×10^{-10} m^2/s°C)(Boudreau 1997); and the near-

seafloor temperature gradient at Sites 03 and 10 of 0.05 °C/mbsf (Erbacher et al. 2004).

More details of diffusion coefficients that incorporate measured formation factors, rather

than being estimated based on the depth of measured salinity or d^{18}O maximums, can be

found in our previous work (Homola et al. 2020; Insua et al. 2014).

Thus while only three parameters are varied, we model 135 unique domains by running each

of the 3 ICs with 15 BCs and 3 *D(z)*s to produce a robust modeled *[Cl](0,z)* profile family

that encompasses the measured data at each site.

Salt Balance of the Modern and LGM Deep Ocean

We approximate the average salinity of the global deep ocean (below 2 km) as the sum of the Atlantic and Pacific deep waters (eq. S1).

$$S_T = (V_A S_A + V_P S_P) / V_T \qquad (S1)$$

Where the average salinity of the total deep Atlantic and Pacific is S_T; the total volume of the deep Atlantic, V_A, and the deep Pacific, V_P, is V_T; and the average salinity of the deep Atlantic and Pacific, respectively, are S_A and S_P.

To examine the sources of deep water-masses, we further separate each basin into a northern, N, and southern, S, deep water component (eq. S2).

$$S_A = (R_{AN} S_{AN} + R_{AS} S_{AS}) V_A \qquad (S2)$$

The ratio of northern or sourced deep waters total deep waters in that basin, R_{AN} and R_{AS} for the north and south Atlantic, respectively, is a volume ratio estimated from zonally averaged published paleosalinity and benthic foraminiferal δ^{13}C, Δ^{14}C, and δ^{18}O data. Vertical, meridional cross sections of Atlantic and Pacific salinities and temperatures below 2 km water depth for the modern and LGM (refs) are used to approximate the ratio of northern to southern sourced water in each basin during the modern and LGM.

The salinities of each deep water source have been inferred from measured (Adkins et al. 2002; Insua et al. 2014) and modeled (Galbraith and Lavergne 2019) studies. We examine published paleosalinity from both measured and modeled studies, incorporating measured data from this study, to calculate the global mean deep ocean salinity during the LGM and its difference from the modern. Inputs and results are included in Table SM.1. When KN223 data is

included, we use a simple, two-source mixing model of the deep Atlantic to calculate the salinity of LGM southern sourced deep water that is consistent with measured salinity and water mass distribution data (eq. S3).

$$S_{AS} = (S_{meas} + f_{AN}S_{AN}) / f_{AS} \qquad (S3)$$

We use the Atlantic cross sections from Oppo et al. (2018) to determine the fractions of northern, f_{AN}, and southern, f_{SN}, sourced bottom water. The average latitude of the measured KN223 sites has bottom water composed of 70 % and 40 % northern sourced deep water during the modern and LGM, respectively (Figure SM.1). Substituting values for each term in eq. 6, we calculate a S_{AS} of 36.7 g/kg from eq. S4.

$$S_{AS} = (36.46 + 0.4*36.1) / 0.6 = 36.7 \qquad (S4)$$

Constants used in these calculations include; seawater density, 1025 kg/m³; global ocean salt mass (constant with time), 4.28 x 10¹⁹ kg; total seawater volume in the modern, 1.02 x 10¹⁸ m³; volume of the Atlantic, 3.1 x 10¹⁷ m³; volume of the Pacific, 7.1 x 10¹⁷ m³; deep water volume equal to 2/3 of total seawater volume; and LGM total seawater volume equal to 98 % of modern total seawater volume.

Table SM.1. Salt balance calculations with their three types of inputs: modeled (green, Galbraith and Lavergne 2019), published measured values (orange, Adkins et al. 2002; Insua et al. 2014), and measured values including those from this study (blue).

| Type	Salinity Data Source	Time	Variable	Unit	Atlantic			Pacific			Global Average Deep Water Salinity (g/kg)	ΔS$_{total}$ (LGM-0) %
					Total	S	N	Total	S	N		
			Deep Water Volume	m3	2.05E+17			4.69E+17				
Modeled	Galbraith and Lavergne 2019	0	Salinity	g/kg	35.0	34.8	35.1	34.7	34.8	34.7	34.79	
			Deep Relative Area	%	100	46	54	100	10	90		
			Deep m_salt	kg	4.84E+18	2.22E+18	2.62E+18	1.10E+19	1.10E+18	9.90E+18		
			Deep Relative Mass Salt	%	10.0	4.6	5.4	22.8	2.3	20.5		3.84
	Galbraith and Lavergne 2019	LGM	Salinity	g/kg	36.3	36.4	35.8	36.1	36.4	36.1	36.18	
			Deep Relative Area	%	100	80	20	100	10	90		
			Deep m_salt	kg	4.92E+18	3.95E+18	9.71E+17	1.12E+19	1.13E+18	1.01E+19		
			Deep Relative Mass Salt	%	10.2	8.2	2.0	23.3	2.3	20.9		
Measured Before KN223 (Published)	Adkins et al. 2002; *Insua et al. 2014*	0	Salinity	g/kg	34.8	34.7	34.9	34.7	34.7	*34.695*	34.73	
			Deep Relative Area	%	100	46	54	100	10	90		
			Deep m_salt	kg	4.82E+18	2.21E+18	2.61E+18	1.10E+19	1.10E+18	9.90E+18		
			Deep Relative Mass Salt	%	10.0	4.6	5.4	22.8	2.3	20.5		4.52
	Adkins et al. 2002; *Insua et al. 2014*	LGM	Salinity	g/kg	36.9	37.1	36.1	36.1	36.2	*36.135*	36.37	
			Deep Relative Area	%	100	80	20	100	10	90		
			Deep m_salt	kg	5.01E+18	4.03E+18	9.79E+17	1.12E+19	1.12E+18	1.01E+19		
			Deep Relative Mass Salt	%	10.4	8.4	2.0	23.3	2.3	21.0		
Measured Including KN223	**KN223,** Adkins et al. 2002; *Insua et al. 2014*	0	Salinity	g/kg	34.8	34.7	34.9	34.7	34.7	*34.695*	34.73	
			Deep Relative Area	%	100	46	54	100	10	90		
			Deep m_salt	kg	4.82E+18	2.21E+18	2.61E+18	1.10E+19	1.10E+18	9.90E+18		
			Deep Relative Mass Salt	%	10.0	4.6	5.4	22.8	2.3	20.5		4.26
	KN223, Adkins et al. 2002; *Insua et al. 2014*	LGM	Salinity	g/kg	36.6	**36.7**	36.1	36.1	36.2	*36.135*	36.27	
			Deep Relative Area	%	100	80	20	100	10	90		
			Deep m_salt	kg	4.96E+18	3.98E+18	9.79E+17	1.12E+19	1.12E+18	1.01E+19		
			Deep Relative Mass Salt	%	10.3	8.3	2.0	23.3	2.3	21.0		
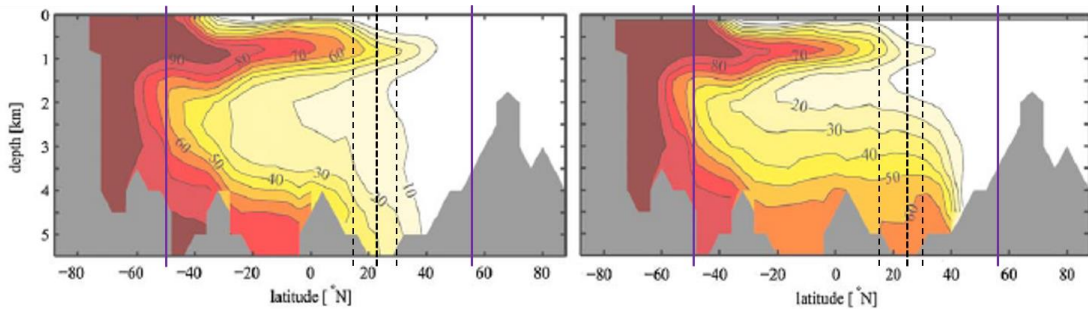
Figure.S1. Modified from Oppo 2018. A meridional, vertical cross section of the western Atlantic for the modern (left) and glacial (right) that shows the percentage of Atlantic water sourced from the southern ocean vs. the north Atlantic. Vertical lines indicate sites used in the salt balance, where purple lines are published locations and the black lines are locations measured in this study (bold centerline is the mean, the northernmost and southernmost latitudes of measured KN223 site locations are shown by the thin dashed lines).