

Mechanisms of Ocean Heat Uptake Along and Across Isopycnals

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12 ABSTRACT: Warming of the climate system accumulates mostly in the ocean and discrepancies
13 in how this is modelled contribute to uncertainties in predicting sea level rise. In this study, regional
14 temperature changes in an atmosphere–ocean general circulation model (HadCM3) are partitioned
15 between excess (due to perturbed surface heat fluxes) and redistributed (arising from changing
16 circulation and perturbations to mixing) components. In simulations with historical forcing, we
17 firstly compare this excess–redistribution partitioning with the spice and heave decomposition, in
18 which temperature anomalies enter the ocean interior either along isopycnals (spice) or across
19 isopycnals (heave, without affecting the temperature-salinity curve). Secondly, heat and salinity
20 budgets projected into thermohaline space naturally reveal the mechanisms behind temperature
21 change by spice and heave linked with water mass generation or destruction. Excess warming
22 enters the ocean as warming by heave in subtropical gyres whereas it mainly projects onto warming
23 by spice in the Southern Ocean and the tropical Atlantic. In subtropical gyres, Ekman pumping
24 generates excess warming as confirmed by Eulerian heat budgets. In contrast, isopycnal mixing
25 partly drives warming and salinification by spice, as confirmed by budgets in thermohaline space,
26 underlying the key role of salinity changes for the ocean warming signature. Our study suggests a
27 method to detect excess warming using spice and heave calculated from observed repeat profiles
28 of temperature and salinity.

29 **1. Introduction**

30 Up to 93% of anthropogenic warming resulting from the increased concentrations of greenhouse
31 gases since the 1950s is stored in the ocean (Rhein et al. 2013) reducing atmospheric warming.
32 The absorption of excess heat (Levitus et al. 2012) that results from anthropogenic warming
33 contributes through thermal expansion to sea-level rise (Church et al. 2011). Prediction of sea-
34 level rise remains poorly constrained due to large uncertainties of ocean heat uptake (Kuhlbrodt and
35 Gregory 2012) and its regional distribution. The absorption of heat anomalies at mid-latitudes is
36 believed to involve along-isopycnal transport, subsequent to subduction by Ekman convergence and
37 geostrophic circulation (Stommel 1979; Church et al. 1991), or to involve an advective-diffusive
38 vertical balance (Munk and Wunsch 1998). This first picture underlines the importance of shallow
39 wind-driven subtropical gyres in heat transport (Talley 2013; Ferrari and Ferreira 2011) and of the
40 adiabatic ventilated thermocline theory (Luyten et al. 1983). Furthermore, the mid-depth cell of the
41 global overturning circulation (Talley 2013) reinforces the along-isopycnal picture of temperature
42 anomalies ventilated at high-latitudes. In this adiabatic cell, density-compensated anomalies of
43 North Atlantic Deep Water flow southward along isopycnals (Mauritzen et al. 2012) and water
44 parcels upwell also along isopycnals in the Southern Ocean (Marshall and Speer 2012). Recent
45 investigations in general circulation models identified the reduction of high-latitude convection and
46 advection in the Southern Ocean as the dominant processes responsible for the ocean heat uptake
47 in CO₂ perturbed experiments (Exarchou et al. 2015; Kuhlbrodt et al. 2015).

48 Under anthropogenic forcing, ocean heat uptake is partly a passive process that follows water-mass
49 ventilation pathways as depicted by (Church et al. 1991). Simulations of temperature anomalies
50 as a passive tracer allow estimation of redistributive anomalies, calculated in models from the
51 residual between total temperature anomalies and the passive tracer (Banks and Gregory 2006;
52 Marshall et al. 2015). Redistributive anomalies largely arise from the changing circulation—
53 due to anthropogenic forcing—of the preindustrial temperature gradient. The decreased Atlantic
54 meridional circulation generates the strongest redistribution warming (cooling) in the subtropical
55 (subpolar) North Atlantic (Lowe and Gregory 2006; Xie and Vallis 2012; Winton et al. 2013).
56 Redistribution warming also occurs in tropical regions and in the Southern Ocean (Chen et al.
57 2019; Dias et al. 2020) contrasting with a prevalent passive warming of the Southern Ocean
58 (Armour et al. 2016; Gregory et al. 2016). In addition, shallow redistribution cooling generates an

59 extra warming by surface fluxes referred to as redistribution feedback (Garuba and Klinger 2016).
60 Once added to the passive anomaly temperature tracer, this feedback forms the excess heat with its
61 deepest penetration in the subpolar North Atlantic (Gregory et al. 2016). Recent efforts distinguish
62 excess and redistributive heat in observations using the water mass transformation framework (Zika
63 et al. 2021) or the similarity between the global ocean uptake of heat and carbon (Bronse laer and
64 Zanna 2020).

65 The spice and heave framework (Bindoff and McDougall 1994) has been used to differentiate the
66 role of air-sea fluxes onto subducted along-isopycnal properties from isopycnal displacements, due
67 either to changes in water mass formation or to dynamical wind-driven changes, in hydrographic
68 sections. Despite being influenced by natural variability, this decomposition revealed strong and
69 equivalent (in temperature and salinity) subsurface patterns likely due to anthropogenic changes
70 and believed to subduct along-isopycnals in large observational datasets of salinity (Durack and
71 Wijffels 2010) and temperature (Häkkinen et al. 2016). The major driver of subducted anomalies
72 often remains difficult to identify being either potentially forced by surface fluxes (Wong et al.
73 1999), by lateral movement of isopycnal in regions of changing surface properties (Lago et al.
74 2016), or by anomalies subducting on fixed lighter isopycnals (Church et al. 1991). Often, spice
75 anomalies are considered to be influenced by surface buoyancy forcing and therefore to penetrate
76 isopycnally below the mixed layer whereas deep transport of properties could also contribute to
77 spice, for example by reducing along-isopycnal upward diffusive transport in the Southern Ocean
78 (Gregory 2000). Another limitation is that global analyses often consider temperature and salinity
79 separately. However there is evidence that considering both together could inform on whether spice
80 trends preferentially result from anomalous heat fluxes in subtropical regions (in “alpha” oceans
81 that are mostly stratified in temperature and where salinity is mostly passive; Durack and Wijffels
82 2010; Carmack 2007) or from high-latitudes regions governed mainly by freshwater fluxes (in
83 “beta” oceans that are mostly stratified in salinity and where temperature becomes mostly passive;
84 Mauritzen et al. 2012).

85 In addition, the water mass transformation framework being in temperature-salinity space can be
86 used to analyse the process-based heat and salinity tendency terms and to link them with the spice
87 and heave decomposition. This framework allowed Walin (1982) to estimate the across-isothermal
88 formation rate of water masses defined in temperature space using surface heat fluxes in the North

89 Atlantic. Such a framework was extended to temperature-salinity space by Speer (1993), who
90 depicts the intensity and direction of water mass transformation due to surface buoyancy forcing
91 as a transformation vector. Moreover, Hieronymus et al. (2014) estimated the effect of subsurface
92 mixing terms on the water mass formation rate. The water mass framework was also applied in
93 density space (Speer and Tziperman 1992) to reveal the predominance of along-isopycnal processes
94 for heat uptake (Saenko et al. 2021).

95 In this study, using a coupled model in a climate change experiment with historical forcing,
96 we first relate excess and redistributive heat to along-isopycnal (density-compensated) temperature
97 anomalies (spice) or to diapycnal warming and water mass readjustment, both resulting in isopycnal
98 displacements (heave). Then, Eulerian heat budgets unveil the mechanisms responsible for regional
99 excess and redistribution warming. Finally, projecting heat and salinity budgets in S - θ space helps
100 to detect which physical process produces warming by spice or heave and, therefore, helps to
101 mechanistically relate the spice and heave decomposition with excess warming.

102 **2. Methods**

103 *a. Temperature Decomposition in Excess and Redistribution*

104 In this study, excess heat (resulting from air-sea flux perturbations) is distinguished from redis-
105 tributed heat. The latter primarily results from oceanic circulation changes and mixing pertur-
106 bations under increasing atmospheric CO₂. We analyse the uptake of excess heat under realistic
107 historical anthropogenic CO₂ forcing. Comparable experiments have previously been done with
108 idealised scenarios of yearly 2% CO₂ increase (Banks and Gregory 2006) or with an abrupt CO₂
109 increase in ocean-only runs (Xie and Vallis 2012; Garuba and Klinger 2016).

110 We use the coupled atmosphere-ocean climate model HadCM3 (Hadley Centre Coupled Model
111 version 3). Following the methodology of (Banks and Gregory 2006), HadCM3 simulates excess
112 heat as a passive anomaly temperature tracer. HadCM3 (Gordon et al. 2000) comprises a rigid-lid
113 ocean model with an horizontal resolution of $1.25^\circ \times 1.25^\circ$ and with 20 unevenly spaced depth
114 levels. The model was spunup for 800 years in the control experiment and a small climate drift
115 was subtracted. Assuming that the drift has no non-linear effect on the evolution, we consider a
116 steady state for the control heat balance.

117 We evaluate the time-mean pre-industrial surface heat flux \overline{Q} over the last 150 years of the control
 118 experiment (Fig. 1a), in which the temperature, θ , follows under the Boussinesq approximation

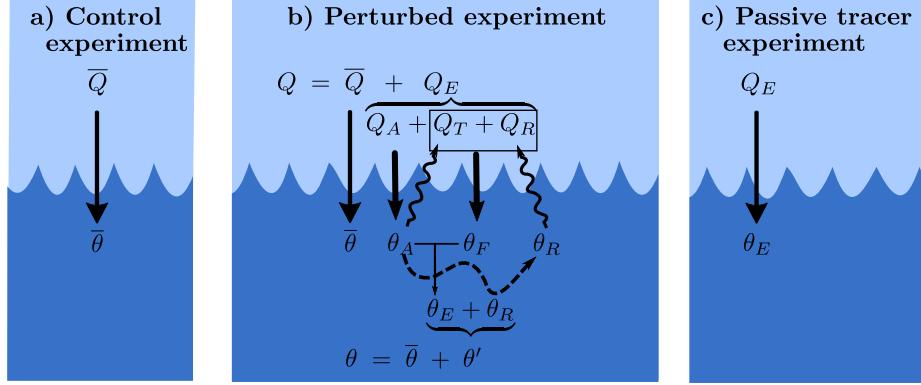
$$c \frac{\partial \overline{\theta}}{\partial t} = \overline{Q} - \nabla \cdot (c \overline{v} \overline{\theta} + \overline{\phi}), \quad (1)$$

119 with the constant c being $\rho_0 c_p$ with a reference density $\rho_0=1026 \text{ kg m}^{-3}$ and the specific heat
 120 capacity $c_p=3998 \text{ J kg}^{-1} \text{ K}^{-1}$ and the overline denotes the unperturbed control steady state. The
 121 last term of the equations (ϕ) represents the nonadvective parameterised subgridscale processes of
 122 the ocean interior: i.e. the isopycnal (ϕ_{iso}) and diapycnal (ϕ_{dia}) diffusion as well as the vertical
 123 mixing terms (ϕ_{vm}), which contains both the convective and mixed layer terms. The advective term
 124 (with the transport, v) comprises the Eulerian and the GM eddy-induced advection. The subgrid
 125 scale GM (Gent and McWilliams 1990) eddy parameterization is implemented using the scheme of
 126 Visbeck et al. (1997) to preserve the spatial dependence of the eddy-induced diffusion coefficient.
 127 The Redi (1982) isopycnal diffusivity is implemented following the scheme of Griffies et al. (1998)
 128 with a constant along-isopycnal diffusion coefficient of $1000 \text{ m}^2 \text{ s}^{-1}$. Within the mixed layer, the
 129 wind-energy mixing parameterisation of Kraus and Turner (1967) is implemented whereas below
 130 the mixed layer, a depth-increasing vertical diffusivity of tracers linearly increases from its shallow
 131 background value of $0.1 \times 10^{-4} \text{ m}^2 \text{ s}^{-1}$ to $1.22 \times 10^{-4} \text{ m}^2 \text{ s}^{-1}$ at 4000 m following Pacanowski and
 132 Philander (1981). Furthermore, the convection scheme of Rahmstorf (1993) is implemented.

133 Following Exarchou et al. (2015), the Eulerian temperature tendency diagnostics [W m^{-3}]
 134 characterise the total heat flux convergence, which results either from varying heat uptake or heat
 135 transport processes. Similarly, salinity (S) tendency diagnostics [psu/s] are calculated with all
 136 diagnostics calculated monthly in Eulerian coordinates with E incorporating the effects of surface
 137 freshwater fluxes

$$\frac{\partial \overline{S}}{\partial t} = \overline{E} - \nabla \cdot (\overline{v} \overline{S} + \overline{\phi}), \quad (2)$$

138 Beginning from the control state, a perturbed experiment (Fig. 1b) is run for 150 years with an
 139 added surface heat flux, Q_A (Fig. 2a). This flux is time-dependent, specified as monthly means
 140 starting in 1860, and is the perturbation to the local surface heat flux caused by the effective
 141 radiative forcing of the climate system, both anthropogenic and natural. It is diagnosed from the



150 FIG. 1. (a) In the pre-industrial control experiment, the surface boundary condition of ocean potential
 151 temperature $\theta = \bar{\theta}$ is the surface heat flux \bar{Q} . (b) In the perturbed experiment, the surface boundary condition of
 152 $\theta = \bar{\theta} + \theta'$ is $\bar{Q} + Q_E$, where θ' is the effect of climate change on ocean potential temperature, and Q_E is the sum
 153 of heat flux forcing Q_A and heat flux feedback. As well as being added to θ , and thus forcing climate change,
 154 the added heat flux Q_A is the surface boundary flux for the passive added heat tracer θ_A , which is initially zero
 155 and purely diagnostic. Climate change alters the SST (the surface field of θ) and consequently changes the
 156 surface heat flux. We distinguish two surface heat flux feedbacks. The direct feedback Q_T is the response of
 157 the atmosphere to the SST change caused by Q_A . The redistribution feedback Q_R arises from the change θ_R in
 158 ocean temperature, and hence in SST, due to redistribution of the control ocean heat content by modified ocean
 159 heat transports. The sum of surface heat flux feedbacks ($Q_T + Q_R$) causes a change θ_F in ocean temperature. (c)
 160 In the passive tracer experiment, the surface excess heat flux $Q_E = Q_A$, and $\theta_E = \theta_A$, because Q_A is not added to
 161 θ , and hence there is no forced climate change. Once $\bar{\theta}$, θ , and θ_E are known, θ_R can be inferred.

142 ECHAM6.3 atmosphere general circulation model with historically varying forcing agents and
 143 prescribed pre-industrial sea surface climate (section 3.1 of Gregory et al. 2020) and thus does
 144 not include the response of the climate system (as described in the next paragraph). Quantities
 145 in the perturbed experiment are denoted without an overline, and primes denote the anomalies
 146 of the perturbed experiment relative to the control experiment. Thus $v = \bar{v} + v'$ and $\theta = \bar{\theta} + \theta'$ in
 147 the perturbed experiment. We use time-averaged variables over the last 50 years of the perturbed
 148 experiment (from 1960 to 2011) relative to the control experiment to quantify the temperature
 149 anomalies throughout our analysis.

162 The temperature of the perturbed experiment, θ , is forced at the surface by $Q = \bar{Q} + Q_E$, while
 163 a separate passive tracer θ_E , called “excess heat”, initialized as zero, is forced by Q_E alone. The

164 “excess surface heat flux” $Q_E = Q_A + Q_T + Q_R$ is the sum of the imposed added heat flux Q_A and
 165 the response $Q_T + Q_R$ of the climate system to the imposed flux. The redistribution feedback heat
 166 flux, Q_R , represents the heat flux change due to the sea surface temperature change arising from the
 167 movement of the background temperature by the circulation change (Garuba and Klinger 2016).
 168 The transport responsible for the circulation changes contains the advective terms as well as the
 169 diffusive and mixing terms. In addition, the atmosphere responds to the temperature change, θ_A ,
 170 due to the added surface heat flux through an additional heat flux: the atmospheric feedback, Q_T ,
 171 that tends to oppose Q_A and to reduce Q_E to approximately a third of the radiative forcing Q_A in
 172 the global mean (Kuhlbrodt and Gregory 2012). The excess heat, θ_E , which is equivalent to the
 173 passive anomaly temperature (PAT in Banks and Gregory 2006) follows

$$c \frac{\partial \theta_E}{\partial t} = Q_E - \nabla \cdot (c\bar{v}\theta_E + cv'\theta_E + \phi_E). \quad (3)$$

174 Using further passive tracers, we decompose $\theta' = \theta_E + \theta_R = \theta_A + \theta_F + \theta_R$, where the last three
 175 quantities are all initialised to zero, and their surface fluxes are Q_A , $Q_T + Q_R$ and zero respectively.
 176 The excess heat added by Q_A is θ_A , and θ_F is the excess heat due to the atmospheric feedbacks $Q_T +$
 177 Q_R . The redistributed heat, θ_R , arises from the effect of changing circulation and parameterised
 178 heat transports, and we calculate it as $\theta_R = \theta' - \theta_E$

$$c \frac{\partial \theta_R}{\partial t} = -\nabla \cdot (cv'\bar{\theta} + c\bar{v}\theta_R + cv'\theta_R + \phi_R). \quad (4)$$

179 The heat redistribution integrated over the whole ocean is zero, which means that the global ocean
 180 heat content change relates to the total heat uptake through $\iiint c\theta' dV = \iiint c\theta_E dV = \iint Q_E dA$. By
 181 construction, the redistribution, θ_R , is unaffected by surface forcing while the redistributive surface
 182 heat fluxes, $Q_T + Q_R$, only modify the excess heat.

183 Our experimental configuration differs from those of Gregory et al. (2016). For their heat-
 184 forced experiment “FAF-heat”, they used method B of FAFMIP (Flux-Anomaly-Forced Model
 185 Intercomparison Project). Surface and atmospheric climate change is prevented in method B,
 186 except for redistribution feedback, so $Q_T = 0$ in the atmosphere–ocean heat flux. Instead, an
 187 estimate \widehat{Q}_T is obtained from previous experiments, and included in the surface flux $Q_A + \widehat{Q}_T$ of
 188 “added heat”. Since redistribution feedback is allowed to occur in method B, the flux of excess

189 heat is $Q_E = Q_A + \widehat{Q}_T + Q_R$, the same as in our case with the replacement of Q_T by \widehat{Q}_T . However,
 190 Gregory et al. (2016) apply Q_R to θ_R , which therefore has a time-dependent ocean volume mean,
 191 instead of to θ_E . By contrast, in our method Q_R is included in the surface flux of θ_E , and our
 192 θ_R is “pure redistribution”, whose surface flux is zero everywhere. In our experiment, all climate
 193 feedbacks are permitted in response to the imposed surface heat flux Q_A . The consequent climate
 194 change includes substantial changes to momentum and freshwater fluxes. Thus, the *results* of the
 195 experiment are more similar to those of “FAF-all”, in which all surface fluxes are perturbed, than
 196 to FAF-heat. On the other hand, our experiment is *technically* the same as FAFMIP FAF-heat
 197 method A, but that case has the substantially different surface flux $Q_A + \widehat{Q}_T$.

198 *b. Spice and Heave Decomposition*

199 Complementing the decomposition into excess and redistribution, which is model-based, we may
 200 also decompose temperature (and salinity) anomalies at each locations into their spice, $\theta|_n$, and
 201 heave, $\theta|_h$, components, following an observationally motivated method (Bindoff and McDougall
 202 1994). Spice relates to along-isopycnal temperature and salinity anomalies which are “density-
 203 compensated” i.e. with no net density change. Spice results from changes of air-sea fluxes where
 204 isopycnals outcrop and from changes in mixing processes along isopycnals. Heave, on the other
 205 hand, results from across-isopycnal anomalies and diabatic heat flux, due for example to diapycnal
 206 mixing or varying water mass formation, and also results from adiabatic water mass rearrangement,
 207 all of which are associated with isopycnal displacements. As done previously, the reference profile,
 208 denoted by overbars, is the depth-average over the last 50 years of the control experiment and the
 209 anomaly with respect to this reference at constant depth is by definition

$$\theta'(t, z) = \theta(t, z) - \bar{\theta}(z) = \theta|_n(t, z) + \theta|_h(t, z). \quad (5)$$

210 Given the background density gradient $\partial\bar{\theta}/\partial\bar{\rho}$ and the density anomaly $\rho'(t, z)$, heave usually
 211 relies on the assumption of small isopycnal displacement, and by a Taylor approximation becomes
 212 (Bindoff and McDougall 1994)

$$\theta|_h(t, z) = \bar{\theta}(\rho(t, z)) - \bar{\theta}(z) \simeq \bar{\theta}(\bar{\rho}(z)) + \frac{\partial\bar{\theta}}{\partial\bar{\rho}}\rho'(t, z) - \bar{\theta}(\bar{\rho}(z)) = \frac{\partial\bar{\theta}}{\partial\bar{\rho}}\rho'(t, z). \quad (6)$$

213 Rather than calculating heave thus, we instead use temperature and salinity profiles to calculate
 214 spice first, as an anomaly from the reference profile along isopycnals, and then infer heave as the
 215 remainder (Doney et al. 2007; Clément et al. 2020). This method removes the potential shallow
 216 residuals of the decomposition that can appear around the mixed layer when using the linearization
 217 of eq.6 applied to the background estimate of $\partial\bar{\theta}/\partial\bar{\rho}$ (Häkkinen et al. 2016)

$$\theta|_n(t, z) = \theta(t, z) - \bar{\theta}(\rho(t, z)), \quad (7)$$

$$\theta|_h(t, z) = \theta'(t, z) - \theta|_n(t, z) = \theta(t, z) - \bar{\theta}(z) - \theta|_n(t, z) = \bar{\theta}(\rho(t, z)) - \bar{\theta}(z). \quad (8)$$

219 Calculations are done under the winter mixed layer (WML) base defined as the deepest mixed
 220 layer over the entire simulation (a definition which gives a unique value at each location).

221 *c. Heat and salinity budgets in thermohaline coordinates*

222 Extending the framework of Walin (1982), Speer (1993) expressed the water mass transformation
 223 (diabatic change of θ and S) due to surface forcing as vectors in S - θ space. Hieronymus et al.
 224 (2014) extended this representation by including the interior (diapycnal and isopycnal) mixing
 225 terms. The transformation vector is written $\mathbf{J} \equiv \mathbf{J}^S(S, \theta), \mathbf{J}^\theta(S, \theta)$. Here \mathbf{J}^S has units of Sv per
 226 °C [with 1 Sv=10⁶ m³ s⁻¹], so $\mathbf{J}^S\Delta\theta$ represents the volume flux in Sv of water with temperature
 227 between θ and $\theta + \Delta\theta$ as it salinifies across the isohaline of salinity S , while \mathbf{J}^θ has units of Sv per
 228 psu, so $\mathbf{J}^\theta\Delta S$ represents the volume flux with salinity between S and $S + \Delta S$ in Sv as water warms
 229 across the isotherm of temperature θ . The convergence of the transformation vector in S - θ space,
 230 integrated over finite ranges in θ and S , equals the formation rate (positive or negative) of water
 231 with properties in those ranges. This formation rate can be expressed either as a volume change
 232 or an outflow (if the transformation is evaluated over a limited domain). Hence, integrating over a
 233 ‘tube’ of fluid with temperature ranging between θ and $\theta + \Delta\theta$, and salinity between S and $S + \Delta S$
 234 with volume $v\Delta\theta\Delta S$, the diabatic convergence across the long sides of the tube produces a change
 235 in volume of $\partial v/\partial t \Delta\theta\Delta S$ and outflow $\Omega\Delta\theta\Delta S$ through the ends of the ‘tube’:

$$\frac{\partial v}{\partial t} \Delta\theta\Delta S + \Omega\Delta\theta\Delta S = -[\mathbf{J}^S(S + \Delta S, \theta) - \mathbf{J}^S(S, \theta)]\Delta\theta - [\mathbf{J}^\theta(S, \theta + \Delta\theta) - \mathbf{J}^\theta(S, \theta)]\Delta S, \quad (9)$$

236 and taking the limit as $\Delta\theta \rightarrow 0$, $\Delta S \rightarrow 0$:

$$\frac{\partial v}{\partial t} + \Omega = -\frac{\partial J^S}{\partial S} - \frac{\partial J^\theta}{\partial \theta}; \quad (10)$$

237 here $\partial v/\partial t$ and Ω are denominated in units of Sv per °C per psu. The HadCM3 model that we
 238 diagnose in this paper only permits virtual salt fluxes at the surface, not mass fluxes of evaporation
 239 or precipitation, so surface mass fluxes cannot help balance the formation and the outflow term Ω
 240 drops out for global integrals.

241 The S - and θ - components of the transformation vector can be related to the material rate of
 242 change of S and θ (the total diabatic forcing) by a simple extension (Hieronymus et al. 2014) of
 243 standard 1-property watermass theory (Walín 1982) according to:

$$J^S = \lim_{\Delta S, \Delta\theta \rightarrow 0} \int_V \frac{DS}{Dt} \frac{\Pi(\theta - \theta')}{\Delta\theta} \frac{\Pi(S - S')}{\Delta S} dV, \quad (11)$$

$$J^\theta = \lim_{\Delta S, \Delta\theta \rightarrow 0} \int_V \frac{D\theta}{Dt} \frac{\Pi(\theta - \theta')}{\Delta\theta} \frac{\Pi(S - S')}{\Delta S} dV. \quad (12)$$

244 The calculation of J^S and J^θ involve the integration of the material rates of change over tubes with
 245 $|S - S'| < \Delta S/2$ and $|\theta - \theta'| < \Delta\theta/2$; this is expressed by the boxcar sampling function $\Pi(X - X') = 1$
 246 for $|X - X'| < \Delta X/2$ and 0 otherwise.

247 The above formulae give the *total* transformation, but we can use eq. 1 and 2 to express the
 248 diabatic changes in terms of the forcing components:

$$\frac{DS}{Dt} = E + \phi_{iso}^S + \phi_{dia}^S + \phi_{vm}^S, \quad (13)$$

$$c \frac{D\theta}{Dt} = Q + \phi_{iso}^\theta + \phi_{dia}^\theta + \phi_{vm}^\theta, \quad (14)$$

249 and separate out the transformation resulting from different processes

$$\mathbf{J} = \mathbf{J}_{surf} + \mathbf{J}_{iso} + \mathbf{J}_{dia} + \mathbf{J}_{vm}, \quad (15)$$

250 where e.g. the contribution to the θ -component of the transformation from isopycnal mixing is

$$J_{iso}^{\theta} = \lim_{\Delta S, \Delta \theta \rightarrow 0} \int_V c^{-1} \phi_{iso}^{\theta} \frac{\Pi(\theta - \theta')}{\Delta \theta} \frac{\Pi(S - S')}{\Delta S} dV.$$

251 When surface mass fluxes can be neglected and a global and sufficiently long time integral is
 252 taken such that the divergence in S - θ space is zero ($\nabla_{S\theta} \cdot \mathbf{J} \equiv \frac{\partial J^S}{\partial S} + \frac{\partial J^{\theta}}{\partial \theta} = 0$), \mathbf{J} can be represented
 253 a streamfunction (Döös et al. 2012; Zika et al. 2012). When both fluid velocity and local tracer
 254 tendencies are appropriately averaged, this streamfunction describes the flow across isotherms and
 255 isohalines (Groeskamp et al. 2014). A non-negligible S - θ divergence is evident in our volume
 256 budget, which is likely partly associated with the numerical mixing resulting from the model's
 257 advection scheme (Holmes et al. 2019) and from errors in our diagnostics (e.g. due to offline
 258 averaging).

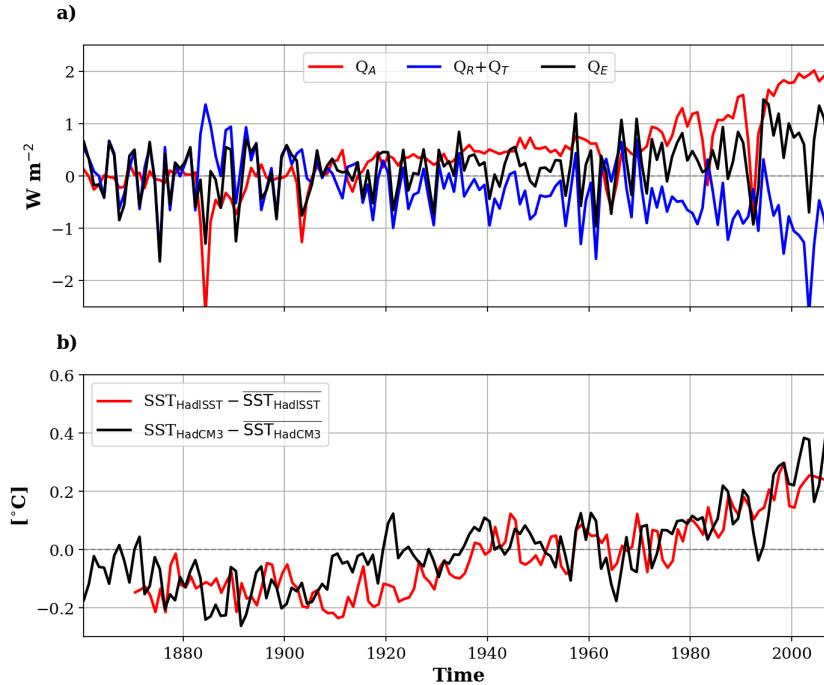
259 Finally, to link the thermohaline budgets with the decomposition presented in Section 2b, we
 260 evaluate the contributions of the spice and heave components to the formation rates by projecting
 261 the transformation vectors from S - θ space into a space whose basis vectors lie along isopycnals
 262 and along S - θ curves (Appendix A), with $\mathbf{J} = \mathbf{J}_{spice} + \mathbf{J}_{heave}$.

263 3. Results

264 In this section, after introducing the atmospheric forcing, we compare the excess-redistribution
 265 and heave-spice decompositions for temperature. The heave-spice decomposition is also applied to
 266 salinity to reveal regional patterns of both heat and salinity budgets. Then, Eulerian heat budgets
 267 describe regionally the prevailing mechanisms behind excess-redistribution warming. Finally, heat
 268 and salinity budgets projected in thermohaline coordinates reveal the processes responsible for
 269 spice-heave warming, that can further be linked to excess warming using results of Eulerian heat
 270 budgets.

279 a. Atmospheric forcing

280 Our experiment aims to reproduce a realistic heat flux forcing under a historical CO₂ scenario.
 281 The timeseries of the global-mean surface heat fluxes (Fig. 2a) reflect the strong increase in surface
 282 added heat flux, Q_A , starting from the 1960s and partly compensated by the redistribution feedback,
 283 Q_R , and the atmospheric feedback, Q_T . The global-mean excess surface heat flux, Q_E , averaged

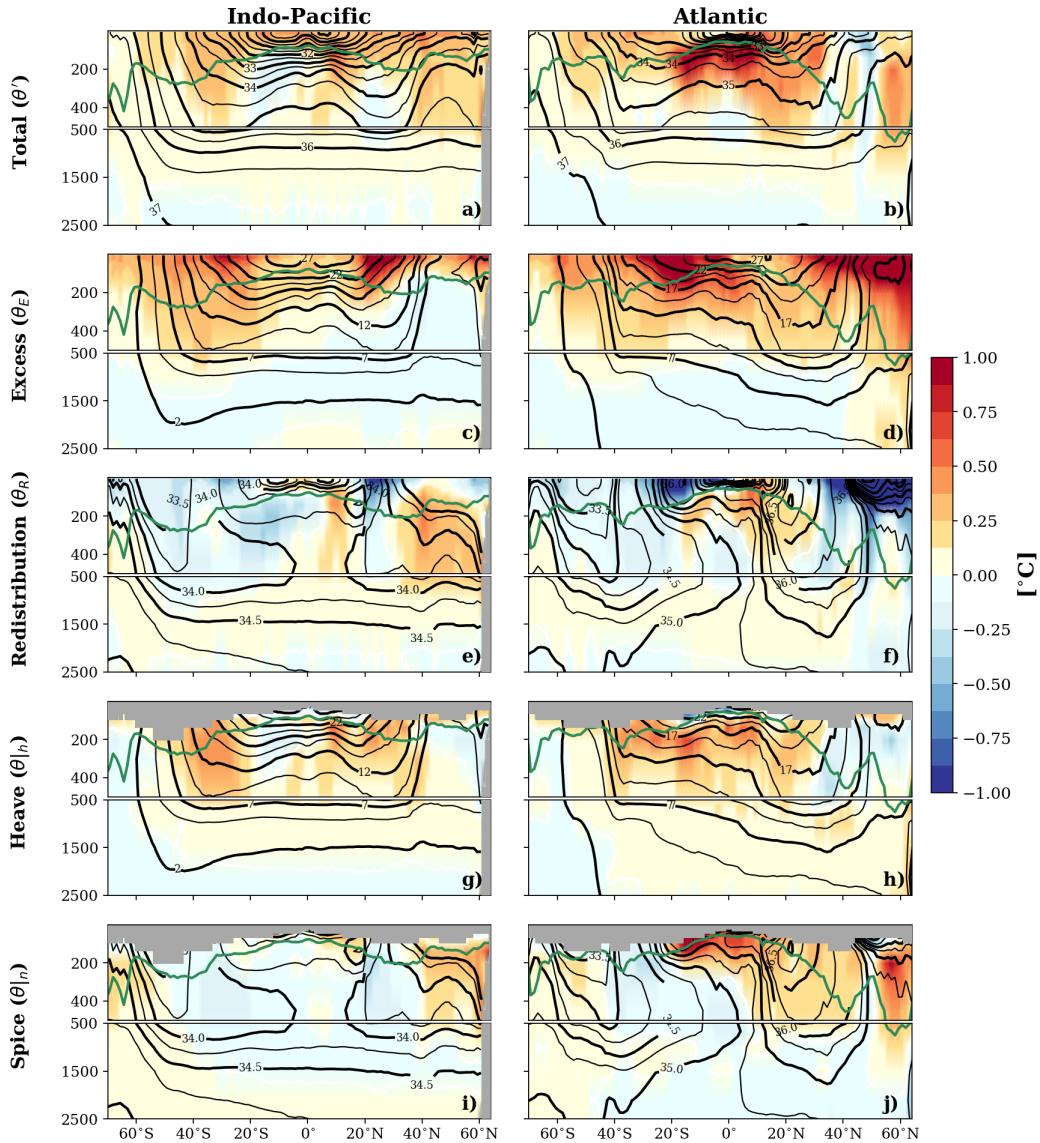


271 FIG. 2. (a) Global-mean excess surface heat flux Q_E (black), surface added heat flux Q_A (red) and sum
 272 of redistribution feedback Q_R and atmospheric feedback Q_T (blue). (b) Global-mean sea surface temperature
 273 relative to the full-period time-average of the perturbed HadCM3 experiment and of the HadISST observations.

284 from 1960 to 2011 is $0.85 W/m^2$. This heat flux somewhat overestimates a recent estimate of
 285 net heating, inferred from observed ocean heat content changes, of $0.52 W/m^2$ from 1960 to 2015
 286 (Cheng et al. 2017) when averaged over the ocean’s surface. Nonetheless, the model surface forcing
 287 simulates sea surface temperature SST anomalies which are sufficiently realistic for the purposes of
 288 our work, seeing that they reproduce well the decadal trends of observed SST anomalies (HadISST
 289 in Fig. 2b; Rayner et al. 2003) and their absolute increase over the past century. HadISST contains
 290 optimally interpolated SSTs from ship data until 1981 complemented by in-situ and satellite SSTs
 291 from 1982. We note that the AOGCM internally generates its own unforced interannual variability,
 292 which cannot be expected to replicate the historical record.

293 *b. Decompositions of temperature anomalies*

294 Contrasting the excess–redistribution and heave–spice temperature decompositions (shown
 295 zonally-averaged in Fig. 3) underlines the varying patterns of ocean heat absorption along isopyc-



274 FIG. 3. Zonally-averaged temperature anomalies for the Indo-Pacific (1st column) and the Atlantic (2nd
 275 column) oceans and their decomposition into either excess (c and d) and redistribution (e and f) or into heave
 276 (g and h) and spice (i and j). The WML base is indicated in green but the variables are shown up to the
 277 shallowest winter mixed layer of 1961-2011 for heave and spice. Black contours indicate various time-averaged
 278 σ_2 isopycnals (1st row), isotherms (2nd and 4th row) and isohalines (3rd and 5th).

296 nals at high latitudes (Fig. 3i-j) versus across isopycnals in subtropics (Fig. 3g-h). It also highlights
 297 the specific mixed regime of the Atlantic north of 20°S with strong warming both across and along
 298 isopycnals (Fig. 3h and j) and where increased salinity becomes prevalent (Fig. 4b).

299 Since the excess heat enters from the surface, its warming effect is strongest in the upper ocean.
300 Excess heat generally causes warming above 700 m (Fig. 3c,d). The deepest penetration of excess
301 warming occurs in the subpolar North Atlantic (> 2500 m) whereas not much deep excess warming
302 appears below 500 m for the rest of the ocean. The largest excess warming appears in the subpolar
303 North Atlantic and in the subtropical South Atlantic (Fig. 3d). In these regions it is amplified by
304 the redistribution feedback (i.e. the response to redistributive surface cooling, Fig. 3f), and the net
305 excess warming mostly overcompensates the redistributive cooling.

306 Redistribution is an indirect result of the surface excess warming. Redistribution mostly cools
307 the ocean above 700 m, except for some subsurface warming in the subtropics (Fig. 3f) and North
308 Pacific (Fig. 3e), and warms the ocean below this depth, but only makes a negligible change to
309 the globally-integrated heat content (in conformance with its definition). Despite using larger heat
310 fluxes resulting from their 4×CO₂ scenario, Garuba and Klinger (2016) observed similar patterns
311 of excess and redistributed heat.

312 In subtropical gyres above 700 m, except in the North Atlantic, heave captures most of the excess
313 warming, probably conveyed from the surface by Ekman downwelling, while the redistributive
314 cooling is mostly by spice (and must therefore be accompanied by freshening). In the North
315 Atlantic, on the other hand, the excess warming due to redistribution feedback mostly projects onto
316 spice above 500 m (Fig. 3j, and must be accompanied by salinification), while redistributive cooling
317 at 30°N and 400 m with warming below (Fig. 3f) projects onto heave (Fig. 3h). In addition, weak
318 warming by heave occurs below 500 m, which is redistribution likely arising from the reduced
319 tropical upwelling due to a reduced overturning (Gregory 2000; Banks and Gregory 2006).

320 The spice patterns agree with previously observed cooling and freshening by spice in the gyres
321 other than the North Atlantic, as well as the warming and salinification of the North Atlantic, over
322 roughly similar periods (Durack and Wijffels 2010; Häkkinen et al. 2016). Equatorward of 30°N
323 in the Atlantic, both heave and spice (Fig. 3h and j) explain some of the excess warming. Warming
324 by heave in the North Atlantic has previously been related to heat transport convergence in both
325 the subtropical and subpolar gyres (Williams et al. 2014; Häkkinen et al. 2015), while present only
326 in the subtropics in our experiment.

327 *c. Temperature anomalies at the WML base*

328 For understanding the uptake of heat under climate change, we are particularly interested in
329 temperature anomalies associated with excess warming at the base of the WML. The WML base
330 (Fig. 3) lies at around 200 m in the extratropics; it is shallower in the tropics (~50–100 m) and
331 deeper in the North Atlantic (~300–500 m). At the WML base, except in the North Atlantic, excess
332 warming and warming by heave are similar in subtropical gyres (green and blue respectively in
333 Fig. 5a, b, see also Fig. 3), while spice is associated with both positive and negative temperature
334 change. However, in the tropical and North Atlantic, excess warming is predominantly by spice at
335 the WML base (Fig. 5b). On the global mean, below the WML base, excess accounts for ~70% of
336 the increased ocean heat content, leaving a substantial component of redistributed warming, while
337 heave accounts for ~107%, which exceeds 100% because of global cooling by spice (Fig. 5c, d).
338 Spice contributes little to the volume-integrated warming below ≈ 500 m where isopycnals flatten
339 so vertical diffusion (which imprints as heave) becomes relatively more important while spice
340 cooling of subtropical gyres continues to be significant.

341 The basin-mean spice effect is warming at the WML base of both Atlantic and Indo-Pacific
342 Oceans (0.21°C and 0.07°C , respectively) but the volume-mean change in ocean heat content by
343 spice (WML–2000 m, Fig. 5c and d) is weakly negative in both basins (-0.2 and -0.5×10^{22} J,
344 respectively). This difference is strongest in the subtropical Atlantic where spice is associated
345 with excess at the WML base (Fig. 5b), with a 2D spatial correlation coefficient, R , of 0.56 (and a
346 p -value < 0.01 as for all reported correlation coefficients) in 20°S – 40°N , but spice does not predict
347 excess below the WML base (Fig. 5d). In this region, there are peaks of warming at 10°S and
348 10°N (Fig. 4a), which are not features of excess warming by spice. In contrast, they coincide with
349 maxima in heave and redistribution (Fig. 4d and f), which are strongly correlated in the subtropical
350 Atlantic, at $R = 0.78$. As opposed to spice warming, the similarities between excess warming and
351 warming by heave previously found in subtropical gyres (except the North Atlantic) persist at the
352 the WML base and below it, with $R = 0.58$ in the Atlantic around 40 – 20°S below the WML base.
353 The excess warming by heave is counteracted both at the WML base and below it by cooling by
354 redistribution and spice, with $R = 0.75$ between them for the heat content in the same region of the
355 Atlantic.

356 Whether temperature anomalies enter the ocean as anomalies that are density-compensated
357 (spice) or not (heave) helps us to interpret long-term stratification changes over the top 2000 m
358 (Fig. 5e and f) and changes of mixed layer depth (Fig. 5g and h). Ekman pumping of excess heat
359 across (horizontal) isopycnals at the center of subtropical gyres projects onto heave, increases the
360 stratification e.g. by $\sim 4\text{--}7\%$ at 30°S (Fig. 5e and f), and reduces the WML depth (Fig. 5g and h),
361 in all but the North Pacific.

362 The behaviour in the tropics and northern extratropics of the Atlantic is again unusual. There is
363 a maximum of excess warming at the WML base of the Atlantic at $20^\circ\text{S}\text{--}0^\circ$ (Fig. 5b, green), which
364 reflects strong intrusion into the ocean interior of heat due to redistribution feedback (not shown).
365 As noted above, this warming is by spice (Fig. 5b, red), with strong imprints by spice in both
366 temperature and salinity (Fig. 4a,b,g,h), and thus enters the ocean along isopycnals before being
367 transported northward (Fig. 3j). This excess warming at $20^\circ\text{S}\text{--}0^\circ$ opposes the substantial shallow
368 redistributive cooling, which is confined above the WML base (Fig. 3f). Acting together, these two
369 effects deepen the WML base (Fig. 5h) and produce a subsurface maximum warming just below
370 the WML base (Fig. 3b) and thus reduce the stratification (Fig. 5f), in a region where stratification
371 is mostly affected by temperature. This region of strong shallow excess and spice warming agrees
372 with the region of observed enhanced spice salinification in Fig. 7c of Durack and Wijffels (2010).

373 In the Labrador and Irminger Seas the combined area-integral subsurface heat content change is
374 3.3×10^{21} J due to excess warming, and 3.0×10^{21} J due to warming by spice. Because this strong
375 excess heat uptake is almost entirely by spice, it has little effect on the density-driven circulation or
376 redistribution (Fig. 4f), in agreement with observation (Mauritzen et al. 2012; Lozier et al. 2019;
377 Zou et al. 2020).

378 In the Southern Ocean, south of subtropical gyres, warming by spice exceeds warming by heave;
379 the latter decreases with increasing latitude to become negligible around 60°S (Fig. 3g–j). Excess
380 warming occurs above ~ 400 m; redistributive warming below (Fig. 3c–f). The spatially-averaged
381 warming by spice of 0.14°C is similar to the excess warming at the WML base (Fig. 5a–b) south
382 of 60°S . However, the spatial variability of warming by spice is negatively correlated with excess
383 heat at the WML base ($R = -0.48$ south of 45°S) and positively correlated with redistributed heat
384 ($R = 0.56$) as expected from Fig. 4f and g. Below the WML base, the correlation between spice and
385 redistribution is even stronger ($R=0.80$ in the Indo-Pacific). Thus, in the Southern Ocean (around

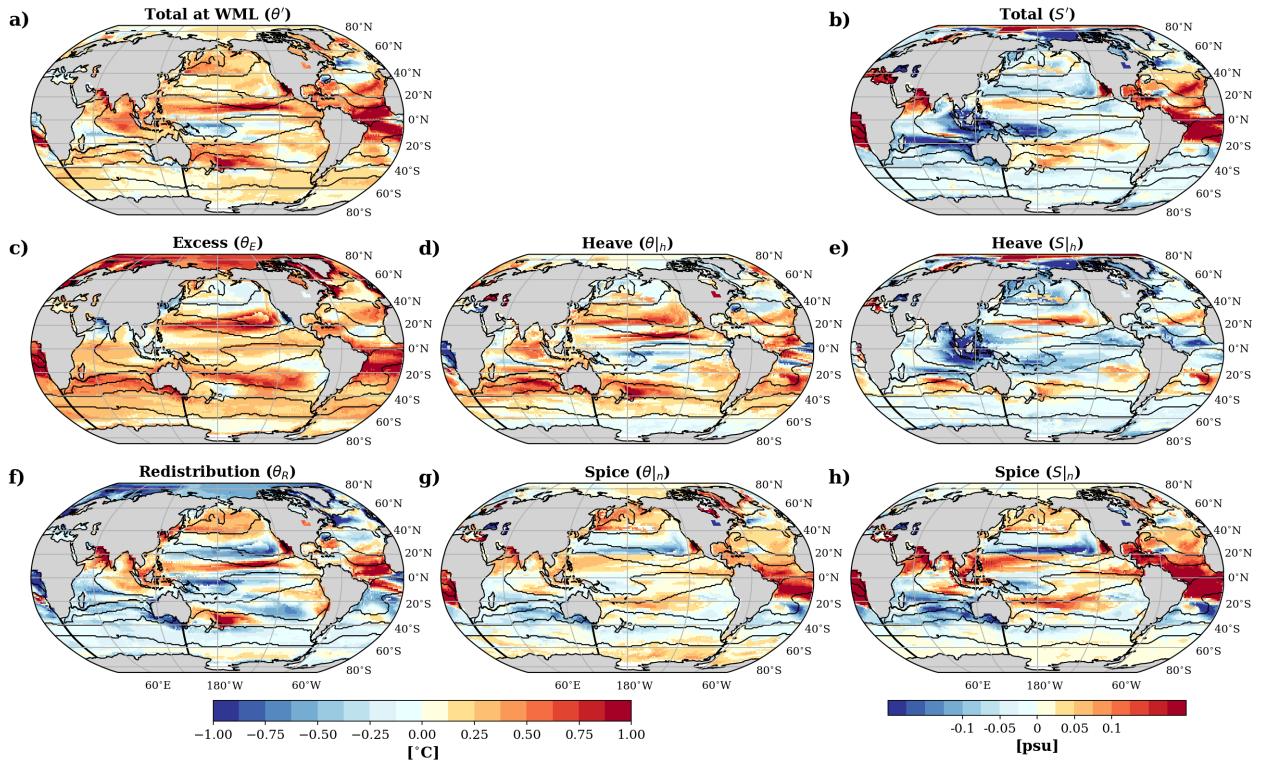
386 60°S) spice captures both shallow excess and deep redistributive warming that are separated around
387 the spatially-varying WML base, discarding any strong correlation with spice at the WML base.
388 Further north (50–40°S), however, heave captures most of the excess heat throughout the water
389 column.

390 Having previously described the 2D spatial correlations, we investigate the large-scale correspon-
391 dence between excess and spice–heave by comparing temperature anomalies spatially-averaged over
392 26 surface patches (Fig. 6a). These patches were previously used to estimate ocean heat content
393 from sea surface temperature assuming steady transport by a Green’s function (Zanna et al. 2019).
394 As expected, the strongest positive and significant correlation of $R = 0.88$ between the excess and
395 heave is found mainly in subtropical gyres (Fig. 6b). For the southernmost patches (the 3 dark
396 red markers in Fig. 6f) and the tropical Atlantic (light red triangles in Fig. 6f), the total anomalies
397 (spice+heave) best represent the excess. This underlines the small contribution of redistribution
398 south of 60°S at the WML base. For the Labrador Sea patch (darkest blue triangle in Fig. 6j), spice
399 best captures the excess warming although it remains half the size of excess. In the other patch of
400 the subpolar Atlantic (lightest blue triangle in Fig. 6j), neither the spice or heave capture the excess
401 warming since the strongest redistributed cooling (Fig. 4f) is unrepresented by the spice–heave
402 decomposition and likely results from the weakening of the Atlantic MOC (Yin et al. 2010; Bouttes
403 et al. 2014).

404 *d. Decompositions of salinity anomalies*

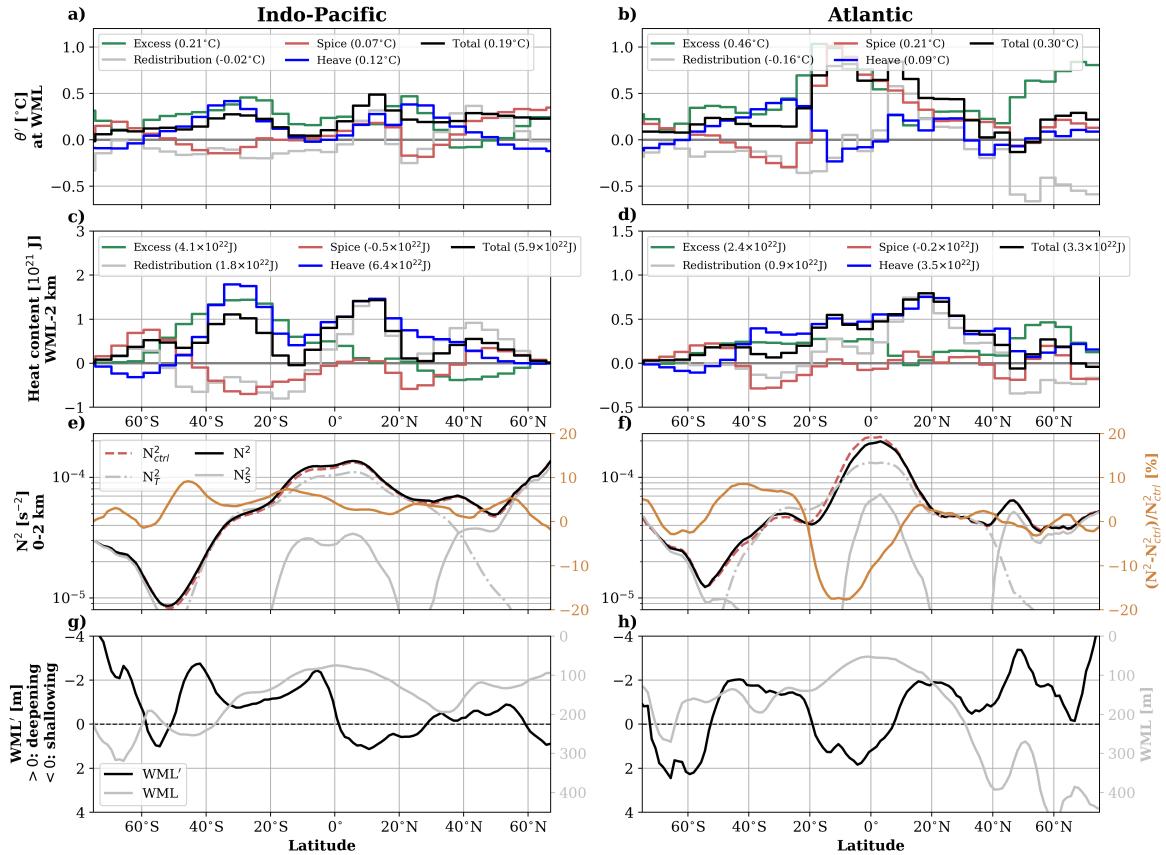
405 We investigate changes in salinity and also decompose them into their heave and spice components
406 (Fig. 4e and h) to elucidate the role of along-isopycnal penetration in creating salinity anomalies
407 and to reveal regional salinity trends, useful for interpreting the thermohaline budgets discussed
408 below. Total and spice salinity intensify in the Atlantic with the deepest spice penetration in the
409 North Atlantic but spice salinity freshens in the Indo-Pacific as expected from Fig. 3j and i. As
410 opposed to temperature, within 40°S–40°N total salinity and its spice component are strongly
411 correlated ($R = 0.81$), which underlines the prevalence of along-isopycnal salinity absorption also
412 described in Lago et al. (2016).

413 Heave salinification (Fig. 4e) in regions of Ekman downwelling marks regions of maximal surface
414 salinity for all subtropical gyres, which are mostly characterised by salinification (Fig. 4b). This



423 FIG. 4. Total temperature anomalies over the past 50 years (a) decomposed in excess (c) and redistribution (f)
 424 and decomposed in heave (d) and spice (g). Total salinity anomalies (b) decomposed in heave (e) and spice (h).
 425 Each component is shown at the WML base. The black contours delimit the surface patches that were used to
 426 estimate ocean heat content from boundary conditions at the sea surface (Zanna et al. 2019).

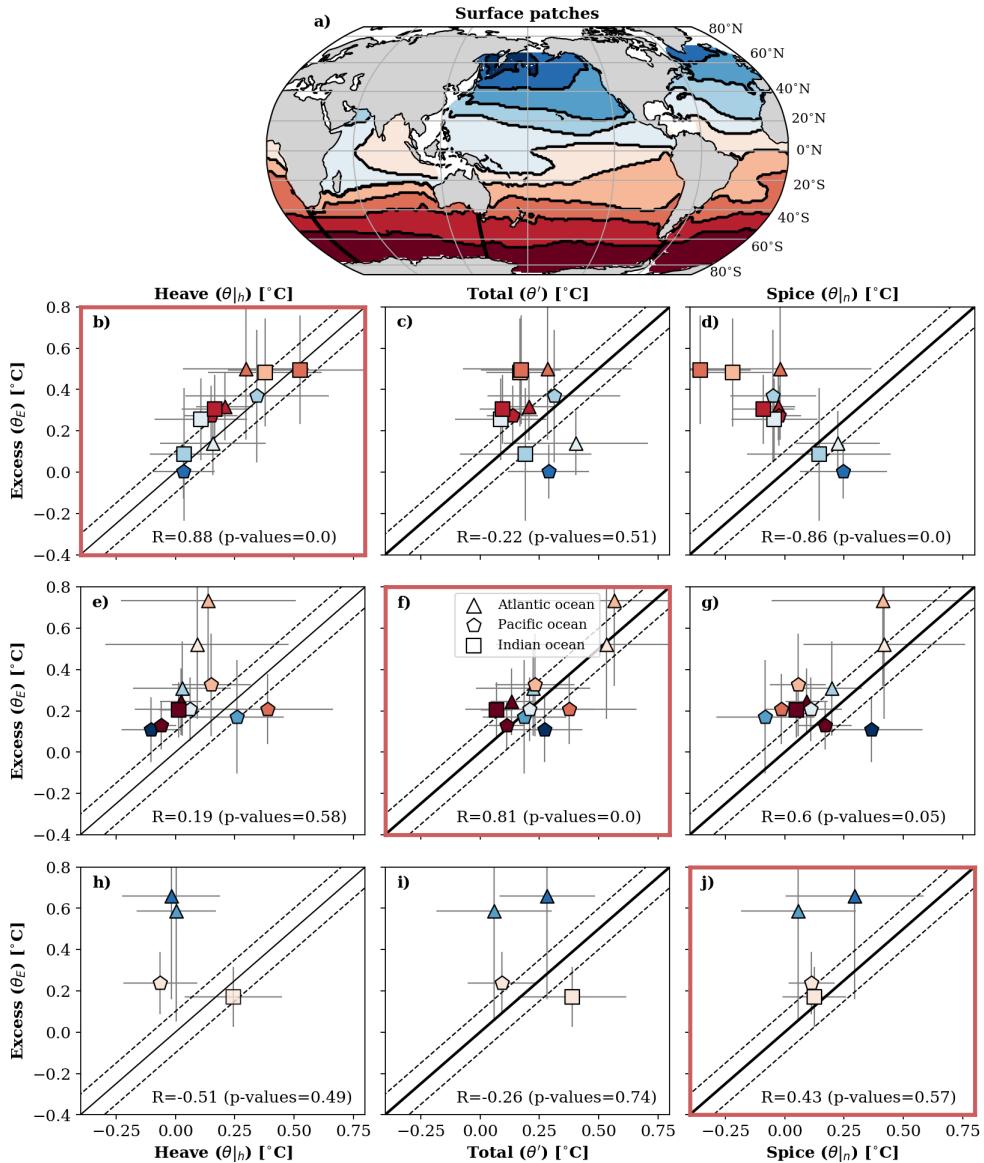
415 heave salinification emphasizes the role of vertical advection that is also present in the North
 416 Atlantic along with the effects resulting from the weakened AMOC potentially captured by spice
 417 (Fig. 4h). Increased (decreased) salinity in the subtropical (subpolar) North Atlantic as well as
 418 the salinity pile-up in the South Atlantic potentially results from AMOC weakening (Levang and
 419 Schmitt 2020; Zhu and Liu 2020). The salinification of the subtropical/tropical Atlantic (Fig. 4b)
 420 with the global freshening of the Pacific at the WML base is consistent with the intensification of
 421 the water cycle in warmer scenarios (Levang and Schmitt 2015) associated with a more evaporative
 422 Atlantic and more precipitative Pacific.



427 FIG. 5. Temperature anomalies (black) at the WML base decomposed into excess (green)/redistribution (grey)
 428 and heave (blue)/spice (red) zonally-averaged across the Indo-Pacific (a) and the Atlantic (b) with their meridional
 429 average indicated in labels. (c) and (d): same as (a) and (b) but for zonally and depth-integrated heat content
 430 from the WML base to 2000 m with their volume integral indicated in labels. Stratification of the control (dashed
 431 red) and perturbed experiments (black) with its temperature (dashed grey) and salinity (grey) components for
 432 the Indo-Pacific (e) and the Atlantic (f). The % difference in stratification of the perturbed relative to the control
 433 experiment is indicated in brown (right y-axis). (g) and (h): Difference (black, left y-axis) between the WML
 434 base of the perturbed (grey, right y-axis) and control experiments.

442 e. Eulerian heat budgets

443 We now investigate Eulerian heat budgets depth-integrated below the WML base to identify the
 444 processes responsible for temperature anomalies and for the warming due to excess and redistributed
 445 heat. The heat budget is qualitatively similar in the control experiment (not shown) and the
 446 perturbed experiment (Fig. 7a and b), because there are large balancing terms in the control, and



435 FIG. 6. (a) Surface patches that were used to estimate ocean heat content from boundary conditions at the sea
 436 surface (Zanna et al. 2019). Excess temperature anomalies spatially-averaged for each patch (with the marker
 437 color corresponding to one patch) and displayed versus heave (1st column), versus total temperature anomalies
 438 (2nd column) and versus spice (3rd column). Subplots b, f and j contain the patches where heave, total anomalies
 439 and spice are the closest to excess, respectively, providing the highest correlation coefficient R . Triangles,
 440 squares, and pentagons represent the surface patches of the Atlantic, Pacific, and Indian oceans, respectively.
 441 Standard deviations are added in grey lines.

447 the perturbations are small by comparison. As previously described for a volume below 120 m in
448 Exarchou et al. (2015), the Southern Ocean dominates the balance, with warming advection (ϕ_{adv}^{θ} ,
449 green) due to the large-scale circulation opposed by cooling eddy-effects (isopycnal diffusion ϕ_{iso}^{θ} ,
450 in blue, and eddy advection, the latter being included in the net ϕ_{adv}^{θ} in Fig. 7) and by cooling
451 convection (included in vertical mixing ϕ_{vm}^{θ} , brown). In the tropics and subtropics, warming by
452 diapycnal mixing (ϕ_{dia}^{θ} , grey) compensates advective cooling due to upwelling.

453 Away from the equator, two peaks of net heat uptake emerge at 45°S and 30°N in the difference
454 of the perturbed experiment with respect to control (black dashed lines, Fig. 7c and d). Poleward
455 of 40°, warming is dominated in both hemispheres by vertical mixing, with a contribution from
456 isopycnal mixing in the southern hemisphere; these are due to relatively small reductions in the
457 cooling due to the same processes in the control. The warming due to vertical mixing around
458 60°S and 60°N is a redistribution due to reduced convective heat loss (Fig. 7g and h). With a
459 warmer surface climate, or with increased surface freshwater flux, convection transports less heat
460 upwards, resulting in deep warming (Manabe et al. 1990), and also weakening the buoyancy-driven
461 overturning circulation. The weakened overturning circulation and reduced easterlies (Fig. 8a)
462 diminish the equatorial cold upwelling (Fig. 8c) and potentially warm the redistribution below
463 400-500 m (Fig. 3e) with a strong advective component (Fig. 7g) that is compensated by an
464 advective full-depth excess cooling (not shown).

465 In addition to the convective parameterization, in the control experiment vertical mixing contains
466 the wind-induced turbulent mixing that opposes and mixes surface fluxes while slightly warming
467 below ~100 m (~500-1000 m) in equatorial (higher latitudes) regions. These surface fluxes
468 comprise the intensified cooling of the non-penetrative component at the shallowest depth and the
469 large warming of the shortwave component below (not shown). This large warming is compensated
470 by the vertical mixing cooling that appears for example at 50°S (Fig. 7a) and that should be affected
471 by changing winds.

472 In the perturbed experiments, the strengthening and lateral shift of the westerlies over the Southern
473 Ocean affect both vertical mixing and advective terms in Exarchou et al. (2015). In our perturbed
474 experiment, a lateral shift occurs in the Atlantic but without strengthening of the westerlies (Fig. 8b).
475 Consistent with reduced cooling subsequent to the weakened westerlies at ~50°S (Fig. 8a and b),
476 turbulent vertical mixing causes subsurface warming by downward redistribution of heat at ~45-

477 50°S (Fig. 7g and h) as further confirmed by analysing the wind-mixing energy flux (not shown)
478 that is strongly reduced at ~50°S. These weakened winds coupled with the increased westerlies
479 (60–65°S) prevail in the Atlantic while occurring 5–10° farther south than in Exarchou et al. (2015)
480 and Morrison et al. (2016).

481 At 40°S in the Indo-Pacific, the westerlies to the south and easterlies to the north induce Ekman
482 convergence and along-isopycnal downwelling of SAMW (Subantarctic Mode Water) and AAIW
483 (Antarctic Intermediate Water) characterised by an advective warming peak (ϕ_{adv}^{θ} in green, Fig. 7c).
484 This peak comprises equal contributions from excess and redistribution (Fig. 7e and g). The wind-
485 driven background circulation transports shallow warm temperature anomalies northwards across
486 isopycnals within the mixed layer (Rintoul and England 2002) and around the WML base as seen
487 from the negative advective peak at 60°S (Fig. 7e and f). This process is most likely represented by
488 the advective excess warming at 40°S (Fig. 7e) and has also been referred to as “passive advection”
489 (Armour et al. 2016). These anomalies then enter the ocean interior along isopycnals below the
490 mixed layer. The redistribution warming at 40°S results from the GM eddy advection perturbation
491 (not shown separately from ϕ_{adv}^{θ}), which warms at depth and opposes the background eddy cooling
492 of the control experiment.

493 Although the peaks of excess and redistributed warming by advection in the Indo-Pacific around
494 40°S should mostly project onto warming by spice as both being along isopycnals, warming by
495 heave mostly prevails at 40°S (Fig. 3g and h) as would be expected from changes in water volumes
496 resulting from wind-driven changes; for example increased volumes of SAMW (Gao et al. 2018)
497 and decreased volumes of AAIW. Our analysis is focussed below the WML base and so may
498 overemphasize this heave contribution while not fully capturing the shallow spice warming in this
499 region due to the local deep WML base (≈ 200 m).

500 In the Indo-Pacific subtropical gyres around 20°S/N (Fig. 7e and g), advective excess warming is
501 mostly compensated by advective redistributed cooling, and the correspondences heave–excess and
502 spice–redistribution are strong (Fig. 5a). Along with this subtropical advective excess warming,
503 salinification by heave in these regions (Fig. 4e), where S as well as θ increases towards the surface
504 and where their anomalies are the strongest, indicates that heave is due to the background downward
505 Ekman pumping of surface anomalies. In addition, weakened subtropical gyres support reduced
506 Ekman downwelling, for example at 20°N in the Pacific (Fig. 8c), as previously noticed in increased

507 CO₂ scenarios (Saenko et al. 2005). This anomalous upwelling causes the shallow redistributed
508 cooling, which appears as spice (for reasons which remain to be elucidated).

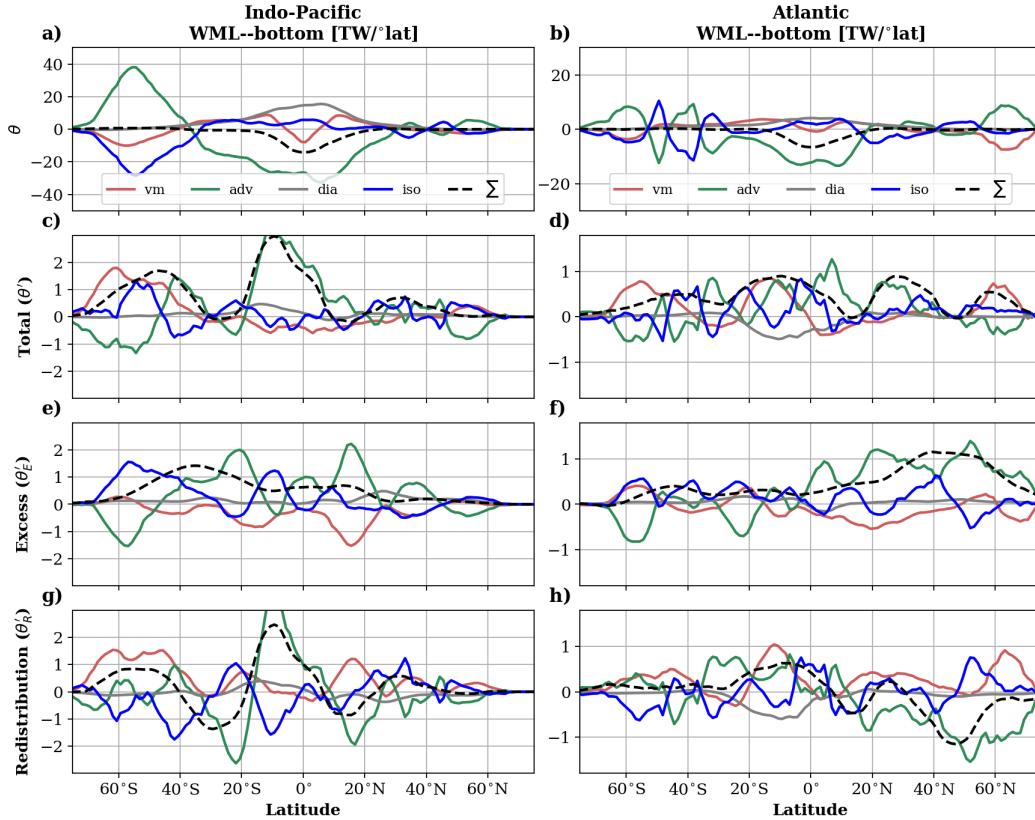
509 In the North Atlantic, the weakening of the meridional overturning circulation reduces northward
510 heat advection, thus giving redistributive advective warming (20°S-20°N) and cooling (20-60°N)
511 (Fig. 7h). The strong excess advective warming north of 20°N (Fig. 7f) is due to redistribution
512 feedback. The excess warming (0-20°N in Fig. 3d), which seems to be advective (Fig. 7f), projects
513 onto both spice and heave (Fig. 3h and j). Spice under the WML base may depict the injection
514 of temperature anomalies by the background and/or perturbed vertical circulation at outcropping
515 isopycnals (20°S-0), which corresponds to the region of highest surface (not shown) and subsurface
516 salinity changes (Fig. 4b). Also in this region and in the North Atlantic with Ekman pumping similar
517 to other subtropical gyres, heave captures the background cross-isopycnal excess heat change due
518 to Ekman flux.

519 The perturbed isopycnal diffusion has a warming effect in the Southern Ocean around 50°S in the
520 Indo-Pacific (ϕ_{iso}^{θ} in blue, Fig. 7c), which opposes the cooling of the control experiment (Fig. 7a).
521 Most of this isopycnal warming occurs in excess heat. It differs from a redistributed warming
522 that would be expected with a reduced temperature gradient along sloping isopycnals that shoal
523 poleward from deep warm to shallow colder waters (Gregory 2000). Therefore, along-isopycnal
524 eddy stirring must contribute to the transport of the warm excess heat downward and equatorward
525 instead of upward and poleward.

526 Redistributed diapycnal mixing warms in the Indo-Pacific around 0-20°S (ϕ_{dia}^{θ} in grey, Fig. 7g),
527 as expected from the enhanced stratification (Fig. 5e) while it cools in the equatorial South Atlantic
528 (Fig. 7h). This cooling is likely due to the sharp negative vertical gradient of redistributive
529 temperature just below the WML base (Fig. 3f) that remains in total temperature anomalies
530 (Fig. 3b), and which contributes to the reduced stratification (Fig. 5f).

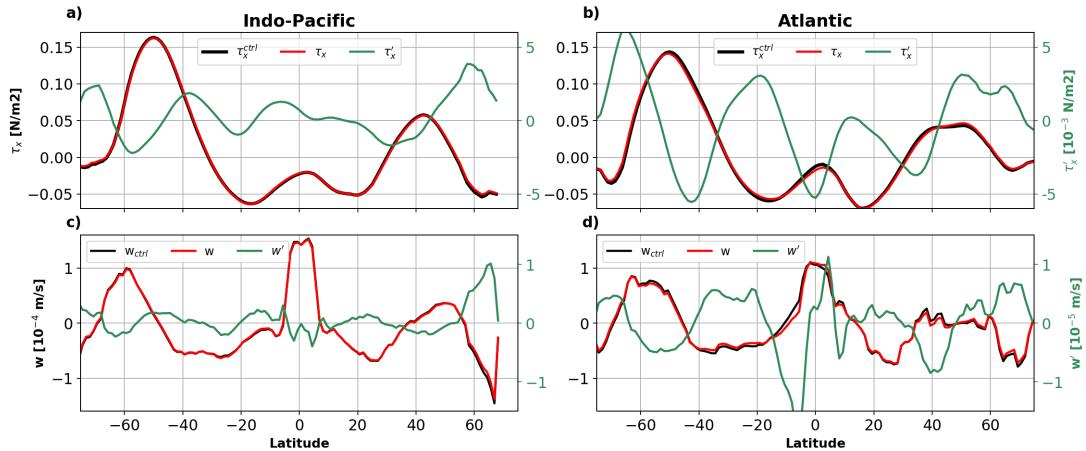
537 *f. Heat and salinity budgets of the control experiment in thermohaline coordinates*

538 We now project heat and salinity budgets onto thermohaline coordinates with the aim of identi-
539 fying the processes that generate warming by spice and heave for the perturbed experiment in the
540 next section. Time-averaged total transformation vectors \mathbf{J} are shown in Fig. 9, panel (e) for the full
541 global ocean in the control experiment and quantify the volume per unit time [in Sv] crossing an



531 FIG. 7. Zonally and depth-integrated heat flux convergences below the WML base of the perturbed experiment
 532 for the Indo-Pacific (left) and the Atlantic (right) oceans. Total temperature θ (a and b), temperature anomalies
 533 θ' (c and d), Excess θ'_E (e and f) and Redistribution θ'_R (g and h).

542 isotherm or an isohaline (by scaling \mathbf{J} by ΔS and $\Delta\theta$, Section 2c). The divergence $\nabla_{S\theta} \cdot \mathbf{J}$ (shading
 543 in Fig. 9e) in S - θ space gives the rates of water mass formation ($\nabla_{S\theta} \cdot \mathbf{J} < 0$) and destruction
 544 ($\nabla_{S\theta} \cdot \mathbf{J} > 0$) in the control experiment. The total transformation vectors \mathbf{J} reflect the two main ther-
 545 mohaline cells described by Döös et al. (2012) and Zika et al. (2012): the shallow tropical Pacific
 546 cell at high temperature and the global conveyor cell that extends to NADW at lower temperature.
 547 These cells should have zero divergence, as they are calculated over the full global ocean, so there
 548 is no outflow Ω in eq. 10 and the control experiment is in steady state after averaging over the
 549 seasonal cycle so the watermass volume v should not change. The non-zero divergence of these
 550 cells may arise partly from numerical mixing and partly from (mostly unavoidable) imperfection
 551 in our diagnostics.



534 FIG. 8. Zonally-averaged zonal wind stress, τ_x , for the perturbed (red) and control (black) experiments (left
 535 y-axis) and their difference (green, right y-axis) for the (a) Indo-Pacific and (b) Atlantic oceans. (c) and (d) same
 536 as in (a) and (b) but for the vertical velocity depth-averaged from the surface to 500 m.

552 The decomposition of the total transformation vectors for the full ocean into the contributions
 553 from the various forcing processes (eq. 15) shows that surface fluxes (Fig. 9a) generally spread water
 554 masses towards their S - θ boundaries (Nurser et al. 1999)—i.e. warming warm waters and cooling
 555 cold waters and similarly freshening fresher waters and salinifying saltier waters—compensated by
 556 both isopycnal and diapycnal mixing terms (Fig. 9b and c) that concentrate water masses toward the
 557 center, i.e. warming cool waters and cooling warm waters. Note that isopycnal diffusion transforms
 558 waters along isopycnals (grey contours show σ_2), while diapycnal diffusion just operates vertically
 559 along the local θ - S curve and so has no preferred alignment relative to isopycnals. Convection
 560 and mixed-layer entrainment \mathbf{J}_{vm} (Fig. 9d) is relatively unimportant, except for cooling at warm
 561 temperatures 25–30°, likely associated with entrainment of upwelling equatorial waters in the
 562 Pacific, and warming of very cold waters associated with convection.

563 Restricting the budget to the volume below the WML base excludes most transformation above
 564 20–25°C (Fig. 9j vs e) and practically all the effects of surface fluxes (Fig. 9f vs a). Isopycnal
 565 and diapycnal mixing is much weakened (Fig. 9g,h, emphasizing the importance of mixing within
 566 the seasonal thermocline. However, the dipole of formation and destruction driven by isopycnal
 567 diffusion is evident in both the full and interior ocean (Fig. 9b, g) and the θ -direction of \mathbf{J} below

568 the WML (Fig. 9g) corroborates the Eulerian heat balance (Fig. 7a and b): i.e. mainly cooling in
569 the Southern Ocean at low temperatures.

570 Flow out of this interior domain across the WML (obduction/subduction) is now permitted and
571 represents a +ve/-ve outflow Ω term in the mass balance (eq. 10), so, in the steady state, positive
572 divergence $\nabla_{S\theta} \cdot \mathbf{J}$ in Fig. 9j may represent θ - S classes that lose mass through mixing in the
573 thermocline, but are resupplied by net subduction, whereas negative divergences (convergences)
574 may represent waters that gain mass through subsurface mixing and hence upwell (obduct) in the
575 global sum. Caution is however required in interpreting these divergences, given the large spurious
576 full-ocean divergences evident in Fig. 9e.

577 *g. Perturbed experiment in thermohaline coordinates*

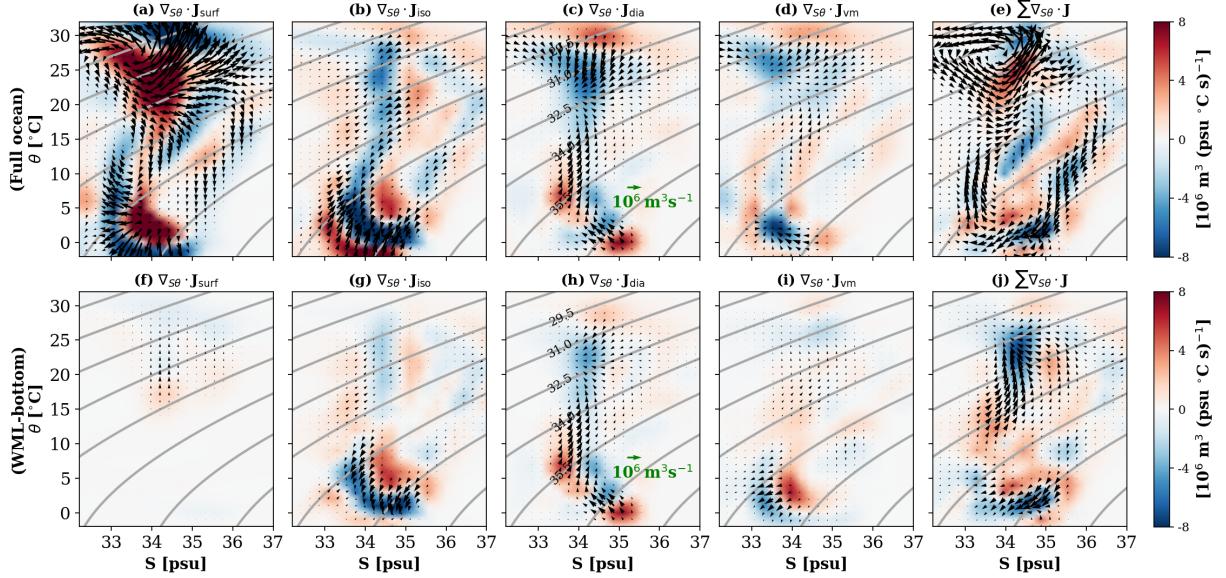
578 The anomalies in the total transformation \mathbf{J}' and in water mass formation $\nabla_{S\theta} \cdot \mathbf{J}'$ in the perturbed
579 experiment relative to the control experiment are shown in Fig. 10 (rightmost panels), for the
580 interior domain below the WML in various ocean basins (different rows). Note that because the
581 ocean is evolving in the historical run, the volume balance (eq. 10) for S - θ tubes now includes
582 inflation/deflation of the ‘tubes’ (non-zero $\partial v / \partial t$); this inflation/deflation depends on the net in-
583 flow/outflow Ω through the WML base and any changes in it, as well as on the transformation below
584 the WML that we describe here. In addition, we relate the changes in water mass formation rates
585 to the spice and heave framework in Fig. 11 by decomposing the anomalies of the transformation
586 vector into their components along isopycnals, $\mathbf{J}'_{\text{spice}}$, and along S - θ curves, $\mathbf{J}'_{\text{heave}}$ (Appendix A).

587 The strongest signals in the interior transformation of Fig. 10 are evident in the N. and S. Atlantic
588 and the N. Indo-Pacific, involving warming and salinification at temperatures between 15 and 25°C,
589 as expected from before in the subtropical regions, and a cooling/warming dipole in the S. Atlantic
590 and S. Indo-Pacific for temperatures below 10°C. S - θ curves averaged over 20° latitude bands i.e.
591 0 – 20° (tropical), 20 – 40° (subtropical), 40 – 60° (subpolar), 60 – 80° (polar) are drawn in Fig. 10
592 (rightmost panels) as dashed red curves for the perturbed run and black lines for the control. The
593 longest curve in each basin is for the tropical band: the curves get shorter moving to subtropical,
594 subpolar and polar regions consistent with the cooler surface waters. The S - θ curves for subtropical
595 regions (where 10°C < θ < 20°C) include the rightmost curve in the N. Atlantic (Fig. 10d); the
596 curve 2nd to right in the S. Atlantic (Fig. 10h), the middle curve in the N. Indo-Pacific (Fig. 10l)

597 and the 2nd from right in the S. Indo-Pacific (Fig. 10p). All these curves and the tropical curves
598 (where $15^{\circ}\text{C} < \theta < 25^{\circ}\text{C}$) show generally increasing θ and S towards the surface except in the
599 S. Indo-Pacific (p).

600 In the N. Atlantic, the warming and salinification below the WML occurring from $\theta=15^{\circ}\text{C}$ to
601 $\sim 27^{\circ}\text{C}$ (Fig. 10d) is primarily achieved by isopycnal mixing (Fig. 10a). This isopycnal warming
602 emerges in the thermohaline representation but is not evident in the depth-integrated Eulerian heat
603 budget of the North Atlantic (Fig. 7d). It presumably results from isopycnal fluxes down across
604 the WML driven by warming and salinification at the surface, or from a potential meridional
605 contribution of isopycnal mixing warming from the South Atlantic (Fig. 10e) as expected from
606 Fig. 3j and d. The \mathbf{J}' in the subtropics is decomposed into heave and spice (Fig. 11a) over the
607 range $5^{\circ}\text{C} < \theta < \sim 27^{\circ}\text{C}$. Since the \mathbf{J}' mostly results from isopycnal diffusion, it expresses as spice
608 rather than heave (note the closeness of the red (spice) and black (total) arrows in Fig. 11a for high
609 S). Therefore, the water mass framework allows to attribute a process of isopycnal warming to
610 the shallow spice warming in the tropical Atlantic at $20^{\circ}\text{S}-20^{\circ}\text{N}$ (Fig. 3j), mainly linked to excess
611 warming (Fig. 5b). Because this spice warming is reminiscent of observations (Durack and Wijffels
612 2010), we hypothesise that isopycnal warming by excess heat may contribute to these observations.
613 Interestingly, low-latitude spice warming along horizontal isopycnals has the unexpected effect
614 of reducing stratification and of increasing locally the WML base at $20^{\circ}\text{S}-0^{\circ}$ (Fig. 5f and h),
615 contrasting with the expected stratification increase of subtropical and tropical regions in a warmer
616 climate.

617 The picture for the cold waters in the Southern Ocean is different. Isopycnal warming and
618 salinification occur over narrower salinity range $S \in [33.5, 35]$ psu and temperature range $\theta \in [2, 8]^{\circ}\text{C}$
619 (Fig. 10m) than vertical mixing warming (Fig. 10o) and, at the same time, over a smaller latitudinal
620 range $45-55^{\circ}\text{S}$ (Fig. 7c) than vertical mixing warming at $45-65^{\circ}\text{S}$. The strong along-isopycnal
621 vertical mixing warming of the S. Indo-Pacific (Fig. 10o) for $\theta \in [0, 10]^{\circ}\text{C}$ at high S should mainly
622 represent the redistributive convective warming around 60°S (Fig. 7g) given that S increases with
623 depth in this region (Fig. 3e). The relatively flat subpolar and polar $S-\theta$ curves in the region
624 unambiguously indicate spice warming as confirmed for $\theta \in [0, 5]^{\circ}\text{C}$ and $S \sim 34.5$ psu in Fig. 11c
625 and d. As a result, we conclude that spice warming at 60°S (Fig. 3i and j) below 300-400 m is
626 most likely linked to redistributive warming due to reduced convection; spice warming at 50°S

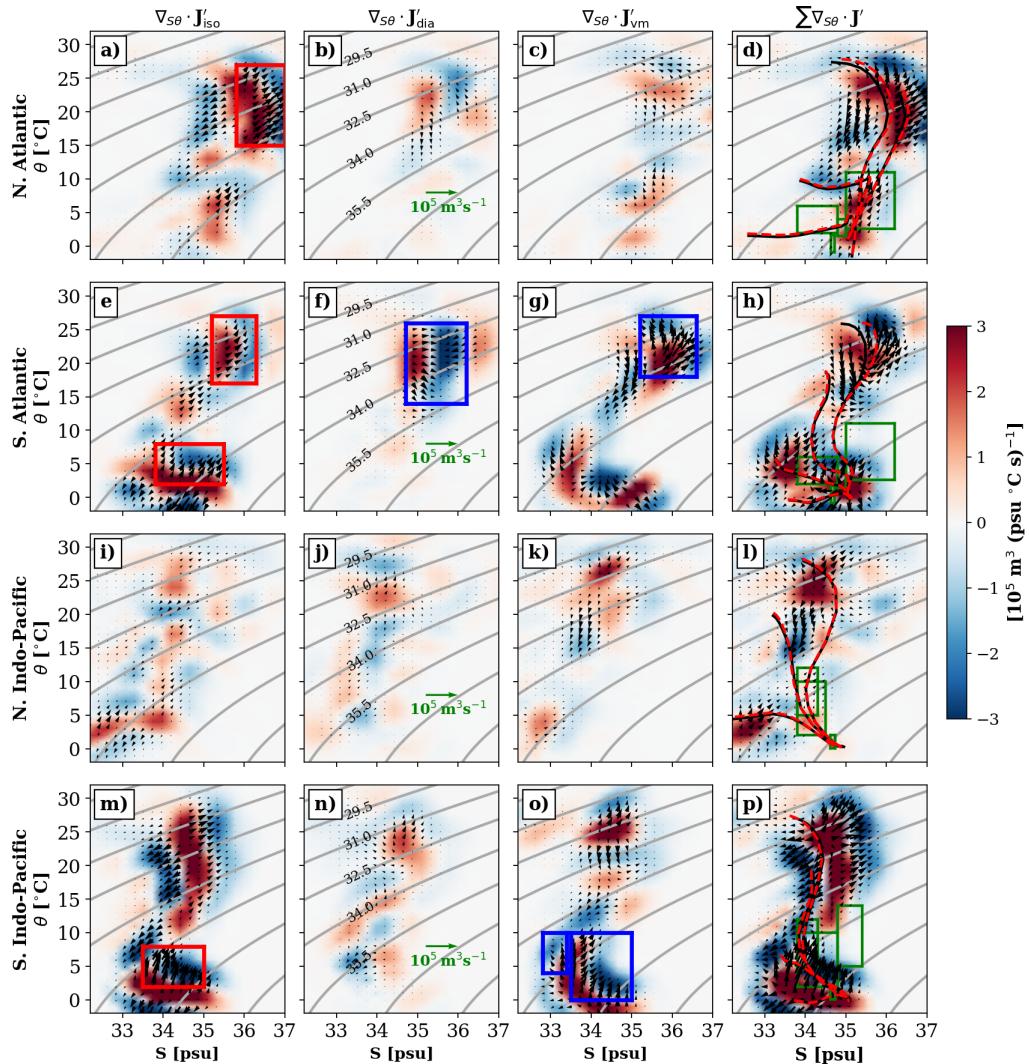


634 FIG. 9. Transformation vector \mathbf{J} and its divergence for the full ocean (1st row) and for the volume below the
 635 WML base (2nd row) for the control experiment. Positive (negative) divergence denotes water mass destruction
 636 (formation). Each column represents the individual effect of the surface fluxes, the isopycnal and diapycnal
 637 mixing and the vertical mixing; the last column represents the sum of all these effects. Grey lines denote σ_2
 638 isopycnals surfaces labelled in the second column.

627 (Fig. 3i), however, is likely linked to excess warming by isopycnal mixing (Fig. 7c). In contrast,
 628 around similar $\theta \in [4, 10]^\circ\text{C}$ but for lower S (~ 33 psu), the wind-driven redistributive vertical mixing
 629 warming (Fig. 10o) related to the shifting of westerlies strongly projects onto heave warming as
 630 seen in Fig. 11d for the S. Indo-Pacific. Consequently, the shallow heave warming above 500 m at
 631 $50\text{-}40^\circ\text{S}$ (Fig. 3g and h) most likely results from a redistributive warming. Overall, both heave and
 632 spice components are important for these cold Southern Ocean waters (Fig. 11c, d) although spice
 633 only seems to capture some of the excess warming.

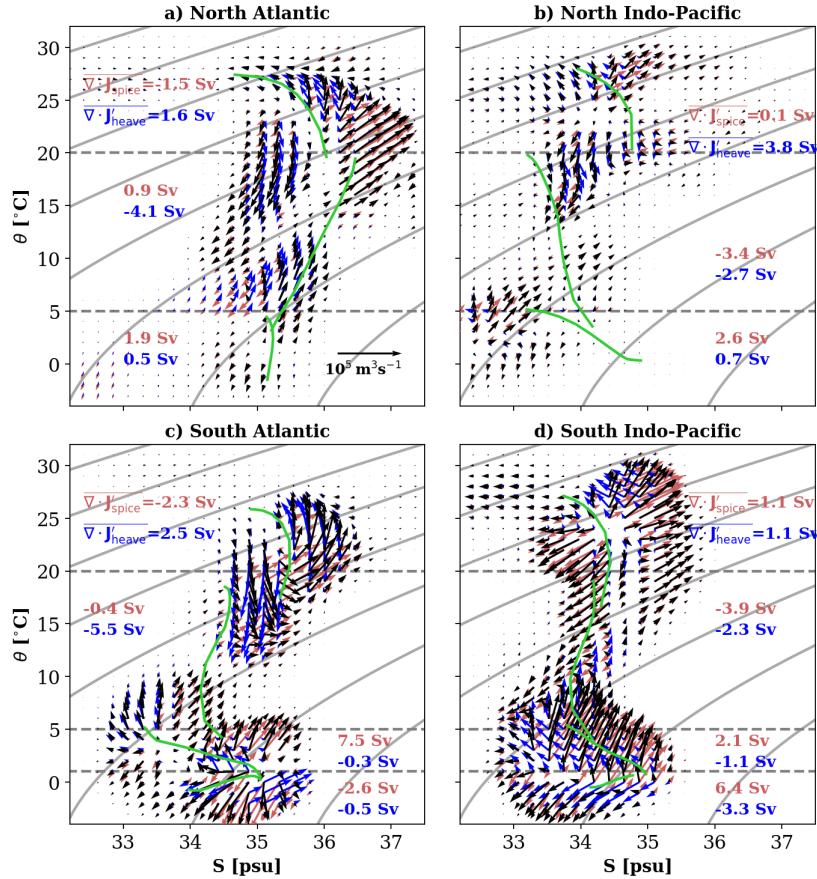
654 4. Conclusions

655 In this work, we study the processes of heat uptake during historical ocean climate change in
 656 a simulation using the HadCM3 AOGCM. Our aim is to make physical connections between the
 657 different views offered by model diagnostics and observationally motivated analysis techniques.
 658 HadCM3 is a typical AOGCM in its formulation; although it was developed more than 20 years ago,



639 FIG. 10. Transformation vector of the anomalies \mathbf{J}' and its divergence of the anomalies for the North and South
 640 Atlantic (first two rows) and the North and South Indo-Pacific (last two rows) below the WML base. The red and
 641 blue boxes represent predictions of excess and redistribution, respectively, based on zonal-averaged θ and S of
 642 Fig. 3. S - θ curves in the last column are averaged across each 20° latitudinal band for the perturbed dashed red
 643 line) and control experiments (black line). The green boxes in the last column delimit the intermediate and deep
 644 water masses (Emery 2001) from the freshest to saltiest in the Atlantic: AAIW, AABW, NADW, and MW and in
 645 the Indo-Pacific: PSIW, AAIW, CDW, and RSPGIW. Grey (brown) lines denote σ_2 isopycnals surfaces labelled
 646 in the first column.

659 its simulations are within the range of and more realistic than some modern AOGCMs (Tett et al.
 660 2022). Thus we expect our qualitative conclusions to apply to other AOGCMs, with quantitative



647 FIG. 11. Transformation vectors of the anomalies \mathbf{J}' (black) and their decomposition in spice along isopycnals
648 (red) and in heave along S - θ curves (blue) for the (a) North and (c) South Atlantic and for the (b) North and
649 (d) South Indo-Pacific below the WML base. The S - θ divergence of the vector decomposition are summed in
650 S - θ space ($\overline{\nabla \cdot \mathbf{J}'_{\text{spice}}}$ and $\overline{\nabla \cdot \mathbf{J}'_{\text{heave}}}$) for various temperature ranges and are indicated in the brown (spice) and
651 blue (heave) captions. These temperature ranges characterise regions of different S - θ curves that are delimited
652 by the horizontal grey dashed lines. S - θ curves (green) of the control experiment are averaged across each 20°
653 latitudinal band and displayed individually for each temperature ranges. The grey lines denote σ_2 isopycnals.

661 differences, for instance due to the rather low vertical resolution of HadCM3 (20 depth layers) and
662 systematic uncertainty in important model parameters (such as isopycnal diffusivity).

663 First, we identified regional similarities between two decompositions of temperature anomalies:
664 the spice and heave decomposition and a partitioning arising either from perturbed surface heat
665 fluxes (excess) or from perturbed circulation (redistribution). Secondly, Eulerian heat budgets
666 revealed the processes responsible for the excess and redistributed warming that, once associated

667 with salinity budgets and projected into thermohaline space, allowed us to attribute the processes
668 driving the warming by spice and heave. This attribution became possible in thermohaline space
669 given the slopes of isopycnals and of $S-\theta$ curves and it revealed along-isopycnal warming patterns
670 undetected in depth-integrated Eulerian heat budgets. This study addresses the patterns and
671 potential drivers of oceanic temperature changes in different frameworks most often used for
672 observations and models. Our work may help to distinguish in observations the contribution of
673 excess heat to warming at the depth of the winter mixed layer base, which could be used in the
674 future to initialise the boundary conditions of passive experiments (Khatiwala et al. 2013; Zanna
675 et al. 2019).

676 Overall, the absorption of excess heat in the diabatic shallow circulation of the subtropical regions
677 (stably-stratified in temperature) occurs across isopycnals via Ekman downwelling and projects
678 onto warming by heave. This relationship, present in all subtropical gyres, is further associated
679 with a redistributive cooling and a cooling due to spice mainly in the Indo-Pacific, and which
680 seems to be associated with a decreased downward Ekman volume flux. In equatorial regions,
681 subsurface across-isopycnal heave warming characterises the decreased overturning circulation or
682 the decreased equatorial cold-water upwelling and the redistributive warming.

683 In contrast to depth-integrated Eulerian heat budgets, moving to thermohaline space reveals the
684 transport by isopycnal mixing of excess heat from the ML and seasonal thermocline across the
685 WML base in the subtropical Atlantic. The absorption of this isopycnal flux generates strong spice
686 warming around and below the WML base that contributes to the along-isopycnal warming and
687 salinification of the shallow tropical Atlantic as opposed to the freshening of the Indo-Pacific. This
688 excess heat within the ML results from the redistribution feedback, which partly compensates the
689 redistributive cooling that is responsible for an unexpected subtropical decreased stratification and
690 deepening mixed layer in the tropical Atlantic. Warming by spice captures the excess heat at the
691 WML base north of 20°S in the subtropical Atlantic. However, it remains within the shallowest
692 500 m without contributing much to the warming of the depth-integrated heat by spice and it should
693 transfer into warming by heave once diapycnally diffused in the ocean interior.

694 The adiabatic middepth cell that outcrops in the high-latitude regions (stably-stratified in salinity)
695 has a strong along-isopycnal flow that transports excess heat downward by advection and isopycnal
696 mixing. Also, the reduced convection at high latitudes (60°N/S) by surface warming reduces the

⁶⁹⁷ along-isopycnal deep heat loss, which primarily contributes to the redistributed warming captured
⁶⁹⁸ by the warming by spice. Warming by spice can thus result from the accumulation and sequestration
⁶⁹⁹ of deep heat by redistribution, indirectly resulting from surface buoyancy forcing.

Projection of the transformation vector in Spice and Heave

This appendix presents how transformation vectors \mathbf{J} given in S - θ space (Section 2c) can be projected in σ - χ space along isopycnals σ and along S - θ curves (denoted χ) to provide the contribution of \mathbf{J} onto spice and heave (Section 2b). Such projection (Fig. A1) reveals which process of the heat and salt budgets predominantly contributes to alter the spice and heave components of temperature and salinity anomalies. The isopycnal angle, Ω_σ , is retrieved from $\tan(\Omega_\sigma) = J_{\text{spice}}^\theta / J_{\text{spice}}^S = -(\alpha_0 \frac{\partial \sigma}{\partial S}) / (\beta_0 \frac{\partial \sigma}{\partial \theta})$ and the angle of the S - θ curve, Ω_χ , follows $\tan(\Omega_\chi) = J_{\text{heave}}^\theta / J_{\text{heave}}^S = (\alpha_0 \frac{\partial \theta}{\partial z}) / (\beta_0 \frac{\partial S}{\partial z})$ when using a normalisation by the domain-averaged thermal expansion coefficient ($\alpha_0 = -\rho^{-1} \partial \rho / \partial \theta$) and saline contraction coefficient ($\beta_0 = \rho^{-1} \partial \rho / \partial S$) as in Huang et al. (2021). The transformation vector \mathbf{J} in S - θ space (J^S, J^θ) is projected in σ - χ space ($\mathbf{J}_{\text{spice}}, \mathbf{J}_{\text{heave}}$)

$$\mathbf{J}^S = \mathbf{J}_{\text{spice}}^S + \mathbf{J}_{\text{heave}}^S \quad (\text{A1})$$

$$\mathbf{J}^\theta = \mathbf{J}_{\text{spice}}^\theta + \mathbf{J}_{\text{heave}}^\theta = \mathbf{J}_{\text{spice}}^S \left(-\alpha_0 \frac{\partial \sigma}{\partial S} / \beta_0 \frac{\partial \sigma}{\partial \theta} \right) + \mathbf{J}_{\text{heave}}^S \left(\alpha_0 \frac{\partial \theta}{\partial z} / \beta_0 \frac{\partial S}{\partial z} \right) \quad (\text{A2})$$

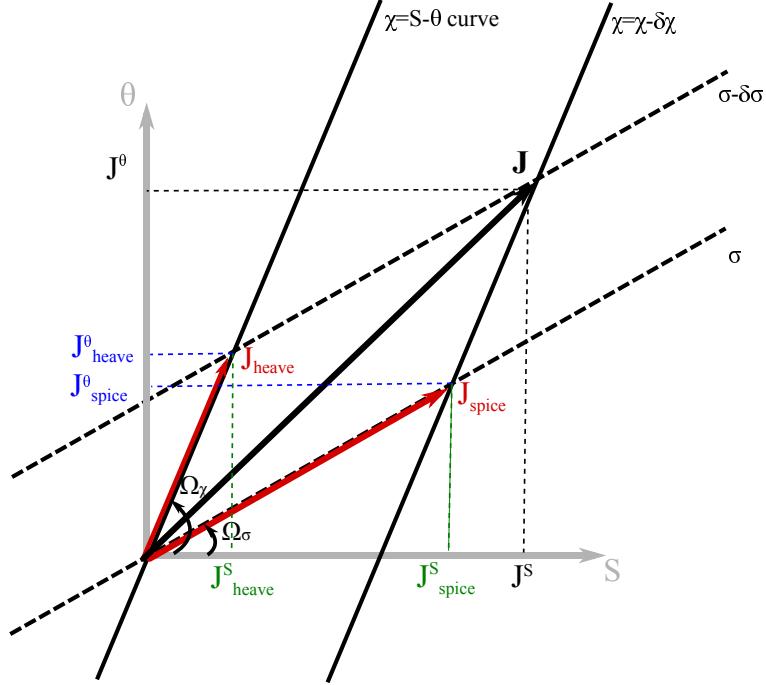
$$\begin{pmatrix} \mathbf{J}^S \\ \mathbf{J}^\theta \end{pmatrix} = \hat{\mathbf{J}}_{\text{spice}}^S \begin{pmatrix} \beta_0 \partial \sigma / \partial \theta \\ -\alpha_0 \partial \sigma / \partial S \end{pmatrix} + \hat{\mathbf{J}}_{\text{heave}}^S \begin{pmatrix} \beta_0 \partial S / \partial z \\ \alpha_0 \partial \theta / \partial z \end{pmatrix} \quad (\text{A3})$$

By introducing $\hat{\mathbf{J}}_{\text{spice}}^S = \mathbf{J}_{\text{spice}}^S (\beta_0 \partial \sigma / \partial \theta)^{-1}$ and $\hat{\mathbf{J}}_{\text{heave}}^S = \mathbf{J}_{\text{heave}}^S (\beta_0 \partial S / \partial z)^{-1}$, this linear system becomes

$$\begin{pmatrix} \mathbf{J}^S \\ \mathbf{J}^\theta \end{pmatrix} = \begin{pmatrix} \beta_0 \partial \sigma / \partial \theta & \beta_0 \partial S / \partial z \\ -\alpha_0 \partial \sigma / \partial S & \alpha_0 \partial \theta / \partial z \end{pmatrix} \begin{pmatrix} \hat{\mathbf{J}}_{\text{spice}}^S \\ \hat{\mathbf{J}}_{\text{heave}}^S \end{pmatrix} \quad (\text{A4})$$

and after a matrix inversion

$$\begin{pmatrix} \hat{\mathbf{J}}_{\text{spice}}^S \\ \hat{\mathbf{J}}_{\text{heave}}^S \end{pmatrix} = \frac{1}{\alpha_0 \beta_0 \left(\frac{\partial \sigma}{\partial \theta} \frac{\partial \theta}{\partial z} + \frac{\partial \sigma}{\partial S} \frac{\partial S}{\partial z} \right)} \begin{pmatrix} \alpha_0 \partial \theta / \partial z & -\beta_0 \partial S / \partial z \\ \alpha_0 \partial \sigma / \partial S & \beta_0 \partial \sigma / \partial \theta \end{pmatrix} \begin{pmatrix} \mathbf{J}^S \\ \mathbf{J}^\theta \end{pmatrix} \quad (\text{A5})$$



719 FIG. A1. Appendix: Projection of the transformation vector \mathbf{J} [Sv] from the S - θ space (J^S, J^θ) onto the σ - χ
 720 space ($\mathbf{J}_{spice}, \mathbf{J}_{heave}$).

715 The spice and heave components of the transformation vector are the first and second term on
 716 the right-hand side of eq.A3, respectively. They are denoted $(J^S_{spice}, J^\theta_{spice})$ and $(J^S_{heave}, J^\theta_{heave})$ in the
 717 S - θ space and can be retrieved from eq.A5:

$$\mathbf{J}_{spice} = \hat{J}^S_{spice} \begin{pmatrix} \beta_0 \partial \sigma / \partial \theta \\ -\alpha_0 \partial \sigma / \partial S \end{pmatrix} \mathbf{i}_\sigma = J^S_{spice} \mathbf{i}_S + J^\theta_{spice} \mathbf{i}_\theta, \quad (\text{A6})$$

$$\mathbf{J}_{heave} = \hat{J}^S_{heave} \begin{pmatrix} \beta_0 \partial S / \partial z \\ \alpha_0 \partial \theta / \partial z \end{pmatrix} \mathbf{i}_\chi = J^S_{heave} \mathbf{i}_S + J^\theta_{heave} \mathbf{i}_\theta \quad (\text{A7})$$

718 with $(\mathbf{i}_S, \mathbf{i}_\theta)$ and $(\mathbf{i}_\sigma, \mathbf{i}_\chi)$, the unit vectors in the S - θ and σ - χ spaces.

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