Supporting Information for

"Surface flux and ocean heat transport convergence contributions to seasonal and interannual variations of ocean heat content"

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1 Heat conservation within an ocean layer of arbitrary depth

To evaluate the drivers of ocean heat content we consider the temperature conservation equation integrated from the ocean free surface η to a depth D.

$$\int_{-D}^{\eta} \frac{\partial T}{\partial t} dz + \int_{-D}^{\eta} \nabla \cdot (\mathbf{u}T) dz = \int_{-D}^{\eta} \frac{1}{\rho_0 c_p} \frac{\partial Q}{\partial z} dz \tag{1}$$

where $\mathbf{u}$ is the three-dimensional velocity field, T is ocean temperature, ρ_0 is a reference density, c_p is the heat capacity of sea water, and Q represents the combined influence of radiation and turbulent fluxes of heat. Expanding the first term in (1) and accounting for time-variations in η and H (Leibniz integral rule) gives the following expression

$$\int_{-D}^{\eta} \frac{\partial T}{\partial t} dz = \frac{\partial}{\partial t} \int_{-D}^{\eta} T dz - T(\eta) \frac{\partial \eta}{\partial t} + T(-D) \frac{\partial (-D)}{\partial t} \tag{2}$$

Similarly, we can expand the second term in (1) into contributions from the horizontal and vertical circulation to give

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$$\int_{-D}^{\eta} \nabla \cdot (\mathbf{u}T) dz = \int_{-D}^{\eta} \nabla_h \cdot (\mathbf{u_h}T) dz + T(\eta)\frac{\partial \eta}{\partial t} - wT|^{-D} \quad (3)$$

where $\mathbf{u_h} = (u, v)$ and we have noted that $w(\eta) = \frac{\partial \eta}{\partial t}$ and $wT|^{-D}$ indicates the product wT evaluated at $-D$. Finally, we can expand the right hand side of (1) to give

$$\int_{-D}^{\eta} \frac{1}{\rho_0 c_p} \frac{\partial Q}{\partial z} dz = \frac{1}{\rho_0 c_p} \left(Q_{net} - Q(-D)\right) \quad (4)$$

where Q_{net} is the net air-sea heat flux across the ocean-atmosphere interface. When D is fixed in time, equations (2)-(4)can be combined to give

$$\frac{\partial H}{\partial t} + \rho_0 c_p \left(\int_{-D}^{\eta} \nabla_h \cdot (\mathbf{u_h}T) dz - wT|^{-D} \right) = Q_{net} - Q(-D) \quad (5)$$

$$H = \rho_0 c_p \int_{-D}^{\eta} T dz \quad (6)$$

where H is ocean heat content integrated to a depth of D. In the case where D is the ocean bottom (D_b), (5) can be simplified to

$$\frac{\partial H_{tot}}{\partial t} = C_{tot} + Q_{net} \quad (7)$$

$$C_{tot} = -\rho_0 c_p \int_{-D_b}^{\eta} \nabla_h \cdot (\mathbf{u_h}T) dz \quad (8)$$

where C_{tot} is the total heat transport convergence within an ocean column. When D is specified to be a time-invariant maximum climatological mixed layer depth (D_{mld}; see main text for definition), turbulent mixing across the lower surface can be considered negligible such that $Q(-D_{mld}) = 0$ resulting in

$$\frac{\partial H_{mld}}{\partial t} = C_{mld} + Q_{net} \quad (9)$$

$$C_{mld} = -\rho_0 c_p \left(\int_{-D_{mld}}^{\eta} \nabla_h \cdot (\mathbf{u_h}T) dz - wT|^{-D} \right) \quad (10)$$

where C_{mld} is the heat transport convergence within the layer bounded by the surface and $-D_{mld}$. Note that C_{mld} also includes the impact of vertical advection across $-D_{mld}$.

2 Application of a Kalman filter to quantify ocean heat transport divergences

Our approach is similar to that described by *Kelly et al.* [2014] but differs in a number of important ways. Firstly, we consider a near-global domain with a spatial resolution of 1 × 1 degrees and focus on the drivers of local heat transport convergences, whereas *Kelly et al.* [2014] focus on meridional transports across zonal sections in the Atlantic. Secondly, we use multiple observation-based estimates of Q_{net} for H to estimate observational uncertainties. Lastly, $\hat{C}$ is treated explicitly within the Kalman filter state transition matrix (along with $\hat{Q_{net}}$, and $\hat{H}$) rather than inferred as an unknown control term. This last step is accomplished by including persistence forecasts of $\hat{C}$ and $\hat{Q_{net}}$ using values from the previous month. Uncertainties in the persistence approximation are estimated from an initial no-Kalman solution and act as a constraint on the variances of $\hat{Q}_{net}$ and $\hat{C}$. By performing this step, we do not have to make any assumptions about the relative magnitude of variances in $\hat{C}$ and $\hat{Q_{net}}$.

Kalman smoother estimates of $\hat{H}_{mld}$ and $\hat{Q}_{net}$ are shown along with smoothed observational estimates and their associated uncertainties in supplementary figure 1a-b for the same illustrative location as figure 2 in the main text. In addition, Kalman smoother estimates of $\hat{C}_{mld}$ are compared with values calculated using a centered-difference approach without a Kalman filter (supplementary figure 1c). These comparisons demonstrate that, within our uncertainty estimates, predictions of $\hat{H}_{mld}$ and $\hat{Q}_{net}$ are consistent with the imposed observational constraints and that $\hat{C}_{mld}$ is highly correlated with the equivalent value estimated as a residual without using a Kalman filter.

2.1 Forward models

In order to apply the Kalman filter, equations (7) and (9) are discretized using a centered difference approximation to give equations of the form

$$H_{t+1} = H_{t-1} + \Delta t[\frac{1}{2}Q_{net,t+1} + Q_{net,t} + \frac{1}{2}Q_{net,t-1} + \frac{1}{2}C_{t+1} + C_t + \frac{1}{2}C_{t-1}] + u_H \quad (11)$$

where the subscript t is month and u_H is a normally distributed random variable with variance σ_H^2 that represents the uncertainty in the forward model. In theory, u_H should be zero as our forward model is an expression of heat conservation. In practice, u_H is specified to be a very small number for numerical stability. Forward predictions of C and Q_{net} are then estimated assuming persistence of values in the previous month.

$$Q_{net,t+1} = Q_{net,t} + u_Q \tag{12}$$

$$C_{t+1} = C_t + u_C \tag{13}$$

The uncertainties u_Q and u_C are specified using output from an initial no-Kalman solution and act as a prescribed constraint on the variance of our solutions for Q_{net} and C.

2.2 Kalman filter equations and state matrices

The equations and solutions to the Kalman RTS smoother are described in detail by *Wunsch* [1996]. In matrix form, our forward model is written

$$x_{t+1} = A_t x_t + \Gamma_t u_t \tag{14}$$

where x is a state vector, A the state transition matrix, Γ an identity matrix (as we assume that uncertainties in our forward model are uncorrelated), and u the uncertainties associated with our forward model. Observational constraints are introduced through the following relationship

$$E_t x_t + n_t = y_t \tag{15}$$

where E is the observation operator matrix, x the state vector, n the uncertainty in observations, and y an observation vector. For our model, these matrices take the following form

$$x_t = \begin{bmatrix} H_t & H_{t-1} & Q_{net,t+1} & Q_{net,t} & Q_{net,t-1} & C_{t+1} & C_t & C_{t-1} \end{bmatrix}^T \tag{16}$$

$$u_t = \begin{bmatrix} u_H & 0 & u_{Q_{net}} & 0 & 0 & u_C & 0 & 0 \end{bmatrix}^T \tag{17}$$

$$y_t = \begin{bmatrix} H_t^{obs} & Q_{net,t}^{obs} \end{bmatrix}^T \tag{18}$$

$$E_t = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{19}$$

$$A = \begin{bmatrix} 0 & 1 & \frac{\Delta t}{2} & \Delta t & \frac{\Delta t}{2} & \frac{\Delta t}{2} & \Delta t & \frac{\Delta t}{2} \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{20}$$

3 Local Ekman forcing of heat content variability

Here, we derive an expression for the local impact of Ekman heat transport convergences (C_{ek}) on ocean heat content variability. Following the same approach that *Gill and Niller* [1973] applied to Ekman density fluxes, we decompose Ekman heat transport convergences into two separate contributions: (i) an upper ocean contribution due to Ekman layer transports across horizontal temperature gradients (C_{ek}^{mld}) and (ii) an ocean interior contribution due to Ekman pumping across vertical temperature gradients (C_{ek}^{int}). Vertically integrating Ekman heat transports from the surface to the bottom of the Ekman layer (z_{ek}) and noting that $\nabla \cdot \mathbf{u_{ek}} = 0$ results in the following expression

$$C_{ek}^{mld} = -\rho_0 c_p \int_{-z_{ek}}^{0} (\mathbf{u_{ek}} \cdot \nabla T)\, dz \tag{21}$$

If we also assume that vertical temperature gradients within the Ekman layer are negligible such that $T(0) = T(-z_{ek})$, this expression simplifies to

$$C_{ek}^{mld} = -\rho_0 c_p \left(\mathbf{U}_{ek} \cdot \nabla T_{ek}\right) \tag{22}$$

where ∇T_{ek} is the horizontal gradient of temperature in the Ekman layer and

$$\mathbf{U}_{ek} = \left(\int_{-z_{ek}}^{0} u_{ek} dz, \int_{-z_{ek}}^{0} v_{ek} dz \right) = \frac{\tau \times \hat{\mathbf{z}}}{\rho_o f} \tag{23}$$

where $\tau = (\tau_x, \tau_y)$ is wind stress at the ocean surface and f is the Coriolis parameter. In the ocean interior, Ekman pumping leads to the vertical displacement of isotherms that can be expressed as an equivalent heat flux, C_{ek}^{int}. We estimate this flux by integrating the heat transport convergence induced by vertical Ekman pumping velocities from the base of the Ekman layer, $-z_{ek}$, to the ocean floor, $-D_b$.

$$C_{ek}^{int} = -\rho_0 c_p \int_{-D_b}^{-z_{ek}} w \frac{\partial T}{\partial z} dz \tag{24}$$

This expression can then be evaluated for the following boundary conditions

$$w(-z_{ek}) = \frac{1}{\rho_0} \text{curl} \left(\frac{\tau}{f} \right) = w_{ek} \tag{25}$$

$$w(-D_b) = 0 \tag{26}$$

under the constraint that w changes linearly with depth such that

$$\frac{\partial w}{\partial z} = \frac{w_{ek}}{D_b - z_{ek}} \tag{27}$$

Expansion of equation (24) using an integration by parts and substitution of the boundary conditions then allows the following simplifications

$$C_{ek}^{int} = -\rho_0 c_p \left(wT|_{-D_b}^{-z_{ek}} - \int_{-D_b}^{-z_{ek}} T \frac{\partial w}{\partial z} dz \right) \tag{28}$$

$$C_{ek}^{int} = -\rho_0 c_p \left(w_{ek} \cdot T_{ek} - [D_b - z_{ek}] \cdot \bar{T} \cdot \frac{w_{ek}}{D_b - z_{ek}} \right) \tag{29}$$

$$\bar{T} = \frac{1}{D_b - z_{ek}} \int_{-D_b}^{-z_{ek}} T dz \tag{30}$$

$$C_{ek}^{int} = -\rho_0 c_p w_{ek} \cdot [T_{ek} - \bar{T}] \tag{31}$$

where T_{ek} is the temperature of the Ekman layer and $\bar{T}$ is the depth-averaged temperature in the ocean interior. Combining equations (22) and (31) gives the following total expression for C_{ek}

$$C_{ek} = C_{ek}^{mld} + C_{ek}^{int} = -\rho_0 c_p \left(\mathbf{U}_{ek} \cdot \nabla T_{ek} + w_{ek} \cdot [T_{ek} - \bar{T}] \right) \tag{32}$$

References

Gill, A., and P. Niller (1973), The theory of the seasonal variability in the ocean, *Deep Sea Research and Oceanographic Abstracts*, *20*(2), 141–177.

Kelly, K. A., L. Thompson, and J. Lyman (2014), The coherence and impact of meridional heat transport anomalies in the atlantic ocean inferred from observations*, *Journal of Climate*, *27*(4), 1469–1487.

Wunsch, C. (1996), *The ocean circulation inverse problem*, Cambridge University Press.

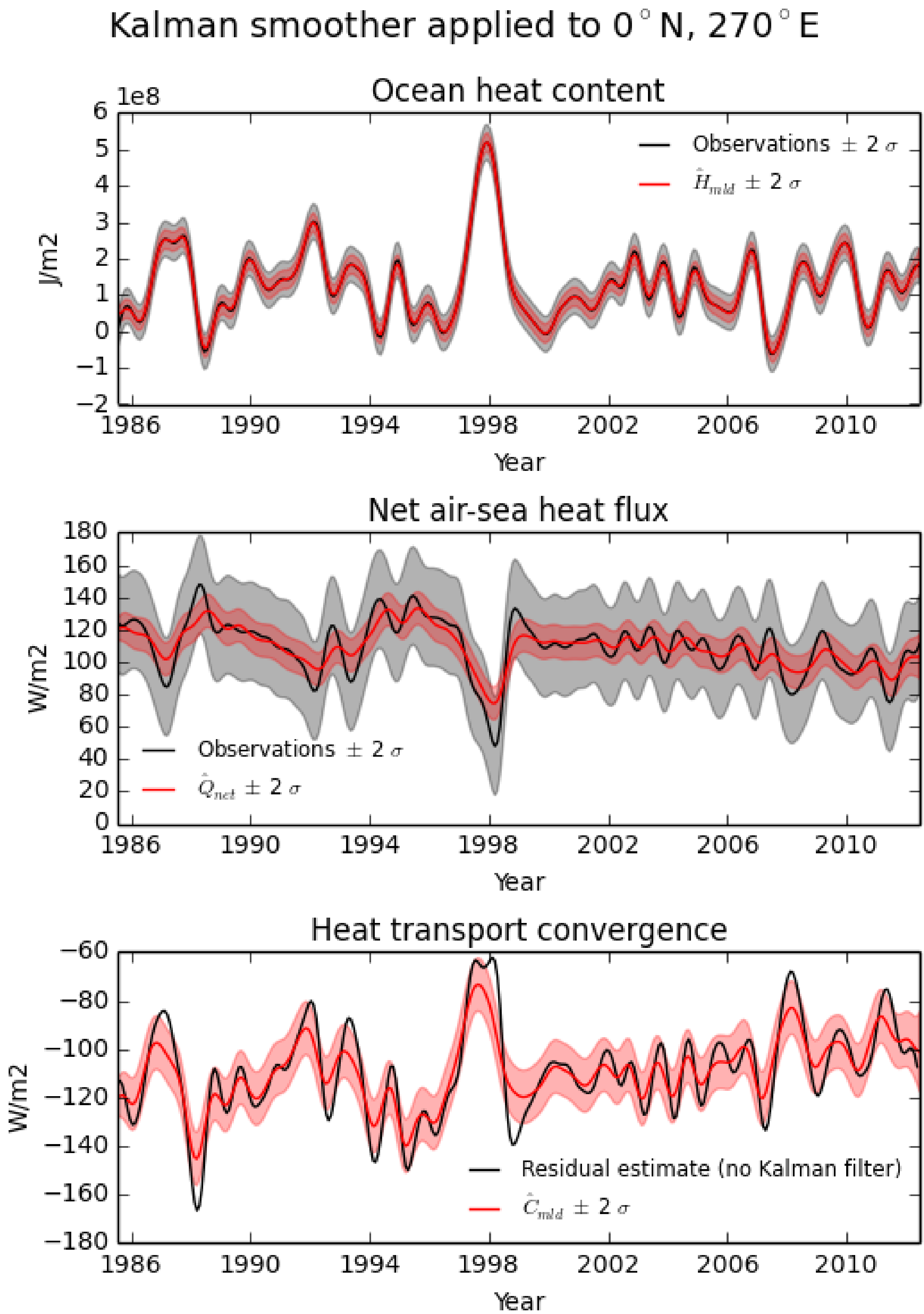

Figure 1. (a-b) Kalman smoother estimates of $\hat{H}_{mld}$ and $\hat{Q}_{net}$ along with smoothed observations their associated uncertainties. (c) Kalman smoother estimate of $\hat{C}_{mld}$ and estimated uncertainty compared with values calculated using a centred-difference approach without a Kalman filter.