Tracking a water mass: under which condition can diffusive processes be ignored?

Eric Deleersnijder, 1st February 2018

Abstract. A highly-idealised, steady-state advection-diffusion model is used to represent the spreading of a water mass under the combined effect of horizontal advection and vertical diffusion. As long as the size of the water patch remains close to its initial value, diffusion is deemed to be negligible. However, in the long run, diffusion can no longer be disregarded. A criterion is established that may be used to roughly estimate the upper bound of the duration of realistic Lagrangian simulation in which diffusive processes can be safely ignored. This time limit depends on the initial size of the water patch under consideration and the vertical (or, more correctly, diapycnal) diffusivity. All of these developments illustrate that all of the components of seawater or aggregates of them, including seawater itself, can be dealt with as passive tracers.

Motivation

Water masses in the ocean may be tracked by means of Eulerian (e.g. Cox 1989, Hirst 1999) or Lagrangian methods aiming at modelling where the water particles under study will go and where they come from. Lagrangian methods are reviewed in van Sebille et al. (2018). In some codes (e.g. Ariane[1]), diffusive processes are ignored, making it easier to address the aforementioned questions. Unfortunately, no criterion seems to exist as to the conditions under which it is legitimate to ignore diffusive processes. Presumably, in a high space/time resolution model, diffusion is less necessary than in a coarse grid model (e.g. Holzer and Primeau 2006, Shah et al. 2017). However, in the long run, diffusive processes should cause the trajectories of water particles to diverge — no matter how small diffusivities may be. Thus, the following question arises: for how long is it acceptable to ignore diffusion?

To address this question, Lagrangian model runs with and without diffusion need be carried out and analysed in depth, possibly by means of tools from dynamical system theory (Gräwe, personal communication, January 2018) or statistical physics. On the other hand, it is plausible that highly idealised models will help inform the design of such numerical studies. Accordingly, the objective of the present working note is to introduce an extremely simple advection-diffusion model admitting an analytical solution from which a criterion as to the importance of diffusion is derived.

A highly idealised problem

According to Griffies (personal communication, January 2018), in a very high resolution ocean model, only vertical (or, more correctly, diapycnal) diffusion need be introduced. This is why the hydrodynamic configuration illustrated in Figure 1 will be considered hereinafter. The domain is two-dimensional and semi-infinite, with $x \in [0,+\infty[$ and $z \in]-\infty,+\infty[$ denoting the horizontal coordinate and the vertical one, respectively. The horizontal

[1] http://www.univ-brest.fr/lpo/ariane

component of the velocity is U (>0) and the vertical velocity is zero. In the vertical direction, transport is purely diffusive and is parameterised by means of a Fourier-Fick formula involving constant diffusivity K (>0). There is no horizontal diffusion. Only the steady-state situation will be investigated.

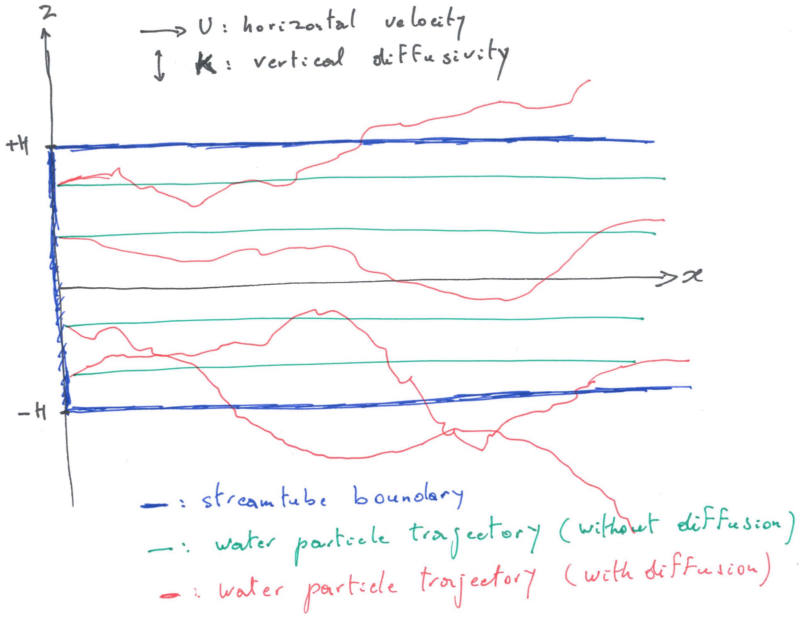

Figure 1. Illustration of the streamtube related to the water mass under study, whose width is $2H$ at $x=0$. Water particle trajectories are illustrated under the assumption that diffusion in disregarded (green) or taken into account (red).

The upstream boundary condition is located at $x=0$. On this boundary, the water mass of interest is located in the interval defined by inequalities $-H<z<H$ (Figure 1). Thus, on the boundary, the width of this patch is $2H$. The objective is to determine the width, hereinafter denoted $\delta(x)$, at any location in the domain. If there is no diffusion, the trajectories of the water particles are straight lines parallel to the x-axis, implying that the width will remain constant, i.e. $\delta(x)=\delta(0)=2H$. If vertical diffusion is present, the water particle trajectory will progressively diverge, causing the water mass of interest of interest to progressively mix with the surrounding water. Therefore, the width of the water patch under study is an increasing function of x. Diffusive processes can be ignored as long as

$$\varepsilon(x) = \frac{\delta(x)-\delta(0)}{\delta(0)} = \frac{\delta(x)-2H}{2H} \tag{1}$$

remains sufficiently small. As $\varepsilon(x)$ is an increasing function of the horizontal coordinate, requiring that $\varepsilon(x) << 1$ is tantamount to requiring that $x << \mathcal{L}$, where $\mathcal{L}$ is a length scale characterising the divergence of the water particle trajectories due to diffusion.

Presumably, length scale $\mathcal{L}$ depends on the key dimensional parameters of the problem, which are U, K and H. Then, dimensional analysis suggests that the sought-after length scale is of the form

$$\mathcal{L} = kU^a K^{-a} H^{1+a} \quad , \tag{2}$$

where k is a suitable dimensionless parameter and a is a real number whose value cannot be determined on the basis of dimensional arguments alone. Therefore, further developments are needed to derive the value of parameter a. The relevant advection-diffusion problem will be solved, paving the way for the explicit estimation of the water mass width $\delta(x)$ and, hence, length scale $\mathcal{L}$.

Analytical expression of the water mass concentration

Establishing analytical expressions in the Lagrangian framework is most likely to be difficult. This is the reason why the Eulerian approach is adopted. The solution obtained in this manner must be equivalent to that of a Lagrangian model: for advection-diffusion problems, there exists a body of theory about the equivalence of the Lagrangian and Eulerian approaches, which has recourse to the Fokker-Planck equation and stochastic differential equations.

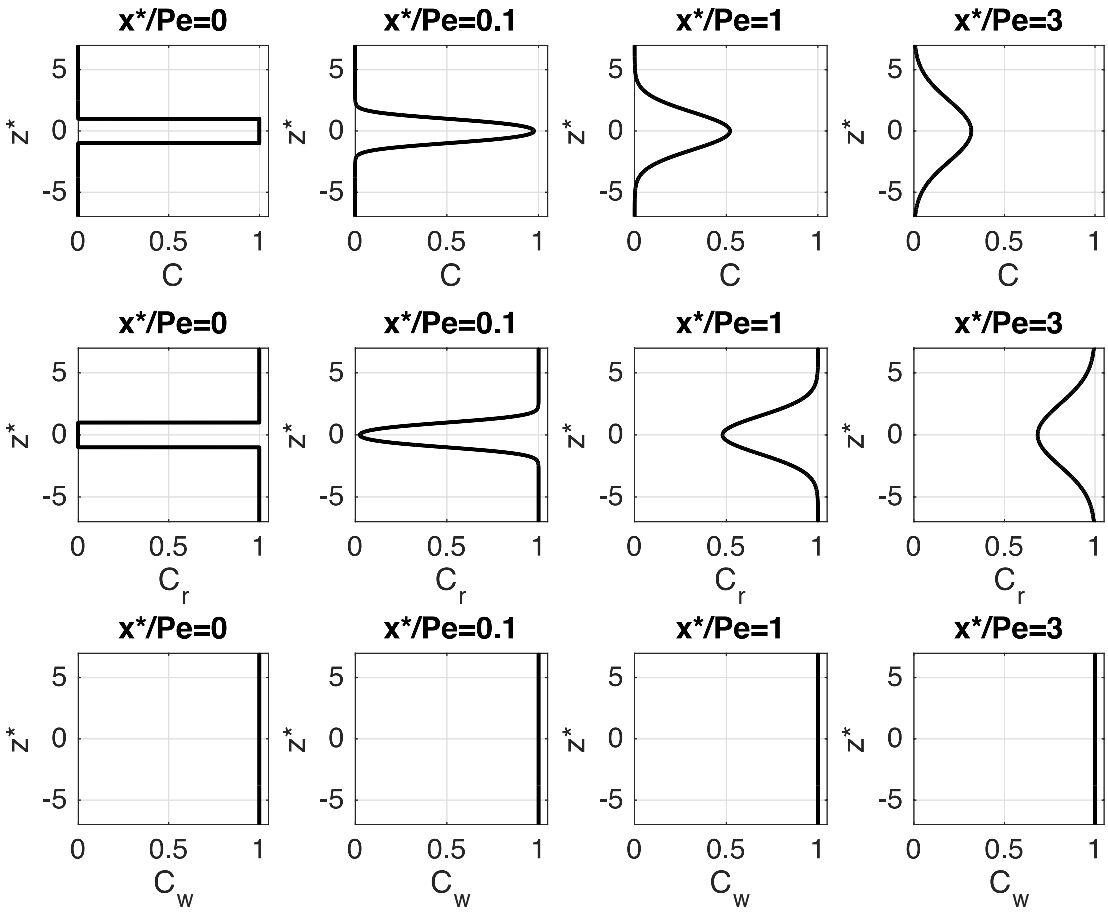

Figure 2. Concentration of the water mass under study, C, the rest of the water, C_r, and seawater itself, C_w, for various values of dimensionless coordinate x^* / Pe. Dimensionless vertical coordinate z^* is used. These profiles are universal in that they depend on neither a dimensional parameter nor a dimensionless one. See also (7)-(9).

Let $C(x,z)$ represent the concentration (defined as a mass fraction) of the water mass under study. It is governed by the following partial differential problem

$$U\frac{\partial C}{\partial x} = K\frac{\partial^2 C}{\partial z^2} \quad , \tag{3}$$

$$C(0,z) = \begin{cases} 1 \text{ if } z \in]-H,+H[\\ 0 \text{ if } z \notin]-H,+H[\end{cases} \tag{4}$$

$$C(x,\pm\infty) < 1 \quad . \tag{5}$$

In the light of the material presented in Appendices A and B, the solution to (3)-(5) is readily seen to be

$$C(x,z) = \frac{1}{2}\,\mathrm{erf}\left(\frac{H-z}{\sqrt{4Kx/U}}\right) + \frac{1}{2}\,\mathrm{erf}\left(\frac{H+z}{\sqrt{4Kx/U}}\right) \tag{6}$$

where "erf" denotes the error function (Appendix A).

Upon using dimensionless space coordinates

$$(x^*,z^*) = \frac{(x,z)}{H} \quad , \tag{7}$$

concentration transforms to

$$C(x^*,z^*) = \frac{1}{2}\,\mathrm{erf}\left(\frac{1-z^*}{\sqrt{4x^*/Pe}}\right) + \frac{1}{2}\,\mathrm{erf}\left(\frac{1+z^*}{\sqrt{4x^*/Pe}}\right) \quad , \tag{8}$$

where

$$Pe = \frac{UH}{K} \tag{9}$$

is the relevant Peclet number. Clearly, viewing the concentration as a function of x^*/Pe and z^* provides a universally valid representation of it (Figure 2).

Width of the water mass patch

When dealing with diffusion, it is customary to quantify the spreading of the particles under study by having recourse to the position variance. In the present case, the latter is defined as

$$\sigma^2(x) = \frac{\int_{-\infty}^{\infty} z^2\, C(x,z)\,dz}{\int_{-\infty}^{\infty} C(x,z)\,dz} \quad . \tag{10}$$

Using (A.6)-(A.8), one easily obtains

$$\sigma^2(x) = \frac{H^2}{3} + \frac{2Kx}{U} \quad . \tag{11}$$

The corresponding width of the water patch is estimated with the help of $\sigma(x)$ in such a way $\delta(0) = 2H$, leading to

$$\delta(x) = 2\sqrt{3}\sigma(x) = 2H\sqrt{1+\frac{6Kx}{UH^2}} \quad (12)$$

Then, spreading estimate $\varepsilon(x)$ reads

$$\varepsilon(x) = \sqrt{1+\frac{6Kx}{UH^2}} - 1 \quad . \quad (13)$$

Criterion for neglecting diffusion

Diffusive effects may be disregarded in the subdomain where $\varepsilon(x)$ is much smaller than unity, i.e.

$$x << \frac{UH^2}{6K} \quad . \quad (14)$$

Thus, length scale (2) is obtained by setting $k = 1/6$ and $a = 1$, yielding

$$\mathcal{L} = \frac{UH^2}{6K} \quad . \quad (15)$$

As such this length scale is of little interest for realistic Lagrangian simulations based on the results of global-scale hydrodynamic models. However, in the present highly-idealised model, there is only advection in the horizontal direction, implying that there is a close relation between the horizontal coordinate and the travel time. Indeed, the time needed to travel from the upstream boundary to point whose coordinate is x is x/U. Combining this piece of information with criterion (14) straightforwardly leads to a criterion regarding the maximum duration of the simulation in which diffusion may be safely ignored

$$\text{simulation duration} << \frac{H^2}{6K} \quad (16)$$

which is equivalent to

$$\text{simulation duration} << \frac{(\text{vertical size of the water mass patch})^2}{6 \times (\text{diapycnal diffusivity})} \quad (17)$$

Discussion

It worth pointing out that the upper bound of the simulation time does not depend on the velocity. This is probably because there is no velocity shear in the present model. If there were shear, things would be much less simple, for there would be some form of shear dispersion — in the horizontal direction. Whether or not it would render (17) completely invalid is hard to predict at this stage.

The upper bound of the simulation time depends of the size of the patch of water under consideration. The larger the size, the longer it takes for spreading to be sufficiently significant, i.e. the longer it takes on average for particles to leave the streamtube under consideration. This is in accordance with elementary physical intuition, but has potentially important consequences on the design of realistic simulations. Indeed, deciding whether or not diffusion can be neglected does not depend on the features of the model only. It also depends on the size of the water mass to be tracked. Presumably, similar considerations hold true for the backward (or adjoint mode), in which it is the origin of the water that is looked for — rather than its future evolution.

Criterion (17) is derived from a highly idealised advection-diffusion model. Whether or not it is relevant to realistic Lagrangian simulations can only be assessed by carrying out actual Lagrangian (high-resolution) simulations in the World Ocean.

For the sake of completeness, it is worth pointing out that the water volume is conserved in the above model, i.e.

$$\int_{-\infty}^{\infty} C(x,z)dz \;=\; 2H \;=\; \int_{-\infty}^{\infty} C(0,z)dz \quad . \tag{18}$$

On the other hand, as pointed out above, the particles of the water mass under study progressively mix with water that surrounded it on the upstream boundary. The concentration of this water, termed the “rest of the water”, is denoted $C_r(x,z)$, and is the solution of the following partial differential problem

$$U\frac{\partial C_r}{\partial x} \;=\; K\frac{\partial^2 C_r}{\partial z^2} \quad , \tag{19}$$

$$C_r(0,z) \;=\; \begin{cases} 0 \text{ if } z \in]-H,+H[\\ 1 \text{ if } z \notin]-H,+H[\end{cases} \tag{20}$$

$$C_r(x,\pm\infty) \;\leq\; 1 \quad . \tag{21}$$

The solution is readily seen to be (Figure 2)

$$C_r(x,z) \;=\; 1 \;-\; \frac{1}{2}\,\mathrm{erf}\!\left(\frac{H-z}{\sqrt{4Kx/U}}\right) \;+\; \frac{1}{2}\,\mathrm{erf}\!\left(\frac{H+z}{\sqrt{4Kx/U}}\right) \;=\; 1 \;-\; C(x,z) \quad . \tag{22}$$

Finally, the water concentration, $C_w(x,z)$, obeys

$$\begin{cases} U\dfrac{\partial C_w}{\partial x} \;=\; K\dfrac{\partial^2 C_w}{\partial z^2} \\ C_w(0,z)=1 \,,\; C_w(x,\pm\infty)=1 \end{cases} \tag{23}$$

which, unsurprisingly, leads to (Figure 2)

$$C_w(x,z) \;=\; C(x,z) \;+\; C_r(x,z) \;=\; 1 \quad . \tag{24}$$

The above results are in agreement with the fact that water masses may be regarded as passive tracers, as has been customarily done in global (e.g. Cox 1989, Hirst 1999) and regional (e.g. Bendtsen et al. 2009) sudies.

Erik van Sebille (personal communication, January 2018) asked questions on a preliminary version of this working note. An attempt is made to answer them in Appendix C.

Appendix A: the error function and some of its properties

The error function is defined by integral

$$\mathrm{erf}(\varsigma) = \frac{2}{\sqrt{\pi}} \int_0^{\varsigma} e^{-\upsilon^2}\, d\upsilon \quad . \tag{A.1}$$

The following properties are readily established:

$$\mathrm{erf}(\varsigma) = -\,\mathrm{erf}(-\varsigma) \quad , \tag{A.2}$$

$$-1 \le \mathrm{erf}(\varsigma) \le 1 \quad , \tag{A.3}$$

$$\lim_{\varsigma \to \pm\varsigma} \mathrm{erf}(\varsigma) = \pm 1 \quad , \tag{A.4}$$

$$\frac{d}{d\varsigma}\mathrm{erf}(\varsigma) = \frac{2e^{-\varsigma^2}}{\sqrt{\pi}} \quad . \tag{A.5}$$

Let λ denote a constant. Then, the integral results below may be seen to hold valid:

$$\int_{-\infty}^{+\infty} \left[\mathrm{erf}(\lambda+\varsigma)+\mathrm{erf}(\lambda-\varsigma)\right] d\varsigma = 4\lambda \quad , \tag{A.6}$$

$$\int_{-\infty}^{+\infty} \varsigma\left[\mathrm{erf}(\lambda+\varsigma)+\mathrm{erf}(\lambda-\varsigma)\right] d\varsigma = 0 \quad , \tag{A.7}$$

$$\int_{-\infty}^{+\infty} \varsigma^2\left[\mathrm{erf}(\lambda+\varsigma)+\mathrm{erf}(\lambda-\varsigma)\right] d\varsigma = 2\lambda + \frac{4\lambda^3}{3} \quad . \tag{A.8}$$

Appendix B: solution of a diffusion equation

Let t and y represent time and a relevant space coordinate. Function $\psi(t,y)$ is the solution of the following diffusion problem in an unbounded domain ($-\infty < y < \infty$)

$$\begin{cases} \dfrac{\partial \psi}{\partial t} = \kappa \dfrac{\partial^2 \psi}{\partial y^2} \\ \psi(0,y) = \Upsilon(-y)\,, \quad \psi(t,\pm\infty) \le 1 \end{cases} \tag{B.1}$$

where diffusivity κ is a positive constant and Υ denotes the Heaviside function, i.e. a function whose value is equal to unity (zero) according to whether its argument is positive (negative). The solution reads

$$\psi(t,y) = \frac{1}{2} - \frac{1}{2}\mathrm{erf}\left(\frac{y}{\sqrt{4\kappa t}}\right) \quad . \tag{B.2}$$

To prove that function (B.2) is the solution of problem (B.1), it is first necessary to show that initial condition is satisfied:

$$y<0:\ \psi(0,y) = \frac{1}{2}-\frac{1}{2}\overbrace{\mathrm{erf}(-\infty)}^{=-1} = \frac{1}{2}+\frac{1}{2} = 1 \tag{B.3a}$$

$$y>0:\ \psi(0,y) = \frac{1}{2}-\frac{1}{2}\underbrace{\mathrm{erf}(+\infty)}_{=1} = \frac{1}{2}-\frac{1}{2} = 0 \tag{B.3b}$$

Then, in the light of (A.3), it is readily seen that function (B.2) is greater or equal to zero and smaller or equal to unity, implying that the "boundary conditions" are met.

To show that (B.2) satisfies the diffusion equation (B.1), the following developments are carried out:

$$\frac{\partial\psi}{\partial t} = \frac{2}{\sqrt{\pi}}\exp\left(-\frac{y^2}{4\kappa t}\right)\underbrace{\frac{\partial}{\partial t}\left(\frac{y}{\sqrt{4\kappa t}}\right)}_{=\frac{-y}{4t\sqrt{\kappa t}}} = -\frac{y}{2t\sqrt{\pi\kappa t}}\exp\left(-\frac{y^2}{4\kappa t}\right) \quad , \tag{B.4}$$

$$\frac{\partial\psi}{\partial y} = \frac{2}{\sqrt{\pi}}\exp\left(-\frac{y^2}{4\kappa t}\right)\underbrace{\frac{\partial}{\partial y}\left(\frac{y}{\sqrt{4\kappa t}}\right)}_{=\frac{1}{2\sqrt{\kappa t}}} = \frac{1}{\sqrt{\pi\kappa t}}\exp\left(-\frac{y^2}{4\kappa t}\right) \quad , \tag{B.5}$$

$$\begin{aligned}\kappa\frac{\partial^2\psi}{\partial y^2} &= \kappa\frac{\partial}{\partial y}\left(\frac{\partial\psi}{\partial y}\right) = \kappa\frac{\partial}{\partial y}\left[\frac{1}{\sqrt{\pi\kappa t}}\exp\left(-\frac{y^2}{4\kappa t}\right)\right] \\ &= \frac{\kappa}{\sqrt{\pi\kappa t}}\underbrace{\frac{\partial}{\partial y}\left[\exp\left(-\frac{y^2}{4\kappa t}\right)\right]}_{=-\frac{y}{2\kappa t}} = -\frac{y}{2t\sqrt{\pi\kappa t}}\exp\left(-\frac{y^2}{4\kappa t}\right)\end{aligned} \tag{B.6}$$

As expected, (B.4) is equal to (B.6). QED.

Presumably, all this is well known.

Appendix C: Questions from Erik van Sebille (January 2018)

Q1:Would it be easy to extend the analysis to 2D (U, V) flow? Would that make any difference? The real ocean of course has two horizontal dimensions.

If U and V are constant, nothing would change, since this may be interpreted as a transformation of the horizontal coordinates. If U and V are not constant, then it will be much more difficult, if not impossible, to obtain an analytical solution. I feel it is not worth trying, since the aim of the analytical approach is to obtain relatively easily a relevant order of magnitude[2] of the maximum duration of the simulation during which diffusion can be ignored.

Q2: Just for the sake of it plugging in some typical numbers for a Lagrangian experiment would get you a simulation duration << (100 m)^2 / 10-4 m^2/s = 10^8 s = O(1 year). That's pretty good news ;-)

Formula (17) contains factor 6 in the denominator, which presumably is too large to be ignored. Thus, the maximum duration is about 6 times smaller. Is this really good news?

Q3: Finally, just to reiterate my own thinking on the question of 'too diffusive or not to diffusive', before I read this note: I was thinking that diffusion is unimportant if the error introduced by not diffusing is of the same order or less than the error introduced by the

[2] It must be borne in mind that dimensional analysis alone does not seem to be sufficient to obtain this order of magnitude.

(linear) interpolation schemes in space and time. My very first PhD student looked a bit into this (Qin et al. 2014).
Good point!

References

Bendtsen J., K.E. Gustafsson, J. Söderkvist and J.L.S. Hansen, 2009, Ventilation of bottom water in the North Sea-Baltic Sea transition zone, *Journal of Marine Systems*, 75, 138-149

Cox M.D., 1989, An idealized model of the World Ocean. Part I: the global-scale water masses, *Journal of Physical Oceanography*, 19, 1730-1752

Hirst A.C., 1999, Determination of water component age in ocean models: application to the fate of North Atlantic Deep Water, *Ocean Modelling*, 1, 81-94

Holzer M. and F. Primeau, 2006, The diffusive ocean conveyor, *Geophysical Research Letters*, 33, L14618, doi: 10.1029/2006GL026232

Qin X., E. van Sebille and A. Sen Gupta, 2014, Quantification of errors induced by temporal resolution on Lagrangian particles in an eddy-resolving model, *Ocean Modelling*, 76, 20-30

Shah S.H.A.M., F.W. Primeau, E. Deleersnijder and A.W. Heemink, 2017, Tracing the ventilation pathways of the deep North Pacific Ocean using Lagrangian particles and Eulerian tracers, *Journal of Physical Oceanography*, 47, 1261-1280

van Sebille E., S.M. Griffies, R. Abernathey, T.P. Adams, P. Berloff, A. Biastoch, B. Blanke, E.P. Chassignet, Y. Cheng, C.J. Cotter, E. Deleersnijder, K. Döös, H. Drake, S. Drijfhout, S.F. Gary, A.W. Heemink, J. Kjellsson, I.M. Koszalka, M. Lange, C. Lique, G.A. MacGilchrist, R. Marsh, C.G. Mayorga Adame, R. McAdam, F. Nencioli, C.B. Paris, M.D. Piggott, J.A. Polton, S. Rühs, S.H.A.M. Shah, M.D. Thomas, J. Wang, P.J. Wolfram, L. Zanna and J.D. Zika, 2018, Lagrangian ocean analysis: fundamentals and practices, *Ocean Modelling*, 121, 49-75