# **Chapter 1 Basic Equations of Marine Flows**



Knut Klingbeil, Eric Deleersnijder, Oliver Fringer, and Lars Umlauf

**Abstract** The modeling of ocean basins, coastal seas, estuaries, and lagoons requires an adequate mathematical description of the state of the fluid in these systems. The state can be characterised by a set of macroscopic variables including density, velocity, temperature, concentrations of salt and other dissolved substances. The evolution of these state variables is governed by partial differential equations derived from physical laws. In this chapter the basic mathematical concepts for formulating the governing equations are summarized and the final set of governing equations is given.

# 1.1 Mathematical Description of Fluids

# 1.1.1 Fluids as Continuous Media

A fluid consists of an extremely large number of ions and molecules. However, it is usually not the microscopic information about all molecules (e.g. position, velocity, interaction), but a finite number of macroscopically averaged quantities that is of interest for the description of a fluid and its motion. Important macroscopic state variables are density  $\rho$ , velocity  $\mathbf{v} = (u, v, w)$ , temperature  $\Theta$ , concentrations of salt *S* and suspended sediment *c*. As long as the mean free path of water molecules is smaller than the smallest scales over which gradients in the fluid occur, the fluid can be

K. Klingbeil (⊠) · L. Umlauf

L. Umlauf e-mail: lars.umlauf@io-warnemuende.de

E. Deleersnijder Université Catholique de Louvain, Ottignies-Louvain-la-Neuve, Belgium e-mail: eric.deleersnijder@uclouvain.be

O. Fringer Stanford University, Stanford, CA, USA e-mail: fringer@stanford.edu

© Springer Nature Switzerland AG 2022 H. Schuttelaars et al. (eds.), *The Mathematics of Marine Modelling*, Mathematics of Planet Earth 9, https://doi.org/10.1007/978-3-031-09559-7\_1

Leibniz Institute for Baltic Sea Research Warnemünde (IOW), Rostock, Germany e-mail: knut.klingbeil@io-warnemuende.de

approximated as a continuous medium. Given that the mean free path of liquid water is  $\mathcal{O}(10^{-10} \text{ m})$  and the smallest flow or density gradients in marine environments occur over scales of  $\mathcal{O}(10^{-3} \text{ m})$ , see e.g. Olbers et al. (2012), the continuum assumption is an extremely good approximation for all motions of interest. Therefore, the resulting state variables can be treated as continuous time-dependent field functions  $\psi(\mathbf{x}, t)$ , with the spatial coordinate  $\mathbf{x} = (x, y, z)$  and time coordinate t.

#### 1.1.2 Integral and Differential Formulations

Volume integration of continuous state variable functions introduced in Sect. 1.1.1 allows for the calculation of physical quantities like mass, momentum, angular momentum and energy. The first principles of classical mechanics and thermodynamics describe the evolution of mass, momentum and energy of a *material volume* of fluid. Material volumes consist of a fixed set of fluid elements bounded by material surfaces that follow the fluid and hence ensure that there is no flow into or out of the material volume. The temporal derivative with respect to the material volume is referred to as the *material derivative*, denoted by D/Dt. The evolution of a state variable  $\psi$  is prescribed by a corresponding source term R, such that the prototype integral budget equation is given by  $\frac{D}{Dt} \int \psi \, dV = \int R \, dV$ . Governing equations for integral flow quantities can be re-formulated in differential form with the help of the Leibniz integral rule. For an arbitrary continuous function  $\psi$  the resulting *Reynolds transport theorem* (Aris 1989) reads

$$\frac{\mathrm{D}}{\mathrm{D}t} \int \psi \,\mathrm{d}V = \int \partial_t \psi \,\mathrm{d}V + \oint \psi \underbrace{\frac{\mathrm{D}\mathbf{x}}{\mathrm{D}t}}_{=\mathbf{y}} \cdot \mathrm{d}\mathbf{A}, \tag{1.1a}$$

$$= \int \left[\partial_t \psi + \nabla \cdot (\mathbf{v}\psi)\right] \mathrm{d}V. \tag{1.1b}$$

In (1.1a), because the material surface moves with the fluid velocity, the material derivative of points on the material surface is equal to the fluid velocity  $\mathbf{v} = D\mathbf{x}/Dt$ . Assuming (1.1b) is satisfied for any material volume, including one that is infinitesimally small, the prototype budget equation in differential form reads

$$\partial_t \psi + \nabla \cdot (\mathbf{v}\psi) = R. \tag{1.2}$$

Formulating the budget equations for mass, momentum and energy in differential form yields a set of coupled nonlinear partial differential equations for the state variables introduced in Sect. 1.1.1.

#### 1.1.3 Averaging of Turbulent Flows

Coupled nonlinear differential equations can exhibit chaotic behaviour with solutions that are very sensitive to disturbances (Lorenz 1963). These solutions describe turbulent flows and exhibit strong fluctuations over a broad range of spatio-temporal scales (Foias et al. 2001). Solving the dynamics of the physical quantities on all scales, i.e. including the turbulent stirring down to the viscous scales, requires an impractical high spatio-temporal resolution. Furthermore, it is usually not one individual turbulent solution that is of interest, but properties of the mean flow. Mean flow quantities can be obtained by the application of a linear averaging operator  $\langle \cdot \rangle$ , commonly over space, time or ensemble realisations. If the operator commutes with the temporal and spatial derivatives, averaging of the prototype Eq. (1.2) yields an equation of identical form for the mean flow quantities, except for an additional turbulent flux  $\tau$  ( $\mathbf{v}$ ,  $\psi$ ) originating from the nonlinearity in the original equation:

$$\partial_t \langle \psi \rangle + \nabla \cdot (\langle \mathbf{v} \rangle \langle \psi \rangle) = \langle R \rangle - \nabla \cdot \underbrace{(\langle \mathbf{v} \psi \rangle - \langle \mathbf{v} \rangle \langle \psi \rangle)}_{=\tau(\mathbf{v},\psi)}.$$
(1.3)

If the averaging operator is also idempotent, i.e.  $\langle \langle \cdot \rangle \rangle = \langle \cdot \rangle$ , it is called a *Reynolds average*. Only for a Reynolds average, e.g. the ensemble mean, the turbulent flux is represented by the correlation of fluctuations (second moments), i.e.

$$\boldsymbol{\tau} \left( \mathbf{v}, \psi \right) = \left\langle \left( \mathbf{v} - \langle \mathbf{v} \rangle \right) \left( \psi - \langle \psi \rangle \right) \right\rangle = \left\langle \mathbf{v}' \psi' \right\rangle \quad \text{for Reynolds averages.}$$
(1.4)

Since turbulent stirring enlarges local gradients and the interfaces where molecular mixing can take place, the net effect of enhanced mixing in turbulent flows motivates to parameterise an unknown turbulent flux as a diffusive flux in terms of an eddy diffusivity and the known mean flow gradient (*eddy viscosity assumption* of Boussinesq).

#### **1.2 Governing Equations**

The governing equations are derived from the physical laws for mass conservation and the budget equations for linear and angular momentum, and energy. They are formulated following the prototype Eq. (1.2). A detailed derivation of each equation is beyond the scope of this book and the reader is referred to the excellent text books by Batchelor (1967), Griffies (2004) and Olbers et al. (2012). In marine modelling, several approximations are applied to simplify the set of equations. A very common approximation is the *Boussinesq approximation* (not to be mistaken for the eddy viscosity assumption of Boussinesq). As described by Young (2010), variations in density are only considered for buoyancy effects in the vertical momentum balance. In all other terms the density is replaced by a constant reference density  $\rho_0$ . The buoyancy follows from a diagnostic *equation of state* which provides the density depending on salinity *S*, temperature  $\Theta$ , and in case of Boussinesq fluids on depth instead of in-situ pressure (Roquet et al. 2015):

$$\rho = \rho(S, \Theta, z). \tag{1.5}$$

With the eddy viscosity assumption of Boussinesq, the set of governing equations for the mean-flow quantities (without brackets for brevity) is presented in the following. The emphasis of the vertical axis in geophysical applications motivates the assumption of *transverse isotropy* and the use of different eddy viscosities and diffusivities for vertical and horizontal turbulent fluxes.

#### 1.2.1 Volume Conservation

Under the Boussinesq approximation it is not mass  $\int \rho \, dV$  anymore, but volume that is conserved. The original prognostic equation for density degenerates to the so-called *incompressibility constraint*,

$$\partial_x u + \partial_y v + \partial_z w = 0, \tag{1.6}$$

enforcing a divergence-free flow.

*Kinematic boundary conditions* further constrain the flow at bounding surfaces by prescribing the diasurface volume flux velocity (Griffies 2004). With the velocity of the bounding surface  $\mathbf{v}_b$  the conditions at a single-valued free surface  $z = \eta(x, y, t)$  and impermeable bottom z = -H(x, y, t) are given by

$$\nabla(z - \eta) \cdot (\mathbf{v} - \mathbf{v}_{b}) = (E - P) \qquad \text{at } z = \eta, \qquad (1.7a)$$

$$\nabla(z+H) \cdot (\mathbf{v} - \mathbf{v}_{b}) = 0 \qquad \text{at } z = -H. \qquad (1.7b)$$

In (1.7a) the volume flux velocity is prescribed in terms of evaporation *E* and precipitation *P*. Alternative formulations are

$$\partial_t \eta + u \partial_x \eta + v \partial_y \eta - w = -(E - P)$$
 at  $z = \eta$ , (1.8a)

$$\partial_t H + u \partial_x H + v \partial_y H + w = 0$$
 at  $z = -H$ . (1.8b)

Boundary condition (1.8a) is used to determine the evolution of the free surface. In contrast, (1.8b) constrains the flow velocity at the bottom in terms of a prescribed bottom topography. The morphological evolution of the bottom  $\partial_t H$  is either neglected or follows from a morphological model (see Chap. 10).

#### 1.2.2 Salt Conservation

Seawater is a mixture of freshwater and salt. The fluid velocity  $\mathbf{v}$  is defined as the center-of-mass (barycenter) velocity of the mixture. The mass fraction of salt in seawater defines the salinity S. The budget equation for salt in differential form reads

$$\partial_t S + \partial_x (uS) + \partial_y (vS) + \partial_z (wS) = \partial_x (K\partial_x S) + \partial_y (K\partial_y S) + \partial_z (v'_t \partial_z S).$$
(1.9)

The diffusive salt flux  $\mathbf{j}_S = (-K\partial_x S, -K\partial_y S, -\nu'_t\partial_z S)$  on the right-hand side parameterizes the mean salt flux relative to the center-of-mass velocity (Beron-Vera et al. 1999; Nurser and Griffies 2019), with horizontal and vertical eddy diffusivities Kand  $\nu'_t$ . For salt there is a discontinuity at the surface and bottom boundaries, with no salt flux through them. Therefore, the analytical boundary condition requires the diffusive salt flux to compensate the advective one associated with (1.7a) and (1.7b):

$$\nabla(z - \eta) \cdot \mathbf{j}_{S} = -(E - P)S \qquad \text{at } z = \eta, \qquad (1.10a)$$
  
$$\nabla(z + H) \cdot \mathbf{i}_{S} = 0 \qquad \text{at } z = -H. \qquad (1.10b)$$

$$(z+H) \cdot \mathbf{j}_S = 0 \qquad \text{at } z = -H. \qquad (1.10b)$$

## **1.2.3** Heat Balance

An excellent representation of the heat of a seawater fluid element is the Conservative Temperature  $\Theta$  (McDougall 2003). From the first law of thermodynamics the corresponding prognostic equation can be derived as

$$\partial_t \Theta + \partial_x (u\Theta) + \partial_y (v\Theta) + \partial_z (w\Theta) = \partial_x (K\partial_x \Theta) + \partial_y (K\partial_y \Theta) + \partial_z (v'_t \partial_z \Theta) + \frac{\partial_z I}{C_p \rho_0},$$
(1.11)

with the specific heat capacity of water at constant pressure  $C_p$  and solar irradiance in I. The boundary condition for the diffusive temperature flux  $\mathbf{j}_{\Theta} =$  $(-K\partial_x\Theta, -K\partial_y\Theta, -\nu'_t\partial_z\Theta)$  with horizontal and vertical eddy diffusivities K and  $v'_t$  reads as

$$\nabla(z-\eta) \cdot \mathbf{j}_{\Theta} = \frac{Q_s}{C_p \rho_0} \qquad \text{at } z = \eta, \qquad (1.12a)$$

$$\nabla(z+H) \cdot \mathbf{j}_{\Theta} = 0 \qquad \text{at } z = -H. \qquad (1.12b)$$

The surface heat flux  $Q_s$  consists of sensible, latent and long-wave radiation contributions.

#### 1.2.4 Momentum Balance

The momentum balance provides prognostic equations for the velocity components. Considering Earth rotation and gravity these can be written as

$$\partial_t u + \partial_x (uu) + \partial_y (vu) + \partial_z (wu) - fv + f_c w$$
  
=  $\partial_x T_{11} + \partial_y T_{21} + \partial_z T_{31} - \partial_x P_{nh} - \partial_x P_{hs},$   
(1.13a)

$$\partial_t v + \partial_x (uv) + \partial_y (vv) + \partial_z (wv) + fu$$
  
=  $\partial_x T_{12} + \partial_y T_{22} + \partial_z T_{32} - \partial_y P_{\text{nh}} - \partial_y P_{\text{hs}},$   
(1.13b)

$$\partial_t w + \partial_x (uw) + \partial_y (vw) + \partial_z (ww) - f_c u$$
  
=  $\partial_x T_{13} + \partial_y T_{23} + \partial_z T_{33} - \partial_z P_{\text{nh}}.$  (1.13c)

In (1.13a)–(1.13c)  $f = 2\Omega \sin \phi$  and  $f_c = 2\Omega \cos \phi$  denote the Coriolis parameters with the spin rate of the Earth  $\Omega$  and latitude  $\phi$ , and  $T_{ij}$  the components of the turbulent stress tensor **T**. Formulations for the stress tensor are given in Sect. 1.2.5. The dynamic pressure is already decomposed into hydrostatic and nonhydrostatic contributions. The hydrostatic pressure contribution is defined by the weight of the water column above,

$$\rho_0 P_{\rm hs}(z) = p_{\rm a} + \rho_0 g(\eta - z) + \int_{z}^{\eta} \left( \rho(z') - \rho_0 \right) g \, \mathrm{d}z', \tag{1.14}$$

with  $p_a$  being atmospheric pressure at the surface and *g* the gravitational acceleration. Dynamic boundary conditions prescribe momentum fluxes through the surface and bottom,

$$\nabla(z - \eta) \cdot \mathbf{T} = \tau_{s} \qquad \text{at } z = \eta, \qquad (1.15a)$$

$$\nabla(z+H) \cdot \mathbf{T} = \tau_{\mathrm{b}}$$
 at  $z = -H$ , (1.15b)

with  $\tau_s$  and  $\tau_b$  being surface and bottom stress vectors defined in opposite direction to the associated momentum fluxes. The bottom stress is usually reconstructed from a logarithmic velocity profile.

### 1.2.5 Common Formulations and Closures

Depending on the application and the scales of interest, different forms of the turbulent fluxes and different closures for the eddy viscosities and diffusivities have to be used.

#### **Nonhydrostatic LES Equations**

The governing equations for *Large eddy simulations (LES)* can be obtained when the averaging operator in (1.3) represents a sufficiently fine spatial filter such that the mean flow quantities still resolve the large energy-containing eddies down to the inertial subrange. Because the horizontal and vertical scales of motion are isotropic within the inertial subrange, the full momentum balance must be solved, which requires the solution of a three-dimensional elliptic Poisson equation for the nonhydrostatic pressure contribution.

In contrast to the large-scale eddies, which strongly depend on the geometry of the domain and thus obey no universal spectrum, the unresolved small-scale eddies are more likely to be homogeneous and isotropic and thus easier to model. The most common approach to modeling the turbulent stress in LES is to assume 3D isotropy for the eddy diffusivity *A* and its flow-dependent calculation following Smagorinsky (1963):

$$T_{ij} = A(\partial_i u_j + \partial_j u_i), \tag{1.16a}$$

$$A = (C_{\mathsf{S}}\Delta)^2 \left(\frac{1}{2}(\partial_i u_j + \partial_j u_i)\frac{1}{2}(\partial_i u_j + \partial_j u_i)\right)^{1/2}.$$
 (1.16b)

In (1.16b) summation is carried out over doubled indices,  $\Delta$  is the filter width and  $C_{\rm S} = \mathcal{O}(0.1)$  is the Smagorinsky constant. Assuming 3D isotropy also implies equal horizontal and vertical eddy diffusivities for tracers, i.e.  $K = v'_t$  in (1.9) and (1.11), which can be calculated in terms of a prescribed turbulent Prandtl number  $Pr_t$ :

$$K = A/Pr_{\rm t}.\tag{1.17}$$

In LES the filter width  $\Delta$  is a measure of the grid size, which must be of  $\mathcal{O}(0.1 \text{ m}) - \mathcal{O}(1 \text{ m})$  to resolve the energy-containing eddies in typical marine applications. Therefore, LES is reserved for small-scale, idealized studies, although its application to real, field-scale problems continues to increase. For a more thorough overview of LES modeling, the reader is encouraged to refer to the texts by Pope (2000) and Rodi et al. (2013).

#### Hydrostatic Shallow Water Equations

In most geophysical applications the vertical scales of motion are much smaller than the horizontal ones. The flows usually take place in horizontal planes without significant vertical acceleration. These considerations motivate the *hydrostatic pressure assumption*, which degenerates the vertical momentum balance by neglecting (1.13c) so that the prognostic integration of w in (1.13c) is replaced by a diagnostic calculation from (1.6), see e.g. Klingbeil and Burchard (2013). Furthermore, the nonhydrostatic pressure contributions in (1.13a) and (1.13b) are neglected, i.e.  $\partial_x P_{nh} = \partial_y P_{nh} = 0$ . In addition,  $f_c w$  is neglected in (1.13a) so that the Coriolis force stays orthogonal to the velocity and does not alter the kinetic energy of a fluid element.

The separation of horizontal and vertical scales also implies different viscosities in the horizontal and vertical direction (*A* and  $v_t$ , respectively). Under this transverse isotropy two formulations of the stress tensor are common (Kamenkovich 1967; Smagorinsky 1993):

$$\begin{bmatrix} T_{11} & T_{21} & T_{31} \\ T_{12} & T_{22} & T_{32} \end{bmatrix} = \begin{bmatrix} 2A\partial_x u & A(\partial_x v + \partial_y u) & v_t \partial_z u \\ A(\partial_x v + \partial_y u) & 2A\partial_y v & v_t \partial_z v \end{bmatrix},$$
(1.18a)

$$A = (C_{\rm S}\Delta)^2 \left( (\partial_x u)^2 + \frac{1}{2} (\partial_x v + \partial_y u)^2 + (\partial_y v)^2 \right)^{1/2}, \qquad (1.18b)$$

or

$$\begin{bmatrix} T_{11} & T_{21} & T_{31} \\ T_{12} & T_{22} & T_{32} \end{bmatrix} = \begin{bmatrix} A(\partial_x u - \partial_y v) & A(\partial_x v + \partial_y u) & v_t \partial_z u \\ A(\partial_x v + \partial_y u) & -A(\partial_x u - \partial_y v) & v_t \partial_z v \end{bmatrix},$$
(1.19a)

$$A = (C_{\rm S}\Delta)^2 \left(\frac{1}{2}(\partial_x u - \partial_y v)^2 + \frac{1}{2}(\partial_x v + \partial_y u)^2\right)^{1/2}.$$
 (1.19b)

The horizontal eddy diffusivity of momentum A is either assumed to be constant, or calculated by the Smagorinsky closures given in (1.18b) and (1.19b), respectively. The horizontal eddy diffusivity for tracers K in (1.9) and (1.11) is usually derived in terms of a prescribed turbulent Prandtl number according to (1.17). Following Umlauf and Burchard (2005), the vertical turbulent diffusivities of momentum  $v_t$  and tracers  $v'_t$  can be obtained from a general algebraic second-moment closure in terms of the turbulent kinetic energy (TKE) k and its dissipation rate  $\varepsilon$ .

#### 1.3 Summary

In this chapter the governing equations for marine flows were presented. For many applications the hydrostatic pressure assumption is valid. The resulting shallow water equations outlined in Sect. 1.2.5 form the basis for many studies and the remaining

chapters. Further details about the numerics of hydrostatic coastal ocean models can be found in Klingbeil et al. (2018).

#### References

- Aris, R. 1989. Vectors. *Tensors and the basic equations of fluid mechanics*. Dover Publications. 978-0-486-66110-0.
- Batchelor, G.K. 1967. An introduction to fluid dynamics. Cambridge University Press.
- Beron-Vera, F.J., J. Ochoa, and P. Ripa. 1999. A note on boundary conditions for salt and freshwater balances. *Ocean Modelling* 1: 111–118.
- Foias, C., O.P. Manley, R. Rosa, and R. Témam. 2001. Navier-Stokes equations and turbulence. In Encyclopedia of mathematics and its applications, vol. 83. Cambridge University Press. https:// doi.org/10.1017/CBO9780511546754.
- Griffies, S.M. 2004. Fundamentals of ocean climate models. Princeton University Press.
- Kamenkovich, V.M. 1967. On the coefficients of eddy diffusion and viscosity in large-scale oceanic and atmospheric motions. *Izvestiya, Atmospheric and Oceanic Physics* 3: 1326–1333.
- Klingbeil, K., and H. Burchard. 2013. Implementation of a direct nonhydrostatic pressure gradient discretisation into a layered ocean model. *Ocean Modelling* 65: 64–77.
- Klingbeil, K., F. Lemarié, L. Debreu, and H. Burchard. 2018. The numerics of hydrostatic structuredgrid coastal ocean models: state of the art and future perspectives. *Ocean Modelling* 125: 80–105.
- Lorenz, E.N. 1963. Deterministic nonperiodic flow. *Journal of the Atmospheric Sciences* 20: 130–141.
- McDougall, T.J. 2003. Potential enthalpy: A conservative oceanic variable for evaluating heat content and heat fluxes. *Journal of Physical Oceanography* 33: 945–963.
- Nurser, A.J.G., and S.M. Griffies. 2019. Relating the diffusive salt flux just below the ocean surface to boundary freshwater and salt fluxes. *Journal of Physical Oceanography* 49: 2365–2376.
- Olbers, D., J. Willebrand, and C. Eden. 2012. Ocean dynamics. Springer.
- Pope, S.B. 2000. Turbulent flows. Cambridge University Press.
- Rodi, W., G. Constantinescu, and T. Stoesser. 2013. *Large-Eddy simulation in hydraulics*. CRC Press.
- Roquet, F., G. Madec, T.J. McDougall, and P.M. Barker. 2015. Accurate polynomial expressions for the density and specific volume of seawater using the TEOS-10 standard. *Ocean Modelling* 90: 29–43.
- Smagorinsky, J. 1963. General circulation experiments with the primitive equations. *Monthly Weather Review* 91 (3): 99–164.
- Smagorinsky, J. (1993). Some historical remarks on the use of nonlinear viscosities. In *Large eddy simulation of complex engineering and geophysical flows*, 3–36. Cambridge University Press. ISBN 9780521131339.
- Umlauf, L., and H. Burchard. 2005. Second-order turbulence closure models for geophysical boundary layers. A review of recent work. *Continental Shelf Research* 25: 795–827.
- Young, W.R. 2010. Dynamic enthalpy, conservative temperature, and the seawater Boussinesq approximation. *Journal of Physical Oceanography* 40: 394–400.