Turbulence modelling in environmental flows
Improving the accuracy of the k-ε model
by a mathematical transformation

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Turbulence modelling in environmental flows

Improving the numerical accuracy of the $k - \varepsilon$ model by a mathematical transformation

Final report

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Cover photo: Dingle bay and Caislean na Mineairde, Ireland
By Aron Dijkstra, 2014
Numerical modelling for environmental flow applications, such as for rivers, lakes, estuaries and coastal flows, faces a trade-off between the numerical accuracy and the required computation time. This trade-off results in grids which typically contain 10 to 100 layers in the vertical direction. Such a grid resolution poses severe limitations to the numerical accuracy of the model. The turbulence model determines a significant part of this accuracy. This research therefore investigates an unexplored method of using transformations to improve the numerical accuracy of two-equation turbulence models at a low resolution.

The $k - \varepsilon$ model is used as starting point for this method. The equation for $\varepsilon$ is transformed to equations for $\omega \sim \varepsilon/k$ and $\tau = k/\varepsilon$. This results in three turbulence models, the $k - \varepsilon$, $k - \omega$ and $k - \tau$ models, which are physically equivalent, but possess different numerical properties. This research identifies these different numerical properties in order to explain when and why a certain transformation is beneficial to the numerical accuracy. The three turbulence models are tested in six cases of homogeneous and stratified flows in a one-dimensional vertical (1DV) numerical model, which is representative for the implementation in the 3D simulation system Delft 3D-FLOW.

It is shown that the $k - \tau$ model yields more accurate results than the $k - \varepsilon$ and $k - \omega$ models in boundary friction dominated flows, such as those found in rivers, partially stratified estuaries and along the coast. This improved performance is explained from the profile of $\tau$, which is linear near the frictional boundary and therefore accurately approximated on a low resolution grid. The profiles of $\varepsilon$ and $\omega$ are hyperbolic near the frictional boundary and therefore not accurately represented on such a grid.

The boundary condition for $\tau$ is well-posed, while no natural boundary conditions for $\varepsilon$ and $\omega$ exist. Dirichlet boundary conditions for $\varepsilon$ and $\omega$ are therefore inaccurate. The Neumann boundary condition is found to be the most accurate alternative boundary condition for $\varepsilon$ and $\omega$. An adjusted Dirichlet conditions used in Delft 3D-FLOW improves on the result of the ordinary Dirichlet condition, but shows bad convergence behaviour, with results being significantly worse at 100 vertical layers than at 10 vertical layers. A new adjusted Dirichlet condition is developed, which has better convergence behaviour, but is still somewhat worse than the Neumann condition.

The $k - \tau$ and $k - \omega$ models contain a number of diffusive terms, the implementation of which may introduce numerical diffusion in the model. Some of these diffusive terms are essential to the stability of the model. Others are optional. It is argued that the choice whether or not to include such optional diffusive terms should be based on both physical and numerical arguments, because the numerical diffusion associated with the implementation of the terms may have a significant desired or undesired effects on the model results.

It is found in the cases in this research that convergence of the turbulence models with increasing grid resolution is typically found between 100 and 1000 grid cells in the vertical direction. One case of temperature modelling of a lake has been tested in which convergence did not occur up to 2000 grid cells. So converged results are generally beyond the range of generally used vertical resolution in 3D models. Within the feasible range of 10 to 100 layers it is found that the results of the turbulence models do not necessarily become more accurate if higher resolution grids are used. So monotonous convergence of the turbulence models is not guaranteed.
The photo on the cover could easily provide the deceiving impression that research into environmental flows, such as the estuarine flow depicted, requires one to go out on a ship to see and touch the water itself. Reality of much of such research is, however, much less romantic as the physical system is schematised to computer models and the development of these computer models is expressed in grids and numerical operators, rather than waves and tides. This research is no different as it focusses on the numerical differences caused by different implementations of the $k - \varepsilon$ turbulence model.

Still, the natural systems of environmental flows have inspired me in this work on numerical modelling details. This research is one of the examples of how the understanding of the physics of the natural systems helps to design better numerical modelling approaches. I hope that the findings of this study also find their way back to the natural system as an improvement of numerical modelling systems that will be used in predicting the future development of such systems.

This research forms my master thesis for Civil Engineering and is part of my double degree in Civil Engineering and Applied Mathematics. The mathematical influences will be clearly visible in this study as both studies have shaped my way of thinking over the past six years. In this thesis, I have tried to connect analytical and numerical analysis of non-linear equations to a physical explanation to make this story appealing to both civil engineers and mathematicians.

I would like to thank Rob Uittenbogaard and Jan van Kester for sharing their wealth of experience and for their great ideas. Our numerous long discussions have motivated me to get to the bottom of the cases in this research, as any of my arguments would always be countered by a critical question. I would also like to thank Henk Schutteelaars for his great interest in this work. Our discussions have helped me to focus my work and have always provided me with new ideas. I would like to thank Julie Pietrzak for helping me to focus the introduction and discussion to this thesis and for making me realise that I could realistically qualify for a position at a top-class research institute. I would also like to express my thanks to Bram van Prooijen for providing valuable advice that has made this thesis much more accessible and precise. Together, Rob, Jan, Henk, Julie and Bram have helped me to give this research an identity that is distinct from any previous study into turbulence modelling.

Finally I would like to thank Herman Kernkamp and Jan Mooiman for their input, support and interest and I would like to express my gratitude to Deltares for giving me the opportunity to work with them for fourteen months during the work on both theses.

I hope that this research will give you some inspiring new insights into the rather unexplored area of using transformations to improve the numerical performance of turbulence models.

Yoeri Dijkstra,
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Turbulence modelling is essential to the modelling of a wide range of processes in environmental flows, which comprise flows in rivers, estuaries, coastal seas and lakes. Turbulence is the dominant mechanism that determines for example how bed friction affects the flow velocity, how heat or salt is distributed over the water column and how fast sediments settle. The accuracy with which turbulence is modelled is therefore of essential importance to the simulation of flow and transport of sediment in a river or estuary and the temperature and biological activity in a lake. The wide range of scales and apparently random nature of turbulent eddies make turbulence notoriously difficult to model and a wide range of turbulence modelling approaches has been developed.

One of the most popular classes of turbulence modelling approaches is that of two-equation turbulence models. Models of this type do not resolve the turbulence itself, but parametrise it by an eddy viscosity, which is calculated from a set of two coupled transport equations. Such a parametrisation allows the model to resolve only the flow on the larger scale, i.e. of the order of decimetres to metres, instead of modelling all scales down to tenths of millimetres. The first equation of the model is generally agreed upon (Mellor and Yamada, 1982) and models the turbulent kinetic energy (TKE), which is denoted by $k$. The exact nature of the second equation is still subject of contention. This equation models a variable that is a function of a length-scale of turbulence, denoted by $l$. Launder and Spalding (1974) have formulated a general form of the equation for a variable $k^m l^n$, where $m$ and $n$ may still be chosen. The resulting $k - k^m l^n$ model is called the general length-scale (GLS) model by Umlauf and Burchard (2003), who have developed an automatic calibration procedure for the model.

Frequently used forms of two-equation models are the $k - \epsilon$ model (Rodi, 1993), where $\epsilon \sim k^{3/2}/l$ is the dissipation of TKE, the $k - \omega$ model (Wilcox, 1993), where $\omega \sim k^{1/2}/l$ is a frequency of turbulence, and the $k - kl$ model (Mellor and Yamada, 1982). Warner et al. (2005) gives a good overview of the ongoing debate on which one of these models is the best, concluding that there is no fundamental theoretical preference for either of these models. Numerous comparisons have been made between the results of the models in a number of cases, but also no single best model has been identified (Warner et al., 2005; Umlauf and Burchard, 2003; Wijesekera et al., 2003).

The numerical accuracy of the models has not been a focal point of the debate. Insight into the numerical accuracy of turbulence models is, however, relevant in light of the trade-off in modelling between the grid resolution and the computational costs. This trade-off has resulted in models using grids with 10 to 50 layers in the vertical direction, which poses severe limitations to the numerical accuracy of turbulence modelling. The numerical implementation of the models therefore becomes an essential part of the modelling process and numerical errors can even dominate over physical inaccuracies.

This study therefore aims at improving the insight into the numerical accuracy of turbulence models and finding a turbulence model implementation that achieves better results at a low grid resolution. Two important components of the numerical accuracy will be investigated: the difference of the model results between a low and high grid resolution and the convergence behaviour. Monotonous convergence would be a desirable property of the model. This would mean that the numerical error decreases when the grid resolution is increased.

One can look to improve the numerical performance of a turbulence model by using a different turbulence model that is believed to have better numerical properties. The several existing turbulence models essentially differ in the length-scale variable and a few terms or boundary conditions. Such an approach does not allow for distinguishing the numerical errors from the analytical differences between two different models. We will therefore look to a comparison between models that contain the same physics and differ only on the numerical aspects.

It could be possible to improve the numerical accuracy by using a more accurate discretisation method. Many
popular numerical simulation systems, such as Delft 3D-FLOW, GOTM and ROMS, use a combination of first-order and second-order accurate numerical operators to discretise their turbulence models. Higher-order discretisation methods or locally higher-order methods (limiters) are available (Zijlema, 1996), but have not been well tested. The downside of using higher-order accurate numerical operators is that require a larger stencil, i.e. more grid points per calculation, and therefore more computational time.

The approach that will be taken in this research uses a mathematical transformation of the dependent variables in the turbulence model. Such a transformation will lead to turbulence models with different length-scale variables, but with the same physical properties. The essential thought behind this approach is that certain length-scale variables possess more favourable numerical properties than others. The use of this method is motivated by the findings of Speziale et al. (1992). They construct the $k - \tau$ model from the $k - \varepsilon$ model by transforming $\varepsilon$ to $\tau \sim 1/k^{1/2}$, which represents a time-scale of turbulence. In homogeneous flows that are dominated by bed friction, this will result in the typical vertical profiles of $\varepsilon$ and $\tau$ sketched in Figure 1. The profile of $\tau$ is linear near the bed and $\tau$ has a well-defined boundary condition at the bed. The profile of $\varepsilon$ on the other hand is hyperbolic and the value of $\varepsilon$ approaches infinity near the bed. The profile and the boundary condition of $\tau$ can be approximated more accurately on a coarse grid than the profile and boundary condition of $\varepsilon$.

We will investigate how much such a transformation can improve the accuracy of the modelled velocity and will investigate whether such a transformation will also improve the results in stratified flows. We will therefore compare three turbulence models in a range of cases including homogeneous and stratified environmental flows. The $k - \varepsilon$ model of Rodi (1993) is used as the basis of the transformation and it will be transformed to the $k - \omega$ and $k - \tau$ models. The $k - \omega$ model is a popular turbulence model in the form of Wilcox (1993). The form of the $k - \omega$ model as a transformation of the $k - \varepsilon$ model is different to this popular form, but still allows us to draw conclusions on the numerical accuracy with which the profile of $\omega$ can be approximated.

The goal of this research is to provide insight into the magnitude of the numerical accuracy at low grid resolutions and the convergence of the $k - \varepsilon$, $k - \omega$ and $k - \tau$ turbulence models by testing these turbulence models in a number of cases of environmental flows in a one-dimensional vertical (1DV) model and comparing the results against measurements. This leads to the following research questions:

1. Can a transformation of the $k - \varepsilon$ model to the $k - \tau$ or $k - \omega$ model improve the numerical accuracy in the simulation of general environmental flows?
2. What properties of the transformed turbulence models are responsible for the differences in numerical accuracy?
3. Does either of the three turbulence model yield monotonous convergence of the results with increasing grid resolution?

Insight into the numerical accuracy will be created by identifying the model properties that explain the differences between the three transformed turbulence models. These properties are identified by testing four cases of simple, but essential flow processes that have been well-studied in earlier research. These cases allow for analysing the mechanisms that determine the behaviour of the turbulence models. This research also includes two additional cases of more complex flows that are more representative of realistic environmental flow cases. These cases are
difficult to analyse because of the interactions between the flow, the stratification and the external sources and sinks of heat or salt. It is nevertheless possible to study the numerical accuracy and convergence behaviour of the turbulence models.

The structure of the report is as follows. The theoretical background behind the use of an eddy viscosity and two-equation models is provided in Chapter 1. The three turbulence models are then given in Chapter 2 and discretised in the 1DV model in Chapter 3. The results of the cases are then presented in Chapter 4 for the first four cases and Chapter 5 for the final two cases. The results are discussed further in Chapter 6. This report closes with conclusions and recommendations.
Turbulence theory and definitions

The foundation of our knowledge of turbulence was laid by Osborne Reynolds in papers from the end of the 19th century. Most notable was the experiment in which he visualised the transition between laminar and turbulent flow. He has related the conditions under which this transition takes place to a dimensionless number, later called the Reynolds number:

$$Re = \frac{\text{inertial forces}}{\text{viscous forces}} = \frac{UL}{\nu},$$

where $U$ and $L$ are typical velocity scales and length-scales and $\nu$ is the kinematic viscosity. The transition between laminar and turbulent flow was found by Reynolds and many researches after him to happen around $Re = O(10^3)$. The environmental flows that will be considered in this thesis have typical dimensions of $U = O(1)\text{ m/s}$, $L = O(10)\text{ m}$ and $\nu = O(10^{-6})\text{ m}^2/\text{s}$ and therefore $Re = O(10^5)$. These flows are clearly turbulent.

Around the same time as Reynolds, Poincaré found that relatively simple non-linear dynamical systems were capable of showing behaviour that resembles randomness, although fully deterministic. However, it was only in 1963 that Lorenz made the connection between this deterministic chaos and turbulence.

Earlier, in 1894, Reynolds already concluded that turbulence is too difficult to understand in all its details and therefore suggested an averaging procedure to remove the turbulent fluctuations from the equations that describe flow and transport. This averaging procedure still forms the starting point of turbulence modelling to date and will be described in Section 1.1 for the equations of flow and transport and in Section 1.2 for the equation of conservation of energy. The Reynolds averaging procedure reveals a turbulence-related term in the equations, known as the Reynolds stress. This term needs a closure assumption to complete the equations. Several types of closure assumptions and turbulence simulation methods will be listed in Section 1.3. Finally, the schematisation of the near-bed region is treated in Section 1.4.

1.1. Reynolds averaging and the equations of motion

Reynolds has suggested a decomposition method that separates the random-like turbulent fluctuations of a flow from the more steady mean flow. This decomposition reads

$$u = \bar{u} + u'$$

for any quantity $u$ and separates it in a mean part $\bar{u}$ and a part which is due to turbulent fluctuations $u'$. The mean is defined as ensemble average, which is the average value of $u$ over infinitely many experiments

$1^O$ is Landau’s order symbol and means ‘of the order of’.
under nearly equal conditions. The ensemble average of the fluctuations $u'\overline{u}$ is therefore zero. This method of decomposition is applied to all unknown variables in the equations for flow and transport.

The flow of water is described by the equations that describe the conservation of mass and momentum, also known as the equations of motion. The momentum equations, or Navier-Stokes equations, are used in a commonly used simplified form in which Coriolis is neglected and the Boussinesq approximation is applied. The Boussinesq approximation states that density differences in the flow can be neglected in all but the gravity term if they are small compared to the density itself. The simplified Navier-Stokes equations read

$$\frac{\partial \overline{u_i}}{\partial t} + \overline{u_j} \frac{\partial \overline{u_i}}{\partial x_j} = - \frac{1}{\rho_0} \frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \nu \frac{\partial \overline{u_i}}{\partial x_j} - \overline{u'_i u'_j} \right) - \frac{\rho}{\rho_0} g \delta_i,3,$$  

(1.1)

where the Einstein convention\(^2\) is used, $i,j \in \{1,2,3\}$ and $\delta_{i,j}$ is the Kronecker delta\(^3\). The variables $u_i$ are the velocity components in $x,y$ and $z$-direction, $p$ is pressure, $\rho$ is density, $\rho_0$ is a constant reference density and $g$ is the acceleration of gravity.

The Reynolds decomposition is applied to these equations by making a decomposition of $u_i$ and $p$. The Reynolds-averaged Navier-Stokes (RANS) equations are then obtained by taking an ensemble average of the Navier-Stokes equations. The RANS equations describe the momentum conservation of the main flow, i.e. without turbulent fluctuations, and read

$$\frac{\partial \overline{u_i}}{\partial t} + \overline{u_j} \frac{\partial \overline{u_i}}{\partial x_j} = - \frac{1}{\rho_0} \frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \nu \frac{\partial \overline{u_i}}{\partial x_j} - \overline{u'_i u'_j} \right) - \frac{\rho}{\rho_0} g \delta_i,3.$$  

(1.1)

The conservation of mass equation is simplified by using the property that water is incompressible. The Reynolds-averaged equations are then obtained by making a decomposition of the velocity and taking the ensemble average. The resulting equation is

$$\frac{\partial \overline{u_i}}{\partial x_i} = 0.$$  

(1.2)

Additional equations are used for the modelling of the transport of a tracer quantity, like temperature, salinity or sediment. Salinity is used as an example here and is modelled according to an advection-diffusion equation. The salinity is also decomposed in a mean and fluctuating part $s = \overline{s} + s'$ and the equation is ensemble averaged. The resulting Reynolds-averaged salinity equation is

$$\frac{\partial \overline{s}}{\partial t} + \overline{u_i} \frac{\partial \overline{s}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \underbrace{D_s \frac{\partial \overline{s}}{\partial x_i}}_{\text{advection}} - \overline{u'_i s'} \right).$$  

(1.3)

The same equation can be used to describe the evolution of the temperature in a body of water without external sources or sinks of heat. A more complete temperature model, which includes external sources and sinks, is used for the case of Lake Vlietland in Section 5.1. This model is the same as in the Delft 3D-FLOW model, see Deltares (2014).

The effect of the salinity and temperature on the density of the flow is described by an equation of state. The UNESCO equation of state (IOC, SCOR and IAPSO, 2010) provides a detailed description of the way in which the density depends on e.g. salinity and temperature, but for the purposes of this thesis a simple linear relation is sufficiently accurate:

$$\rho(s) = \rho_0 + \beta s,$$

where $\beta$ is a constant with magnitude $\beta = 7.6 \cdot 10^{-4}$ kg/(m$^3$ psu) for salinity and $\beta = -0.1 \cdot 10^{-4}$ kg/(m$^3$°C) for temperature. The UNESCO equation of state is used for the Lake Vlietland case.

\(^2\)Summation takes place over indices that occur twice in a term, see Appendix A.1 for a more elaborate explanation.

\(^3\)\(\delta_{i,j} = 1\) for $i = j$ and $\delta_{i,j} = 0$ for $i \neq j$.\n
The above equations form a set of five Reynolds-averaged differential equations for five mean flow variables \( \overline{u}_i \) (\( i = 1, 2, 3 \)), \( \overline{p} \) and \( \overline{\tau} \). The equations contain some remaining unknowns which are correlations of turbulent fluctuations. The first type of correlation is \( \overline{u}_i' \overline{u}_j' \), which is known as the Reynolds stress:

\[
R_{ij} = -\overline{u}_i' \overline{u}_j'.
\]

Note that the Reynolds stress is alternatively defined as \( \rho_0 \overline{u}_i' \overline{u}_j' \), which has the dimension of a stress. However, for simplicity, \( \overline{u}_i \overline{u}_j' \) is used. The other correlation is of the form \( \overline{u}_i' \overline{s}_{ij}' \).

The problem of relating the unknown correlation terms to mean flow properties is called the closure problem. Several methods for solving this closure problem are treated in Section 1.3. First, however, the averaging procedure is repeated on the equation that describes the conservation of energy.

1.2. The energy equation

The law of conservation of energy provides insight into the nature of turbulence when it is separated in an equation for the mean flow and the turbulent fluctuations. The Reynolds averaging procedure is therefore applied to the energy equation. The following definitions will be used:

- \( k = \overline{u}_i' \overline{u}_i' \) turbulent kinetic energy (TKE)
- \( K = \overline{u}_i \overline{u}_i \) mean kinetic energy

The energy balance for the mean flow may be obtained by taking the dot product of the RANS equations with the velocity vector. This results in the following equation for the kinetic energy of the mean flow

\[
\frac{\partial K}{\partial t} + u_j \frac{\partial K}{\partial x_j} = -R_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\rho}{\rho_0} u_i u_j g - \frac{1}{\rho_0} \frac{\partial p u_i}{\partial x_j} - \frac{\partial (\overline{u}_i' \overline{u}_i') u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \nu \frac{\partial K}{\partial x_j} \right) - \nu \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}.
\]

The energy balance for fluctuations is obtained by first finding the momentum balance for fluctuations by subtracting the RANS equations from the Navier-Stokes equations. Next, the dot product of this set of equations with the vector of velocity fluctuations is taken. This yields the energy equation for the kinetic energy of the turbulent fluctuations

\[
\frac{\partial k}{\partial t} + u_j \frac{\partial k}{\partial x_j} = R_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\rho}{\rho_0} u_i u_j' - \frac{1}{\rho_0} \frac{\partial p' u_i}{\partial x_j} - \frac{\partial (\overline{u}_i' \overline{u}_i') u_i'}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \nu \frac{\partial k}{\partial x_j} \right) - \nu \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}.
\]

The first term on the right-hand side, \( R_{ij} \frac{\partial u_i}{\partial x_j} \), occurs in both energy equations; as a sink in the mean energy and as a source in the turbulent energy. So it acts as an energy exchange from the mean motion to the turbulent motion. This Reynolds stress term dominates the dissipation of energy of the mean motion, while viscous dissipation dominates the dissipation of energy in the turbulent kinetic energy equation. So we see energy being transferred from the mean motion to the turbulent motion by the a term involving the Reynolds stress. This energy of the turbulent motion is then converted to heat by viscous dissipation. This chain of processes is referred to as the energy cascade.

The energy cascade can be used to connect the large scales of the mean motion to the small scales of the turbulent fluctuations. Energy is transferred from the large to the small scale at a rate of \( \mathcal{O}(U/L) \), where \( U \) and \( L \) are velocity and length scales of the mean motion. This rate is based on dimensional arguments, see Pope (2000) for more information. The same amount of energy should be dissipated by viscous dissipation on the small scales. So we also find a dissipation rate \( \varepsilon \) equal to \( \mathcal{O}(U^2/L) \).

The range between the large and the small scales is called the inertial range. This stretches approximately from the scale of \( \mathcal{O}(0.1) \) m to the Kolmogorov scale of \( \mathcal{O}(0.1) \) mm for environmental flows. The energy in this range can be described as a function of the wave frequency of turbulent eddies, which is related to the inverse of the size of the eddies. In 1941 Kolmogorov derived such an equation for the energy density \( E \) as a function of the
frequency $f$ of turbulent eddies on the basis of self-similarity and isotropy of turbulent eddies (Kolmogorov, 1991, reprinted translation). This equation can be written as

$$E(f) = \alpha\varepsilon^{2/3} f^{5/3},$$  \hspace{1cm} (1.6)

where $\alpha$ is a constant. This equation has been confirmed in measurements, see Figure 2.

The energy density spectrum $E$ is described in three different directions. The spectrum in all directions is approximately the same for turbulence in the inertial range. This property of equal turbulence properties in different directions is called isotropy. The flow at larger turbulent length-scales (i.e. lower frequency) is anisotropic and the spectrum is different in different directions, see Figure 2.

![Turbulence power spectrum](image)

Figure 2: Turbulence power spectrum (energy per unit frequency) from measurements in the Elkhorn Slough estuary, CA, USA. The components indicate spectrum in the streamwise (solid), transverse (dashed) and vertical (dotted) direction. The line $f^{5/3}$ is also shown. Figure adapted from Monismith (2010).

1.3. Turbulence modelling

The closure problem that was introduced in Section 1.1 requires that the effect of turbulence is expressed in terms of properties of the mean flow. Several methods exist to either solve for the turbulent fluctuations themselves or solve the closure problem. Pope (2000) mentions the following classes of turbulence models:

- Direct numerical simulation (DNS)
- Large eddy simulation (LES)
- PDF models
- Reynolds stress modelling (RSM)
- Eddy viscosity models

This thesis uses turbulence models in the class of eddy viscosity models. A short overview of the other models is also given below to motivate the use of these eddy viscosity models for environmental applications.

1.3.1. DNS and LES

DNS and LES are turbulence simulation methods, i.e. they resolve the turbulent fluctuations. The Reynolds averaging procedure is not required for these methods. In DNS all turbulent spatial scales are resolved from
the large scale \( O(L) \) to the Kolmogorov scale \( \lambda_{kolm} \). The amount of computational cells required to capture all these scales is, by dimensional analysis,

\[
\frac{L}{\lambda_{kolm}} = O \left( \left( \frac{UL}{\nu} \right)^{3/4} \right) = O \left( Re^{3/4} \right).
\]

So the number of grid points for three spatial dimensions, a temporal dimension and a Courant number near unity is of the order of \( Re^{3} \). The Reynolds number for typical environmental applications is of order of \( 10^5 \), which makes DNS not computationally feasible.

LES requires that the scales are resolved down to a scale in the inertial range. The turbulence on the sub-grid level is then modelled under the assumption that it is isotropic, which is more accurate than the modelling of anisotropic turbulence on larger scales. LES is sometimes used in civil engineering applications, especially for rapidly varying flows around structures. However, the method is computationally intensive for larger scale applications.

### 1.3.2. PDF models

Probability density function (PDF) models start from the observation that the mean velocity and \( u'_i u'_j \) are the mean and covariance of a stochastic variable with a certain probability density function \( f \) that may differ in all directions and in time. Such models need a closure for a turbulent length scale which may be provided either deterministically or stochastically. Solving these stochastic models is generally done using Lagrangian particle methods which are time consuming, but provide insight into the turbulence itself. For more information, see Pope (2000).

### 1.3.3. Reynolds stress models (RSM)

Reynolds stress models (RSM) and eddy viscosity models are turbulence modelling methods, i.e. they only close the Reynolds stresses and do not resolve the turbulence itself.

Reynolds stress modelling uses an exact (i.e. based on the Navier-stokes equations) transport equation for the Reynolds stress. The resulting equations are given below to illustrate the complexity of the model. The equations in abstract form read

\[
\frac{\partial u'_i u'_k}{\partial t} + u_j \frac{\partial u'_i u'_k}{\partial x_j} = P_{ik} + B_{ik} - \Phi_{ik} + D_{ik} - \varepsilon_{ik}, \quad i, k \in \{1, 2, 3\}
\]

where \( P_{ik} \) and \( B_{ik} \) are production terms related to mean shear and buoyancy. \( \Phi_{ik} \) are pressure-strain correlations, responsible for the distribution of stresses between the several components \( u'_i u'_j \). \( D_{ik} \) are turbulent and viscous transport or diffusion terms and \( \varepsilon_{ik} \) is viscous dissipation.

The more detailed form of the equations is given by (Umlauf, 2001)

\[
\frac{\partial R_{ik}}{\partial t} + u_j \frac{\partial R_{ik}}{\partial x_j} = -R_{ij} \frac{\partial u_i}{\partial x_j} - R_{jk} \frac{\partial u_i}{\partial x_j} - \frac{g}{\rho_0} \delta_{i3} \delta_{j3} u'_k + \frac{g}{\rho_0} \delta_{i3} \delta_{j3} u'_k + \frac{1}{\rho_0} \left( \frac{\partial u'_i}{\partial x_k} + \frac{\partial u'_k}{\partial x_i} \right) - \frac{\partial u'_i u'_j u'_k}{\partial x_j} - \frac{1}{\rho_0} \left( \frac{\partial u'_i p'}{\partial x_k} + \frac{\partial u'_k p'}{\partial x_i} \right) + \nu \frac{\partial^2 u'_i u'_k}{\partial x_j^2} + 2\nu \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_k}{\partial x_j}.
\]

This equation still contains correlations of fluctuations that are not resolved and need further closure assumptions. If closures are used at this point, this is called second-order RSM. Higher-order RSM are obtained by formulating more equations for the unknown terms, but also these higher-order RSM need closure assumptions. The second-order Reynolds stresses model needs six equations, which are added to the five that were already found in Section 1.1. The great number of equations and associated computational time required to solve them make the Reynolds stress models less popular in environmental flow modelling than the simpler eddy viscosity models.
1.3.4. The eddy viscosity hypothesis

Boussinesq introduced the eddy viscosity hypothesis in 1877 (Boussinesq, 1877), stating that the ‘deviatoric Reynolds stress’ equals the ‘mean rate of strain’, or

\[-u'_i u'_j + \frac{2}{3} k \delta_{i,j} = \nu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) .\]

In other words: the correlations of the fluctuating velocity components are assumed to be equal to a Fickian diffusion term that contains the velocity gradient and a diffusion or dispersion coefficient \( \nu_t \), which is known as the eddy viscosity. This is analogous to the way that the molecular viscosity is treated in the stress-rate-of-strain relation for Newtonian fluids. The assumption is reasonable if, following the mean flow, the characteristics of turbulence and the gradients of the mean flow change slowly. This is the case for example for shear flows, channel flows and boundary layer flows (Pope, 2000).

The above hypothesis can be simplified for two-dimensional boundary layer flows, where the velocity is mainly in \( x \)-direction, while the gradients are greatest in the \( z \)-direction. These conditions hold generally in environmental applications, because the water depth is much smaller than the length or width of the water system. The hypothesis then reduces to only one dominant Reynolds stress component and reads

\[\overline{u'w'} = -\nu_t \frac{\partial u}{\partial z} .\] (1.7)

The closure problem is now transformed into the problem of finding an expression for the eddy viscosity. Prandtl suggested in 1825 to use his mixing-length hypothesis to describe the eddy viscosity. He observed from a dimensional analysis that \( \nu_t \) can be expressed as product of a length-scale of turbulent eddies \( l \) and a velocity scale \( U \). He chose a velocity scale which is equal to the velocity changes over a distance equal to the typical eddy size (Prandtl, 1825):

\[U = l \frac{\partial u}{\partial z},\]
\[\nu_t = l U = l^2 \frac{\partial u}{\partial z} .\]

Alternatively, the eddy viscosity hypothesis can be derived from the second-order Reynolds stress model (Canuto et al., 2001). These RSM equations can be simplified for boundary layer applications and reduce to Equation 1.7. This method additionally provides an expression for the eddy viscosity:

\[\nu_t = c_\mu k^{1/2} l,\] (1.8)

where \( c_\mu \) is a stability function, which depends on stratification. \( k \) is the turbulent kinetic energy, which was introduced in Equation 1.5, and \( l \) is a length-scale of turbulence. The term \( k^{1/2} \) has the dimension of a velocity scale so that Equation 1.8 can also be regarded as a form of the mixing-length hypothesis.

A similar method can be used to close the correlations of density and velocity fluctuations. This leads to an expression which involves an eddy diffusivity \( D_t \) and a mean density gradient

\[\overline{u'_i \rho'} = -D_t \frac{\partial \rho}{\partial x_i} .\] (1.9)

The dominant correlation for boundary layer applications is \( \overline{w' \rho'} \).

The eddy diffusivity \( D_t \) has a similar form to the eddy viscosity:

\[D_t = \frac{\nu_t}{\sigma_\rho} = \frac{c_\mu k^{1/2} l}{\sigma_\rho},\] (1.10)

where \( \sigma_\rho \) is the Prandtl-Schmidt number that relates the eddy viscosity to the eddy diffusivity.

The turbulent kinetic energy \( k \) and length-scale \( l \) are still unknown quantities. Both variables can be closed by either an algebraic equation or a differential equation. Three types of models are used in practice (Burchard, 2002).
1. zero-equation models:
These are also called algebraic viscosity models. In this type of model both \( k \) and \( l \) are calculated by using an algebraic equation. The easiest zero-equation models are based on a constant eddy viscosity. In more advanced versions TKE is calculated from local equilibrium between production and dissipation, where dissipation is determined from an equation for a macro length-scale \( l \). For well known classes of flows, including open channel flows, the specification of \( l \) is described by many authors and the mixing-length model yields quite accurate results.

2. one-equation models:
TKE is calculated by using a transport equation. The rate of dissipation in this equation is again closed by an algebraic equation for a macro length-scale.

3. two-equation models:
Both variables are calculated by using transport equations.

This thesis uses the class of two-equation models. These models will be presented in Chapter 2.

### 1.4. Near-bed flow

Many environmental flows are shallow water flows which are affected by bed friction. The near-bed region is an area where the velocity changes quickly in the vertical direction. This requires a high vertical resolution in numerical modelling, which is generally not feasible for simulations of large domains. The area closest to the bed is therefore not resolved, but modelled by using the assumptions that are presented below.

We introduce dimensionless wall coordinates to simplify the equations for near wall flows. In the following it is assumed that the flow is predominantly in the \( x \)-direction. The transformation to dimensionless variables reads

\[
\begin{align*}
\zeta^+ &= \frac{z u_*}{\nu}, \\
u^+ &= \frac{u}{u_*},
\end{align*}
\]

where \( u_* \) is the shear velocity which is defined as

\[
u_* = \left( \frac{|\tau|}{\rho} \right)^{1/2} \]

The shear velocity is a frequently used parametrisation of the shear stress \( \tau \) along the boundary. This shear stress can be decomposed into a viscous and a turbulent part according to

\[
\tau = -\rho \nu \frac{\partial u}{\partial z} + \rho u' w',
\]

The near-bed region can be divided into several layers according to the dominant contribution to the shear stress, see Figure 3a. The viscous effects dominate in the viscous sublayer \((z^+ < 5)\) and the shear stress follows from the molecular viscosity \( \tau = -\rho \nu \frac{\partial u}{\partial z} \). The size of the ‘roughness determining elements’, such as the ripples and small dunes on the bed, is typically larger than the thickness of this layer. The numerical modelling of the viscous sublayer would therefore require grid cells that are smaller than the size of these elements. Such high resolution is not feasible for large domains and the viscous sublayer is therefore not resolved.

The turbulent effects dominate in the inner layer \((30 < z^+ < 100)\) and the shear stress is described by \( \tau = \rho u' w' \). The correlation of fluctuating components is closed by the eddy viscosity hypothesis and mixing-length hypothesis. The mixing-length close to the boundary can be closed by the law of the wall. This law states that the length-scale of turbulent eddies near the bed is limited by the distance to the bed according to \( l = \kappa z \), where \( \kappa \) is the Von Kármán constant with a value of 0.4. The shear stress then reads

\[
\tau = \rho u' w' = \rho \nu t \frac{\partial u}{\partial z} = \rho \left( \kappa z \frac{\partial u}{\partial z} \right)^2.
\]
The classic logarithmic velocity profile follows from this expression if it is assumed that the shear stress is constant in the vertical direction. This approximation holds approximately in the inner layer. The velocity profile in the inner layer reads:

\[ u^+ = \frac{1}{\kappa} \ln(z^+) + B. \]  

(1.12)

A value of \( B = 5.5 \) is found empirically for boundary layers and pipe flow. Nezu and Rodi (1986) find that \( B = 5.29 \) applies for the inner layer in open channel flow and find that this profile holds to up to 20% of the water depth.

Two terms in Equation 1.12 have not been defined properly: the meaning of the term ‘distance to the bed’ and the way in which the roughness of the bed is incorporated in the velocity profile. These two subjects will be discussed below.

The distance to the bed is a difficult notion, because the bed level changes strongly from place to place and in time due to moving ripples and dunes. As these ripples and dunes are not resolved by the model, a less variable definition of the bed level is used. Hinze (1975) defines the bed level \( z = 0 \) as the average of the height of the roughness determining elements, see Figure 3b. This level is in the inner layer so that he suggests to assume a logarithmic velocity profile of the form:

\[ u^+(z^+) = \frac{1}{\kappa} \ln(z^+ + k^+_e) - \Delta u^+ + B. \]

This velocity profile equals Equation 1.12 with a shift in the \( z \) direction to include the net effect of the roughness determining elements on the velocity. So this shift parametrises the effect of the bed roughness.

Based on various observations Hinze (1975) locates the origin of the logarithmic profile (i.e. such that \( u^+(z^+) = 0 \)) at \( z^+ = -k^+_e \), where \( k_e \) is some roughness parameter, and defines

\[ \Delta u^+ = \frac{1}{\kappa} \ln(k^+_e) - 0.4 \]

and \( B = 4.9 \).

The roughness height is generally not parametrised by \( k_e \), but by a roughness height \( z_0 \). This roughness height is defined in terms of the Nikuradse height \( k_s \). Hinze (1975) uses the following relations between these three roughness-related variables on a rough bed:

\[ z_0 = \frac{k_s}{30} = \frac{k_e}{9}. \]

The near-bed velocity profile can then be written in normal coordinates as:

\[ \frac{u(z)}{u^*} = \frac{1}{\kappa} \ln \left( 8.78 + \frac{29.3z}{k_s} \right) \approx \frac{1}{\kappa} \ln \left( 9 + \frac{z}{z_0} \right). \]

(1.13)

The velocity at the level \( z = 0 \) is thus \( u(0) = \frac{u^*}{\kappa} \ln(9) \).

Most authors and numerical models use other definitions of the bed level. A popular choice is to define \( z = 0 \) in such a way that the logarithmic velocity profile reduces to

\[ \frac{u(z)}{u^*} = \frac{1}{\kappa} \ln \left( \frac{z}{z_0} \right), \]

and lies a distance \( 9z_0 \) below the adopted definition. This definition is not favourable, because the velocity is negative for \( z \in (0, z_0) \) and undefined in \( z = 0 \) itself. Moreover, this velocity profile is not well approximated in the numerical simulation, see Appendix B.3.

Another frequently used assumption is to set \( z = 0 \) such that \( u(0) = 0 \), which lies a distance \( 8z_0 \) below the definition of Equation 1.13 that is adopted here.
1.5. Turbulence models in this research

Turbulent variations of the flow range from motions on a large scale to motions on a very small scale. Current models for environmental applications cannot resolve turbulence up to such small scales, because of limited computational power. It is therefore that parametrisations of turbulence are being used. The process of Reynolds-averaging leads to equations for the mean flow, which contain a Reynolds stress term that needs to be parametrised in terms of mean flow properties. This research uses the eddy viscosity hypothesis to parametrise the Reynolds stress and a roughness coefficient to parametrise the effect of small-scale bed topography on the flow.

The eddy viscosity is parametrised by two variables: the turbulent kinetic energy and a length-scale of turbulence. We will use two transport equations to calculate these two variables in terms of mean flow quantities. The transport equations will be introduced in the next chapter.
Two-equation models

The theory of turbulence modelling in the previous chapter has introduced the concept of the eddy viscosity to parametrise the effect of turbulence on the mean flow. This eddy viscosity needs to be expressed in terms of mean flow properties in order to capture some of the complex dependencies of turbulence on the flow. Two-equation models are a popular way of capturing some of such complex dependencies, but still be sufficiently simple to solve in a limited amount of computational time. Two-equation models consist of transport equations for turbulent kinetic energy $k$ and for a length-scale variable $l$ to determine the eddy viscosity according to

$$\nu_t = c_\mu k^{1/2}l.$$ 

There exists consensus on the form of the TKE equation (Mellor and Yamada, 1982), but the form of the length-scale equation is subject of discussion. Almost never is the length-scale equation used as an equation for $l$ itself. Rather, the equation uses a variable which is related to the length-scale. We will use the $k - \varepsilon$ model of Rodi (1993) and transform this model to a $k - \omega$ and $k - \tau$ model which are mathematically identical to this $k - \varepsilon$ model. The $k - \varepsilon$ model is chosen because it is a widely used model. The $k - \omega$ model is a popular alternative to the $k - \varepsilon$ model. The transformed version of the $k - \omega$ model differs from the popular version of the model by Wilcox (1993), but it is still possible to comment on the suitability of $\omega$ as a variable for the numerical accuracy of the turbulence model. The $k - \tau$ model has not been used extensively, but is conceptually promising. The linear profile of $\tau$ near frictional boundaries is expected to be an advantage to the numerical accuracy.

The equations for $k$, $\varepsilon$, $\omega$ and $\tau$ will be presented in Sections 2.1 and 2.2. A general length-scale (GLS) model will also be presented in Section 2.2 to highlight the similarities, but also the differences between different two-equation models. The equations contain a number of coefficients, the values of which will be presented in Section 2.3. The boundary conditions of the models will be given in Section 2.4.

2.1. TKE equation

An equation for TKE was already derived from the Reynolds averaged Navier-Stokes equations in Section 1.2. This equation still contains some unknown correlations of turbulent fluctuations, which require closure assumptions before the equation can be used. The closure procedure is explained by Mohammadi and Pironneau (1994).
The closed equation reads

\[
\frac{Dk}{Dt} = \frac{\partial}{\partial x_j} \left( \left( \nu + \nu_t \sigma_k \right) \frac{\partial k}{\partial x_j} \right) + \nu_t M^2 - \frac{\nu_t}{\sigma_k} N^2 - \varepsilon,
\]

(2.1)

where \( D_k \) represents viscous and turbulent transport, \( P_k \) and \( B_k \) are production by shear and buoyancy respectively and \( \varepsilon \) is dissipation. \( \sigma_k \) is the Schmidt number that relates the eddy viscosity to the eddy diffusivity of TKE and is usually a constant \( \sigma_k = 1 \). Moreover

\[
M^2 = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \frac{\nu_t}{\nu} \delta_{ij} \frac{\partial u_i}{\partial x_j},
\]

\[
N^2 = -\frac{g}{\rho_0} \frac{\partial \rho}{\partial z},
\]

\( N \) is also called the Brunt-Väisälä or buoyancy frequency. The variables \( M \) and \( N \) contain the forcing of the turbulence models by the flow and stratification: \( M \) contains the forcing by the velocity shear and \( N \) the forcing by vertical density gradients. Another possible forcing of the turbulence models comes from the boundary conditions.

The energy dissipation rate \( \varepsilon \) is related to the length-scale which is calculated in the second transport equation.

### 2.2. Length-scale equation

The appropriate equation for the length-scale is subject of debate and as a result several different alternatives are available. The debate often features a preference for a different variable that is related to the length-scale, such as \( \varepsilon \) or \( \omega \), which will be defined below. However, these variables can be transformed into one-another and the discussion could equally well be on the question which terms should be included in the equations. The several alternatives take a similar form of the local production and dissipation terms, but take different diffusive terms. We will first present the \( k - \varepsilon \) model of Rodi (1993) and the transformations to the \( k - \omega \) model and \( k - \tau \) model. We will then return to the matter of explaining the differences between the several alternative two-equation models when discussing the GLS model.

All length-scale related variables are proportional to \( k^m l^n \), where \( m \) and \( n \) can be chosen arbitrarily as long as \( n \neq 0 \). One popular variable for the length-scale equation is \( \varepsilon \), which is the dissipation of TKE. This can be related to a macro length-scale of turbulence by using the energy spectrum of Equation 1.6. The relation is then (Burchard, 2002)

\[
\varepsilon = \frac{c_{\mu}^{3/4} k^{3/2}}{l}.
\]

(2.2)

Other choices for the length-scale variable are \( \omega \), which is a frequency of turbulent eddies, and \( \tau \), which is a time-scale of turbulence. They are defined as

\[
\omega = \frac{1}{c_{\mu} k} = \frac{1}{c_{\mu}^{1/4} k^{1/2}}
\]

(2.3)

\[
\tau = \frac{k}{\varepsilon} = \frac{l}{c_{\mu}^{3/4} k^{1/2}}.
\]

(2.4)

The definition of \( \omega \) uses a scaling by \( c_{\mu} \) true to the notation of Wilcox (e.g. Wilcox (1993)) who has developed the contemporary variants of the \( k - \omega \) model.

The eddy viscosity then equals

\[
\nu_t = c_{\mu} \frac{k^2}{\varepsilon} = \frac{k}{\omega} = c_{\mu} k \tau.
\]
2.2. Length-scale equation

2.2.1. Rate of dissipation \( \varepsilon \)

The rate of dissipation of TKE, \( \varepsilon \), is the most popular choice for the length-scale equation. The version of the model by Rodi (1993) is commonly used and reads

\[
\frac{D\varepsilon}{Dt} = \frac{\partial}{\partial x_j} \left( \frac{\nu + \nu_t}{\sigma_{\varepsilon}} \frac{\partial \varepsilon}{\partial x_j} \right) + \frac{\varepsilon}{k} c_{\varepsilon 1} \nu_t M^2 - \frac{\varepsilon}{k} \frac{\nu_t}{\sigma_{\rho}} N^2 - \frac{\varepsilon^2}{c_{\varepsilon 2}} \frac{\tau}{k},
\]

with the following values of the coefficients:

\[
c_{\varepsilon 1} = 1.44, \quad c_{\varepsilon 2} = 1.92 \quad \text{and} \quad \sigma_{\varepsilon} = 1.3.
\]

The appropriate value of \( c_{\varepsilon 3} \) is subject of discussion and is presented in Section 2.3.

2.2.2. Turbulence time-scale \( \tau \)

The \( k - \tau \) model is derived by Speziale et al. (1992) as a transformation of the \( \varepsilon \)-equation, but has not been used for environmental applications. The variable \( \tau \) models a typical time-scale of turbulent eddies. The equation reads

\[
\frac{D\tau}{Dt} = \frac{\partial}{\partial x_j} \left( \frac{\nu + \nu_t}{\sigma_{\tau}} \frac{\partial \tau}{\partial x_j} \right) + \frac{\tau}{k} c_{\tau 1} \nu_t M^2 - \frac{\tau}{k} \frac{\nu_t}{\sigma_{\rho}} N^2 - \frac{\tau^2}{c_{\tau 2}} \frac{\varepsilon}{k} \frac{\nu_t}{\sigma_{\varepsilon}} \frac{\partial \varepsilon}{\partial x_j} \left( \frac{1}{\sigma_{\varepsilon}} \right),
\]

The derivation of the \( k - \tau \) model is given in Appendix A.3. This model deviates from the equation of Speziale et al. (1992) at a few points, because they used a different version of the \( k - \varepsilon \) model to derive their \( k - \tau \) model. The most important difference is that they do not include buoyancy in their model. No versions of the \( k - \tau \) model with buoyancy effects have been published previously.

The coefficients of the \( k - \tau \) model are

\[
c_{\tau 1} = 1 - c_{\varepsilon 1} = -0.92, \\
c_{\tau 2} = 1 - c_{\varepsilon 2} = -0.44, \\
c_{\tau 3} = 1 - c_{\varepsilon 3}.
\]

The signs of the coefficients are so that the ‘production’ term \( P_{\tau} \) actually acts as sink of \( \tau \). This can be explained by realising that production of dissipation \( \varepsilon \) results in a faster dissipation of turbulent eddies and therefore a smaller time-scale \( \tau \) of turbulence. Even though \( P_{\tau} \) acts as a sink, it will still be called a production term because of the parallels with the \( \varepsilon \)-equation. Likewise the ‘dissipation’ term \( \varepsilon_{\tau} \) is a source of \( \tau \).

2.2.3. Turbulence frequency \( \omega \)

The idea for modelling a turbulence frequency \( \omega \) goes back to Kolmogorov in 1942. His formulation of the \( \omega \)-equation was probably based on dimensional analysis, rather than derivation from a conservation equation (Warner et al., 2005). The contemporary version is developed by Wilcox (1993) and Umlauf and Burchard (2003), who have added a buoyancy term to the equation.
The formulation by Umlauf and Burchard (2003) is

\[ \frac{D\omega}{Dt} = \frac{\partial}{\partial x_j} \left( \left( \nu + \frac{\nu_t}{\sigma_\omega} \right) \frac{\partial \omega}{\partial x_j} \right) + \frac{\omega}{k} \left( c_{\omega_1} \nu_t M^2 - c_{\omega_3} \frac{\nu_t}{\sigma_p} N^2 - c_{\omega_2} \omega k \right). \] (2.7)

Alternatively, the \( \omega \)-equation can be derived as a transformation of the \( \varepsilon \)-equation. The equation then reads

\[ \frac{D\omega}{Dt} = \frac{\partial}{\partial x_j} \left( \left( \nu + \frac{\nu_t}{\sigma_\omega} \right) \frac{\partial \omega}{\partial x_j} \right) + \frac{\omega}{k} \left( c_{\omega_1} \nu_t M^2 - c_{\omega_3} \frac{\nu_t}{\sigma_p} N^2 - c_{\omega_2} \omega^2 \right) \]

\[ + \frac{2}{k} \left( \nu + \frac{\nu_t}{\sigma_\omega} \right) \frac{\partial \omega}{\partial x_i} \frac{\partial k}{\partial x_i} - \frac{\omega}{k} \frac{\partial}{\partial x_j} \left( \left( \frac{1}{\sigma_\varepsilon} - \frac{1}{\sigma_k} \right) \nu_t \frac{\partial k}{\partial x_j} \right). \] (2.8)

The derivation of this equation is given in Appendix A.2.

The latter form of the equation will be used in this research. This version of the \( k - \omega \) model adds a cross-diffusion term, \( D_{k\omega} \), and a term involving diffusion of TKE, \( D_{kk} \), to Equation 2.7. It is subject of the discussion whether the additional diffusion terms should be included. This discussion will be continued below in Section 2.2.4.

The values of the coefficient also differ between versions. Table 2.1 presents two sets of values; one that results from the transformation of the \( k - \varepsilon \) model and one used in the \( k - \omega \) model of Wilcox (1993).

<table>
<thead>
<tr>
<th>Transformed from ( \varepsilon )-equation</th>
<th>( \sigma_k )</th>
<th>( \sigma_\omega )</th>
<th>( c_{\omega_1} )</th>
<th>( c_{\omega_2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wilcox (1993)</td>
<td>1.0</td>
<td>1.3</td>
<td>0.44</td>
<td>0.083</td>
</tr>
<tr>
<td>Wilcox (1993)</td>
<td>2.0</td>
<td>2.0</td>
<td>0.56</td>
<td>0.083</td>
</tr>
</tbody>
</table>

Table 2.1: Two sets of coefficients of the \( \omega \)-equation.

2.2.4. General length-scale model \( \psi \)

The idea of formulating a model for a general length-scale variable of the form \( k^m l^n \) with arbitrary choice for \( m \) and \( n \) was first suggested by Launder and Spalding (1974). This model is called the general length-scale (GLS) model by Umlauf and Burchard (2003), who have developed an automatic calibration procedure for the model. The general length-scale variable is called \( \psi \) and is defined as

\[ \psi = (c_\psi)^p k^m l^n \]

Table 2.2 shows how certain choices of \( p, m \) and \( n \) reduce the GLS model to some other published length-scale models.

<table>
<thead>
<tr>
<th>( \psi )</th>
<th>Two-equation model by</th>
<th>( p )</th>
<th>( m )</th>
<th>( n )</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \varepsilon )</td>
<td>Rodi (1993)</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>( \tau )</td>
<td>Speziale et al. (1992)</td>
<td>-2</td>
<td>2</td>
<td>-1</td>
<td>GLS from differs from Speziale et al. (1992)</td>
</tr>
<tr>
<td>( \omega )</td>
<td>Wilcox (1993)</td>
<td>-1</td>
<td>2</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>( k\tau )</td>
<td>Zeierman and Wolfshtein (1986)</td>
<td>-1</td>
<td>2</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>( kl )</td>
<td>Mellor and Yamada (1982)</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>GLS from differs from Mellor and Yamada (1982)</td>
</tr>
</tbody>
</table>

Table 2.2: choices of \( p, m, n \) for some well-known length-scale equations.
The general form of the transport equation for $\psi$ is

$$
\frac{D\psi}{Dt} = \frac{\partial}{\partial x_j} \left( \frac{\nu}{\sigma_\psi} \frac{\partial \psi}{\partial x_j} \right) + \frac{\psi}{k} c_\psi \frac{\nu}{\sigma} N^2 - \frac{\psi}{k} c_\psi^2 \varepsilon - B \psi - c_\psi \psi.
$$

(2.9)

The model contains several parameters that need to be calibrated. These parameters are $(c_\mu)^p$, $\sigma_k$, $\sigma_\psi$, $c_\psi^1$, $c_\psi^2$, $c_\psi^3$. Moreover, the Schmidt number $\sigma_k$ in the $k$-equation and the Prandtl-Schmidt number $\sigma_\rho$ are unknown. Umlauf and Burchard (2003) describe the possibility of adding $m$ and $n$ to this list and so calibrate the modelled variable itself. This is called polymorphism.

The polymorphism in the GLS model is not the same as a transformation of the model. To illustrate this we again compare the $k - \varepsilon$ model with the two presented versions of the $k - \omega$ model. The $k - \varepsilon$ model and the $k - \omega$ model of Equation 2.7 are polymorphisms of the GLS model, but not mathematical transformations. The converse is true for the $k - \varepsilon$ model and the $k - \omega$ model of Equation 2.8.

Similar differences between the GLS polymorphism version and the transformed version hold for all choices of the length-scale variable; the transformed version contains one or more additional diffusive terms. These diffusive terms are central to the debate on which two-equation turbulence model is best. A good summary of this debate is provided by Warner et al. (2005). In light of this debate, Kantha and Carniel (in press) respond to the GLS model by proposing a similar model, but now with the addition of one diffusive term for certain choices of $m$ and $n$. This model is called the universal length-scale (ULS) model by Warner et al. (2005).

There is no clear theoretical or practical preference for one particular model and the performance of the turbulence model depends as much on the values of the coefficients, choices for stability functions (see Section 2.3) or wall functions (see below) and, as will be shown in this research, the numerical implementation.

The exclusion of the additional diffusive terms in the GLS model has implications on the stability of the turbulence model for choices of the length-scale that use a positive value of $n$, which is for example the case for $\psi = \tau$. The GLS model needs so called wall functions to guarantee the stability. This is not needed in the ULS model.

### 2.3. Coefficients

The two-equation turbulence models can be tuned with 7 coefficients: $\sigma_k$, $\sigma_\psi$, $c_1$, $c_2$, $c_3$, $c_\mu$ and $\sigma_\rho$, where the last three of these coefficients may depend on stratification. Umlauf and Burchard (2003) and Burchard (2002) provide an overview of experimental and theoretical results on which these parameters may be calibrated.

The parameter values that are used in this study are summarised in Table 2.3. The values are based on Rodi (1993) and Deltares (2014). We will provide a brief comment on the inconsistency of these parameter values and on the value of the buoyancy-related variable $c_3$ below.

<table>
<thead>
<tr>
<th></th>
<th>$k - \varepsilon$</th>
<th>$k - \tau$</th>
<th>$k - \omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_1$</td>
<td>1.44</td>
<td>-0.44</td>
<td>0.44</td>
</tr>
<tr>
<td>$c_2$</td>
<td>1.92</td>
<td>-0.92</td>
<td>0.92</td>
</tr>
<tr>
<td>$c_3$, stable</td>
<td>0</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$c_3$, unstable</td>
<td>1.44</td>
<td>-0.44</td>
<td>0.44</td>
</tr>
<tr>
<td>$c_\mu$</td>
<td>0.09</td>
<td>0.09</td>
<td>0.09</td>
</tr>
<tr>
<td>$\sigma_\rho$</td>
<td>0.7</td>
<td>0.7</td>
<td>0.7</td>
</tr>
<tr>
<td>$\sigma_k$</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$\sigma_\psi$</td>
<td>1.3</td>
<td>1.3</td>
<td>1.3</td>
</tr>
</tbody>
</table>

Table 2.3: Parameter values for the turbulence models.
The parameter values such as mentioned in the table are inconsistent with the assumption of a logarithmic velocity profile near the boundary. This inconsistency can be expressed in a so called compatibility relation (Umlauf, 2001). A new type of derivation of this relation is given in Appendix A.4. The compatibility relation reads

\[ \sqrt{c_{\mu}} = \frac{\kappa^2}{\sigma_\varepsilon (c_2 - c_1)}. \]  

(2.10)

The substitution of the values yields 0.3 on the left-hand side and 0.27 on the right-hand side; the values are not consistent with this condition.

Abid and Speziale (1993) recommended that "this constraint should be made use of more carefully in the future formulation of second-order models". However, this appeal did not lead to a revision of the \( k - \varepsilon \) model. The version of the \( k - \omega \) model by Wilcox (1988) does satisfy the compatibility relation.

The effects of density stratification are contained within the three parameters \( c_{\mu}, \sigma_\rho \) and \( c_3 \). The value of these coefficients is debated in literature. There is a multitude of damping functions or stability functions that relate \( c_{\mu} \) and \( \sigma_\rho \) to the Richardson number, \( Ri = \frac{N^2}{M^2} \), or \( N^2 \) and \( M^2 \) separately, see e.g. Burchard and Bolding (2001) or Umlauf et al. (2007) for an overview of some of these functions. Stability functions are not used in this research conform to the implementation in Delft 3D-FLOW.

The value of the parameter \( c_3 \) is assigned different values for stable stratification and unstable stratification. The values of \( c_3 \) are not determined directly from measurements, but follow from a combination of measurements in stratified flows and the values for \( \sigma_\rho \) and \( c_{\mu} \) (Umlauf, 2001). The value of \( c_3 \) in stably stratified flows is determined by the critical Richardson number. This number expresses the threshold above which all turbulence is destroyed by buoyancy in local equilibrium flows. These are flows in which the diffusive terms of the turbulence models are negligible. The critical Richardson number can be expressed in terms of the model parameters and reads

\[ Ri_c = \frac{N^2}{M^2} = \sigma_\rho \frac{c_{r1} - c_{r2}}{c_{r3} - c_{r2}}. \]

The derivation is given in Appendix D.2. The critical Richardson number is measured and simulated in LES and DNS and should be between 0.13 and 0.25, although some authors find values of \( Ri_c = O(1) \) (Gerz and Schumann, 1995). The present model settings yield a value \( Ri_c = 0.175 \), which is within the measured range.

The value \( c_{\varepsilon 3} = 1 \) is chosen for unstable stratification by Burchard and Petersen (1999) and Burchard and Bolding (2001). A value of \( c_{\varepsilon 3} = c_{\varepsilon 1} = 1.44 \) is used in Delft 3D-FLOW (Deltares, 2014). In general, however, the modelling of unstable stratification is seen as a weak point of two-equation models and needs further testing (Warner et al., 2005). It is considered a weak point, because the essential physics is missing; unstable stratification is a convective process, but is modelled by dispersive and local terms in the turbulence model.

### 2.4. Boundary conditions

The boundary conditions of the turbulence models at the bed and the surface will be presented in this section. These two boundary conditions are sufficient, because the models will only be used in the vertical dimension. This section focusses on the boundary condition at the bed. The boundary condition at the free surface is addressed in short at the end of the section. We will see that the the equations for \( k \) and \( \tau \) have natural boundary conditions, while the equations for \( \varepsilon \) and \( \omega \) do not. Several possibilities for these last two models are therefore discussed.

The TKE has a natural value of \( k = 0 \) at the bed, because the mean and fluctuating flow velocity reduce to zero at the bed and \( k \) is defined as the correlation of velocity fluctuations. The actual value of TKE at the level \( z = 0 \) however is unequal to zero, because \( z = 0 \) is not located exactly at the bed, see Section 1.4. The boundary condition for \( k \) is derived from the assumption that production and dissipation of TKE are in balance at \( z = 0 \). This assumption reads

\[ \nu_t M^2 = \varepsilon. \]
This can be used to derive the boundary condition for $k$ by assuming that the logarithmic velocity profile of Equation 1.13 holds at the bed and by using the law of the wall that was introduced in Section 1.4 and reads $l = \kappa(z + 9z_0)$. We then find

$$M^2|_{z=0} = \left(\frac{\partial u}{\partial z}\right)^2|_{z=0} = \left(\frac{u_\ast}{9\kappa z_0}\right)^2$$

$$\nu_t|_{z=0} = c_\mu \frac{k^2}{\varepsilon}|_{z=0}$$

$$\varepsilon|_{z=0} = c_{3/4} k^{3/2} \frac{\kappa}{l}|_{z=0} = c_{3/4} k^{3/2} \frac{\kappa}{9\kappa z_0},$$

and the boundary condition for $k$ becomes

$$k|_{z=0} = \frac{u_\ast^2}{\sqrt{c_\mu}}.$$ (2.11)

The rate of dissipation $\varepsilon$ does not have a natural boundary condition at the bed, because of its hyperbolic nature, so that $\varepsilon \to \infty$ at the bed. However, a Dirichlet boundary condition can still be prescribed at $z = 0$. This is true because of two reasons. Firstly, $z = 0$ is not situated at the bed so that $\varepsilon$ has a large, but finite value at $z = 0$. Secondly, $z = 0$ is defined in the inner layer (see Section 1.4). The flow has a high Reynolds number in this layer so that the $k - \varepsilon$ model is valid; corrections would be needed for low Reynolds number flows. The latter condition ensures that the definition of $\varepsilon$ in terms of $l$ is still valid. The Dirichlet condition follows from the definition of $\varepsilon$ in Equation 2.2 and the above assumptions:

$$\varepsilon|_{z=0} = \frac{|u_\ast|^3}{9\kappa z_0}.$$ (2.12)

The large gradient of $\varepsilon$ near the bed is badly approximated in the numerical simulation. It is therefore more accurate to prescribe a gradient near the bed than to prescribe the actual value (Burchard and Petersen, 1999). A Neumann formulation is therefore preferred. The Neumann condition is derived by taking the derivative of $\varepsilon$ near the bed and evaluating this derivative at $z = \frac{1}{2} \Delta z$. The condition is evaluated at this level, because this is where the condition is implemented in the numerical simulation. The Neumann condition reads

$$\frac{\partial \varepsilon}{\partial z} \bigg|_{z=\frac{1}{2} \Delta z} = - \frac{(c_\mu)^{3/4} k^{3/2}}{\kappa(9z_0 + \frac{1}{2} \Delta z)^{3/2}}$$

$$\approx - \frac{|u_\ast|^3}{\kappa(9z_0 + \frac{1}{2} \Delta z)^{3/2}}.$$ (2.13)

The last expression 2.14 is the most common formulation of the Neumann condition and is used in this thesis. However, formulation 2.13 is more exact as it uses $k$ at the level $z = \frac{1}{2} \Delta z$ instead of at $z = 0$.

The boundary conditions for $\omega$ follow from the transformation of the above boundary conditions;

$$\omega|_{z=0} = c_{\mu}^{-1/4} \frac{\sqrt{k}}{9\kappa z_0},$$

$$\frac{\partial \omega}{\partial z} \bigg|_{z=\frac{1}{2} \Delta z} = c_{\mu}^{-1/4} \frac{\sqrt{k}}{\kappa(9z_0 + \frac{1}{2} \Delta z)^{3/2}}.$$ (2.16)

Again the Neumann condition is more accurate than the Dirichlet condition and we will use the Neumann condition.

The value of $\tau$ at the bed is zero and its gradient of $\tau$ is linear near the bed and therefore accurately approximated in the numerical simulation. It is therefore not necessary to use a Neumann condition for $\tau$ and a Dirichlet
condition for $\tau$ will be used in this research. Both types of boundary conditions are given here for completeness.

\begin{align}
\tau|_{z=0} &= \frac{\kappa}{\mu^{3/4} \sqrt{k}} 9 z_0, \\
\frac{\partial \tau}{\partial z} \bigg|_{z=\frac{1}{2} \Delta z} &= \frac{\kappa}{\mu^{3/4} \sqrt{k}} 
\end{align}

(2.17) (2.18)

The same boundary conditions are being used at the surface. A separate roughness value $z_0$ is used at the surface for this purpose. This value is zero in this thesis.

Throughout this thesis we will use the Neumann conditions for the $k - \varepsilon$ and $k - \omega$ models and the Dirichlet condition for the $k - \tau$ model, unless it is mentioned otherwise. Some calculations have been done with the Dirichlet condition for the $k - \varepsilon$ model, in which case this is mentioned specifically.

The three turbulence models and the boundary conditions that have been introduced in this chapter are solved numerically in a 1DV model. The next chapter will therefore restrict the models to 1DV and present the numerical implementation.
This chapter treats the numerical implementation of the three turbulence models in a one-dimensional vertical model. The numerical implementation is based on a trade-off between the order of accuracy, the robustness and the computational time. This has led to a numerical implementation in which robustness is essential and the accuracy is of first-order or second-order in the case of Delft 3D-FLOW, and in fact many other models for environmental flows. Such first-order or second-order accuracy means that the numerical errors can be of significant importance on typical grids that are used for 2D and 3D modelling.

This research uses a 1DV model, but many of the concepts and results in 1DV can be transferred to 3D simulations. The turbulence models in 3D hydrostatic models for environmental flows are essentially 1DV models with the possible addition of advection of turbulent energy; the gradients of velocity, density and turbulent energy that drive the turbulence models are predominantly in the vertical direction.

The model equations in 1DV are presented in Section 3.1 together with the definition of the grid. We will then treat the discretisation method of the momentum equation in Section 3.2. Section 3.3 shows a number of methods that are used to treat the positivity and non-linearity of the turbulence models. The turbulence models are then implemented in Section 3.4.

3.1. 1DV equations and grid definition

The model used in this research is a one-dimensional model in vertical direction (1DV). This implies that all quantities are assumed to be uniform in the horizontal direction. Consequently, from the continuity equation it follows that \( w = 0 \). These assumption allow us to greatly simplify the equations. Additionally, the momentum equation in \( z \)-direction reduces to the hydrostatic pressure equation. The three momentum equations reduce to

\[
\frac{\partial u}{\partial t} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x} + \frac{\partial}{\partial z} \left( (\nu + \nu_t) \frac{\partial u}{\partial z} \right),
\]

\[
\frac{\partial v}{\partial t} = -\frac{1}{\rho_0} \frac{\partial p}{\partial y} + \frac{\partial}{\partial z} \left( (\nu + \nu_t) \frac{\partial v}{\partial z} \right),
\]

\[
\frac{\partial p}{\partial z} = -\rho g.
\]
The boundary conditions of this model are quadratic slip conditions of the form
\[
\nu \left. \frac{\partial u}{\partial z} \right|_{z=0} = u_*,b \left| u_*,b \right|,
\]
\[
\nu \left. \frac{\partial u}{\partial z} \right|_{z=h} = u_*,s \left| u_*,s \right|,
\]
where the subscripts denote the shear velocity which is due to bed shear \( b \) or surface shear \( s \).

At most one constituent is modelled in the cases treated here: either salinity or temperature. The relation between density and temperature or salinity can be approximately linear and both can be modelled by the equation
\[
\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial z} \left( \nu + \nu_t \sigma \frac{\partial \rho}{\partial z} \right).
\]
(3.4)

The equation takes no-flux conditions at the bed and surface.

The case of Lake Vlietland additionally uses a model for temperature exchange with the air and the UNESCO equation of state. The model is the same as used in Delft 3D-FLOW, see Deltares (2014). The case of estuarine flow uses a fixed density gradient in the \( x \)-direction and an advection term in the transport equation 3.4. This equation then becomes
\[
\frac{\partial \rho}{\partial t} + \nu_x \frac{\partial \rho}{\partial x} = \frac{\partial}{\partial z} \left( \nu + \nu_t \sigma \frac{\partial \rho}{\partial z} \right).
\]
(3.5)

The above equations and the three turbulence models are solved on a staggered grid such as shown in Figure 4. The unknowns \( u, v \) and \( p \) are defined in the cell centres and \( \nu_t, k \) and the length-scale variable \( \varepsilon, \omega \) or \( \tau \) are defined on the interfaces. The water depth is assumed to be constant in time. The grid can be non-equidistant, but most grids in this research are equidistant. Non-equidistant grids will be used in a part of Sections 4.2 and 4.3, where it will be mentioned specifically that non-equidistant grids are used.

The sizes of grid cells are denoted by \( \Delta z_i \) for distances between cell interfaces and \( \Delta z_{i-1/2} \) for distances between cell centres. Subscripts \( i \) denote the vertical position on the grid. Superscripts \( n \) denote the time level.

### 3.2. Discretisation of the momentum equation

The momentum equation in the \( x \)-direction, Equation 3.1, is first transformed before it is implemented according to a Hermite method (Stelling, 1995). The numerical model solves for \( \phi = \frac{\partial u}{\partial z} \) instead of \( u \). This procedure is explained below. The equation is time integrated by using the implicit Euler method
\[
\frac{u_{i+1/2}^{n+1} - u_{i+1/2}^n}{\Delta t} = \frac{1}{\Delta z_{i+1}} \left( \hat{\nu}_i^{n+1} \phi_i^{n+1} - \hat{\nu}_i^n \phi_i^n \right) = \frac{1}{\rho_0} \left( \frac{\partial p}{\partial x} \right)_{i+1/2}^n, \quad i = 0, \ldots, I - 1
\]
where the symbol $\hat{\nu}$ is used for the sum of molecular and eddy viscosity. Subtracting the equations for two neighbouring cells yields:

$$
\frac{(u_{i+1/2} - u_{i-1/2})^{n+1} - (u_{i+1/2} - u_{i-1/2})^n}{\Delta t} - \frac{1}{\Delta z_{i+1}} (\hat{\rho}_{i+1/2}^{n+1} \phi_{i+1}^{n+1} - \hat{\rho}_{i-1/2}^{n} \phi_{i}^{n+1}) \\
+ \frac{1}{\Delta z_{i}} (\hat{\rho}_{i}^{n+1} \phi_{i}^{n+1} - \hat{\rho}_{i-1}^{n} \phi_{i-1}^{n+1}) = - \frac{1}{\rho_0} \left( \frac{\partial p}{\partial x} \right)^n_{i+1/2} + \frac{1}{\rho_0} \left( \frac{\partial p}{\partial x} \right)^n_{i-1/2}.
$$

The spatial discretisation is done according to the central differences method;

$$
\phi_i = \frac{u_{i+1/2} - u_{i-1/2}}{\Delta z_{i-1/2}}.
$$

The final discretised momentum equation is

$$
\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} - \frac{1}{\Delta z_{i+1}} (\hat{\rho}_{i+1/2}^{n+1} \phi_{i+1}^{n+1} - \hat{\rho}_{i-1/2}^{n} \phi_{i}^{n+1}) + \frac{1}{\Delta z_{i}} (\hat{\rho}_{i}^{n+1} \phi_{i}^{n+1} - \hat{\rho}_{i-1}^{n} \phi_{i-1}^{n+1}) = - \frac{1}{\rho_0} \left( \frac{\partial p}{\partial x} \right)^n_{i+1/2} + \frac{1}{\rho_0} \left( \frac{\partial p}{\partial x} \right)^n_{i-1/2}.
$$

### 3.3. Linearisation, decoupling and positivity

The turbulence models form a system of two coupled non-linear equations and compute positive quantities, TKE and the length-scale variable. The techniques for treating the non-linearity and guaranteeing positivity are outlined below.

The two equations of the turbulence model are solved independently. As a result, the equations should be solved iteratively to obtain an accurate numerical approximation of the coupled system. However, if the time step is small compared to the time-scale of changes in the modelled system, the error resulting from not iterating is small; the time stepping then acts approximately as iterative solving. This is the approach that is taken in Delft 3D-FLOW and in this research.

The numerical implementation is implicit in time. This requires non-linear terms to be linearised, so that only linear terms are used in the implicit calculation. Two ways of linearising the discretised equations are used: the Picard and the Newton method. The Picard method takes a linear part of a term at the new time level, leaving the rest at the old level. For example for the term $\varepsilon^2$ in the $\varepsilon$-equation this would yield $\varepsilon^{n+1} \varepsilon^n$. The Newton method for a function $f(x)$ is defined as

$$
f(x) \approx f(x^n) + \frac{d}{dx} f (x^n + \alpha (x^{n+1} - x^n)) \bigg|_{\alpha=0}
$$

This would result in the following linearisation of $\varepsilon^2$:

$$
\varepsilon^2 = (\varepsilon^n)^2 + \frac{d}{dx} (\varepsilon^n + \alpha (\varepsilon^{n+1} - \varepsilon^n)) \bigg|_{\alpha=0}^2
= (\varepsilon^n)^2 + 2(\varepsilon^{n+1} - \varepsilon^n) \varepsilon^n
= 2\varepsilon^n \varepsilon^{n+1} - (\varepsilon^n)^2
$$

Mohammadi and Pironneau (1994) show that the $k - \varepsilon$ model with the boundary conditions introduced in Section 2.2 has a positive solution. Such a positive solution is also a desired property in the numerical solution. Patankar (1980, p.145) stresses the importance of positivity in a footnote in his section on positivity as follows:

"For many readers, this seemingly minor topic may turn out to be the most valuable information in this book. In practical computations, it is quite common to encounter erroneous results such as negative mass fractions and negative turbulence kinetic energy. These have such a devastating effect on the rest of the calculation [...] that they must be prevented at all costs."
We will adopt a numerical method that guarantees positivity. To illustrate this method, consider the following transport equation to which a time-stepping method is applied:

\[
\frac{X^{n+1} - X^n}{\Delta t} = P_1 - S_1 + P_2 X^{n+1} - S_2 X^n + 1, \quad P_1, P_2, S_1, S_2 \geq 0. \tag{3.7}
\]

The quantity \( X \) denotes a some quantity, e.g. \( k, \varepsilon, \omega \) or \( \tau \), and \( P_1, P_2, S_1, S_2 \) are positive semi-definite scalar or matrix coefficients. The \( P \) denotes source (production) terms and the \( S \) denotes sink terms.

In order to analyse positivity we rewrite the equation to

\[
X^{n+1} = (I - \Delta t P_2 + \Delta t S_2) (X^n + \Delta t P_1 - \Delta t S_1)^{-1}. \tag{3.8}
\]

Positivity is guaranteed if both factors on the right-hand side are positive. This is generally not the case and the discretisation is altered in two ways to ensure positivity. Firstly, it is required that \( P_2 = 0 \). All sources of the system should thus be treated explicitly in time (i.e. use \( X^n \) only). Secondly, \( S_1 \) is changed according to the quasi-implicit method by Patankar (1980);

\[
S_{1,\text{new}} = S_1 (X^n)^{-1} X^{n+1}. \tag{3.9}
\]

The system now becomes

\[
\frac{X^{n+1} - X^n}{\Delta t} = P_1 - (S_2 + S_1 (X^n)^{-1}) X^{n+1}, \quad P_1, S_1, S_2 \geq 0.
\]

The new expression for \( X^{n+1} \) becomes

\[
X^{n+1} = (I + \Delta t S_1 (X^n)^{-1} \Delta t S_2) (X^n + \Delta t P_1)^{-1},
\]

which is always positive.

### 3.4. Discretisation of the turbulence models

The equations for \( k, \varepsilon, \omega \) and \( \tau \) are implemented numerically by using the above methods and first-order and second-order accurate numerical approximations. The \( k - \varepsilon \) method is discretised according to the same method as in Delft 3D-FLOW. The other turbulence models are currently not implemented in Delft 3D-FLOW.

#### 3.4.1. Discretisation of the TKE equation

The TKE equation 2.1 in 1DV reduces to

\[
\frac{\partial k}{\partial t} = \frac{\partial}{\partial z} \left( \left( \nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial z} \right) + \frac{\nu_t M^2}{\rho_k} - \frac{\nu_t N^2}{\rho_k} - \varepsilon. \tag{3.8}
\]

The diffusion, production and buoyancy terms are non-linear as \( \nu_t \) is non-linear in \( k \). The terms are linearised by taking the eddy viscosity at the old time level (Picard’s method).

The diffusion term is time-integrated according to a \( \theta \)-scheme (\( \theta \in [0, 1] \))

\[
D_{k,i}^n = \frac{1}{\Delta z_{i+1/2}} \left[ \left( \nu + \frac{\nu_t}{\sigma_k} \right)^{n+1/2} \left( \theta \frac{k_{i+1}^{n+1} - k_i^n}{\Delta z_i} + (1 - \theta) \frac{k_i^n - k_{i-1}^n}{\Delta z_i} \right) - \left( \nu + \frac{\nu_t}{\sigma_k} \right)^{n+1/2} \left( \theta \frac{k_{i+1}^{n+1} - k_i^n}{\Delta z_{i+1}} + (1 - \theta) \frac{k_i^n - k_{i+1}^n}{\Delta z_{i+1}} \right) \right], \tag{3.9}
\]
3.4. Discretisation of the turbulence models

where

\[
\nu_{t,i+1/2} = \frac{\nu_{t,i} + \nu_{t,i+1}}{2}.
\]

This discretisation is unconditionally stable for \( \theta \in [\frac{1}{2}, 1] \) and second-order accurate for \( \theta = \frac{1}{2} \). All computations use \( \theta = 1 \), in accordance with the standard setting of Delft 3D-FLOW. This setting is not the most accurate, but is certain to prevent numerical oscillations, or wiggles, from this term.

It can be verified that the discretisation of the above term with \( \theta = 1 \) satisfies the positivity criterion of Section 3.3. Consider the operator \( -D_{n,k,i}^n \) above as a matrix with elements that correspond to \( k_{i-1}, k_i \) and \( k_{i+1}, i.e. \) in the same way that it would be implemented numerically. This matrix is diagonally dominant, real, symmetric and has only non-negative elements on the diagonal. It then follows that the matrix is positive semi-definite and that \( D_{n,k,i}^n \) is negative semi-definite. So the operator \( D_{n,k,i}^n \) is an \( S_2 \) term in Equation 3.7, and positivity is guaranteed.

The discretised production term becomes

\[
P_{\varepsilon,n}^n = \nu_{t,i}^n M_k^2.
\]

The dissipation term is a sink and the buoyancy term may be a sink for TKE in the case of stable stratification and can cause \( k \) to become negative. The terms are therefore treated quasi-implicitly (see Section 3.3). The buoyancy term is a source of TKE in the case of unstable stratification and does not need the quasi-implicit method.

\[
B_{\varepsilon,n}^n = \begin{cases} 
-\frac{\nu_{t,i}^n N^2}{\sigma_p} \frac{k_n^{i+1}}{k_i^n} & \text{if } N^2 > 0; \text{ stable stratification} \\
-\frac{\nu_{t,i}^n N^2}{\sigma_p} & \text{if } N^2 < 0; \text{ unstable stratification}. 
\end{cases}
\]

\[
\varepsilon_n^i = \begin{cases} 
2\varepsilon_n^{i+1} \frac{k_n^{i+1}}{k_i^n} - \varepsilon_i^n, & k - \varepsilon \text{ model} \\
\varepsilon_n^{i+1}, & k - \omega \text{ model} \\
\frac{k_n^{i+1}}{k_i^n}, & k - \tau \text{ model.}
\end{cases}
\]

3.4.2. Discretisation of the \( \varepsilon \)-equation

The equation for \( \varepsilon \) of Equation 2.5 reduces to the following 1DV form

\[
\frac{\partial \varepsilon}{\partial t} = \frac{\partial}{\partial z} \left( \left( \nu + \frac{\nu_t}{\sigma_p} \right) \frac{\partial \varepsilon}{\partial z} \right) + \varepsilon \frac{c_{\varepsilon,1} \nu_t M^2}{k} - \frac{\varepsilon}{k} \frac{c_{\varepsilon,3} \nu_t}{\sigma_p} N^2 - \frac{c_{\varepsilon,2} \varepsilon^2}{k} - B_{\varepsilon} \varepsilon. \tag{3.10}
\]

The production and buoyancy terms \( P_{\varepsilon} \) and \( B_{\varepsilon} \) can be simplified by using \( \nu_t = c_\mu \frac{\nu^2}{k} \). The terms then become linear in \( k \) and independent of \( \varepsilon \).

The discretisation of the diffusion term is similar to the \( k \)-equation (Equation 3.9). The production is discretised according to

\[
P_{\varepsilon,n}^n = c_{\varepsilon,1} c_\mu k_n^n M_k^2.
\]
The discretisation of the buoyancy term is similar to the TKE-equation; ensuring positivity by using the quasi-implicit method

\[
B_{\varepsilon,i}^n = -c_{\varepsilon 3} \left[ \frac{k_i^n}{\varepsilon_i^n} \right] \frac{\varepsilon_i^{n+1}}{\varepsilon_i^n} \quad \text{if } c_{\varepsilon 3} N^2 > 0 \\
\frac{k_i^n}{\varepsilon_i^n} \quad \text{if } c_{\varepsilon 3} N^2 < 0.
\]

The dissipation term is non-linear and is linearised by using a Newton method, see Section 3.3. The non-linear part of the term is $\varepsilon^2$. The $k$ that appears in the term is taken at the old time level so that the $k - \varepsilon$ model equations are solved independently. The derivation of the Newton linearisation of $\varepsilon^2$ has been given above so that the term reads

\[
\varepsilon_{\varepsilon,i}^n = c_{2\varepsilon} \frac{2\varepsilon_{\varepsilon,i}^{n+1}}{k_i^n} - c_{2\varepsilon} \left( \frac{\varepsilon_{\varepsilon,i}^n}{k_i^n} \right)^2.
\]

3.4.3. Discretisation of the $\omega$-equation

The equation for $\omega$, Equation 2.8, in 1DV reduces to

\[
\frac{\partial \omega}{\partial t} = \frac{\partial}{\partial z} \left( \left( \nu + \frac{\nu_t}{\sigma_\omega} \right) \frac{\partial \omega}{\partial z} \right) - \frac{\omega}{k} \left[ \frac{\omega}{k} \frac{\nu_t}{\sigma_\omega} N^2 - c_{\omega 3} \omega^2 \right] \varepsilon_\omega \\
+ \frac{2}{k} \left( \nu + \frac{\nu_t}{\sigma_\omega} \right) \frac{\partial \omega}{\partial k} \frac{\partial k}{\partial z} - \frac{\omega}{k} \frac{\partial}{\partial z} \left( \left( \frac{1}{\sigma_\varepsilon} - \frac{1}{\sigma_k} \right) \nu_t \frac{\partial k}{\partial z} \right),
\]

where

\[
D_{k\omega} = \frac{2}{\sigma_\omega} \left( \frac{1}{\omega_i^n} \frac{\partial k}{\partial z} \right) \left\{ \omega_{i+1}^{n+1} - \omega_i^{n+1} \right\} \quad \text{if } \frac{1}{\omega_i^n} \frac{\partial k}{\partial z} |_{i} > 0 ,
\]

\[
D_{k\omega} = \frac{2}{\sigma_\omega} \left( \frac{1}{\omega_i^n} \frac{\partial k}{\partial z} \right) \left\{ \omega_{i-1}^{n+1} - \omega_i^{n+1} \right\} \quad \text{if } \frac{1}{\omega_i^n} \frac{\partial k}{\partial z} |_{i} < 0 .
\]
The molecular viscosity is neglected in this term, because it may cause numerical instabilities. The molecular viscosity is included in the $D_{kk}$ term as $\frac{\nu}{\sigma_k} \frac{\partial k}{\partial z}$. If $k$ goes to zero, then it follows from the positivity of $k$ that $\frac{\partial k}{\partial z}$ also goes to zero. However, numerically $\frac{\partial k}{\partial z}$ is not necessarily small when $k_i$ goes to zero, especially on coarse grids. The term $D_{kk}^{3.4.4.}$ can then grow to infinity. The molecular viscosity is generally small compared to the eddy viscosity, so it is neglected.

The $D_{kk}$ term can also become unstable for similar reasons as explained above. No solution to this has been found yet and therefore the $D_{kk}$ term is neglected. It is expected that this term is generally rather small because the factor $\frac{1}{\sigma_k} - \frac{1}{\sigma_k}$ in front of the term is only 0.2 with the current parameter settings. The term is unimportant in the cases that have been investigated for this research.

### 3.4.4. Discretisation of the $\tau$-equation

The equation for $\tau$, Equation 2.6, in 1DV reduces to

$$
\frac{\partial \tau}{\partial t} = \frac{\partial}{\partial z} \left( \frac{\nu}{\sigma_{\tau}} \frac{\partial \tau}{\partial z} \right) + \frac{\nu}{\sigma_{\tau}} \frac{\partial \tau}{\partial z^2} - \frac{\nu}{\sigma_{\tau}} \frac{\partial \tau}{\partial z} - \frac{\nu}{\sigma_{\tau}} \frac{\partial \tau}{\partial z} \left( \frac{1}{\sigma_{\tau}} - \frac{1}{\sigma_k} \right) \frac{\partial k}{\partial z},
$$

(3.13)

The diffusion of $\tau$, $D_{\tau}$, is again discretised according to Equation 3.9. The production and buoyancy terms are quadratic in $\tau$ and a Picard method is used to linearise the terms:

$$
P_{\tau,i} = c_{r1} c_{\mu} M^2 \frac{\partial \tau}{\partial z}^2 + c_{r2},
$$

$$
B_{\tau,i} = \begin{cases} 
-c_{r3} \frac{\nu}{\sigma_{\tau}} N^2 \tau_i \frac{\partial \tau}{\partial z} & \text{if } c_{r3} N^2 > 0 \\
-c_{r3} \frac{\nu}{\sigma_{\tau}} N^2 (\tau)^2 & \text{if } c_{r3} N^2 < 0
\end{cases}
$$

The currently used values of $c_{r3}$ for stable and unstable stratification guarantee that $c_{r3} N^2$ is positive under all conditions, because $c_{r3} < 0$ if $N^2 < 0$ and $c_{r3} > 0$ if $N^2 > 0$. The case in which it is negative is mentioned for completeness.

The $D_{\tau\tau}$ and $D_{k\tau}$ terms are discretised according to a first-order upwind scheme. This is motivated by the observation that $\tau \frac{\partial k}{\partial z}$ and $k \frac{\partial \tau}{\partial z}$ have the dimension of a velocity. The terms are discretised together to ensure that the transport in one direction:

$$
D_{\tau k,i}^n - D_{\tau k,i}^{n+1} = \frac{c_{\mu}}{\sigma_{\tau}} \left( \tau_i \frac{\partial k}{\partial z} - k_i \frac{\partial \tau}{\partial z} \right) \frac{\tau_i^{n+1} \Delta z_i}{\Delta z_i^{n+1}} \frac{k_i^{n+1} - k_i^n}{\Delta z_i},
$$

if $\tau_i \frac{\partial k}{\partial z} - k_i \frac{\partial \tau}{\partial z} > 0$,

$$
D_{\tau k,i}^n - D_{\tau k,i}^{n+1} = \frac{c_{\mu}}{\sigma_{\tau}} \left( \tau_i \frac{\partial k}{\partial z} - k_i \frac{\partial \tau}{\partial z} \right) \frac{\tau_i^{n+1} \Delta z_i}{\Delta z_i^{n+1}} \frac{k_i^{n+1} - k_i^n}{\Delta z_i},
$$

if $\tau_i \frac{\partial k}{\partial z} - k_i \frac{\partial \tau}{\partial z} < 0$.

(3.14)

where

$$
\frac{\partial k}{\partial z}_i = \frac{1}{2} \left( \frac{k_i^n - k_{i+1}^{n+1}}{\Delta z_{i+1}} + \frac{k_{i-1}^n - k_i^n}{\Delta z_i} \right),
$$

$$
\frac{\partial \tau}{\partial z}_i = \frac{1}{2} \left( \frac{\tau_i^n - \tau_{i+1}^{n+1}}{\Delta z_{i+1}} + \frac{\tau_{i-1}^n - \tau_i^n}{\Delta z_i} \right).
$$

The amount of numerical diffusion is smaller when the $D_{\tau\tau}$ and $D_{k\tau}$ are discretised together than when they are treated separately. The upwind scheme introduces numerical diffusion with numerical diffusion coefficient $D_{num}$:

$$
D_{num} = \frac{1}{2} \Delta z \left| \tau_i^n \frac{\partial k}{\partial z} - k_i^n \frac{\partial \tau}{\partial z} \right|.
$$
An alternative to (3.14) is to discretise $D_{k\tau}$ according to the first-order upwind scheme and $D_{\tau\tau}$ according to a midpoint scheme. However, this method was not stable for the Vlietland case of Section 5.1.

The molecular viscosity is neglected in the discretisation (3.14) for the same reasons as for the $k - \omega$ model. Likewise the $D_{kk}$ term is neglected.
Model properties in basic flow processes

The four cases that will be discussed in this chapter are used to analyse how the properties of the three model implementations affect the numerical accuracy. Such analysis is possible because the cases represent simple flow processes that are well-understood from measurements or previous modelling studies.

River, estuarine and coastal flows are often dominated by bed friction. We will therefore start with two cases in which bed friction governs the flows. We will consecutively treat a stationary channel flow and a tidal flow. Stratification is important for modelling the water quality of lakes and the flow and transport in estuaries. We will therefore test two basic cases of stratified flows. The first is the mixing of a stably stratified water column by wind stress. The second is the mixing of an unstably stratified water column. The cases are selected to match experiments by Price (1979) and Deardorff et al. (1969) and can be compared with the results of, amongst others, Warner et al. (2005) and Burchard and Petersen (1999) who tested the $k - \varepsilon$ and Mellor & Yamada turbulence models for these cases.

The cases are all tested for a range of grid resolutions in order to test the convergence and sensitivity to the grid resolution. The results are analysed by a number of tools. Firstly, the shape of the vertical profiles of TKE and the turbulence length-scale are used to comment on the numerical accuracy, because linear profiles are exactly represented in a numerical discretisation, whereas rapidly varying or curvy profiles require many layers before the numerical simulation is accurate. Secondly, the individual terms in the turbulence equations are analysed. This can, in some cases, help to simplify the turbulence models to a balance of fewer terms which are easier to analyse. Lastly, it is shown by Burchard and Petersen (1999) that the boundary condition for the $k - \varepsilon$ model has a great effect on the results. Several boundary conditions are therefore analysed.

4.1. Stationary uniform open channel flow

The first case is a homogeneous stationary uniform open channel flow driven by a fixed pressure gradient. As a result, the water level gradient and bed level gradient are the same. Such a flow is a simplification of a typical lowland river, see Figure 5. The simulation of the vertical profile of river flow is for example important for predicting the transport of sediments. The bed load sediment transport depends on the velocity gradient near the bed and the suspended sediment transport depends on the vertical structure of the flow. Vertical velocity profiles in rivers can also be used for studies into the spreading of a pollutant or cooling water discharge from industrial areas. The case of open channel flow additionally represents a class of bed friction dominated flows, which are also found in estuaries and along the coast. The results of this case can therefore be applied in a wide range of cases.

The average velocity in such a flow is predicted by Chézy’s law. This law describes a basic balance between a
pressure gradient and friction without resolving the vertical flow structure. The equation reads

\[ \pi = C \sqrt{h \frac{\partial \zeta}{\partial x}}, \]

\[ = \sqrt{\frac{gh \frac{\partial \zeta}{c_f \partial x}}}, \]

where \( C \) is the Chézy bed roughness coefficient (in m^{1/2}/s). Alternatively, \( c_f \) is a dimensionless friction coefficient and \( \frac{\partial \zeta}{\partial x} \) the water level gradient.

The results of this case are expressed in a dimensionless velocity \( q^* \) defined as

\[ q^* = \frac{\pi}{C \sqrt{h \frac{\partial \zeta}{\partial x}}}, \]

\[ = \sqrt{c_f \frac{\pi}{\sqrt{gh}} \frac{\partial \zeta}{\partial x}}, \]

and should be equal to unity according to Chézy’s law.

### 4.1.1. Measurements

Before presenting the results of the 1DV model, we will comment on the validity of Chézy’s law for use in 3D simulations. The Chézy or \( c_f \) roughness parameters originate from 1D and 2D horizontal modelling of rivers, seas and estuaries. The parameters are also frequently used for computations that involve the vertical dimension, because of the experience with these roughness values. However, the parameters need to be converted to a roughness height \( z_0 \), which is a suitable roughness parameter for water column simulations (i.e. 1DV, 2DV or 3D). Such conversion needs an assumption for the vertical velocity profile. The logarithmic profile is commonly used for this conversion. The expression for \( z_0 \) then reads

\[ z_0 = h \exp \left( -1 - \frac{C}{\sqrt{g}} \right), \]

\[ = h \exp \left( -1 - \frac{C}{\sqrt{c_f}} \right). \]

However, measurements by Coles (1956) and Nezu and Rodi (1986) suggest that open channel flow profiles deviate from this logarithmic velocity profile by an amount that is often parametrised by Coles’ wake law \( W(z) \).

\[ W(z) = \frac{2\Pi}{\kappa} \sin^2 \left( \frac{1}{2} \pi \frac{z}{h} \right), \]

where \( \Pi \) is an empirical parameter. Nezu and Rodi (1986) adopt a value \( \Pi = 0.2 \) for applications to river flow, but find a scatter in the measurements with \( \Pi \in [0.1, 0.25] \).
The resulting velocity profile is then

$$u(z) = \frac{u^*}{\kappa} \ln \left( \alpha + \frac{z}{z_0} \right) + u_\ast W(z). \quad (4.1)$$

From the measurements it is therefore not expected that the dimensionless velocity \( q^* \) equals unity as is stipulated by Chézy’s law, but rather

$$q^* \approx 1 + \frac{\sqrt{g}}{C\kappa} \Pi = 1 + \frac{\sqrt{\nu}}{\kappa} \Pi. \quad (4.2)$$

The derivation of Equation 4.2 from Equation 4.1 is presented in Appendix B.2.

Please note that the logarithmic profile is also not expected from the numerical 3D computation. The logarithmic profile does for example not satisfy the no-stress boundary condition that is prescribed for the velocity at the surface. The profile is also not fixed in the turbulence models.

### 4.1.2. Results

The numbers that will be used for the numerical test case are

$$\frac{\partial \zeta}{\partial x} = 5 \cdot 10^{-5},$$

$$\h = 5 \text{ m},$$

$$C' = 60 \text{ m}^{1/2} \text{s}^{-1} \text{ or } c_f = 2.8 \cdot 10^{-3},$$

where \( \frac{\partial \zeta}{\partial x} \) is the water level gradient. These dimensions are typical for average river flow conditions in the Netherlands. The grid is equidistant and the simulation time is sufficient for a steady flow to develop. The expected value of the dimensionless velocity according to Equation 4.2 is \( q^* = 1.025 \) for this set-up.

The dimensionless velocity predicted by the three turbulence models is plotted against the number of layers in Figure 6. Two types of boundary conditions for the \( k - \varepsilon \) model are included: the Dirichlet and the Neumann conditions. Some alternatives to the Dirichlet and the Neumann boundary conditions of the \( k - \varepsilon \) model are presented and tested in Appendix B.1.

![Open channel flow - layer convergence](image)

Figure 6: Dimensionless velocity \( q^* \) plotted against the number of layers for several turbulence models in the 1DV code. Note that the horizontal axis does not scale consistently with the number of layers in order to show the results for a wide range of grid resolutions.

The figure shows that all model results converge between 100 and 1000 layers. Such resolution is rarely achieved in numerical modelling studies. Instead, the domain of 10 to 100 layers is more realistic for most modelling studies. The \( k - \varepsilon \) model with Dirichlet boundary condition performs worst with a value of \( q^* \) of 1.34 at 10
layers and 1.12 at 100 layers. The Neumann boundary condition yields significantly better results with a rather more constant value of 1.05 between 10 to 100 layers. The $k - \omega$ model shows a similar trend with a value of 1.07 for 10 to 100 layers, both showing the same result of 1.02. The $k - \tau$ model shows the least sensitivity to the number of layers, with the results varying only 1% between 3 and 2000 layers.

All models eventually converge to a value of the dimensionless velocity of approximately 1.02, which is within the range of values that might be expected on the basis of the measurements by Nezu and Rodi (1986).

The results can be explained by looking at the profiles of the turbulence parameters in Figure 7. The figure shows the profiles of TKE, the length-scale rewritten to $\tau$, $\nu_t$ and $u$ of the three turbulence models at 10 layers compared to the result of the $k - \tau$ model at 2000 layers, which is nearly identical to the other models at 2000 layers. The $k - \varepsilon$ model in this figure uses Neumann boundary conditions.

The profiles of TKE simulated by all three models are similar and are already close to the converged result at 10 layers. The profiles of the calculated value of $\tau$ however differs between the three models. The $k - \tau$ model follow the converged result near the bed but deviates significantly from it near the surface. The reverse holds for the $k - \varepsilon$ model. The value of $\tau = k/\varepsilon$ at the bed in the $k - \varepsilon$ model is larger than the converged value due to the Neumann boundary condition. The value is smaller than the converged value further up in the water column, but the model performs better than the $k - \tau$ model near the surface. A similar result holds for the $k - \omega$ model. The results observed in $\tau$ carry over to the results of $\nu_t$, with the $k - \tau$ model corresponding closely to the converged result near the bed and the $k - \varepsilon$ and $k - \omega$ models only performing better than the $k - \tau$ model near the surface.

The reason for these results can be found in the shape of the profiles of $k$, $\tau$, $\varepsilon$ and $\omega$. The profiles of $\tau$, $\varepsilon$ and $\omega$ are shown in Figure 8. The profile of $k$ and $\tau$ are almost linear near the bed. Their gradients are therefore represented exactly by the numerical operators. Such exactness follows from the truncation error of a
4.1. Stationary uniform open channel flow

The numerical operator. In order to illustrate this, we calculate the truncation error of a simple first-order accurate Euler approximation of $\tau$:

$$\left( \frac{\partial \tau}{\partial z} \right)_i = \frac{\tau_{i-1} - \tau_i}{\Delta z_i}$$

The truncation error follows from substituting the Taylor series of $\tau$ around $\tau_1$ in this approximation. This Taylor series reads

$$\tau_{i-1} = \tau(z_i) - \frac{\partial \tau}{\partial z}(z_i) \Delta z_i + \frac{1}{2} \frac{\partial^2 \tau}{\partial z^2}(z_i) \Delta z_i^2 + \text{higher-order terms},$$

where the subscripts denote numerically calculated values and the suffix $(z_i)$ denotes an evaluation of the exact solution. The truncation error is the difference between the numerical and exact derivative and becomes

$$\left( \frac{\partial \tau}{\partial z} \right)_i - \frac{\partial \tau}{\partial z}(z_i) = \frac{1}{2} \frac{\partial^2 \tau}{\partial z^2}(z_i) \Delta z_i + \text{higher-order terms}.$$  

The higher-order terms also contain a combination of higher derivatives of $\tau$ and powers of $\Delta z_i$. The error becomes zero if $\tau$ is linear, because $\frac{\partial^2 \tau}{\partial z^2}$ and all higher derivatives are zero.

The profile of $\epsilon$ on the other hand behaves as $1/z$ near the bed, see Figure 8. The truncation error is then dependent on the grid size $\Delta z_i$ with a coefficient

$$\frac{1}{2} \frac{\partial^2 \epsilon}{\partial z^2} \sim \frac{1}{z^3},$$

which becomes large near the bed. The higher derivatives in the higher-order terms can even become larger near the bed than this term. A similar reasoning holds for $\omega$ which behaves as $1/z^2$ near the bed and produces an even larger truncation error. The reverse holds near the surface, where the profiles of $\epsilon$ and $\omega$ show less curvature, while the profile of $\tau$ shows more curvature.

The terms that contain the gradient of $\epsilon$, $\tau$ and $\omega$ are $D_\epsilon$, $D_\tau$, and $D_\omega$. These terms are of the same order of magnitude as the local production and dissipation terms, so that the gradients have a significant influence in the equations. An inaccurate approximation of the gradients therefore leads to an inaccurate prediction of the velocity.

The $k-\tau$ model is clearly better at predicting the average velocity and velocity profile at low grid resolution than the other two turbulence models. It must therefore be concluded that it is more important to have an accurate representation of turbulence near the bed than it is near the surface. This can be explained by considering the momentum equation for a stationary 1DV flow:

$$\frac{\partial}{\partial z} \left( \frac{\partial u}{\partial z} \right) = -\frac{1}{\rho} \frac{\partial p}{\partial x}.$$
The right-hand side is a prescribed constant pressure gradient, so that the Reynolds stress \( R = \nu_t \frac{\partial u}{\partial z} \) has a linear profile. The numerical implementation of the momentum equation ensures that such linear profile of \( R \) is reproduced exactly in the simulation. The velocity gradient is large near the bed so that a small error in the eddy viscosity near the bed must result in a significant error in the velocity gradient and the velocity. Conversely, the velocity gradient is small near the surface so that an error in the eddy viscosity has only a weak effect on the velocity.

Summarising, the \( k - \tau \) model is better than the other turbulence models at low resolution, because the profiles of \( k \) and \( \tau \) are linear and therefore exact in the numerical simulation in the area where the velocity gradient is largest.

### 4.1.3. Non-equidistant grid

Platzek et al. (2014) discuss the performance of the \( k - \varepsilon \) model for one particular type of non-equidistant grid that is frequently encountered with a z-layer model in computations with a gently sloping bed: a grid that is equidistant except for a very thin bottom layer, see Figure 9. Platzek et al. (2014) show that the velocity profile is badly reproduced on such grids and propose a solution in which the lowest two grid cells are averaged. This test will be repeated for the \( k - \tau \) model on a grid that uses a bottom cell height of 1% of the water depth and 9 cells of the same height on top, each 11% of the water depth. The solution by Platzek et al. (2014) results in a grid with the two bottom-most cells having a thickness of 6% of the depth each and 8 equidistant cells on top.

Figure 9: Small bottom cells in a 2DV model with gently sloping bed.

The accuracy of the \( k - \tau \) model for predicting the flow velocity is affected more severely than the \( k - \varepsilon \) model by such small bed cells. The results are given in Figure 10. From the figure it is clear that the turbulence model is not affected by the small bottom layer. Likewise \( \frac{\partial u}{\partial z} \) is not affected by the small bottom layer, as there are no differences in \( k \), \( \tau \) and \( \nu_t \). The errors in the velocity profile thus originate from the numerical integration procedure that transforms \( \frac{\partial u}{\partial z} \) to \( u \). The numerical integration in the bottom cell follows from the following equation:

\[
 u_{I-3/2} = u_{I-1/2} + \Delta z_{I-1/2} \left. \frac{\partial u}{\partial z} \right|_{I-1},
\]

which would be exact if \( \left. \frac{\partial u}{\partial z} \right|_{I-1} \) represents the average velocity gradient in the interval \( [I-1/2, I-3/2] \). The velocity gradient is approximately proportional to the inverse of \( z \): \( \frac{\partial u}{\partial z} \sim \frac{1}{z} \). For equidistant cells this gradient is defined in the middle of the interval, which is a reasonable approximation of the average (but not exact, see Appendix B.3). For the non-equidistant grid under consideration the gradient \( \left. \frac{\partial u}{\partial z} \right|_{I-1} \) is defined very close to the bed and is considerably larger than the average gradient.

The adjusted grid does not display these large errors for two reasons. Firstly, the great disproportionality between the cell sizes is reduced, so the that numerical velocity gradient is closer to the average velocity gradient in the cell. Secondly, the unequal cells are found one cell higher than in the original grid. The velocity gradient higher in the water column is smaller than near the bed, so that the errors in the numerical integration have less effect on the velocity profile.

Platzek et al. (2014) also suggest a change in the discretisation of the \( k - \varepsilon \) model. Such a change is not advised for the \( k - \tau \) model, because the errors in the velocity profile do not originate from the turbulence model.
4.2. Tidal flow

Tidal flow is a dynamic variant of the open channel flow discussed above. The tidal flow is so slow that the boundary layer is almost always fully developed or, in other words, the time derivatives of the turbulent quantities are small. The flow can therefore also be regarded as a quasi-stationary flow. The only exception to this is the flow around slack tide, i.e. the moment in time when the depth-averaged flow velocity is zero. The dynamics of the flow around slack tide is the topic of this section.

For certain settings of tidal flow in a straight channel De Boer and De Nijs (2006, pers. comm.) have found that the Delft 3D-FLOW implementation of the $k-\varepsilon$ model erroneously produces very little turbulence for some time after slack tide. This problem can be seen in Figure 12 between 15 and 16 hours. The figure is a reproduction of a similar figure by Uittenbogaard and Van Kester (2006, pers. comm.). It is especially clear in the profile of $\nu_i$ at 2 metres above the bed. The profile is not smooth as is expected, but shows some stagnation followed by a sharp transition after slack tide. The problem is also visible in the velocity signal, which deviates

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Figure 10: TKE, $\tau$, $\nu_i$ and $u$ for the $k-\tau$ model with 10 equidistant layers, a non-equidistant grid with small bottom layer and the non-equidistant improved grid according to Platzek et al. (2014).

Figure 11: Tidal flow consisting of a single semi-diurnal constituent with prescribed velocity amplitude.
from the sinusoidal profile after slack tide.

A correct simulation of the dynamics around slack tide is important for the transport of suspended sediment transport. Sediments tend to settle on shallow areas around slack tide, because of lack of turbulence. An overprediction of the settling rate around slack tide has profound effects on the predicted sediment transport on the long term.

We will consider an $S_2$, i.e. 12-hour period, tidal flow in a straight, infinitely wide channel. The following numbers will be used:

- $h = 10$ m
- $C = 50$ m$^{1/2}$s$^{-1}$
- $\overline{w}(t) = \cos(\omega t)$ [ms$^{-1}$]
- $\omega = 1.45 \times 10^{-4}$ s$^{-1}$
- $\Delta z = 1$ m, (i.e. 10 layers)

These results are found with a 1DV model using the boundary conditions that were implemented in Delft 3D-FLOW version 3.54.05, which are Dirichlet conditions for $k$ and $\varepsilon$ at the bed and surface. The Dirichlet condition of $\varepsilon$ at the bed is adjusted in Delft 3D-FLOW by changing the diffusive term $D_{n,\varepsilon,I-1}$ in the $\varepsilon$-equation, see Appendix B.1.

4.2.1. Problem analysis

The eddy viscosity profile after slack tide can be considered to consist of two parts: a parabolic decreasing part and a part that builds up from the bed, see Figure 13. The parabolic part is the profile that corresponds to a fully developed boundary layer flow. This parabolic eddy viscosity decreases when the flow approaches slack tide, but continues to decrease after slack tide. The increase of the eddy viscosity after slack tide takes the form of a signal that originates from the bed and then propagates upward through the water column before reaching the fully developed parabolic profile. Clearly, there is a different balance of terms in the turbulence model that governs this build-up of the eddy viscosity than that governs the fully developed flow.

For the $k - \varepsilon$ model in this case, however, the eddy viscosity only decreases after slack tide and the part that builds up from the bed is delayed. This problem is not visible when using the $k - \tau$ model. We can therefore gain understanding of this problem by comparing the terms in the TKE equation of the $k - \varepsilon$ and $k - \tau$ models.

Figure 14 shows these terms at time $t = 15.3$ h, 20 minutes after slack tide. The panel displaying $\frac{\partial k}{\partial t}$ confirms that the TKE at the bed starts to increase in the $k - \tau$ model, while it still decreases in the $k - \varepsilon$ model. The figure also shows that the dissipation in the $k - \varepsilon$ model is greater than the production and diffusive flux of TKE at the first cell interface above the bed; the lowermost point in the figure. As a result the TKE, $k_{I-1}$, and the eddy viscosity, $\nu_{I-1}$, become zero at these points and the increasing bed shear stress cannot propagate upwards to build-up the TKE and eddy viscosity profiles. This results in a flow that is not affected by bottom friction and an almost uniform flow velocity.

We need to look further back in time to trace the origin of the differences between the $k - \varepsilon$ and $k - \tau$ model that were outlined above. For example looking at the time $t = 15.2$ h, 12 minutes after slack tide, shows only minor differences between the terms in the equations of both turbulence models. Slight differences exist, but all terms have a similar shape and sign. So these small differences must be the cause of the unrealistic behaviour of the $k - \varepsilon$ model. Figure 15 illustrates this by presenting a time series of the terms in the TKE-equation one cell interface above the bed after slack tide. The production of TKE, $D_k + P_k$, starts to exceed dissipation in the $k - \tau$ model around $t = 15.1$ h, while the dissipation is just larger than the production in the $k - \varepsilon$ model. Apparently, this small excess of dissipation drives the $k - \varepsilon$ model towards another dynamic equilibrium, which is not characterised by $P_k \approx \varepsilon$, as is expected, but by $P_k = 0$ and $D_k = \varepsilon$.

The latter equilibrium of $D_k$ and $\varepsilon$ is the balance between the upward transport of TKE and dissipation. This
Figure 12: Time series of $u$, $\nu_t$, TKE and $\varepsilon$ at 0, 2, 5 and 9 meters above the bed. Adapted from (Uittenbogaard and Van Kester, 2006, pers. comm.)
Figure 13: Schematic image on the evolution of the eddy viscosity after slack tide. The eddy viscosity profile consists of two parts: one parabolic decreasing part and a part that builds up from the bed.

Figure 14: Terms in TKE equation (diffusion, production, dissipation and residual) at $t = 15.3$ h, 20 minutes after slack tide. Note that the lowest point in this plot is at one cell interface above the bed; point $I - 1$. The dissipation exceeds the production and diffusion in the $k - \varepsilon$ model, resulting in a negative $\frac{D_k}{\partial t}$.

is coherent with the explanation given above: the turbulence propagating upward from the bed is inhibited by the dissipation so that the turbulence production vanishes.

This new dynamic equilibrium is not stable for the entire tidal period. The velocity profile in the new dynamic equilibrium is uniform in all but the bottom layer; the velocity in this point remains small. As a result, the gradient $\frac{\partial u}{\partial z}$ grows larger with time due to the increase of $u$. So the production term $P_k$ grows with time up to the point where $D_k + P_k > \varepsilon$ and the equilibrium becomes unstable as can be seen from Figure 15.

The further development of this instability is easily explained: if TKE increases, the eddy viscosity increases and in turn the production of TKE grows further. This positive feedback mechanism drives the sudden transition back to the correct dynamic equilibrium $P_k \approx \varepsilon$.

The attraction properties of the ‘wrong’ equilibrium condition are not fully understood; it acts as an attractor for some period of time, but no cases have been found where the solution approximates this equilibrium so closely that it cannot return to the correct solution at some point during the tidal cycle.

4.2.2. Possible solutions

The above analysis shows that turbulence during slack tide is sensitive to small numerical errors, which may drive the system into another temporarily stable dynamic equilibrium. As a result even small changes in the
A convenient way to show whether or not the model switches to another dynamic equilibrium is to plot a time series of $u_\ast$, see Figure 16. In the wrong dynamic equilibrium the velocity profile is uniform at all cells but the bottom cell. As a consequence, the velocity in the bottom cell, and therefore $u_\ast$, follows a well defined trajectory. The trajectory of $u_\ast$ in the wrong equilibrium state is found by forcing $P_k = 0$ at all times.

1. **The $k-\tau$ model**
   It was shown in Section 4.1 that the $k-\tau$ model performs well near the bed for the case of open channel flow and that this performance is almost independent of the number of layers. So the error near the bed is sufficiently small for the system to remain at the right dynamic equilibrium. The model results show that, for the case under consideration, the $k-\tau$ model shows no sign of the problem with three or more layers.

2. **Number of layers**
   From the problem analysis it follows almost trivially that increasing the number of layers solves the problem, because the numerical error should reduce with an increasing number of layers. For the case under consideration, the problem is only just visible if 15 layers are used and has completely disappeared for 20 layers. Such dependence of the model behaviour on the grid resolutions is not a favourable property of a model. Conversely, a reduction of the number of layers increases the time interval during which the wrong dynamic equilibrium is pursued.

3. **Boundary condition of $\varepsilon$**
   The boundary condition for $\varepsilon$ near the bed is topic of discussion in literature. Burchard and Petersen (1999) showed that a Neumann boundary condition for $\varepsilon$ is better at reproducing a logarithmic profile near the bed. The open channel flow case of Section 4.1 also showed that the Neumann boundary condition
is better than the Dirichlet boundary condition. The following boundary conditions for $\varepsilon$ are considered:

\[
\varepsilon|_{z=0} = \frac{u_3^3}{9z_0\kappa}, \quad \text{with correction to } D_\varepsilon; \quad \text{(D3D, see also Appendix B.1)}
\]

\[
\varepsilon|_{z=0} = \frac{u_3^3}{9z_0\kappa}, \quad \text{without corrections;} \quad \text{(DIR)}
\]

\[
\frac{\partial \varepsilon}{\partial z} \bigg|_{z=\frac{1}{2} \Delta z} = -\frac{u_3^3}{\kappa(9z_0 + \frac{1}{2} \Delta z)^2}, \quad \text{(NEU1)}
\]

\[
\frac{\partial \varepsilon}{\partial z} \bigg|_{z=\frac{1}{2} \Delta z} = -\varepsilon^{3/4} \frac{k^{3/2}}{\kappa(9z_0 + \frac{1}{2} \Delta z)^2}. \quad \text{(NEU2, see also Appendix B.1)}
\]

Figure 16 shows the results in terms of $u_*$ and with 10 layers. Both Neumann boundary conditions perform well and show almost no shift to the alternative dynamic equilibrium. The model with the DIR boundary condition shows some distortion, but less than that with D3D boundary condition. Note however that the use of the DIR boundary condition underestimates the amplitude of $u_*$ compared to the alternative boundary conditions.

![Figure 16: Time series of $u_*$ using 10 layers for several boundary conditions of the $k-\varepsilon$ model.](image)

The problem of the delayed build-up of turbulence after slack tide is likely to be restricted to simple symmetric tidal flows. Any asymmetry in the tide will cause an asymmetry in turbulent mixing. This will create an exchange flow, i.e. a flow component that is non-zero after averaging over the tidal time-scale. The shear of this exchange flow will cause a persisting amount of turbulence around slack tide, see Dijkstra (2014). The problems that are observed in the tidal flow case are therefore not likely to be found in practical situations.

### 4.3. Wind over a stably stratified lake

The next two cases will treat mixing processes in stably and unstably stratified water columns. A frequently used test case for testing mixing in stably stratified fluids is wind over a stably stratified lake. A number of papers discuss measurements of this case (Kato and Philips, 1969; Linden, 1975; Price, 1979) and model studies (Luyten et al., 1996; Burchard and Petersen, 1999; Burchard and Bolding, 2001). Wind straining of a stably stratified water column is an important source of mixing in lakes, estuaries and along the coast. In lakes for example it has influence on the heat distribution in the water and therefore the ecology of the lake. Straining of a stably stratified water column by flow instead of wind is also important in estuarine and coastal flows and shows some similarities with the physics in this case.

We will consider a stably stratified infinitely deep lake with no flow. At $t = 0$ the wind starts to blow over the surface of the lake at a constant speed, thereby building a layer where velocity shear dominates stratification and the water is well mixed; the mixed-layer depth $D_{ml}$, see Figure 17.
4.3. Wind over a stably stratified lake

The following numbers will be used

$$h = 100 \text{ m},$$
$$u_{10} = 4 \text{ m/s}$$ wind speed at 10 metres above the surface,
$$T = 3 \text{ days}$$ end time of simulation,
$$\left. \frac{\partial \rho}{\partial z} \right|_{t=0} = -0.02 \text{ kg/m}^4$$ linear initial density gradient; $30^\circ \text{C}$ at surface and $10^\circ \text{C}$ at bed.

The depth of the lake in the numerical simulation is not infinite, but still much larger than the depth of wind influence so that the bed friction is negligible.

The wind stress velocity follows from the relation by Smith and Banke (1975) and reads

$$u_{*,w} = \rho_{\text{air}} u_{10}^2 \left( 0.63 + 0.66 u_{10} \right) \cdot 10^{-3}$$
$$= 1.6 \cdot 10^{-5} \text{ m/s}.$$  

The wind speed and stratification are such that the wind influence penetrates less than 25 metres into the water column before $t = T$. The bottom half of the lake is therefore unimportant and contains only 4 equidistant grid cells. The upper half of the water column contains 10 to 1000 equidistant cells. Based on data by Kato and Philips (1969), Price (1979) suggested the distance of wind influence $D_m$ equals

$$D_m = 1.05 u_{*,w} \left( \frac{t}{N_0} \right)^{1/2},$$ (4.3)

where $N_0$ is the buoyancy frequency at $t = 0$, which is defined as

$$N_0 = \sqrt{\frac{g}{\rho_0} \left. \frac{\partial \rho}{\partial z} \right|_{t=0}}.$$  

4.3.1. Results

The development of the mixed-layer depth in time is investigated by using the $k-\varepsilon$, $k-\tau$ and $k-\omega$ models. The mixed-layer depth is defined as the lowermost point of the thermocline. There is almost no turbulence below the thermocline, so the lowermost point of the thermocline corresponds well to the uppermost grid point where $k < 10^{-8} \text{ m}^2/\text{s}^2$. A similar definition of $D_m$ is used by Warner et al. (2005).

Figure 18 shows a time series of the mixed layer depth for 25 and 100 layers in the upper half of the water column. The graphs only show cell interface levels; the results are not interpolated between grid points. This means that 2 metre variations between the models are to be expected for the case of 25 layers, because a cell is 2 metres high. The results of the turbulence models are similar and correspond well to Equation 4.3.
Figure 18: Time series of $D_m$ for the $k-\varepsilon$, $k-\tau$ and $k-\omega$ models a) for 25 and b) for 100 layers in the upper 50 m.

Figure 19: $h - D_m$ after 3 days for the $k-\varepsilon$, $k-\tau$ and $k-\omega$ models and for several numbers of layers. Note that the horizontal axis does not scale consistently with the number of layers in order to show the results for a wide range of grid resolutions.

The convergence of the mixed-layer depth at $t = T$ is plotted in Figure 19. The error bars indicate the cell height and therefore some measure of expected numerical uncertainty. The results have converged within the uncertainty of one cell thickness once 200 or more layers are used in the upper part of the water column. The converged result shows values that are $O(0.1 \text{ m})$ smaller than the estimate by Price (1979), which is so small that this is no reason to retune the model parameters.

The three models behave nearly identically in this case. The balance of the terms in the turbulence models will again be used to explain this. This balance shows that the diffusive terms in both the TKE and length-scale equations are negligible. This means that gradients of turbulence quantities are unimportant, so that the eddy viscosity follows from the local values of the production and dissipation terms. Such state is therefore
4.4. Unstable stratification by bed heating

Unstable stratification occurs frequently in natural systems. It occurs for example in estuaries when the flood tide advects salt water over fresh water (Simpson et al., 1990). It is also seen in lakes when the air cools the surface of warmer water, e.g. in the evening. Another source of unstable stratification in lakes is the heating of the surface of water with a temperature below $4^\circ C$; below this temperature water becomes more dense when heated. This makes unstable stratification an important process in the simulation of freezing and thawing of ice on lakes.

Deardorff et al. (1969) performed measurements on the mixing of unstable temperature stratification. In these experiments the temperature at the surface of a tank with water was kept constant at $T_{surf}$, while the temperature at the bottom was kept at $T_{b,stable} < T_{surf}$ until a stationary stably stratified state was reached. Then, at $t = 0$, the temperature under the bed was changed to $T_{b,unstable} > T_{surf}$ by letting hot water flow under the tank. This forces convective mixing in the water column. There is no background flow.

![Figure 20: Heating the bottom of a tank with stably stratified water to create unstable stratification.](image)

It has been remarked that two-equation turbulence models such as the ones used here, are not capable of modelling unstable stratification sufficiently well, because they do not contain the physics of convective mixing of unstable stratification. Burchard and Petersen (1999) however show in a 1DV model that the $k - \varepsilon$ model is nevertheless capable of reproducing the measurements of the mixed layer depth and the density profiles. However, the model does so by modelling an advection dominated process by a combination of diffusive transport and local production.

The experiment is repeated with the 1DV model and the dimensions of the numerical model correspond to the
4. Model properties in basic flow processes

Laboratory dimensions of Deardorff et al. (1969):

- $h = 0.36$ m
- $T_{surf} = 39^\circ C$
- $T_{b, stable} = 21.5^\circ C$
- $T_{b, unstable} = 43.4^\circ C$

Both the papers by Deardorff et al. (1969) and Burchard and Petersen (1999) are not clear about the rate at which heat diffuses through the bottom of the tank and how this should be implemented in a numerical simulation. The heat diffusion through the bottom in DPM is implemented by adding $n_{bed}$ extra cells below bed level and solving a heat diffusion equation in these cells. At the lower boundary of this grid extension $T_{b, stable}$ or $T_{b, unstable}$ is prescribed and the upper boundary, i.e. the interface bed-water, connects to the heat equation that is solved in the flow. The additional parameters are calibrated as follows:

- $n_{bed} = 2$, number of additional cells below bed level,
- $D_b = 7.5 \cdot 10^{-8}$ m$^2$/s rate of diffusion through the bed,
- $\Delta z_{I+1} = \Delta z_{I+2} = 0.001$ m height of cells below bed level.

The experiments and a theoretical analysis by Deardorff et al. (1969) suggest that the mixed-layer builds-up according to the relation

\[
\frac{1}{3} \zeta^{2/3} + \frac{2}{3} \zeta^{-1/3} = 1 + 0.047 t^* ,
\]

where

\[
\zeta = 1 - \frac{D_m(t)}{h},
\]

\[
t^* = C_2 \left. \frac{\partial T}{\partial z} \right|_{0} (T_{b, unstable} - T_{b, stable})^{-2/3} t 
\approx 0.0028t .
\]

4.4.1. Results

The mixed-layer depth for the unstable stratification case is defined as the upper side of the thermocline; the mixed-layer now builds up from the bed instead of from the surface. Numerically this is the lowermost point such that $k < 10^{-8}$ m$^2$/s$^2$.

Figure 21 shows the results of the simulation on a grid of 100 layers. The black line roughly represents the data and theoretical results by Deardorff et al. (1969); their theoretical result and measurements were close together. The figure shows that the models behave similarly, but the response to the heat input through the bed is different. The $k - \tau$ and $k - \varepsilon$ models respond immediately, which is closest to the results of Deardorff et al. (1969), while $k - \omega$ models responds slower. This response time depends on the grid resolution, see Table 4.1.

<table>
<thead>
<tr>
<th>$k - \tau$</th>
<th>10</th>
<th>25</th>
<th>50</th>
<th>75</th>
<th>100</th>
<th>200</th>
<th>300</th>
<th>500</th>
<th>1000 layers</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k - \varepsilon$</td>
<td>$\infty$</td>
<td>60</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$k - \omega$</td>
<td>$\infty$</td>
<td>80</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>80</td>
<td>140</td>
<td>160</td>
</tr>
<tr>
<td>$k - \omega$</td>
<td>$\infty$</td>
<td>360</td>
<td>180</td>
<td>140</td>
<td>120</td>
<td>120</td>
<td>140</td>
<td>140</td>
<td>140</td>
</tr>
</tbody>
</table>

Table 4.1: Response time (s) of mixing with the three models at several grid resolutions.

The response time expresses the problem of the turbulence model to start-up from a completely still situation. A closer look at the turbulence models even shows that the turbulence production remains zero if the eddy
viscosity is zero initially. The $k - \tau$ and $k - \varepsilon$ models at all resolutions show an eddy viscosity which has a magnitude of about $10^{-14}$ m$^2$/s at the bed at $t = 0$, while this is much smaller in the $k - \omega$ model.

The boundary conditions for the length-scale variable play an important part in the response of the model. A high value of $\tau$ at the bed makes sure that any TKE at the bed results in an eddy viscosity that is sufficient to start-up turbulent mixing. The value of $\tau$ in the $k - \tau$ model should approach infinity at the bed and attains a value of the order of $10^6$ s at $t = 0$ in the model for all grid resolutions. A similar equivalent value of $\tau$ at the bed is attained in the $k - \varepsilon$ model with a Neumann boundary condition for resolutions up to 100 layers, but this value decreases to $10^4$ s for 1000 layers. This is because the Neumann boundary condition prescribes the gradient instead of the actual value of $\varepsilon$ at the bed. The equivalent value of $\tau$ at the bed in the $k - \omega$ model is almost equal to zero. It is likely that this explains the long response times for the $k - \varepsilon$ model at high resolution and for the $k - \omega$ model at any grid resolution.

It is likely that the bad response of the models at 10 and 25 layer is due to an inaccurate representation of the gradients of $k$, $\varepsilon$, $\tau$ and $\omega$, which all have a hyperbolic-type shape near the bed.

The shape of the curves in Figure 21 after turbulence has picked-up is almost fully controlled by the parameters of the sub-bed cells and therefore the rate at which heat is made available to the water. These parameters are therefore calibrated so that the models roughly fit the measured data. The three turbulence models react to this parameter set with a similar rate of heat diffusion.

The dependence of $D_m$ on the grid resolution at the end time is shown by Figure 22. All models have nearly converged at 1000 layers, but the models converge to different values. This is to be expected considering the different response times of the model and therefore the different total amounts of heat that enter the model.
Figure 22: $D_m$ after 800 s for the $k - \varepsilon$, $k - \tau$ and $k - \omega$ models for 10 to 1000 layers. Note that the horizontal axis does not scale consistently with the number of layers in order to show the results for a wide range of grid resolutions.
5

Results with complex flow processes

The previous chapter treated simple flow situations in which the properties of the different turbulence models could be analysed and the differences could be coupled to the numerical implementation of the models. This becomes more difficult for more complex flow situations, because the non-linear interactions between the processes obscure the reasons for the differences between the model results. It is for the same non-linear relations that the results of the more complex flow cases are difficult to predict on the basis of the results of the previous cases. These complex cases are included to gain some first experience with these versions of the $k - \tau$ and $k - \omega$ models for more realistic situations.

Two cases will be tested in the 1DV model. The first concerns the temperature in a lake forced by measured wind and air temperature data. The second concerns the flow in a well-mixed to partially stratified estuary, which is dominated by the tide and stratification.

5.1. Temperature modelling in Lake Vlietland

Uittenbogaard and Aparicio-Medrano (2011) model the temperature in the southern part of Lake Vlietland near Leiden, the Netherlands. They use the DPM model with the $k - \varepsilon$ turbulence model and compare the results against measurements. They find a good correspondence between the model results and the measurements. Similar good results with a 1DV lake temperature model are obtained in several cases by Goudsmitt et al. (2002). The temperature in lakes is important for simulating the ecology of the lake. It serves for example the prediction of algae blooms in lakes.

The model involves the heat-flux model that is implemented in Delft 3D-FLOW (Deltares, 2014) and wind and temperature data from meteorological observations in 2009.

![Figure 23: Wind and heat exchange affecting the flow and stratification in a lake.](image)
The temperature in the lake was measured during the summer of 2009 with an accuracy of 0.1 °C and sampling interval of 5 minutes. The measurements were obtained by a number of temperature loggers that were attached to a buoy. The temperature was measured at 5 minute intervals for 6 months at a depth of 0.1, 4.1, 5.6, 7.1, 8.1, 9.6, 10.6 and 16.1 metres below the surface. The water level in the lake was fairly constant.

The parameter values are

\[ h = 36 \text{ m}, \]
\[ \text{Stanton number} = 1.3 \cdot 10^{-3}, \]
\[ \text{Dalton number} = 1.0 \cdot 10^{-3}, \]
\[ \text{Number of layers} = 200. \]

The Stanton number is a parameter that determines the heat exchange between air and water which is due to the wind and the Dalton number parametrises the degree of evaporation. Both parameters are calibration parameters of the temperature model, see Deltares (2014).

We will first consider the temperature evolution over the year by using daily values of the measured and modelled temperature at 10.00 AM, following the study by Uittenbogaard and Aparicio-Medrano (2011). Next, a more detailed image of the temperature evolution during a few days is discussed.

5.1.1. Results over one year

The simulated temperature by the \( k-\varepsilon \) and \( k-\tau \) models in the lake throughout the year 2009 is presented in Figure 24. A similar figure for the \( k-\omega \) model is given in Appendix F. The lake starts to stratify around day 100, which is in April, due to heating at the surface. The measurements are not shown in the figure, because measurements are too sparse, only 8 locations in the vertical, to provide an accurate contour-plot. The main thermocline is established in late April (around day 120) at approximately 15 metres below the surface and stays there throughout the summer. The lake becomes well-mixed again in late Autumn by a combination of wind mixing and cooling from the surface.

The most important difference between the results with the \( k-\varepsilon \) and \( k-\tau \) models is the location of the main thermocline. This main thermocline is situated lower in the water column with the \( k-\tau \) and \( k-\omega \) models than with the \( k-\varepsilon \) model. The measured thermocline is situated between the results of the \( k-\tau \) and \( k-\varepsilon \) models at a resolution of 200 layers.

The mean error is calculated according to several methods and is summarised in Table 5.1 for a grid with 200 layers. The \( k-\varepsilon \) is clearly better in all three error measures. It can however not be concluded that the \( k-\varepsilon \) model is better than the other models. A different calibration of the model parameters or a different grid resolution may favour the other models. We will therefore measure the performance of the model by its sensitivity to the grid resolution. Figure 25 shows the root mean square error for several grid resolutions. The error of the \( k-\varepsilon \) model shows a stronger dependence on the grid resolution than the other two models. The \( k-\tau \) model seems to converge towards 500 layers, but then shows changing results between 500 and 1000 layers.

The variations of the results for different resolutions correspond to variations of the level of the thermocline. The thermocline moves upward with an increasing number of layers in all the models. The three models produce similar results for 20 to 50 layers. A further increase in the number of layers sees the level of the thermocline rise with 5 metres in the \( k-\varepsilon \) model between 50 layers and 2000 layers and about 2 metres in the \( k-\tau \) and \( k-\omega \) models.

Such similarity of the results of the \( k-\tau \) and \( k-\omega \) models and deviations from the results of the \( k-\varepsilon \) model were not observed in the earlier cases. It may be hypothesised that this is the result of the removal of the \( D_{kk} \) from the \( k-\tau \) and \( k-\omega \) models, so that they are not exact transformations of the \( k-\varepsilon \) model (see Section 3.4). This is however not the case as is explained in Appendix F. The \( D_{kk} \) term has little influence on the trends that were explained above.
5.1. Temperature modelling in Lake Vlietland

![Simulated temperature profiles](image)

Figure 24: Simulated temperature profile at one location in southern lake Vlietland in 2009 a) using the $k-\tau$ model, b) using the $k-\varepsilon$ model and c) the difference plot $(k-\varepsilon)-(k-\tau)$. The grid contains 200 layers.

<table>
<thead>
<tr>
<th></th>
<th>$k-\tau$</th>
<th>$k-\varepsilon$</th>
<th>$k-\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean error ($^\circ$C)</td>
<td>1.9</td>
<td>0.1</td>
<td>1.8</td>
</tr>
<tr>
<td>Mean absolute error ($^\circ$C)</td>
<td>2.2</td>
<td>1.3</td>
<td>2.1</td>
</tr>
<tr>
<td>Root mean square (RMS) error ($^\circ$C)</td>
<td>3.2</td>
<td>1.6</td>
<td>3.1</td>
</tr>
</tbody>
</table>

Table 5.1: Errors in simulated temperature compared to the measurements. The grid contains 200 layers.

![RMS error graph](image)

Figure 25: Root mean square error of the three models for 20 to 2000 layers.

5.1.2. Results over a few days

Some more details are revealed by looking at the temperature evolution over a few days in 40 minute intervals. This is presented in Figure 26 by showing the Richardson number:

$$Ri = \frac{N^2}{M^2}$$
The Richardson number denotes the balance between buoyancy and velocity shear in the TKE equation. A negative Richardson number denotes mixing due to unstable stratification and a positive Richardson number denotes turbulence damping by stable stratification. The highest Richardson number, i.e. the strongest influence of buoyancy, is found near the thermocline. The scale restricted to $Ri \in [-3, 3]$ for clarity.

![Richardson number diagrams](image)

Figure 26: The Richardson number in the range $[-3, 3]$ for the days 181 to 186, i.e. the first days of July, in the model results of the $k-\tau$ and $k-\varepsilon$ model and the difference between these results. The model uses 200 layers.

The figure shows a daily event of convective mixing at the surface, which is due to cooling of the surface during night time. Both the $k-\varepsilon$ model and the $k-\tau$ model reproduce these convective mixing events, but the rate of mixing differs. This is especially clear just after $t = 184$ days where the $k-\varepsilon$ model produces much less mixing than the $k-\tau$ model. The reason for this particular difference does probably not originate from different properties of the models in simulating convective mixing. Rather, the behaviour between $t = 183.5$ and $t = 184$ days is more likely to be the cause, because the $k-\varepsilon$ model results still show a secondary pycnoline at $z = 33$ m, while the $k-\tau$ model does not. The measurements do not provide a decisive answer to which model is closest to the truth, because of lack of spatial resolution.

The differences between the models in the behaviour near the surface during these daily warming and cooling events is essential for the temperature of the lake on the time-scale of a year. However, such near-surface behaviour is strongly influenced by the temperature in the whole layer above the main thermocline. It is
therefore difficult to relate the results to the properties of the turbulence models.

Concluding the above observations, the three turbulence models reproduce the same features on a yearly time-scale as well as a daily time-scale, however they produce quantitatively different results on both time-scales.

5.2. Estuarine circulation

The flow in an estuary consists mainly of a tidal and a river flow that are affected by density differences due to salt and possibly sediment stratification. It therefore combines the flow processes of the tidal flow with those of stably and unstably stratified flows. Estuarine flow is simplified to a 1DV problem by the same method that is employed by Burchard and Hetland (2010). They prescribe a tidal velocity and frequency, a river discharge and a fixed horizontal density gradient which is caused by differences in salinity only.

![Figure 27: The flow in an estuary is reduced to the combination of a simple tidal flow and a fixed horizontal density gradient.](image)

This case simulates one of the processes that is responsible for creating stratification in a well-mixed or partially stratified estuary. This process is the straining of the density field by the velocity and is visualised conceptually in Figure 28. During the ebb tide, the fresher water from the riverine side of the estuary moves faster at the surface than near the bed, because the flow velocity is higher at the surface than near the bed. Lighter fresh water therefore moves over heavier salt water and creates a stably stratified water column. The reverse holds during the flood tide, leading to a potentially unstably stratified water column. The amount of mixing increases as a consequence of this tendency for unstable stratification. The water column is therefore more likely to become well-mixed than unstably stratified.

![Figure 28: Straining of a well-mixed water column by the ebb flow velocity.](image)

The flow and stratification in the estuary induce an exchange flow. The exchange flow is a residual flow, i.e. it has a non-zero contribution after averaging over the tidal time-scale, and has a depth-averaged contribution of zero. The exchange flow is typically seaward near the surface and landward near the bed. The exchange flows are typically much smaller than the typical tidal velocity, but can nevertheless be responsible for a significant part of the transport of constituents such as salt and sediments (Jay and Musiak, 1994; MacCready, 2004). Turbulence modelling is important for the prediction of the exchange flows, because the variations of turbulence over the tidal period determine a large part of the exchange flow. Details on how the exchange flows are created are provided by Geyer and MacCready (2014) and Dijkstra (2014).
The model parameters are

\[ h = 25 \text{ m}, \]
\[ C = 60 \text{ m}^{1/2}/\text{s}, \]
\[ \frac{\partial p}{\partial x} = 10^{-4} \text{ kg/m}^4, \]
\[ T = 12 \text{ h} \quad \text{Tidal period}, \]
\[ \hat{u} = 1 \text{ m/s} \quad \text{Depth-averaged } M_2 \text{ tidal velocity amplitude}, \]
\[ u_{\text{river}} = 0 \text{ m/s} \quad \text{depth-averaged river velocity}. \]

The parameters fall in the parameter space that is covered by the study of Burchard and Hetland (2010) for this case, so that the results of this study could be verified against their results.

5.2.1. Results

The results of the simulation of one tidal period with the \( k - \tau \) model are summarised in Figure 29, which shows the velocity, salinity, eddy viscosity, TKE shear production and TKE buoyancy production. The figure corresponds closely to Figure 2 of Burchard and Hetland (2010). The figure shows that the water columns stratifies during ebb (negative velocity), leading to a negative buoyancy production. The water column mixes during flood leading to a positive buoyancy production and higher peak eddy viscosity than during ebb. The magnitude of the shear production and buoyancy production reveals that this case is dominated by bed friction in the lower half of the water column.

The three turbulence models produce qualitatively the same results. They, for example, produce the same shapes of the profiles of the tidal velocity, exchange flows, salinity and eddy viscosity. The quantitative differences between the three models are small on all aspects given in Figure 29.

The buoyancy production displays an interesting ‘stepwise profile’. This appears when the lower part of the water column is already mixed, while the upper part of the water column is still stratified. It is outside the scope of this research to investigate this behaviour in detail, but it is found in all three turbulence models. It is also found in the GOTM model with the \( k - \varepsilon \) model with the same settings as used here. Such a stepwise profile is not observed by Burchard and Hetland (2010), who use GOTM with a \( k - \varepsilon \) model and a stability function to relate the parameters \( c_\mu, \sigma_p \) and \( c_3 \) to the degree of stratification.

The quantitative differences between the results of the three models and the convergence of the results are measured by the exchange flow magnitude. Figure 30 shows the mean absolute exchange flow, i.e.

\[ \int_0^h |u_{\text{exchange}}| \, dz, \]

where \( u_{\text{exchange}} \) is the exchange flow velocity.

The models all converge monotonously to approximately the same result. The \( k - \tau \) model shows the best convergence with a deviation from the converged result of 5% at 10 layers and less than 1% at 100 layers. The \( k - \varepsilon \) shows a deviation of 9% at 10 layers and still 5% at 100 layers and the \( k - \omega \) model displays a numerical error of 15% at 10 layers and 6% at 100 layers.

It is likely that part of the result can be explained by the results of the open channel flow case, where the \( k - \tau \) model also performed best because the profile of \( \tau \) is linear near the bed. Figure 29 shows that the effect of buoyancy at the bed is negligible compared to the effect of shear production so that we find approximately a homogeneous channel flow near the bed.

The result is extremely sensitive to small changes in the implementation. An example of this sensitivity to a small change in the Neumann boundary condition of the \( k - \varepsilon \) model is presented in Appendix G. This sensitivity exemplifies that some aspects of the numerical accuracy are still not fully understood and that experience with a model implementation is of crucial importance in order to gain trust in the numerical accuracy and robustness.
Figure 29: Results of the estuarine flow case with the $k - \tau$ model with 200 layers.

Figure 30: Magnitude of the mean absolute exchange flow at several grid resolutions in all three turbulence models.
Discussion

One of the main challenges in numerical modelling is in finding a balance between numerical accuracy and computational time. An important part of the numerical accuracy of an environmental flow model is determined by the numerical accuracy of the turbulence model. We have been investigating how a transformation of the modelled variables in a turbulence model can lead to a higher numerical accuracy at a smaller number of layers. We have therefore identified the properties of the transformed turbulence models that are responsible for the improved results.

This approach differs from most earlier research into the differences between two-equation turbulence models. Most earlier research has focussed on the ongoing debate on which two-equation turbulence model is the best model. The debate centres around the question which length-scale variable should be chosen for the second equation of the two-equation turbulence model. This question has been approached from a theoretical point of view by e.g. Mellor and Yamada (1982) and Wilcox (1993), who motivate their different choices of turbulence model by providing different closure assumptions. A modelling point of view has been taken by e.g. Warner et al. (2005), Umlauf and Burchard (2003) and Wijesekera et al. (2003). In their studies they have compared different two-equation turbulence models for a range of cases.

The numerical accuracy has not been a focal point in this debate. As a result, the numerical accuracy and convergence properties of the turbulence model implementations are largely unknown. Additionally, the choice for a turbulence model is purely based on physical grounds and not on numerical aspects. As an example, the freedom of the length-scale variable in the GLS model can result in a user-defined length-scale variable, which assumes a vertical profile that is badly reproduced on a low resolution numerical grid. This is potentially one of the reasons that Umlauf and Burchard (2003) and Warner et al. (2005) find worse results with the ‘optimal’ calibrated GLS parametrisation than with other turbulence models. Burchard and Bolding (2001) include the computational economy and physical soundness as two of their five requirements on a turbulence model; reflecting a trade-off between accuracy and computational time, but not considering numerical accuracy. These requirements do not stress that the accuracy of a model can be compromised, because physically sound terms or variables are badly approximated in the numerical simulation.

It is unfortunate that the length-scale variable has become the focal point of the debate. The choice of one length-scale variable over the other is only of limited significance from a physical perspective. Indeed, models with different length-scales can be made physically equivalent by adjusting some diffusive terms and coefficients. The results of this research show however that the length-scale variable is a useful tool for improving the numerical performance. A better result can be attained at a lower resolution by adjusting the length-scale variable to suit the numerical computation.

We have been investigating two aspects of numerical accuracy: the accuracy at a low grid resolution and the monotonicity of convergence. These properties will be discussed in Sections 6.1 and 6.2. Finally, we will discuss
the costs and benefits of implementing the $k - \tau$ model in Section 6.3.

6.1. Numerical accuracy

The results of the six cases that have been investigated in this research can be generalised by understanding how the properties of the turbulence models influence the numerical accuracy. We have identified three categories of properties that affect the numerical accuracy:

1. the approximation of gradients,
2. the type of boundary conditions and
3. the implementation of diffusive terms.

Below we will discuss how these properties relate to the numerical accuracy of the results at a low grid resolution.

The gradient of $\tau$ can be approximated with a higher degree of accuracy in bed friction dominated flows than the gradients of $\varepsilon$ and $\omega$. The profile of $\tau$ is linear near the frictional bottom boundary, while the profiles of $\varepsilon$ and $\omega$ are hyperbolic. The gradients of $\tau$ are therefore exactly represented in the numerical computation, while the gradients of $\varepsilon$ and $\omega$ are not exact. This was also shown by Speziale et al. (1992) for the area closest to the bed. This research builds upon this result by showing that the numerical advantages of the linear profile of $\tau$ extend through a significant part of the water column. It has also been found that it is most important to have an accurate representation of the gradients in the area where the velocity gradient is greatest. This is near the bed in bed friction dominated flows. In the case of stationary uniform open channel flow, this results in an average velocity in the $k - \tau$ model which varies only by 1% between 10 and 2000 layers. The result of the $k - \varepsilon$ model with Neumann boundary condition varies by 3% in this range and the result of the $k - \omega$ model varies by 6%.

The small improvement of the velocity simulation by the $k - \tau$ model in bed-friction dominated flows can become significant when studying the transport of constituents, such as salt or sediments. The bed-load sediments transport for example strongly depends on the velocity gradient near the bed. The importance of bed friction is not restricted to homogeneous flows. Also estuarine and coastal flows rely strongly on an accurate representation of the near-bed layer (Prandle, 1982; Souza, 2013). The approximation of this layer affects the accuracy of the modelling of stratification in these systems. This could possibly lead to an amplification of numerical error made at the bed and therefore lead to a greater advantage of the $k - \tau$ model over the $k - \varepsilon$ and $k - \omega$ models. The estuarine flow case in this study suggests that this is realistic, because the differences between the three turbulence models are twice as large in this case as in the open channel flow case; the estuarine exchange flow velocity varies by 5% between 10 and 2000 layers in the $k - \tau$ model, 9% in the $k - \varepsilon$ model and 15% in the $k - \omega$ model.

No clear advantage or disadvantage of either turbulence model has been found for general stratified flows. The profiles of the three length-scale variables possess a similar degree of curvature, so that the approximation has a similar degree of accuracy. In some cases of stably stratified flows, the approximation of the gradients of the turbulence variables is unimportant, because the turbulence models are governed by local production and dissipation terms. An example is the case of wind over a stably stratified lake.

The $k - \tau$ model has natural boundary conditions. This means that its Dirichlet boundary condition is well-defined at the bed. The $k - \varepsilon$ and $k - \omega$ models do not possess such natural boundary conditions; the values of $\varepsilon$ and $\omega$ become infinite at the frictional boundary. Dirichlet conditions cannot nevertheless be defined for these models, but this can result in large errors. The open channel flow cases sees over 25% variation of the results between 10 and 2000 layers with Dirichlet conditions for $\varepsilon$ and $\omega$. The results can be improved by implementing a correction to the Dirichlet condition for $\varepsilon$ that is used in Delft 3D-FLOW. This boundary condition results in a variation of the velocity in the open channel flow case of 5% between 10 and 2000 layers. However, the results become worse when increasing the number of layers between 10 and 100 and only improve of more than 100 layers are used. Such convergence behaviour is not a favourable model property. A new correction to the Dirichlet condition of $\varepsilon$ has been developed and it shows promising results of monotonous convergence in the open channel flow case. It is however not better than the Neumann boundary condition for $\varepsilon$. 
The Neumann boundary condition for $\varepsilon$ and $\omega$ has been shown to be a better alternative boundary condition in bed friction dominated flows (Burchard and Petersen, 1999), but there are some individual cases in which this condition is worse. One such case is that of unstable stratification in this research. Turbulence production should be started in this case by small disturbances in the level of TKE at the bed. The Neumann boundary conditions for $\varepsilon$ and $\omega$ create a value of these variables which is too large near the bed. Any small disturbance in the level of TKE is damped by these levels of dissipation so that turbulence does not start. This case is very specific, as any other disturbance of the flow would be sufficient to start turbulence production. However, this case shows that the lack of natural boundary conditions for $\varepsilon$ and $\omega$ can result in odd behaviour in certain situations. Similar problems have not been identified with the natural Dirichlet boundary condition for $\tau$.

Speziale et al. (1992) criticise the Neumann boundary condition of the $k-\varepsilon$ model, because it has ‘no theoretical or experimental justification’. The Neumann condition for $\varepsilon$ and $\omega$ is however practical and its advantages over the Dirichlet condition outweigh the disadvantages. The Neumann condition can therefore best be seen a useful numerical alternative to the Dirichlet condition, rather than a different physical boundary condition.

Some of the diffusive terms in the turbulence models are essential to their stability, while others are optional. The choice on which diffusive terms to include should be based on both physical and numerical considerations. The term $D_{\tau \tau}$ is an essential term for the stability of the $k-\tau$ model (Umland and Burchard, 2003; Kantha and Carniel, in press). The details of its implementation, however, also show why diffusive terms should be included for both physical and numerical reasons. If the $D_{\tau \tau}$ term were to be implemented with a second-order accurate central differences approach, it would lead to a factor two reduction of the mixed layer thickness in the unstable stratification case for a low grid resolution (see Appendix E). The results do converge to the correct result if more than 1000 layers are used. This implies that the numerical diffusion generated by the first-order implementation that has been used for $D_{\tau \tau}$, is actually required to find the correct result at low grid resolution. It is speculated that, for this case, a minimum level of diffusion is required above which the local production and dissipation govern the behaviour of the system. This minimum level of diffusion is found from physical diffusion at a high-resolution or from numerical diffusion at a lower resolution.

So the numerical diffusion that is incorporated in a model by implementing certain diffusive terms can be of essential importance to obtaining accurate results at a low resolution. Such dependence has only been experienced with the $D_{\tau \tau}$ term in this research. The other diffusive terms $D_{k \tau}, D_{k \omega}, D_{kk}$ have not proven essential to the qualitative behaviour of the results in the present test cases. The general physical and numerical importance of these terms is unknown and could not be discerned from the cases in this research.

There are some differences between the results of the three turbulence models that cannot be explained by the above three properties. An example of such unexplained behaviour is the case of Lake Vlietland tested in this research. This case involves the modelling of the temperature of a lake driven by variable wind and air temperature data. Even though the qualitative results of the models are similar, the quantitative results show significant deviations between the $k-\varepsilon$ model on the one hand and the $k-\tau$ and $k-\omega$ models on the other hand. The main difference on a seasonal time-scale is the depth of the main thermocline. This depth varies with the grid resolution; the thermocline moves upward if the grid resolution increases. The $k-\omega$ and $k-\tau$ models see the thermocline moving about 2 metres between 50 and 2000 layers with the thermocline around 15 metres below the surface. The $k-\varepsilon$ model shows the largest variation of the level of the thermocline, which moves about 5 metres between 50 and 2000 layers. Such a large variation is not acceptable.

The results of the lake case do not converge up to 2000 layers for all turbulence models. Especially the $k-\varepsilon$ model still shows a strong change between 1000 and 2000 layers of 0.5 metre movement of the thermocline. Based on these results it can even be argued that an increase of the grid resolution does not increase the numerical accuracy at all.

This raises concerns on degree to which the two-equation turbulence models can be used for computations of temperature evolution from a numerical perspective. This adds to concerns of e.g. Martin (1985) and Hodges et al. (2000) on the capability of these models to capture stratification sufficiently well for the application to temperature modelling in lakes and oceans. On the other hand, Burchard and Bolding (2001), Goudsmit et al. (2002) and Uittenbogaard and Aparicio-Medrano (2011) find good results with their two-equation turbulence models for these applications. The present results mainly raise the question on whether the good results with
these models are due to the correct modelling of the physics or whether they are a direct consequence of the
calibration of the parameters in the temperature model. This can be tested by repeating the simulations at a
number of grid resolutions to test the robustness of the results to the grid resolution.

6.2. Monotonicity of convergence

The previous discussion has only considered the performance of a turbulence model at a low resolution compared
to its converged result. The convergence behaviour of the model is another aspect of the numerical accuracy.
The models converge between 100 and 1000 layers in all cases, except for the case of Lake Vlietland. This
means that convergence of the turbulence models is not reached in most 3D models. Numerical errors are
therefore an inherent part of the turbulence model. Hence, monotonous convergence of the turbulence model
is a desirable property.

Monotonous convergence means that the variation of the result between two grid sizes always has the same sign
and that this variation decreases with the grid resolution. This implies that an increase of the grid resolution
improves the result. However, not all results in this research show monotonous convergence. Two problems
associated with such non-monotonous convergence can be identified.

1. It is not possible to extrapolate the result to the expected converged result on the basis of a few results
   at low resolution.

2. The result may seem to converge already at some low resolution, while the real converged result differs
   strongly from this apparently converged result.

The convergence is not monotonous in the open channel flow case. The first problem associated with non-
monotonous convergence listed above is for example visible with the $k-\varepsilon$ model with the Delft 3D-FLOW
boundary condition (Appendix B.1) and the $k-\tau$ model in the open channel flow case; an extrapolation of
the result at 10, 20 and 50 layers would lead to a result that differs from the converged result. The second
problem occurs in the $k-\varepsilon$ model with a Neumann boundary condition in the same case; the small variation
of the result between 10 and 100 layers seems to indicate an almost converged result, while the converged result
differs significantly.

This research has made a first step in investigating the convergence behaviour of turbulence models. This has
not been studied systematically before, so that little is known about such convergence behaviour. It has been
shown that monotonicity of convergence is not guaranteed even for relatively simple flow situations. This means
that it is generally not possible to estimate the converged model result on the basis of one or a number of low
resolution results. It also means that a grid refinement does not necessarily lead to an improved result.

6.3. Implementation of the $k-\tau$ model

The results have shown a clear advantage of the $k-\tau$ model over the $k-\varepsilon$ and $k-\omega$ models for bed friction
dominated flows, while the results are similar the other tested cases. The implementation of the $k-\tau$ model
does however pose some challenges. Most importantly there is a lack of experience with the $k-\tau$ model
implementation. This experience is required to gain trust that the $k-\tau$ model gives accurate and stable results
in all cases. The necessity of experience is shown by the examples of high and unexpected sensitivity of the
results to small changes in implementation in Appendix E and G. Small changes to the implementation might
be required to establish robust and accurate results for all cases.

It is likely that the $k-\tau$ model yields worse results in existing model schematisations, i.e. calibrated model
schematisations of a certain system that are ready for use when required. This is because the model coefficients,
such as roughness values, are tuned to yield the best performance with the currently implemented turbulence
model. The implementation of the $k-\tau$ model implementation would therefore mean that such existing
schematisations should be recalibrated. This raises the question on whether the costs of implementing the
$k-\tau$ model weigh-up against the benefits. This means that the implementation of the $k-\tau$ model is most
efficient for new model schematisations or together with other major changes to a numerical code.
A transformation of the $k-\varepsilon$ turbulence model to the $k-\tau$ model results in an improvement of the numerical accuracy in boundary friction dominated flows, such as flows in rivers, partially stratified estuaries and near-coastal flows. A 3% to 5% more accurate velocity prediction can be achieved by employing the $k-\tau$ model instead of the $k-\varepsilon$ model with Neumann boundary conditions in the range of 10 to 100 cells in the vertical direction in such cases. The $k-\varepsilon$, $k-\tau$ and $k-\omega$ models show a similar numerical accuracy in other tested cases of buoyancy dominated flows.

The results have been explained by identifying three types of differences between the three models. The most important difference between the three models is the vertical profile shape of the length-scale related variable, i.e. $\varepsilon$, $\tau$ or $\omega$. A high numerical accuracy is obtained if this profile is approximated accurately in the area where the velocity gradient is largest. This is near the frictional boundary in boundary friction dominated flows. The profile of $\tau$ is linear in this area, which results in an exact numerical approximation of this profile. The profiles of $\varepsilon$ and $\omega$ are hyperbolic and cannot be approximated accurately on a coarse grid. Similar clear advantages of the shape of $\varepsilon$, $\tau$ or $\omega$ have not been found for buoyancy dominated flows. In these cases the approximation was either of a similar accuracy for all three variables or the shape of the profiles was unimportant, because the local production and dissipation terms were dominant.

The boundary conditions are a second difference between the models. The $k-\tau$ model has a natural Dirichlet boundary condition, while the $k-\varepsilon$ and $k-\omega$ models do not, because the value of $\varepsilon$ and $\omega$ approaches infinity near the bed. Dirichlet conditions for $\varepsilon$ and $\omega$ can nevertheless be prescribed, but these yield inaccurate results in friction dominated flows. The Neumann boundary condition is a practical alternative for $\varepsilon$ and $\omega$ to improve the numerical accuracy in most cases. The Neumann condition results in an erroneous value of $\varepsilon$ and $\omega$ at the boundary, but these errors are only of importance in some cases with no sources of turbulence production except for at the boundary. The advantages of the Neumann conditions over the Dirichlet conditions outweigh the disadvantages.

The third type of differences between the models is in the implementation of the diffusive terms. Some diffusive terms are essential to the stability of the turbulence model, such as the term that was named $D_{\tau\tau}$ in the $\tau$-equation. Other diffusive terms are optional. The choice whether or not to include these terms should be motivated by both physical and numerical considerations, because the terms induce both physical effects and numerical effects, such as numerical diffusion.

Convergence of the result is generally found between 100 and 1000 layers, which is typically beyond the range of feasible grid resolutions for 3D environmental modelling. No convergence has been found up to 2000 layers in one of the test cases, in which the water temperature in a lake was simulated. This means that numerical errors are an inherent part of a turbulence model.

Within the typically feasible range of 10 to 100 layers, it is not guaranteed that the numerical error is reduced if the grid resolution is increased. Monotonous convergence of the results has been found in some of the test cases, but not all. Monotonously converging results are for example not found in the apparently simple case of homogeneous open channel flow.

So the results of this research confirm that numerical errors are an inherent part of the model, its implementation and the grid. An increase of the numerical resolution within the range of feasible resolutions does not necessarily reduce the error. Instead one can consider changes to the implementation of the model to improve its accuracy. One method of doing this is by a mathematical transformation of the $k-\varepsilon$ model to the $k-\tau$ model, which improves the accuracy for some cases of environmental friction dominated flows, while it attains a similar accuracy for other tested cases.
Recommendations regarding the implementation of turbulence models

The $k - \tau$ model shows a clear advantage over the $k - \varepsilon$ model in bed friction dominated flows. The model results with the $k - \tau$ model are less sensitive to the grid resolution and are better than the results with the $k - \varepsilon$ model at low resolution. The $k - \tau$ model has shown similar, or arguably better, results for the tested cases of buoyancy dominated flows.

There are some critical notes regarding the implementation of the $k - \tau$ model. Firstly, there is a lack of experience with the implementation. Further testing is required to establish whether the implementation is accurate and robust in complex 1D, 2D and 3D models. Secondly, the $k - \tau$ model is likely to yield worse results in existing calibrated model schematisations, because the coefficients are calibrated to give the best performance with the currently implemented turbulence model. A recalibration of the model may be required to obtain equally accurate results with the $k - \tau$ model. Finally, the improvements brought by the $k - \tau$ model are only small; 3% to 5% improvements in the prediction of the velocity were achieved in the bed friction dominated cases in this research. However, larger improvements are to be expected in the prediction of tracer quantities, such as salt and sediment. These arguments lead to the advise to not replace the $k - \varepsilon$ model by the $k - \tau$ model in existing modelling software.

There is a great opportunity to implement the $k - \tau$ model in new modelling software developments or together with major changes to an existing software package, such as the development of DFLOW-FM at Deltares. Few existing calibrated model schematisations exist in this case or existing model schematisations need to be recalibrated because of other major changes. The only argument against the $k - \tau$ model is then the lack of experience with the model.

The $k - \tau$ model that has been used here is identical to the $k - \varepsilon$ model in terms of the physics that is implemented. It can therefore be regarded as a different implementation of the $k - \varepsilon$ model. This would mean that model users still select to use the better known $k - \varepsilon$ model, while the model solves the transformation to the $k - \tau$ model. Such an approach could, however, lead to confusion. It is therefore recommended to provide the $k - \tau$ model as a separate option in numerical simulation packages.

It is recommended to use the Neumann boundary condition for $\varepsilon$ with the $k - \varepsilon$ model. This boundary condition yields a major improvement compared to the Dirichlet condition in bed friction dominated flows. The Neumann condition leads to a bad numerical approximation of the actual value of $\varepsilon$ at the boundary, but this only affects the flow and stratification in some specific cases.

The corrected Dirichlet boundary condition for $\varepsilon$ that is used in Delft 3D-FLOW is not recommended. It provides more accurate results than the original Dirichlet condition, but the convergence behaviour in the case of open channel flow is severe. In the present 1DV simulations, the corrected Dirichlet condition has no advantages over the Neumann condition, which is advised as the alternative. If one wants to use a Dirichlet condition for $\varepsilon$ it is recommended to look into the accuracy of a new correction to the Dirichlet condition that has been developed and is promising in stationary uniform open channel flow, but not better than the Neumann condition.

It is not recommended to use any variant of the $k - \omega$ model for bed friction dominated flows. The profile of $\omega$ in these flows is not accurately approximated on the numerical grid. There are no arguments against using the $k - \omega$ model for other situations and the version of the $k - \omega$ model that was used in this research performs similarly, or arguably better, than the $k - \varepsilon$ model.
Recommendations for further research

It is unfortunate that the ongoing debate on which turbulence model is best has focussed on the length-scale variable that should be chosen for the model. There is little reason to choose one variable over the other from a physical perspective. Indeed, the equation of any length-scale variable can always be transformed to a physically equivalent equation in another variable. The choice of variable is a useful instrument for improving the numerical implementation of a turbulence model. The use of $\tau$ is for example numerically better than $\varepsilon$ or $\omega$ in boundary friction dominated flows. If all two-equation turbulence models are transformed to the same variables, the only differences would be in the diffusive terms and coefficients.

For these reasons, the use of the general length-scale model is only recommended for research purposes. This model allows the user the freedom to choose an arbitrary length-scale variable. The freedom of the length-scale variable requires the user to understand how the choice of length-scale variable affects both the physical accuracy as well as the numerical accuracy and therefore requires an in-depth knowledge of turbulence modelling. The use of the automatic calibration procedure that chooses the length-scale of the GLS model is not recommended as it does not take numerical aspects into account.

It is recommended to take both physical and numerical considerations into account in deciding which diffusive terms to include certain in the length-scale equation (e.g. $D_{k\tau}$, $D_{kk}$). It is possible that the physical considerations that motivate the inclusion of such a term are compromised by numerical errors associated with the implementation of the term on coarse numerical grids. The opposite can also hold; numerical diffusion can also be required in order to obtain more accurate results. An example of this has been shown in Section 4.4 and Appendix E.

Little is known about the convergence behaviour of the turbulence models and how this is influenced by the numerical implementation. The results converge between 100 and 1000 layers in most cases that were tested in this study, which is beyond the generally employed resolution in 3D models. Convergence is therefore a relevant subject of study. Convergence does not seem to be guaranteed. In cases where the turbulence model does converge, monotonous convergence is not guaranteed. It is recommended to conduct further research into these convergence issues. A particular question of interest would be how the numerical implementation of the turbulence model affects the convergence behaviour. A starting point for such research would be to compare the convergence of the results of several cases in a number of numerical simulations systems.

The numerical errors associated with turbulence modelling have implications for the calibration of a model. If a model is calibrated on measurements, this means that the calibration compensates for the numerical error. Calibration parameters, such as the bed roughness, therefore only have a meaning in combination with a certain numerical model and grid resolution. This numerical error may behave very different from the physical system. This limits the predictive capability of the calibrated model. It is important to be aware that the calibration is tied to the model implementation and resolution and that the unknown behaviour of the numerical error reduces the accuracy of the model.


This appendix provides the details of the notation and derivations used in this thesis. Section A.1 provides a further explanation to the Einstein summation convention that is used in Chapters 1 and 2. The transformations from the \( k - \varepsilon \) model to the \( k - \omega \) and \( k - \tau \) models are presented in Sections A.2 and A.3. Finally, a new derivation is given of the inconsistency of the model parameters that was treated in Section 2.3.

A.1. Einstein convention

The Einstein notation convention is often used to shorten the mathematical notation of vector equations. To illustrate the method, let us consider two vectors in three-dimensional space \( u = (u_1, u_2, u_3) \) and \( x = (x_1, x_2, x_3) \). The Einstein convention prescribes that one should sum over indices that occur twice in one term. For example the index \( j \) occurs twice in the term \( u_j \frac{\partial u_i}{\partial x_j} \) and one should sum over \( j = 1, 2, 3 \), i.e.

\[
\frac{\partial u_i}{\partial x_j} = u_1 \frac{\partial u_i}{\partial x_1} + u_2 \frac{\partial u_i}{\partial x_2} + u_3 \frac{\partial u_i}{\partial x_3}, \quad \text{where } i \in \{1, 2, 3\}.
\]

Another example is the term \( R_{ij} \frac{\partial u_i}{\partial x_j} \), where \( R_{ij} \) is the \( 3 \times 3 \)-matrix of Reynolds stresses. Both \( i \) and \( j \) occur twice and the term can be expanded to

\[
R_{ij} \frac{\partial u_i}{\partial x_j} = R_{1,1} \frac{\partial u_1}{\partial x_1} + R_{1,2} \frac{\partial u_1}{\partial x_2} + R_{1,3} \frac{\partial u_1}{\partial x_3} + R_{2,1} \frac{\partial u_2}{\partial x_1} + R_{2,2} \frac{\partial u_2}{\partial x_2} + R_{2,3} \frac{\partial u_2}{\partial x_3} + R_{3,1} \frac{\partial u_3}{\partial x_1} + R_{3,2} \frac{\partial u_3}{\partial x_2} + R_{3,3} \frac{\partial u_3}{\partial x_3}.
\]

A.2. Derivation of \( \omega \)

The version of the \( k - \omega \) model that is used in this thesis is transformed from the \( k - \varepsilon \) model. We will show the derivation of the \( \omega \)-equation from the \( \varepsilon \)-equation. The following definitions will be used:

\[
\omega = \frac{1}{c_\mu} \frac{\varepsilon}{k},
\]

\[
\nu^k = \nu + \frac{\nu_t}{\sigma_k},
\]

\[
\nu^\varepsilon = \nu + \frac{\nu_\varepsilon}{\sigma_\varepsilon}.
\]
The $k$-equation and $\varepsilon$-equation are repeated from Equations 2.1 and 2.5:

\[
\frac{Dk}{Dt} = \frac{\partial}{\partial x_j} \left( \left( \nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) + \frac{\nu_t M^2}{\sigma_k} - \frac{\nu_t N^2}{-B_k}, \quad D\omega = \frac{\partial}{\partial x_j} \left( \left( \nu + \frac{\nu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right) + \frac{\varepsilon}{k} c_{\varepsilon 1} \nu_t M^2 - \frac{\varepsilon}{k} c_{\varepsilon 3} \sigma_\rho N^2 - c_{\varepsilon 2} \frac{\varepsilon^2}{\sigma_\varepsilon}.
\]

First the definition of $\omega$ is substituted in the $\varepsilon$-equation

\[
\frac{D}{Dt} (c_\mu \omega) = c_\mu \frac{\partial}{\partial x_j} \left( \nu^e \frac{\partial}{\partial x_j} (k \omega) \right) + c_\mu \omega (c_{\varepsilon 1} P_k + c_{\varepsilon 3} B_k - c_{\varepsilon 2} c_\mu k \omega).
\]

This is then rewritten by using the product rule for differentiation and by substituting the TKE-equation.

\[
\frac{\omega}{k} \frac{D}{Dt} k + \frac{D}{Dt} \omega = D_\varepsilon + \omega (c_{\varepsilon 1} P_k + c_{\varepsilon 3} B_k - c_{\varepsilon 2} c_\mu k \omega),
\]

\[
\frac{k}{\omega} \frac{D}{Dt} \omega = \frac{1}{\omega} D_\varepsilon + c_{\varepsilon 1} P_k + c_{\varepsilon 3} B_k - c_{\varepsilon 2} c_\mu k \omega - D_k - P_k - B_k + c_\mu k \omega,
\]

\[
= \frac{1}{\omega} D_\varepsilon - D_k + (c_{\varepsilon 1} - 1) P_k + (c_{\varepsilon 3} - 1) B_k - (c_{\varepsilon 2} - 1) c_\mu k \omega.
\]

The diffusion terms $D_\varepsilon$ and $D_k$ can be expanded to

\[
\frac{\omega}{k} \left( \frac{1}{\omega} D_\varepsilon - D_k \right) = \frac{\partial}{\partial x_j} \left( \nu^e \frac{\partial}{\partial x_j} \omega \right) + \frac{2}{k} \nu^e \frac{\partial}{\partial x_j} \frac{\partial k}{\partial x_j} + \frac{\omega}{k} \frac{\partial}{\partial x_j} \left( (\nu^e - \nu^k) \frac{\partial k}{\partial x_j} \right).
\]

The resulting equation for $\omega$ is

\[
\frac{D}{Dt} \omega = \frac{\partial}{\partial x_j} \left( \nu^e \frac{\partial}{\partial x_j} \omega \right) + \frac{2}{k} \nu^e \frac{\partial}{\partial x_j} \frac{\partial k}{\partial x_j} + \frac{\omega}{k} \frac{\partial}{\partial x_j} \left( \left( \frac{1}{\sigma_\varepsilon} - \frac{1}{\sigma_k} \right) \nu_t \frac{\partial k}{\partial x_j} \right) + \cos_{\varepsilon 1} (c_{\varepsilon 1} - 1) P_k + \cos_{\varepsilon 3} (c_{\varepsilon 3} - 1) B_k - c_\mu (c_{\varepsilon 2} - 1) \omega^2.
\]

### A.3. Derivation of $\tau$

The equation for $\tau$ can be derived from the $\varepsilon$-equation in a similar manner as in the previous section. The following definitions will be used.

\[
\tau = \frac{k}{\varepsilon}, \quad \nu^k = \nu + \frac{\nu_t}{\sigma_k}, \quad \nu^e = \nu + \frac{\nu_t}{\sigma_\varepsilon}.
\]

The definition of $\tau$ is substituted in the equation for $\varepsilon$ to obtain

\[
\frac{D}{Dt} \left( \frac{k}{\tau} \right) = \frac{\partial}{\partial x_j} \left( \nu^e \frac{\partial}{\partial x_j} \left( \frac{k}{\tau} \right) \right) + \frac{1}{\tau} (c_{\varepsilon 1} P_k + c_{\varepsilon 3} B_k - c_{\varepsilon 2} \frac{k}{\tau}).
\]
This is again rewritten by using the product rule for differentiation and by substituting the TKE-equation, Equation 2.1.

\[
\frac{-k}{\tau^2} \frac{D\tau}{Dt} + \frac{1}{\tau} \frac{Dk}{Dt} = D_x + \frac{1}{\tau} \left( c_{11} P_k + c_{13} B_k - c_{22} \frac{k}{\tau} \right),
\]

\[
-\frac{k}{\tau} \frac{D\tau}{Dt} = \tau D_x + c_{11} P_k + c_{13} B_k - c_{22} \frac{k}{\tau} - D_k - P_k - B_k + \frac{k}{\tau},
\]

\[
= \tau D_x - D_k + (c_{11} - 1)P_k + (c_{13} - 1)B_k - (c_{22} - 1)K. 
\]

The diffusion terms \( D_x \) and \( D_k \) can be expanded to

\[
\tau D_x - D_k = -\tau \frac{\partial}{\partial x_j} \left( \nu^e \frac{k}{\tau^2} \frac{\partial \tau}{\partial x_j} \right) + \tau \frac{\partial}{\partial x_j} \left( \nu^e \frac{1}{\tau} \frac{\partial k}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left( \nu^e \frac{\partial k}{\partial x_j} \right).
\]

The first term in this group of diffusion terms can be rewritten further to

\[
-\tau \frac{\partial}{\partial x_j} \left( \nu^e \frac{k}{\tau^2} \frac{\partial \tau}{\partial x_j} \right) = -k \frac{\partial}{\partial x_j} \left( \nu^e \frac{\partial \tau}{\partial x_j} \right) - \frac{1}{\tau} \nu^e \frac{\partial \tau}{\partial x_j} \frac{\partial k}{\partial x_j} + 2 \frac{k}{\tau^2} \nu^e \frac{\partial \tau}{\partial x_j} \frac{\partial \tau}{\partial x_j}.
\]

The second term can similarly be rewritten to

\[
\tau \frac{\partial}{\partial x_j} \left( \nu^e \frac{1}{\tau} \frac{\partial k}{\partial x_j} \right) = \frac{\partial}{\partial x_j} \left( \nu^e \frac{\partial k}{\partial x_j} \right) - \frac{1}{\tau} \nu^e \frac{\partial k}{\partial x_j} \frac{\partial \tau}{\partial x_j}.
\]

So that the diffusion term becomes

\[
\tau D_x - D_k = -k \frac{\partial}{\partial x_j} \left( \nu^e \frac{\partial \tau}{\partial x_j} \right) - \frac{2}{\tau} \nu^e \frac{\partial \tau}{\partial x_j} \frac{\partial k}{\partial x_j} + 2 \frac{k}{\tau^2} \nu^e \frac{\partial \tau}{\partial x_j} \frac{\partial \tau}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \nu^e \frac{\partial k}{\partial x_j} \right).
\]

The resulting equation for \( \tau \) is

\[
\frac{D\tau}{Dt} = \frac{\partial}{\partial x_j} \left( \nu^e \frac{\partial \tau}{\partial x_j} \right) + 2 \nu^e \frac{\partial \tau}{\partial x_j} \frac{\partial k}{\partial x_j} - \frac{2}{\tau} \nu^e \frac{\partial \tau}{\partial x_j} \frac{\partial k}{\partial x_j} - \frac{1}{\tau} \nu^e \frac{\partial \tau}{\partial x_j} \frac{\partial \tau}{\partial x_j} + \frac{\tau}{k} \frac{\partial}{\partial x_j} \left( \frac{1}{\sigma_k} - \frac{1}{\sigma_k} \right) \left( \nu^e \frac{\partial k}{\partial x_j} \right)
\]

\[
= \frac{\tau}{k} (c_{11} - 1)P_k - \frac{\tau}{k} (c_{13} - 1)B_k + (c_{22} - 1).
\]

### A.4. Inconsistency of model parameters

It can be derived that the generally accepted values of the parameters in the \( k - \varepsilon \) model are inconsistent. This inconsistency is discussed e.g. by Umlauf (2001) who refers to Abid and Speziale (1993) and Launder et al. (1975). Below, a new derivation of the inconsistency is presented.

Consider the near-bed layer of a stationary, uniform, homogeneous flow. The flow velocity is assumed to be logarithmic in vertical direction. The velocity is assumed to have the following profile

\[
u(z) = \frac{u^*}{\kappa} \ln \left( \frac{z}{z_0} \right).
\]

This is still consistent with the velocity profile of Equation 1.13, which adds 9 to the term in the \( \ln \), by shifting the definition of \( z \). The above profile is used in this derivation for simplicity.

The \( k - \varepsilon \) model is

\[
\frac{\partial}{\partial z} \left( \frac{\nu_k}{\sigma_k} \frac{\partial k}{\partial z} \right) + \nu_k M^2 - \varepsilon = 0,
\]

\[
\frac{\partial}{\partial z} \left( \frac{\nu_e}{\sigma_e} \frac{\partial \varepsilon}{\partial z} \right) + \frac{\varepsilon}{k} (c_1 M^2 - c_2 \varepsilon) = 0,
\]
where
\[
M^2 = \left( \frac{\partial u}{\partial z} \right)^2, \\
= \left( \frac{u_*}{\kappa} \right)^2 \frac{1}{z^2}, \quad \text{and} \\
\nu_t = \frac{k^2}{\varepsilon}.
\]

It is assumed that the solutions have the simple form
\[
k = \mu z^\alpha \quad \text{where } \mu \neq 0, \\
\varepsilon = \lambda z^\beta \quad \text{where } \lambda \neq 0.
\]

(A.1)

It will be verified that this assumption is consistent with the assumption that the Reynolds stress is constant close to the bed, which is a generally adopted assumption (Pope, 2000).

These profiles can be substituted in the \( k - \varepsilon \) equations to yield
\[
(3\alpha - \beta - 1)\alpha \frac{c_\mu}{\sigma_k} \frac{\mu^3}{\lambda^2} z^{3\alpha - 2} + c_\mu \frac{\mu^2}{\lambda} \left( \frac{u_*}{\kappa} \right)^2 z^{2\alpha - 2} - \lambda \beta^2 = 0, \\
(2\alpha - 1)\beta \frac{c_\mu}{\sigma_\varepsilon} \mu^2 z^{3\alpha - 2} + c_1 c_\mu \mu \left( \frac{u_*}{\kappa} \right)^2 z^{2\alpha - 2} - c_2 \lambda^2 \frac{z^{2\beta}}{\mu} = 0.
\]

The unique solution to this equation is
\[
\alpha = 0, \quad \beta = -1 \\
\mu = \pm (c_1 - c_2) \sigma_\varepsilon \left( \frac{u_*}{\kappa} \right)^2, \\
\lambda^2 = c_\mu \mu^2 \left( \frac{u_*}{\kappa} \right)^2.
\]

The profiles of \( k \) and \( \varepsilon \) are then
\[
k(z) = -\sigma_\varepsilon \left( \frac{u_*}{\kappa} \right)^2 (c_1 - c_2) \approx 3.7 u_*^2, \quad \text{(A.2)} \\
\varepsilon(z) = -\sqrt{c_\mu} \sigma_\varepsilon \left( \frac{u_*}{\kappa} \right)^3 (c_1 - c_2) \frac{1}{z} \approx 2.7 \frac{u_*^3}{z}. \quad \text{(A.3)}
\]

The resulting profile of the eddy viscosity is
\[
\nu_t = -\sqrt{c_\mu} \sigma_\varepsilon (c_2 - c_1) \left( \frac{u_*}{\kappa} \right) z.
\]

The assumptions and results above are consistent with the assumption that production of TKE balances dissipation of TKE and the law of the wall. Using this, the usual boundary conditions for TKE and \( \varepsilon \) can be derived. These boundary conditions are:
\[
k(z) = \frac{u_*^2}{\sqrt{c_\mu}} \approx 3.3 u_*^2, \quad \text{(A.4)} \\
\varepsilon(z) = \frac{u_*^3}{\kappa z} \approx 2.4 \frac{u_*^3}{z}. \quad \text{(A.5)}
\]
The so called compatibility relation is found by relating A.2 to A.4 and A.3 to A.5. This relation reads

\[ \sqrt{c_\mu} = \frac{\kappa^2}{\sigma_\varepsilon (c_2 - c_1)} \].

However, with the general parameter values for the \( k - \varepsilon \) model this relation is not satisfied as

\[ \sqrt{c_\mu} = 0.30 \] and
\[ \frac{\kappa^2}{\sigma_\varepsilon (c_2 - c_1)} = 0.27 \].

**A.4.1. Verification of the assumptions**

The assumed profiles of \( k \) and \( \varepsilon \) can be verified by checking the implications that the above calculated \( \nu_t \) has on the flow. We therefore use the relation

\[ \nu_t \frac{\partial u}{\partial z} = R_{xz} \].

The original logarithmic velocity profile is retrieved if the Reynolds stress \( R_{xz} \) is constant. Integrating \( \frac{\partial u}{\partial z} \) from \( z_0 \) to \( z \) yields

\[ u(z) = -\frac{\kappa R_{xz}}{\sqrt{c_\mu \sigma_\varepsilon (c_2 - c_1) u_*}} \ln \left( \frac{z}{z_0} \right) \].

The original velocity profile is retrieved if

\[ R_{xz} = -\sqrt{c_\mu \sigma_\varepsilon (c_2 - c_1)} \left( \frac{u_*}{\kappa} \right)^2 = u_*^2 \]

which is indeed the near-bed shear stress.

So the assumed profiles are consistent with the constant stress assumption and therefore realistic.
Further analysis of the open channel flow case

This appendix provides some additional analyses of the open channel flow case that help to further understanding this case. Firstly, we will present some additional boundary conditions of the $k$ – $\varepsilon$ model than the Dirichlet and Neumann conditions that were presented in Section 4.1. The error that is caused by the Dirichlet condition can be measured and can be minimised by adapting the boundary condition. Two such adaptations will be tested together with an adaptation to the Neumann condition.

Secondly, we will spend some more attention on the wake law and roughness formulation and the implications it has on the conversion from a 1D or 2D horizontal model to a model that resolves the vertical dimension.

Finally, we will show that part of the error in the determination of the velocity is irrespective of the turbulence model, but originates from the process of numerically integrating $\frac{\partial u}{\partial z}$ to obtain $u$. This error depends on the roughness and roughness formulation.

B.1. Analysis of boundary conditions for $\varepsilon$

We have seen that the Dirichlet boundary condition results in large errors in the open channel flow simulation. The reason for this is that the Dirichlet boundary condition yields the wrong value of the flux of $\varepsilon$ in the lowest grid cell. The exact flux can be determined by applying the law of the wall. This yields

$$
\frac{\nu}{\kappa} \frac{\partial \varepsilon}{\partial z} \bigg|_{z = \frac{1}{2} \Delta z} = -\frac{u^4}{9 \Delta z + \frac{1}{2} \Delta z}.
$$

(B.1)

Similarly we have

$$
\nu \big|_z = (z + 9 \Delta z)\kappa |u_*|,
$$

$$
\varepsilon \big|_z = \frac{|u_*|^3}{(z + 9 \Delta z)\kappa}.
$$

B.1.1. Error caused by the normal Dirichlet condition

It can now be derived how well the flux is approximated by the Dirichlet boundary condition of the $\varepsilon$-equation. The normal implementation of the flux in the term $D_{\varepsilon}$ equals

$$
\frac{\nu}{\kappa} \frac{\partial \varepsilon}{\partial z} \bigg|_{J-1/2} = \frac{1}{2} (\nu_{J-1}^n + \nu_{J}^n) \frac{\varepsilon_{J-1}^{n+1} - \varepsilon_J^{n+1}}{h_I}.
$$
This can be rewritten by using the above expressions for \( \nu_t \) and \( \varepsilon \).

\[
\nu_t \left. \frac{\partial \varepsilon}{\partial z} \right|_{I-1/2} = \left( (9z_0 + \Delta z)\kappa \left| u_* \right| + 9z_0 \kappa \left| u_* \right| \right) \frac{1}{h_I} \left( \frac{\left| u_* \right|^3}{(9z_0 + \Delta z)\kappa} - \frac{\left| u_* \right|^3}{9z_0 \kappa} \right)
\]

\[
= u_*^t (9z_0 + \frac{1}{2}\Delta z) \frac{1}{\Delta z} \left( \frac{9z_0}{(9z_0 + \Delta z)9z_0} - \frac{9z_0 + \Delta z}{(9z_0 + \Delta z)9z_0} \right)
\]

\[
= -u_*^t \left( \frac{9z_0 + \frac{1}{2}\Delta z}{(9z_0 + \Delta z)9z_0} \right).
\]

The error between the exact flux B.1 and the numerical flux reduces to a simple expression if it is assumed that \( \Delta z \gg 9z_0 \). The error is

\[
\nu_t \left. \frac{\partial \varepsilon}{\partial z} \right|_{z=\frac{1}{2}\Delta z} - \nu_t \left. \frac{\partial \varepsilon}{\partial z} \right|_{I-1/2} \approx u_*^t \left( \frac{1}{2\Delta z} - \frac{\frac{1}{2}\Delta z}{9z_0 \Delta z} \right)
\]

\[
\approx \frac{u_*^t}{9z_0}.
\]

This error is generally large, because \( 9z_0 \) is small.

**B.1.2. Correction by Van Kester (1994)**

This error can be reduced by adjusting the discretisation of the flux near the bed. This approach has been taken by Van Kester (1994) and implemented in Delft 3D-FLOW. The adjustment to the flux implementation reads

\[
\nu_t \left. \frac{\partial \varepsilon}{\partial z} \right|_{z=\frac{1}{2}\Delta z} = \nu_t \left. \frac{\partial \varepsilon}{\partial z} \right|_{I-1/2} \text{\ changed to } \frac{\varepsilon_{I+1}^{n+1} - \varepsilon_I^{n+1}}{h_I}.
\]

(B.2)

One can again derive a simple expression for the difference between the exact flux and the numerical approximation of the flux:

\[
\nu_t \left. \frac{\partial \varepsilon}{\partial z} \right|_{z=\frac{1}{2}\Delta z} - \nu_t \left. \frac{\partial \varepsilon}{\partial z} \right|_{I-1/2} = \frac{u_*^t}{9z_0 + \frac{1}{2}\Delta z} \approx \frac{u_*^t}{\Delta z} \text{ assuming } \Delta z \gg 9z_0.
\]

This error is much smaller than the error in the original implementation assuming \( \Delta z \gg 9z_0 \).

**B.1.3. Further improvement of the Dirichlet condition**

The approximation of the flux can be improved further by setting the error between the exact and numerical flux to zero and deriving the corresponding expression for \( \nu_t \) that should be used in the formulation of the flux.

We therefore set

\[
\nu_t \left. \frac{\partial \varepsilon}{\partial z} \right|_{z=\frac{1}{2}\Delta z} - \nu_t \left. \frac{\partial \varepsilon}{\partial z} \right|_{I-1/2} = 0
\]

\[
\Leftrightarrow \frac{u_*^t}{9z_0 + \frac{1}{2}\Delta z} + \frac{u_*^t}{\kappa} \frac{1}{(9z_0 + \Delta z)9z_0} = 0.
\]
This equation can be solved to find the optimal formulation of the eddy viscosity.

\[ \nu_t = |u_*| \kappa \frac{(9z_0 + \Delta z)9z_0}{9z_0 + \frac{1}{2}\Delta z} \approx 2|u_*|\kappa 9z_0 \quad \text{assuming } \Delta z >> 9z_0. \]

So the implementation of the flux changes to

\[ \nu_t \left. \frac{\partial \varepsilon}{\partial z} \right|_{z=\frac{1}{2} \Delta z} = \frac{2\nu_{t,I}}{h_I} (\varepsilon_{n+1}^{I-1} - \varepsilon_{n+1}^I). \quad (B.3) \]

The fact that the error between the exact and numerical flux near the bed is zero does not mean that the error in the open channel flow case also vanishes. The flux at other levels than the bottom cell also contains errors. It would not be realistic to adjust the implementation of the flux in a similar manner at these levels, because the law of the wall is no longer valid here. Both corrected formulations yield much better results than the original Dirichlet boundary condition as will be shown below.

### B.1.4. Alternative Neumann boundary condition

Burchard and Petersen (1999) show that a Neumann boundary condition yields significantly better results than the Dirichlet boundary condition in approximating boundary layer flow with few layers. In this section an improved method for determining the Neumann boundary condition is presented. The generally used form of the Neumann boundary condition is

\[ \left. \frac{\partial \varepsilon}{\partial z} \right|_{z=\frac{1}{2} \Delta z} = \frac{|u_*|}{\kappa(\frac{1}{2} \Delta z + 9z_0)^2}. \]

An improvement can be derived by going back to the derivation of this boundary condition. The boundary condition is derived from the relation of \( \varepsilon \) to a typical turbulent length-scale and the law of the wall;

\[ \varepsilon(z) = c_{\mu}^{3/4} \frac{k(z)^{3/2}}{l} = \frac{c_{\mu}^{3/4}}{\kappa(z + 9z_0)} k(z)^{3/2}. \]

The boundary condition follows from taking the derivative with respect to \( z \). This yields

\[ \frac{\partial \varepsilon}{\partial z} = \frac{3^{3/4}}{\kappa} \left( \frac{3 \sqrt{k(z) k'(z)} - k(z)^{3/2} (9z_0 + z)}{(9z_0 + z)^2} \right). \]

The discretisation of this boundary condition reads

\[ \left. \frac{\partial \varepsilon}{\partial z} \right|_{z=\frac{1}{2} \Delta z} = \frac{3^{3/4}}{\kappa} \left( \frac{3 \sqrt{\frac{1}{2} (k_{I-1} + k_I)(k_{I-1} - k_I)} (9z_0 + \frac{1}{2} \Delta z) \Delta z}{(9z_0 + \frac{1}{2} \Delta z)^2} - \frac{(\frac{1}{2} (k_{I-1} + k_I))^{3/2} (9z_0 + \frac{1}{2} \Delta z)^2}{(9z_0 + \frac{1}{2} \Delta z)^2} \right). \]

This boundary condition is only applied at the bed. A similar approach might be valid at the surface.

### B.1.5. Results with the alternative boundary conditions

The boundary conditions are applied to the open channel flow case of Section 4.1. The results are presented in Figure 31. The boundary condition of Van Kester (1994) is called ‘Dirichlet JvK’ and the results compare well to the results of Delft 3D-FLOW which employs the same boundary conditions. The results of Delft 3D-FLOW are only included up to 20 layers.

The newly defined ‘optimal’ correction to the Dirichlet condition is denoted by ‘Dirichlet YMD’. This condition is better than the JvK condition as the error is a bit smaller and the results converge monotonously. The Neumann condition, however, is still generally better than the any of the Dirichlet conditions. The newly defined Neumann condition ‘Neuman YMD’ is only slightly better than the original.
B.2. Conversion of Chézy roughness to $z_0$

The Chézy roughness and $c_f$ roughness parameter are a roughness parametrisations that were developed for 1DH and 2DH modelling. These roughness parameters need to be converted to a $z_0$ roughness value for use in vertical dimension resolving models. Such conversion needs the assumption of a vertical velocity profile. To this end it is generally assumed that the velocity profile is logarithmic. However, this assumed profile does not correspond to measurements and output of the turbulence models. As a result, the average velocity of a 3D computation does not correspond to the Chézy equation. There are two reasons for this discrepancy:

1. the two-equation turbulence models do not reproduce the logarithmic profile, but are closer to the wake law suggested by measurements, and
2. the location of $z = 0$ is defined differently to the implicit definition in the Chézy equation.

The contributions of both sources are quantified below. We will illustrate this by using the Chézy roughness value. Similar derivations hold for the $c_f$ roughness value.

If one assumes that the result of the turbulence models does indeed correspond to the wake law, the velocity profile from the 1DV calculation corresponds to

$$u(z) = \frac{u_*}{\kappa} \ln \left( \alpha + \frac{z}{z_0} \right) + u_* \mathcal{W}(z),$$

where $\alpha$ parametrises the location of $z = 0$ and Coles’ wake function $\mathcal{W}$ is given by (Coles, 1956)

$$\mathcal{W}(z) = \frac{2\pi}{\kappa} \sin^2 \left( \frac{1}{2} \frac{z}{h} \right).$$

The average velocity is obtained by integrating this velocity profile from $z = 0$ to $z = h$ and dividing by $h$

$$\bar{u} = \frac{u_*}{\kappa} \left( \frac{z_0}{h} \alpha \ln \left( 1 + \frac{h}{\alpha z_0} \right) + \ln \left( \alpha + \frac{h}{z_0} \right) - 1 \right) + \frac{u_* \Pi}{\kappa}. \tag{B.4}$$

This equation predicts the same average velocity as the Chézy equation if $\alpha = 0$ and $\Pi = 0$.

B.2.1. Influence of the wake law on $q^*$

The wake law adds a contribution $\frac{u_* \Pi}{\kappa}$ to the average velocity in equation B.4. The addition to the dimensionless discharge $\Delta q^*$ is then

$$\Delta q^* = \frac{u_* \Pi}{\kappa} \frac{1}{C \sqrt{h \frac{\partial C}{\partial z}}}. $$
According to the Chézy equation and the logarithmic velocity profile the following relations hold

\[ C = \frac{\sqrt{g}}{\kappa} \left( \ln \left( \frac{h}{z_0} \right) - 1 \right), \]

\[ \bar{u} = \frac{u_s}{\kappa} \left( \ln \left( \frac{h}{z_0} \right) - 1 \right), \]

which together results in

\[ \frac{C}{\sqrt{g}} = \frac{\bar{u}}{u_s}. \]

Substituting this yields the following equation for \( \Delta q^* \)

\[ \Delta q^* = \frac{\bar{u}}{C} \frac{\sqrt{g}}{\kappa C} \Pi \]

\[ = (1 + \Delta q^*) \frac{\sqrt{g}}{\kappa C} \Pi \]

\[ = \frac{\sqrt{g}}{\kappa C} \Pi + \mathcal{O} \left( \left( \frac{\sqrt{g}}{\kappa C} \Pi \right)^2 \right). \]

This adds 2.5% to the dimensionless discharge in the case of Section 4.1.

### B.2.2. Influence of \( \alpha \) on \( q^* \)

It was explained in Section 1.4 that a value of \( \alpha = 0 \) is not realistic and principally wrong on the interval \([0, z_0)\), because the flow would reverse there. We use \( \alpha = 9 \), which has the same effect as moving the \( z \)-coordinate with \( 9z_0 \) compared to \( \alpha = 0 \). So the integration of the velocity profile with \( \alpha = 9 \) from \( z = 0 \) to \( z = h \) equals the integration of the profile with \( \alpha = 0 \) from \( z = 9z_0 \) to \( z = h + 9z_0 \). We therefore ‘miss’ the discharge in the bottom \( 9z_0 \) metres and find an extra \( 9z_0 \) metres at the top of the water column.

The net difference of the average velocity between the profiles with \( \alpha = 0 \) and \( \alpha = 9 \) is

\[ \Delta u = \bar{u}_{\alpha=9} - \bar{u}_{\alpha=0} = \frac{u_s}{\kappa} \left( \frac{9z_0}{h} \ln \left( \frac{1 + \frac{h}{9z_0}}{\frac{h}{9z_0} + 1} \right) \right) \]

\[ \approx \frac{u_s}{\kappa} \frac{9z_0}{h} \ln \left( \frac{h}{9z_0} \right) \quad \text{if} \quad z_0 \ll h. \]

The difference in dimensionless discharge \( q^* \) is

\[ \Delta q^* \approx \frac{9z_0}{h} \quad \text{if} \quad z_0 \ll h. \]

The influence of \( \alpha \) is thus typically small if the roughness height is small compared to the water depth. The difference is less than 1% in the case of Section 4.1.

### B.3. Difference operator for logarithmic profile

The momentum equation solves for \( \frac{\partial u}{\partial z} \). This gradient is then integrated numerically to obtain \( u \). This integration operator causes the errors in the velocity with in the case of the small bottom cell in Section 4.1. It also produces an error for equidistant grids. This error depends on the roughness formulation and the grid resolution and is quantified below.

A logarithmic profile over a rough bed is of the form

\[ u(z) = \ln(\alpha + \beta z), \]
where $\alpha$ and $\beta$ are positive constants.

The error caused by the numerical integration can be quantified as the difference between the exact average velocity and the numerically calculated average velocity. The exact average velocity can be calculated from the above logarithmic profile. The numerically calculated average velocity is calculated by taking the exact derivative of the logarithmic profile and then taking the numerical integral of this derivative. In a mathematical notation, the error $\Delta \pi$ reads

$$\Delta \pi = \pi_{\text{exact}} - \pi_{\text{numerical}}$$

$$= \frac{1}{I} \sum_{i=1}^{I} \left( u_{i-1/2} - J_i \left( \frac{\partial u}{\partial z} \right) \right),$$

where the numerical integration operator, $J_i$, on a staggered grid is given by

$$J_i \left( \frac{\partial u}{\partial z} \right) = u_{1/2} + \sum_{i=1}^{I} \Delta z \frac{\partial u}{\partial z} \bigg|_i,$$

and where $u_{1/2}$ is given by a boundary condition.

Table B.1 shows the values of $\Delta q^* = \Delta \pi/\pi$ for the stationary flow case. Note that the numerically calculated velocity is smaller than the exact velocity. The error is rather small, but does not disappear for $\alpha = 0$. This is another reason for not using $\alpha = 0$.

<table>
<thead>
<tr>
<th>Number of layers</th>
<th>$\Delta q^*$ using $\alpha = 9z_0$</th>
<th>$\Delta q^*$ using $\alpha = z_0$</th>
<th>$\Delta q^*$ using $\alpha = 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.2%</td>
<td>1.3%</td>
<td>1.3%</td>
</tr>
<tr>
<td>20</td>
<td>1.3%</td>
<td>1.4%</td>
<td>1.4%</td>
</tr>
<tr>
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<td>1.2%</td>
<td>1.4%</td>
<td>1.4%</td>
</tr>
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</tr>
<tr>
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<td>0.2%</td>
<td>1.0%</td>
<td>1.5%</td>
</tr>
<tr>
<td>10,000</td>
<td>0.0%</td>
<td>0.1%</td>
<td>1.5%</td>
</tr>
</tbody>
</table>

Table B.1: Error for the open channel flow case which is due to the numerical integration.
The $k - \omega$ model in the tidal flow case

The $k - \omega$ model was not treated in Section 4.2. The results of this model will therefore be presented in this appendix. The time series of $u_*$ is plotted in Figure 32. The results of the Dirichlet condition show a small disturbance of the flow after slack tide. This is not as worse as with the Dirichlet condition of the $k - \varepsilon$ model. The results with the Neumann condition show no lag in the turbulence production after slack tide.

![Figure 32: Time series of $u_*$ using 10 layers and two boundary conditions of the $k - \omega$ models.](image)

The figure also shows that the amplitude of $u_*$ is underpredicted if the Dirichlet condition is used. This agrees with the result of the open channel flow case, which shows that the Dirichlet condition is inaccurate for predicting the velocity profile.
Wind over stable stratification: analytical solution & critical Richardson number

The case of wind straining over an infinitely deep stably stratified lake was introduced in Section 4.3. The numerical experiments show that the diffusive terms are negligibly small, but that they must be included to capture the effect of the deepening of the mixed layer. We will derive analytical solutions that use these observations. It will be shown in Section D.1 that the equation for the rate of deepening can be approximated closely by an analytical solution. Section D.2 will show some properties of the flow in this condition of local equilibrium. It will be shown that the critical Richardson number governs the flow in local equilibrium conditions.

D.1. Solution for $D_m(t)$

The depth of wind influence propagates as a shock wave down through the water column. The profile of TKE is approximately linear in the mixed layer with $k = \frac{u^2 \nu \sigma}{\sqrt{c}}$ at the surface $z = h$ and $k = 0$ at the mixed-layer depth $h - D_m$. The TKE is zero below this level if the lake is considered infinitely deep. The TKE profile is thus given by

$$k(z, t) = \begin{cases} \frac{u^2 \nu(z-h+D_m(t))}{\sqrt{c}} & \text{if } z > h - D_m \\ 0 & \text{if } z \leq h - D_m \end{cases} \quad (D.1)$$

The Rankine-Hugoniot shock conditions can be used to determine the velocity of propagation of the shock. We therefore integrate the TKE equation over the shock from $z_1 < D_m$ to $z_2 > D_m$, and separate the domain into the parts $[z_1, D_m(t)]$ and $[D_m(t), z_2]$. The TKE profile is a continuously differentiable function in both domains so that it is allowed to interchange integration and differentiation. The resulting equation is

$$\frac{\partial}{\partial t} \int_{z_1}^{D_m(t)} k \, dz + \frac{\partial}{\partial t} \int_{D_m(t)}^{z_2} k \, dz = \int_{z_1}^{z_2} \frac{\partial}{\partial z} \left( \frac{\nu_t \partial k}{\sigma_k \partial z} \right) + P + B - \varepsilon \, dz.$$

The numerical results show that local equilibrium holds approximately, i.e. $P + B - \varepsilon = 0$. The equation now reduces to

$$\frac{\partial}{\partial t} \int_{z_1}^{D_m(t)} k \, dz + \frac{\partial}{\partial t} \int_{D_m(t)}^{z_2} k \, dz = \nu_t \frac{\partial k}{\sigma_k \partial z} \bigg|_{z_1}^{z_2}.$$
The Rankine-Hugoniot shock equations are obtained using Leibniz’ rule and by letting $z_1, z_2 \to D_m(t)$. The equations yield an ordinary differential equation for the propagation velocity of the shock

$$\frac{\partial D_m(t)}{\partial t} = \frac{\left( \frac{\nu}{\sigma_k} \frac{\partial k}{\partial z} \right)_{z_2} - \left( \frac{\nu}{\sigma_k} \frac{\partial k}{\partial z} \right)_{z_1}}{k_{z_2} - k_{z_1}}.$$

The velocity of the shock follows from the TKE profile D.1 and the profile for $\tau$ D.3, which is derived in the next section;

$$\frac{\partial D_m(t)}{\partial t} = c_{\mu} \tau(t, z_1) \frac{\partial k}{\partial z}(t, z_1) = \frac{u_{*, w}^2}{\sigma_k} \left( \frac{N^2}{\sigma_{\rho}} \left( \frac{c_{3, \tau} - c_{1, \tau}}{c_{1, \tau} - c_{2, \tau}} \right) \right)^{-1/2} \frac{1}{D_m(t)}.$$

The solution is obtained by using separation of variables:

$$D_m(t) = \sqrt{\frac{2}{\sigma_k}} \left( \frac{c_{1, \tau} - c_{2, \tau}}{\sigma_{\rho} c_{3, \tau} - c_{1, \tau}} \right)^{1/4} u_{*, w} \sqrt{\frac{t}{N}} = 0.98 u_{*, w} \sqrt{\frac{t}{N}}.$$

This is a fairly close approximation to the expression by Price (1979), who finds 1.05 as a coefficient instead of 0.98.

**D.2. Local equilibrium & critical Richardson number**

The two-equation turbulence models can be solved analytically if the diffusion terms are neglected. This is approximately true in the case of wind over a stable stratified lake. The structure of the $k - \tau$ model is especially suited for constructing this analytical solution, because the $\tau$-equation decouples from the TKE equation. We therefore consider the $k - \tau$-model without diffusive terms and with fixed values of $M^2$ and $N^2$. The system is of the form

$$\frac{\partial k}{\partial t} = \alpha k \tau - \beta \frac{k}{\tau},$$

$$\frac{\partial \tau}{\partial t} = \gamma \tau^2 - \delta.$$

The constants $\alpha, \beta, \gamma, \delta$ are given by

$$\alpha = c_{\mu} M^2 - c_{\mu} \frac{N^2}{\sigma_{\rho}},$$

$$\beta = 1,$$

$$\gamma = c_{1, \tau} c_{\mu} M^2 - c_{3, \tau} c_{\mu} \frac{N^2}{\sigma_{\rho}},$$

$$\delta = c_{2, \tau}.$$
1. \((k, \tau) = \left(0, \sqrt{\frac{\beta}{\gamma}}\right)\); laminar flow,

2. \(k\) undetermined and \(\tau = \sqrt{\frac{\beta}{\gamma}} = \sqrt{\frac{\beta}{\gamma}}\).

The second equilibrium is called \textit{local equilibrium}. Note that this can only exist if \(\alpha\) is positive. It then implies that

\[
\begin{align*}
Ri_c &= \frac{N^2}{M^2} = \frac{\sigma_p}{c_3} \left( \frac{c_3 - c_1}{c_1 - c_2} \right), \quad \text{and} \\
\tau &= \left( \frac{c_2}{c_1} \frac{N^2}{\sigma_p} \left( \frac{c_3 - c_1}{c_1 - c_2} \right) \right)^{-1/2}.
\end{align*}
\]

The profile of \(\tau\) is a constant in local equilibrium.

The Richardson number in local equilibrium is called the critical Richardson number, because it marks a shift in the behaviour of the equations before equilibrium is reached. Turbulence decays on the long-term if \(Ri < Ri_c\) and it grows if \(Ri > Ri_c\).

This can be illustrated by solving the equations. The equation for \(\tau\) does not depend on \(k\) so that the equations can be solved consecutively. The solution to this system is

\[
\begin{align*}
\tau(t) &= \sqrt{\frac{\delta}{\gamma}} \tanh \left( \sqrt{\gamma \delta} \left( K_1 + t \right) \right), \\
k(t) &= K_2 \tanh \left( \sqrt{\gamma \delta} \left( K_1 + t \right) \right) \cosh \left( \sqrt{\gamma \delta} \left( K_1 + t \right) \right)^{\beta/\delta - \alpha/\gamma},
\end{align*}
\]

where \(K_1\) and \(K_2\) are constants depending on the initial conditions. The \(\tanh\)-function goes to 1 for \(t \to \infty\), while the \(\cosh\)-function goes to infinity. So the behaviour of the solution of \(k\) depends on the sign of the power \(\beta/\delta - \alpha/\gamma\):

\[
k(t) \rightarrow \begin{cases} 
0 & \text{if } \beta/\delta - \alpha/\gamma < 0 \\
K_2 & \text{if } \beta/\delta - \alpha/\gamma = 0 \\
\infty & \text{if } \beta/\delta - \alpha/\gamma > 0
\end{cases}.
\]

This can be rewritten to a condition on the Richardson number.

\[
k(t) \rightarrow \begin{cases} 
0 & \text{if } Ri < Ri_c \\
K_2 & \text{if } Ri = Ri_c \\
\infty & \text{if } Ri > Ri_c
\end{cases}.
\]

Note that the unstable case \(k \to \infty\) will not occur in practice, because the increasing amount of mixing will reduce the stratification and therefore the Richardson number. So if \(Ri > Ri_c\) the system is still likely to move towards the equilibrium \(Ri = Ri_c\).
Unstable stratification: sensitivity to implementation

The results of the case of unstable stratification of Section 4.4 can be very sensitive to small changes to the implementation. It was for example already explained that the boundary conditions have a significant effect on the response time of the models to the unstable stratification. We will show how the results change if a different implementation of the $D_{\tau \tau}$ term in the $k - \tau$ model is used in this appendix.

The alternative implementation of the $D_{\tau \tau}$ term uses central difference operators instead of upwind operators. We will first repeat the term

$$D_{\tau \tau} = 2 \frac{1}{\tau} \left( \nu + \nu_t \right) \frac{\partial \tau}{\partial x_j} \frac{\partial \tau}{\partial x_j}.$$

The alternative implementation reads

$$D_{\tau \tau,i}^{n} = 2 \left( \frac{k^n}{\sigma_{\tau}} \right) \frac{1}{4} \left( \frac{\tau^n_i - \tau^n_{i-1}}{h_{i+1}} + \frac{\tau^n_{i+1} - \tau^n_i}{h_i} \right) \left( \frac{\tau_{i+1}^{n+1} - \tau^n_i}{\tau^n_i} \right)^2.$$

The results of the $k - \tau$ model with this term are plotted in Figures 33 and 34. The mixed layer depth is approximately halved at 100 layers. The results improve if a 1000 layer grid is used. The above implementation is second-order accurate, but produces less accurate results than the first-order implementation in Section 4.4.

The numerical diffusion that is associated with the first-order upwind implementation is clearly required to get accurate results. The most likely explanation for the results is that the amount of diffusion in the turbulence model is limiting the mixed layer depth if the amount of diffusion is small. However, if the amount of diffusion is large, the mixed layer depth is limited by local production and dissipation terms. The upwind implementation produces sufficient numerical diffusion to obtain a system that is dominated by local terms, which are independent of the grid resolution. The second-order implementation is governed by diffusive terms.

The $D_{k\tau}$ and $D_{kk}$ terms have hardly any effect on the mixed-layer depth.
E. Unstable stratification: sensitivity to implementation

Figure 33: Time series of $D_m$ for the $k - \tau$ model with different implementation of the $D_{\tau\tau}$ for 100 layers.

Figure 34: $D_m$ after 800 s for the $k - \tau$ model with different implementation of $D_{\tau\tau}$. Note that the horizontal axis does not scale consistently with the number of layers in order to show the results for a wide range of grid resolutions.
Additional results Vlietland case

This appendix provides some additional results on the case of Section 5.1. We will first look at the temperature profile such as predicted by the $k-\omega$ model. It will then be shown that the $D_{kk}$ term, which is not implemented in the $k-\omega$ and $k-\tau$ models, cannot explain the differences between these models and the $k-\varepsilon$ model. Finally, we will show how the critical Richardson number may be used in this case to comment on the balance of the terms in the turbulence model.

A contourplot of the temperature over the course of a year is shown in Figure 35. The figure compares the result of the $k-\omega$ model and the $k-\tau$ model at 200 layers. Both models yield approximately the same results. This is consistent with the errors presented in Section 5.1, which also shows that the two models produce similar results.

The differences between the $k-\omega$ or $k-\tau$ model and the $k-\varepsilon$ model cannot be attributed to the $D_{kk}$ term which is not implemented, see also Section 3.4. This can be tested by setting $\sigma_\varepsilon = \sigma_k$; in this case they are both set to 1.0. The $D_{kk}$ term then vanishes from the equations.

Figure 36 shows the results in terms of the RMS error between the simulated temperature and the measurements. The figure shows a similar trend as the results of Section 5.1 that the $k-\varepsilon$ model results behave different than the $k-\omega$ and $k-\tau$ model results. So the differences between the models are not explained by the $D_{kk}$ term.

Finally, we will look at the relation between the Richardson number and turbulence. The theory of local equilibrium laid out in Appendix D.2 stated that a flow in local equilibrium tends to laminar flow if the Richardson number is greater than the critical Richardson number of 0.175. Figure 37 shows the fraction of grid cells at each time step with turbulent flow plotted against the Richardson number. Two grid resolutions are shown: 200 and 2000 layers. It is expected that a flow in local equilibrium has a very abrupt transition around the critical Richardson number, which is marked by the black vertical line in the figure.

Some transition is visible around the critical Richardson number, but the diffusive terms are still strong enough to have some turbulence even at a Richardson number of eight. The figures of 200 and 2000 layers compare well, except for the behaviour of the $k-\tau$ model. It has a tendency to go to local equilibrium at a high grid resolution. This tendency of the $k-\tau$ model to local equilibrium starts from 1000 layers and corresponds to the jump in the RMS error in Figure 25 in Section 5.1. This behaviour is not well understood.
**Figure 35:** Simulated temperature profile at one location in southern lake Vlietland in 2009 with 200 layers a) using the $k-\omega$ model, b) using the $k-\tau$ model and c) the difference plot $(k-\tau) - (k-\omega)$.

**Figure 36:** Root mean square error of the three models for 20 to 2000 layers with $\sigma_e = \sigma_k = 1$ so that the $D_{kk}$ term drops from the equations.
Figure 37: Fraction of turbulent grid cells ($\nu_t > 10^{-5} \text{ m}^2/\text{s}$) as a function of the Richardson number. Top: 200 layers. Bottom: 2000 layers.
Estuarine flow: sensitivity to implementation

We will treat one example of extreme sensitivity of the results of the estuarine flow case to the implementation of the turbulence model in this appendix. This example involves the implementation of the Neumann boundary condition of the $k-\varepsilon$ model. The implementation of the Neumann boundary condition of the $k-\varepsilon$ model that is used in this report reads

$$\frac{\varepsilon_{I-1}^{n+1} - \varepsilon_I^n}{h_I} = -\frac{|u_\ast|^3}{\kappa \left(\frac{1}{2}h_I + \alpha z_0\right)^2}.$$ 

The parameter $\alpha$ has a value of 9, which follows from the definition of the bed level, see Section 1.4.

Alternatively one can choose $\alpha$ equal to zero or one.

$$\frac{\varepsilon_{I+1}^{n+1} - \varepsilon_I^n}{h_I} = -\frac{|u_\ast|^3}{\kappa \left(\frac{1}{2}h_I\right)^2},$$

$$\frac{\varepsilon_{I-1}^{n+1} - \varepsilon_I^n}{h_I} = -\frac{|u_\ast|^3}{\kappa \left(\frac{1}{2}h_I + z_0\right)^2}.$$ 

In this appendix we only vary $\alpha$ in the turbulence model and not in the momentum equation. The three conditions are similar if $z_0$ is much smaller than the bottom cell height.

Similarly one can neglect $z_0$ in the Dirichlet boundary condition of the $k-\tau$ model:

$$\tau_I^{n+1} = 0.$$ 

It is unexpected that these small differences in the boundary condition change the convergence behaviour of the turbulence models in the case of estuarine flow. Figure 38 shows the exchange flow magnitude at several grid resolutions with the three boundary conditions of the $k-\varepsilon$ model. Whereas the results converge nicely for $\alpha = 9$, they tend to diverge for $\alpha = 0$ and $\alpha = 1$. This behaviour is not understood.
Figure 38: Magnitude of the mean absolute exchange flow at several grid resolutions for the \( k - \varepsilon \) and \( k - \tau \) models and some variations of the boundary conditions.