Simulatie MOdellen voor de NATte Waterstaat

Technical Documentation WAQUA

Simona-reportnr. 98-01
Simulatie MModelen voor de NAtte Waterstaat

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Preface

Until the appearance of this report the technical documentation of WAQUA consisted of a number of papers published in proceedings and journals, and of several thesis. The current work is a collection and update of that information. The documentation is, in its final form, meant to be the starting point for maintenance, restructuring, and extending the WAQUA program. Modifications in and extensions to WAQUA must also be documented in the technical documentation such that consistency of the program is guaranteed. A consequence is that new functionalities are integrated in the system and not added as a separate and independent part (which happened in the implementation of the Riemann invariant type of boundary, see the last chapter). The documentation should show the context in which a modification or extension will be made.

The current work describes in general terms the mathematical-physical formulation, i.e. the basic equations of the WAQUA program. Subsequently it presents the finite difference approximations which are used, how flooding and drying of tidal flats is computed and the general solution method of the system of equations. In order to serve as a starting point for maintenance, restructuring, and extending the WAQUA program several aspects have to be described. For example the sequence of initialisation and the calls to all the subroutines in the computation program. As the main subroutines are very compactly written a detailed description of the equations which are considered is required. In other words the gap between the system documentation and the technical documentation should be reduced.

The current technical documentation is not finished, which is, of coarse, natural for an evolving system. At this moment, however, extra improvements as suggested above have to be made. For the near future it is recommended that the gap mentioned above is reduced. During the writing of the documentation it appeared that some parts required improvement. These and other recommendations are collected in the chapter with recommendations and are a good suggestion for improvements.

Projectmanager
SIMONA*SYS
H.H. ten Cate
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<td>depth-averaged concentration</td>
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<td>$C_{2D}$</td>
<td>2D Chézy coefficient</td>
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<td>wind drag coefficient</td>
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<td>horizontal dispersion</td>
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<td>radius of the Earth</td>
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<td>$S$</td>
<td>depth averaged salinity</td>
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<td>$T_{TH,\text{surface}}$</td>
<td>Thatcher Harleman return time for the surface layer</td>
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<td>$U$</td>
<td>depth averaged velocity in the $\xi$-direction</td>
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<td>averaged wind speed at 10 m above free surface</td>
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<td>velocity in the $\eta$-direction</td>
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</tr>
<tr>
<td>$V$</td>
<td>depth averaged velocity in $\eta$-direction</td>
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<tr>
<td>$w$</td>
<td>velocity in the $z$-direction</td>
<td>m/s</td>
</tr>
<tr>
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<td>m/s</td>
</tr>
<tr>
<td>$W_{\eta}$</td>
<td>component of surface wind $W$ in $\eta$-direction</td>
<td>m/s</td>
</tr>
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<td>component of surface wind $W$ in $\lambda$- direction</td>
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<td>$\Delta y$</td>
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<td>Von Karman constant</td>
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</tr>
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<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
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<td>--------</td>
<td>--------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
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<td>horizontal eddy viscosity ($\xi$- and $\eta$-direction)</td>
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<td>$\nu_l$</td>
<td>turbulent eddy viscosity</td>
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<td>shear stress</td>
<td>kg/m$^2$</td>
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<td>$\tau_{bottom,x}$</td>
<td>shear stress at bed in x-direction</td>
<td>kg/m/s$^2$</td>
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<tr>
<td>$\tau_{bottom,y}$</td>
<td>shear stress at bed in y-direction</td>
<td>kg/m/s$^2$</td>
</tr>
<tr>
<td>$\tau_{surface,x}$</td>
<td>shear stress at surface in x-direction</td>
<td>kg/m/s$^2$</td>
</tr>
<tr>
<td>$\tau_{surface,y}$</td>
<td>shear stress at surface in y-direction</td>
<td>kg/m/s$^2$</td>
</tr>
<tr>
<td>$\xi, \eta$</td>
<td>horizontal, curvilinear spatial co-ordinates</td>
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<td>$\zeta$</td>
<td>water level above some horizontal plane of reference (datum)</td>
<td>m</td>
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<tr>
<td>$\Omega$</td>
<td>earth rotation vector</td>
<td>1/s</td>
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</table>
I Introduction

As part of the Ministry of Transport, Public Works and Water Management, the National Institute of Coastal and Marine Management (RIKZ) and the Institute for Inland Water Management and Wastewater Treatment (RIZA) provide advice and information on subjects related to the sustainable use of rivers, estuaries, coasts and seas. To gain knowledge on the behaviour of the Dutch coastal waters in physical and ecological sense RIKZ and RIZA make use of an extended monitoring program. Besides that, modelling efforts are made as well to understand the coastal environment.

During most part of this century the use of physical scale models was common practice. Owing to increasing computer power these scale models have been replaced by mathematical models. In Dutch engineering practice one dimensional models for the calculation of water levels and flow were already used in the first half of this century for the closure of the Southern Sea (Lorentz, 1926). At that time calculations were made by hand.

At the end of the sixties two dimensional models were introduced for the simulation of well-mixed estuaries. Based on the work of (Leendertse, 1967) the WAQUA-system has been developed. WAQUA is used for two-dimensional hydrodynamic and water quality simulation of well-mixed estuaries, coastal seas and rivers (WAQUA, 1992). In the beginning of the eighties major improvements have been made on the robustness of the WAQUA-system by (Stelling, 1984).

The processing part of WAQUA is based on the shallow water equations. These equations are in most cases sufficiently accurate in predicting water levels along the Dutch coastline. The North Sea and the various Dutch estuaries can be characterised by the fact that the length of the surface waves are much larger than the depth of these water areas.

In 1992 the WAQUA-system has been redesigned according to SIMONA. Today the WAQUA-processor is able to interact with other SIMONA models for short waves, sediment transport, morphodynamics and ecological processes.

WAQUA can simulate the hydrodynamics and the distribution of dissolved substances in geographical areas based on rectilinear, curvilinear or spherical co-ordinates. In the second half of the eighties boundary fitted curvilinear co-ordinates have been introduced to improve the representation of complex geometries and to gain resolution in areas of interest, without considerably increasing the computational costs. Based on the work of (Willemsse et al., 1986) the WAQUA-system has been modified to support curvilinear grids.

The choice between the above mentioned co-ordinate systems should be made in a very early stage of the modelling project, because it is vital for all model input preparing activities. The choice is governed by the characteristics of the area to be modelled. In general rectilinear co-ordinates will be applied. A curvilinear grid however may be more favourable in cases where the area of interest is much smaller than the complete model area, or when the physical characteristics of the area demand small grid sizes on certain locations.
and allow at the same time larger grid sizes in other areas. This may be the case in river applications when an extensive winter bed is present. Rectilinear and curvilinear models covering a relatively large part of the globe produce less accurate results due to the sphere shape of the earth. For such models spherical co-ordinates is an adequate option.

The geographical areas in WAQUA are bounded by any combination of closed boundaries (land) and open boundaries. Open boundaries force the flows in the model by water levels, velocities, Riemann invariants, discharges or distributed discharges, given either as time-varying data or Fourier/harmonic functions of phase and amplitude at given frequencies, or as a table, relating discharge with water level values. The system accounts for sources of discharge, such as rivers or outfalls, for tidal flats, for islands and dams, movable barriers or sluices and weirs. For the computation of dissolved substances only during inflow the concentrations at the open boundaries are prescribed by boundary data.
2 The Model Equations

In this chapter we will derive from the conservation laws for mass, momentum and concentration the depth-averaged shallow-water equations and the depth-averaged advection-diffusion equation for dissolved matter. This set of partial differential equations in combination with an appropriate set of initial and boundary conditions is solved on a finite difference grid by the WAQUA system. The discretizations in space and time are described in Chapter 3, 4 and 5. The boundary conditions are discussed in Chapter 6.

Starting point for the derivation of the depth-averaged shallow water equations are the so-called Navier-Stokes equations for fluid flow, see e.g. (Malvern, 1969). In Sections 2.2 and 2.3 the basic equations of WAQUA will be derived for rectangular co-ordinates. In Sections 2.4 and 2.5 a description is presented of respectively the transformation of the equations to orthogonal curvi-linear boundary-fitted co-ordinates and to spherical co-ordinates. In Section 2.6, we will derive an equation for the horizontal pressure terms in which a barotropic and a baroclinic part can be recognised. Finally, Section 2.7 is devoted to structures in WAQUA.

2.1 Definition

The WAQUA system is used for modelling two-dimensional free surface flow and transport of well-mixed estuaries, coastal seas and rivers. The physical domain in the vertical direction is depicted in Figure 2.1. The vertical water boundaries are defined as follows. The free surface is represented by the function \( z(x,y,t) \) at position \((x,y)\) and time \(t\), which is the distance between the surface and a plane of reference. This function is called the water level. The bottom is described by the function \( d(x,y) \), which gives the depth below the plane of reference. The function \( H(x,y,t) = z(x,y,t) + d(x,y) \) is called the total water depth of the domain.

![Figure 2.1. Water area with bottom and free surface.](image-url)
WAQUA is a depth-averaged flow and transport model. In the derivation of the depth-averaged 2D equations from the 3D equations we will frequently use Leibniz' rule:

\[
\int_{-d(x)}^{\zeta(x,t)} \frac{\partial f(x,z)}{\partial x} \, dz = \frac{\partial}{\partial x} \left( \int_{-d(x)}^{\zeta(x,t)} f(x,z) \, dz \right) - f(x, \zeta(x,t)) \frac{\partial \zeta}{\partial x} - f(x, -d(x)) \frac{\partial d}{\partial x} \quad (2.1.1)
\]

The depth-averaged velocities are defined by

\[
U = \frac{1}{H} \int_{-d}^{\zeta} u \, dz \quad (2.1.2a)
\]

\[
V = \frac{1}{H} \int_{-d}^{\zeta} v \, dz \quad (2.1.2b)
\]

and the depth-averaged concentration is defined by

\[
C = \frac{1}{H} \int_{-d}^{\zeta} c \, dz \quad (2.1.2c)
\]

### 2.2 The Hydrodynamic Equations in Rectangular Co-ordinates

Starting point of our derivation are the Reynolds-averaged, time-dependent incompressible Navier-Stokes equations. This does not mean that the density is constant, but rather that the density is independent of the pressure. The density may vary due to variations of temperature or salinity. Reynolds decomposition followed by some averaging or low-pass filtering operator yields Reynolds stresses in the right-hand side of the momentum equations, see e.g. (Rodi, 1980). In Cartesian co-ordinates the Reynolds-averaged equations in three dimensions read

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (2.2.1)
\]

\[
\frac{\partial u}{\partial t} + \frac{\partial u^2}{\partial x} + \frac{\partial uv}{\partial y} + \frac{\partial uw}{\partial z} = F_x \quad (2.2.2a)
\]

\[
\frac{\partial v}{\partial t} + \frac{\partial uv}{\partial x} + \frac{\partial v^2}{\partial y} + \frac{\partial vw}{\partial z} = F_y \quad (2.2.2b)
\]

\[
\frac{\partial w}{\partial t} + \frac{\partial uw}{\partial x} + \frac{\partial vw}{\partial y} + \frac{\partial w^2}{\partial z} = F_z \quad (2.2.2c)
\]

with \( u, v, w \) the velocity components in \( x, y \) and \( z \)-direction respectively. The \( z \) is positive upward. \( F_x, F_y, \) and \( F_z \) represent the components of the external forces.
Forces of interest are:

- the gravity force,
- the Coriolis force,
- the pressure,
- the unbalance (force) in Reynolds stresses.

The forces for tide generation are not included explicitly in the equations. Their effect is represented in the open boundary conditions.

We make use of the Boussinesq approximation. The influence of variable density appears only in the baroclinic pressure term. In the other terms we assume a constant reference density $\rho_0$.

The contribution of the different forces to $F_x$, $F_y$ and $F_z$ are respectively:

**Gravity:**

\[
F_x = 0 \\
F_y = 0 \\
F_z = -g
\]  
(2.2.3a)

with $g$ the acceleration of gravity.

**Coriolis:**

The coriolis term brings into account the effect of earth rotation:

\[
F_x = 2\Omega_1 v - 2\Omega_2 w \\
F_y = 2\Omega_1 w - 2\Omega_2 u \\
F_z = 2\Omega_2 u - 2\Omega_3 w
\]  
(2.2.3b)

with $\Omega = (\Omega_1, \Omega_2, \Omega_3)$ the earth rotation vector.

**Pressure:**

\[
F_x = -\frac{1}{\rho_0} \frac{\partial p}{\partial x} \\
F_y = -\frac{1}{\rho_0} \frac{\partial p}{\partial y} \\
F_z = -\frac{1}{\rho_0} \frac{\partial p}{\partial z}
\]  
(2.2.3c)

with $p$ the pressure.
Friction:

The ensemble averaging of the Navier Stokes equations introduces a force which represents the unbalance of the Reynolds stresses:

\[
F_x = \frac{1}{\rho_0} \left[ \frac{\partial R_{xx}}{\partial x} + \frac{\partial R_{yx}}{\partial y} + \frac{\partial R_{zx}}{\partial z} \right]
\]

\[
F_y = \frac{1}{\rho_0} \left[ \frac{\partial R_{yx}}{\partial x} + \frac{\partial R_{yy}}{\partial y} + \frac{\partial R_{zy}}{\partial z} \right]
\]

\[
F_z = \frac{1}{\rho_0} \left[ \frac{\partial R_{zx}}{\partial x} + \frac{\partial R_{zy}}{\partial y} + \frac{\partial R_{zz}}{\partial z} \right]
\]  

(2.2.4a)

The Reynolds stresses are determined with a so-called turbulence closure model using the eddy-viscosity concept, for details see e.g. (Rodi, 1980). This concept expresses the Reynolds-stress components as the product between a flow-dependent eddy viscosity coefficient \( \nu_t \) and the corresponding components of the mean rate-of-deformation tensor being the symmetric part of the mean-velocity gradient. In tensor notation the eddy viscosity concept may be expressed as:

\[
R_{ij} = \rho_0 \nu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]  

(2.2.4b)

Also the effect of the molecular viscosity is expressed in this way but the value of the turbulent eddy viscosity coefficient \( \nu_t \) is usually much larger than the molecular viscosity and the contribution of the molecular viscosity is neglected.

The forces due to turbulence are relatively unimportant for large scale flows of vertically well-mixed water bodies. For deriving the depth-averaged equations we assume a spatially-constant eddy viscosity. Using the continuity equation, the forces for the unbalance of the Reynolds stresses simplify to

\[
F_x = \nu_t \left[ \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right]
\]

\[
F_y = \nu_t \left[ \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right]
\]

\[
F_z = \nu_t \left[ \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right]
\]  

(2.2.4c)

Boundary conditions for the stresses along the free surface and the bottom are coupled with the wind stress and the bottom stress.
Before applying vertical integration of the equations, the momentum equation for the vertical velocity component \( w \) in Eq. (2.2.2c) will be simplified. WAQUA is applied for flows where the characteristic horizontal length scales (dimensions of the flow domain and wavelengths) are much larger than the vertical length scale (the water depth). The flows are boundary-layer type of flows. The motion of a fluid particle is therefore mainly horizontal and the vertical accelerations are neglected with respect to the gravity. From linear wave theory it can be found that a long shallow water wave results if the ratio of water depth to wave length is less than about 0.05 (Vreugdenhil, 1994).

Also the effect of the vertical stresses and the Coriolis force are small compared to the acceleration of gravity. The vertical momentum equation is reduced to the hydrostatic pressure relation:

\[
\frac{\partial p}{\partial z} = -\rho g \quad (2.2.5)
\]

For an extended description of this simplification called the “shallow water approximation” one is referred to (Vreugdenhil, 1994).

In this section we assume that the density \( \rho \) is constant and equal to \( \rho_0 \), which is specified by the user. In Section 2.6 we give an equation of state relating the local density to the values of temperature and salinity. An expression will be derived for the horizontal components of the pressure force which will contain gradients of the density, the so-called baroclinic pressure gradients. In this section we restrict ourselves to the component due to gradients in the free surface level, the so-called barotropic pressure gradients.

For constant density:

\[
p(x, y, z, t) = \int_{z}^{\zeta(x, y, t)} \rho_0 g dz' + p_{atm} = \rho_0 g(\zeta(x, y, t) - z) + p_{atm} \quad (2.2.6)
\]

where \( p_{atm} \) is the atmospheric pressure. In the derivation which follows we neglect the gradients of the atmospheric pressure. They are included in the WAQUA system for space and time varying wind and pressure, which assumes a spherical co-ordinate system. Substituting (2.2.6) in the horizontal pressure gradients and neglecting the atmospheric pressure yields:

\[
\frac{1}{\rho_0} \frac{\partial p}{\partial x} = g \frac{\partial \zeta}{\partial x} \quad (2.2.6a)
\]

\[
\frac{1}{\rho_0} \frac{\partial p}{\partial y} = g \frac{\partial \zeta}{\partial y}
\]

As horizontal dimensions are large, the vertical velocity component is an order of magnitude smaller than the horizontal components: \( |w| \ll (|u|, |v|) \). The Coriolis force in the horizontal momentum equations is reduced to
\[ F_x = 2\Omega_x \nu \]
\[ F_y = -2\Omega_y \mu \]  \hspace{1cm} (2.2.7a)

with \( \Omega \) the angular speed of the rotation of the earth, and \( \phi \) the geographic latitude. Making use of the oceanographic notation \( f = 2\Omega \sin \phi \) the Coriolis force becomes

\[ F_x = f \nu \]
\[ F_y = -f \mu \]  \hspace{1cm} (2.2.7b)

The assumptions discussed before yield the following horizontal momentum equations:

\[ \frac{\partial u}{\partial x} + \frac{\partial \nu}{\partial y} + \frac{\partial w}{\partial z} = 0 \]
\[ \frac{\partial u}{\partial t} + \frac{\partial u^2}{\partial x} + \frac{\partial \nu u}{\partial y} + \frac{\partial \nu w}{\partial z} - g \frac{\partial \zeta}{\partial x} - f \nu - \nu_{\Delta u} = 0 \]  \hspace{1cm} (2.2.8)
\[ \frac{\partial \nu}{\partial t} + \frac{\partial \nu u}{\partial x} + \frac{\partial \nu^2}{\partial y} + \frac{\partial \nu w}{\partial z} + g \frac{\partial \zeta}{\partial y} + f u - \nu_{\Delta v} = 0 \]

The so-called "depth-averaged shallow water equations" are derived by integrating of Eq. (2.2.8) over the total water depth from bottom to free surface. This leads to loss of information on the vertical distribution of the horizontal flow velocity. We split the horizontal flow velocities in a depth-averaged part and fluctuations:

\[ u = U + u', \nu = V + \nu' \]  \hspace{1cm} (2.2.9a)

with

\[ \int_{-d}^{\zeta} u \, dz = 0, \int_{-d}^{\zeta} \nu \, dz = 0 \]  \hspace{1cm} (2.2.9b)

Now we will integrate the system (2.2.8), i.e. the continuity and momentum equations, over the depth. First we will consider the continuity equation.

\[ \int_{-d}^{\zeta} \left( \frac{\partial u}{\partial x} + \frac{\partial \nu}{\partial y} + \frac{\partial w}{\partial z} \right) \, dz = 0 \]  \hspace{1cm} (2.2.10)

Using Leibniz' rule (2.1.1), integration of the first term gives

\[ \int_{-d}^{\zeta} \frac{\partial u}{\partial x} \, dz = \frac{\partial}{\partial x} \int_{-d}^{\zeta} u \, dz - u(-d) \frac{\partial d}{\partial x} - u(\zeta) \frac{\partial \zeta}{\partial x} \]  \hspace{1cm} (2.2.11a)
and we can write (2.2.11a) as

$$\int \zeta \frac{\partial u}{\partial x} \, dz = \frac{\partial HU}{\partial x} - u(\zeta) \frac{\partial \zeta}{\partial x} - u(-d) \frac{\partial d}{\partial x}$$  \hspace{1cm} (2.2.11b)$$

Similarly we have:

$$\int \zeta \frac{\partial v}{\partial y} \, dz = \frac{\partial HV}{\partial y} - v(\zeta) \frac{\partial \zeta}{\partial y} - v(-d) \frac{\partial d}{\partial y}$$  \hspace{1cm} (2.2.11c)$$

Integration of the last term of (2.2.10) leads to

$$\int \zeta \frac{\partial w}{\partial z} \, dz = w(\zeta) - w(-d)$$  \hspace{1cm} (2.2.11d)$$

If we assume that a water particle will not leave the water area (the so-called kinematic relation), we obtain

$$w(\zeta) = \frac{d\zeta}{dt} = \frac{\partial \zeta}{\partial t} + u(\zeta) \frac{\partial \zeta}{\partial x} + v(\zeta) \frac{\partial \zeta}{\partial y}$$  \hspace{1cm} (2.2.12a)$$

Similarly, if we neglect the slow variation of the bottom in time (i.e. \(\partial d / \partial t = 0\)), then at the bottom \(z = -d(x,y)\) the kinematic boundary condition reads:

$$w(-d) = -u(-d) \frac{\partial d}{\partial x} - v(-d) \frac{\partial d}{\partial y}$$  \hspace{1cm} (2.2.12b)$$

With (2.2.11) - (2.2.12) the integration of the continuity equation results in:

$$\frac{\partial \zeta}{\partial t} + \frac{\partial}{\partial x} (HU) + \frac{\partial}{\partial y} (HV) = 0$$  \hspace{1cm} (2.2.13)$$

Eq. (2.2.13) is the well-known depth-averaged continuity equation.

For the derivation of the depth-averaged momentum equation in x-direction we will only pay attention to the partial derivatives in x-direction and in z-direction. The integration of the partial derivative in the y-direction is similar as for the partial derivative in the x-direction.

$$\int \zeta \frac{\partial u}{\partial t} \, dz = \frac{\partial}{\partial t} \int \zeta \, du \, dz - u(\zeta) \frac{\partial \zeta}{\partial t} = \frac{\partial HU}{\partial t} - u(\zeta) \frac{\partial \zeta}{\partial t}$$  \hspace{1cm} (2.2.14a)$$

$$\int \zeta \, f v \, dz = fHV$$  \hspace{1cm} (2.2.14b)$$
\[ \begin{align*}
\int_{-d}^\zeta g \frac{\partial \zeta}{\partial x} \, dz &= gH \frac{\partial \zeta}{\partial x} \\
\int_{-d}^\zeta \left( \frac{\partial u^2}{\partial x} + \frac{\partial uv}{\partial y} + \frac{\partial uv}{\partial z} \right) \, dz &= \frac{\partial HU^2}{\partial x} - u^2(\zeta) \frac{\partial \zeta}{\partial x} - u^2(-d) \frac{\partial d}{\partial x} \\
&\quad - \frac{\partial HVU}{\partial y} - uv(\zeta) \frac{\partial \zeta}{\partial y} - uv(-d) \frac{\partial d}{\partial y} \\
&\quad + w(\zeta)u(\zeta) - w(-d)u(-d) + \frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{yy}}{\partial y} \\
\end{align*} \] (2.2.14c)

with

\[ T_{xx} = \int_{-d}^\zeta (u - U)^2 \, dz \quad \text{and} \quad T_{yy} = \int_{-d}^\zeta (v - V)^2 \, dz \] (2.2.14e)

The integration terms at the free surface and the bed cancel due to the kinematic boundary conditions (2.2.12).

Depth-averaging the three-dimensional Reynolds-averaged momentum equations discards the mean vertical exchange of horizontal momentum, such as induced by tidal motions, flow over bed topography, wind, vertical stratification, etc. These effects are contained in the stresses \( T_{xx} \) and \( T_{yy} \). To close the system of equations the stresses have to be expressed as functions of the depth-averaged velocities. A well-known approximation is to assume that \( T_{xx} \) and \( T_{yy} \) will have the same behaviour as molecular viscosity and it leads to an additional viscosity (dispersion) term in the right-hand side. The eddy viscosity in the depth-averaged equations is increased compared to the one appearing in the three-dimensional equations. For the applications of the WAQUA system these terms must be of secondary importance because otherwise the 3D system TRIWAQ should be used.

Finally we have to integrate the Laplace operator. First we integrate the horizontal second order derivative. By using Leibniz’ rule twice, this results in:

\[ \begin{align*}
\int_{-d}^\zeta v_i \frac{\partial^2 u}{\partial x^2} \, dz &= v_i \frac{\partial^2 HU}{\partial x^2} - v_i \frac{\partial}{\partial x} \left( u(\zeta) \frac{\partial \zeta}{\partial x} \right) - v_i \frac{\partial}{\partial x} \left( u(-d) \frac{\partial d}{\partial x} \right) \\
&\quad - v_i \frac{\partial u(\zeta)}{\partial x} \frac{\partial \zeta}{\partial x} - v_i \frac{\partial u(-d)}{\partial x} \frac{\partial d}{\partial x} \\
\end{align*} \] (2.2.14e)

Integration of the vertical viscosity term gives

\[ \begin{align*}
\int_{-d}^\zeta v_i \frac{\partial^2 u}{\partial z^2} \, dz &= v_i \frac{\partial u}{\partial z} (\zeta(x,y,t) - v_i \frac{\partial u}{\partial z} (-d(x,y)) \\
\end{align*} \] (2.2.14f)
The shear stresses at the free surface and bottom in the $x$-direction are combined:

$$\frac{\tau_{\text{surface}}}{\rho_0} = v_i \frac{\partial u}{\partial z} (\zeta(x,y,t)) - v_i \frac{\partial u}{\partial x} \frac{\partial \zeta}{\partial x} (\zeta(x,y,t)) - v_i \frac{\partial u}{\partial y} \frac{\partial \zeta}{\partial y} (\zeta(x,y,t))$$  \hspace{1cm} (2.2.15a)

$$\frac{\tau_{\text{bottom}}}{\rho_0} = v_i \frac{\partial u}{\partial z} (\bar{d}(x,y)) + v_i \frac{\partial u}{\partial x} \frac{\partial \bar{d}}{\partial x} (\bar{d}(x,y)) + v_i \frac{\partial u}{\partial y} \frac{\partial \bar{d}}{\partial y} (\bar{d}(x,y))$$  \hspace{1cm} (2.2.15b)

Without wind forcing the shear stress at the free surface should be zero. With wind, the wind stress is coupled to the wind velocity:

$$\tau_{\text{surface}} = \tau_{\text{wind}} = C_d \rho_{\text{air}} |\bar{u}_{10}| u_{10} = C_d \rho_{\text{air}} |\bar{u}_{10}|^2 \sin \psi$$  \hspace{1cm} (2.2.16)

where $\rho_{\text{air}}$ is the air density, $C_d$ the wind stress coefficient, $u_{10}$ the wind speed at 10 metres above the water surface and $\psi$ the angle between the wind direction and the positive $y$-direction. To close the system of equations, the bottom stress has to be expressed in the depth-averaged velocities. The following semi-empiric quadratic relation is applied:

$$\tau_{\text{bottom}} = \frac{\rho_0 g U^2}{C_{\text{2D}} x (U^2 + V^2)}$$  \hspace{1cm} (2.2.17)

with $C_{\text{2D}}$ the Chézy coefficient of flow resistance. It takes into account bottom roughness and may be a function of the water depth, see Section 6.2. We remark that in WAQUA the Chézy coefficient depends on the coordinate direction, either $x$- or $y$-direction. This makes it possible to take into account subgrid bottom topography (ripples) which are perpendicular to one of the coordinate directions. When transport of constituents is involved and one of the constituents is salt, then a correction may be applied to the bottom roughness. For a detailed description we refer to Section 6.2.

As mentioned above the residual terms $T_{xx}$ and $T_{xy}$ have the same behaviour as molecular viscosity. Therefore we will use in the depth-integrated equations $\nu_{\text{m}}$ instead of $\nu_{\text{t}}$ in the horizontal mixing terms. This coefficient now represents: molecular viscosity, turbulence and dispersion due to vertical variations of the horizontal flow field. The stress terms are of secondary importance and in WAQUA simplified to a 2D Laplace operator. This is a consistent way of modelling. The horizontal viscosity terms are necessary to be able to reproduce large-scale eddies.

By subtracting the integrated continuity equation (2.2.13) from the integrated momentum equation a non-conservative expression can be obtained for the momentum equation (2.2.14).
\[
\frac{\partial U}{\partial t} + U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} = -g \frac{\partial \zeta}{\partial x} + fV + V H \left( \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} \right) + \frac{\tau_{\text{wind}y} - \tau_{\text{bottom}y}}{H} \tag{2.2.18}
\]

In a similar way we can derive the depth-averaged momentum equation in the y-direction.

Summarizing, the system of equations becomes

\[
\frac{\partial \zeta}{\partial t} + \frac{\partial}{\partial x} (H U) + \frac{\partial}{\partial y} (H V) = 0 \tag{2.2.19a}
\]

\[
\frac{\partial U}{\partial t} + U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} = -g \frac{\partial \zeta}{\partial x} + fV + V H \left( \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} \right) + \frac{\tau_{\text{wind}y} - \tau_{\text{bottom}y}}{\rho_0 H} \tag{2.2.19b}
\]

\[
\frac{\partial V}{\partial t} + U \frac{\partial V}{\partial x} + V \frac{\partial V}{\partial y} = -g \frac{\partial \zeta}{\partial y} - fU + V H \left( \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} \right) + \frac{\tau_{\text{wind}x} - \tau_{\text{bottom}x}}{\rho_0 H} \tag{2.2.19c}
\]

The equations (2.2.19a-c) are known as the shallow-water or 2D long-wave equations. They accurately describe tidal waves in rivers and seas, flood waves in rivers, but also oscillations in harbour basins.

The system of equations is hyperbolic, because the viscosity terms are of secondary importance. In 1D the system of shallow water equations has two characteristics. Without friction, the quantities that are conserved, the so-called Riemann invariants, are given by:

\[
R^+ = u + \sqrt{g(\zeta + d)}
\]

\[
R^- = u - \sqrt{g(\zeta + d)} \tag{2.2.20}
\]

The characteristic wave propagation velocity is \(\sqrt{g(\zeta + d)}\). In 2D the characteristic lines turn into characteristic surfaces, see (Gerritsen, 1982).

### 2.3 The Transport Equation in Rectangular Co-ordinates

The flow in rivers and coastal seas often transports dissolved substances and/or heat. In this section we will derive the depth-averaged transport equation. The equation is consistent with the depth-averaged continuity equation (2.2.19a).

Starting point is the Reynolds-averaged 3D advection-diffusion equation:

\[
\frac{\partial c}{\partial t} + \frac{\partial uc}{\partial x} + \frac{\partial vc}{\partial y} + \frac{\partial wc}{\partial z} = \frac{\partial D_x \partial c}{\partial x^2} + \frac{\partial D_y \partial c}{\partial y^2} + \frac{\partial D_z \partial c}{\partial z^2} \tag{2.3.1}
\]
In Eq. (2.3.1) \( c \) is the concentration of a dissolved substance and \( D_t \) is the turbulent eddy diffusivity coefficient. The turbulent mixing is assumed to be isotropic, but is still dependent on position and time. Now we will integrate Eq. (2.3.1) over the total water depth in the same way as has been done in the previous section. This leads to loss of information of the vertical distribution of the concentration. We split the concentration in a depth-averaged part and fluctuations:

\[
c = C + c' \tag{2.3.2}
\]

with

\[
\oint_{-d} c' dz = \oint_{-d} (c - C) dz = 0 \tag{2.3.3a}
\]

\[
\oint_{-d} \frac{\partial c}{\partial t} dz = \oint_{-d} c \frac{\partial c}{\partial t} dz = -c(\zeta) \frac{\partial c}{\partial t} + \frac{\partial HC}{\partial t} - c(\zeta) \frac{\partial c}{\partial t} \tag{2.3.3b}
\]

\[
\oint_{-d} \left( \frac{\partial uc}{\partial x} + \frac{\partial vc}{\partial y} + \frac{\partial wc}{\partial z} \right) dz = \oint_{-d} \frac{\partial HUC}{\partial x} - uc(\zeta) \frac{\partial c}{\partial x} - uc(-d) \frac{\partial d}{\partial x} - \frac{\partial HVC}{\partial y} - vc(\zeta) \frac{\partial c}{\partial y} - vc(-d) \frac{\partial d}{\partial y}
+ w(\zeta)c(\zeta) - w(-d)c(-d) + \frac{\partial F_{sx}}{\partial x} + \frac{\partial F_{sy}}{\partial y} \tag{2.3.3c}
\]

\[F_{sx} = \oint_{-d} (u - U)(c - C) dz \text{ and } F_{sy} = \oint_{-d} (v - V)(c - C) dz. \tag{2.3.3d}\]

The integration terms at the free surface and the bed cancel due to the kinematic boundary conditions (2.2.12).

Depth-averaging the advection-diffusion equation discards the mean vertical exchange of matter, such as induced by vertical variations of the horizontal flow field, the so-called Taylor shear dispersion. These effects are contained in the fluxes \( F_{sx} \) and \( F_{sy} \). To close the system of equations the fluxes have to be expressed as functions of the depth-averaged concentrations. A well-known approximation is to assume that \( F_{sx} \) and \( F_{sy} \) have the same mathematical formulation as molecular diffusion and this leads to an additional diffusion (dispersion) term in the right-hand side. The eddy diffusion coefficient in the depth-averaged equations is increased compared to the one appearing in the three-dimensional equations. Therefore we will use in the depth-integrated equations \( D_H \) instead of \( D_t \) in the horizontal mixing terms, see Eq. (2.3.6a).
In WAQUA the additional horizontal dispersion may be estimated following (Elder, 1959):

\[
D_{disp_x} = \frac{C_{disp} H |U| \sqrt{g}}{55.0} \\
D_{disp_y} = \frac{C_{disp} H |V| \sqrt{g}}{55.0}
\]

(2.3.4)

where 55.0 is an average Chézy-coefficient and \( C_{disp} \) is a constant specified by the user in the input file. For the applications of the WAQUA system these terms must be of secondary importance. If the vertical shear is really important, the 3D mathematical model TRIWAQ should be used.

Finally we have to integrate the Laplace operator. First we integrate the horizontal second order derivative. By using Leibniz' rule twice, this results in:

\[
\int_{-d}^{\zeta} D_i \frac{\partial^2 c}{\partial x^2} dz = D_i \frac{\partial^2 H C}{\partial x^2} - D_i \frac{\partial}{\partial x} (c(\zeta) \frac{\partial \zeta}{\partial x}) - D_i \frac{\partial}{\partial x} (c(-d) \frac{\partial d}{\partial x}) \\
- D_i \frac{\partial c}{\partial x} \frac{\partial \zeta}{\partial x} = D_i \frac{\partial c}{\partial x} (-d) \frac{\partial d}{\partial x}
\]

(2.3.5a)

Integration of the vertical diffusion gives:

\[
\int_{-d}^{\zeta} D_i \frac{\partial^2 c}{\partial z^2} dz = D_i \frac{\partial c}{\partial z} (\zeta(x, y, t)) - D_i \frac{\partial c}{\partial z} (-d(x, y))
\]

(2.3.5b)

The diffusion terms at the free surface in (2.3.2b) are combined. In WAQUA it is assumed that there is no exchange through the free surface. Also the exchange through the bottom is zero.

The depth-averaged advection-diffusion equation is given in conservative form by:

\[
\frac{\partial H C}{\partial t} + \frac{\partial H U C}{\partial x} + \frac{\partial H V C}{\partial y} = \frac{\partial}{\partial x} \left( H \left( D_H + D_{disp} \right) \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( H \left( D_H + D_{disp} \right) \frac{\partial C}{\partial y} \right) + S
\]

(2.3.6)

where \( S \) is the sum of the local source and sink terms defined by

\[
S = S_{IN} C_{IN} - S_{OUT} C
\]

(2.3.7)

with

\[
C_{IN} \quad \text{concentration of global source} \\
Q_{IN} \quad \text{global source per unit area in (m/s)} \\
Q_{OUT} \quad \text{global sink per unit area in (m/s)}
\]
2.4 Model Equations in Curvi-linear Co-ordinates

In Section 2.2 and 2.3 we derived the equations of WAQUA in rectilinear co-ordinates. In the following chapters we describe the finite difference method to discretize the governing equations. Discretization of the equations on an equidistant rectilinear grid has some drawbacks:

- the poor representation of coastlines, river bends, navigation channels,
- no grid refinement possible.

Therefore, especially for river engineering applications, a boundary-fitted curvi-linear co-ordinate transformation was introduced in WAQUA (Willemse et al., 1986). Curvilinear grids make it possible to follow the horizontal geometry smoothly. The transformation introduces local grid refinement, e.g. to use a fine grid in the summer bed and a more coarse grid in the winter bed. On a rectilinear grid the deep channels are more often aligned at 45 degrees to the computational grid, which introduces artificial wall friction, see (Weare, 1979).

By the use of an orthogonal transformation, the transformed equations are very similar to the original equations and the finite difference method developed by (Stelling, 1984) for rectilinear grids, may be applied. We define our co-ordinate transformation as:

\[ x = X(\xi, \eta) \]
\[ y = Y(\xi, \eta) \]  
(2.4.1)

The transformation coefficients from the Cartesian co-ordinate system \((x, y)\) to the orthogonal curvilinear system \((\xi, \eta)\) are:

\[ g_{\xi\xi} = \left( \frac{\partial x}{\partial \xi} \right)^2 + \left( \frac{\partial y}{\partial \xi} \right)^2 \]
\[ g_{\eta\eta} = \left( \frac{\partial x}{\partial \eta} \right)^2 + \left( \frac{\partial y}{\partial \eta} \right)^2 \]  
(2.4.2)

The grid lines \(\xi = \text{constant}\) and \(\eta = \text{constant}\) form an orthogonal mesh if:

\[ \frac{\partial x}{\partial \xi} \frac{\partial x}{\partial \eta} + \frac{\partial y}{\partial \xi} \frac{\partial y}{\partial \eta} = 0 \]  
(2.4.3)

The determinant of the Jacobian of the transformation is denoted by:

\[ J = \left| \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \xi} \frac{\partial x}{\partial \eta} \right| = \sqrt{g_{\xi\xi}g_{\eta\eta}} = \sqrt{g}. \]  
(2.4.4)
WAQUA is often applied for complex geometries. Then the above defined co-ordinate transformation can not be prescribed analytically. By numerically solving a set of Poisson equations, see (Willemse et al., 1986) a curvi-linear grid can be generated from a desired grid in the physical space. A further discussion on curvi-linear grid generation is beyond the scope of this report and we refer to (Thompson et al., 1980). The curvilinear grid, which is the output of a grid generator, e.g. RGFGGRID, must be given to the WAQUA system as input file.

(Verboom et al., 1983) gives an extended description of the transformation of the depth-averaged shallow water equations to an orthogonal curvilinear grid, see also (Willemse et al., 1986). The velocities in WAQUA follow the covariant directions but have the same velocity scale as the original Cartesian counterparts. Here we only present the result of the transformation.

Writing the continuity equation (2.2.19a) in orthogonal curvilinear co-ordinates yields:

\[
\frac{\partial \xi}{\partial t} + \frac{1}{\sqrt{g \cdot \xi}} \frac{\partial}{\partial \xi} \left( HU \sqrt{g \eta \eta} \right) + \frac{1}{\sqrt{g \cdot \eta}} \frac{\partial}{\partial \eta} \left( HV \sqrt{g \xi \xi} \right) = 0
\]  

(2.4.5a)

and for the momentum equations (2.2.19b-c) we have:

\[
\frac{\partial U}{\partial t} + \frac{U}{\sqrt{g \xi \xi}} \frac{\partial U}{\partial \xi} + \frac{V}{\sqrt{g \eta \eta}} \frac{\partial U}{\partial \eta} + \frac{UV}{\sqrt{g \xi \xi}} + \frac{V^2}{\sqrt{g \eta \eta}} \frac{\partial}{\partial \xi} \left( f + \frac{g}{\sqrt{g \xi \xi}} \right) - \frac{v}{\sqrt{g \eta \eta}} \frac{\partial}{\partial \eta}
\]

\[
+ g \frac{U}{C^2_{2\eta \xi}} \frac{U^2 + V^2}{H} = \frac{\rho_0 C_d W_0}{\rho_0 H} \frac{W_0 \xi + W_0 \eta}{\sqrt{g \xi \xi}} \frac{\partial}{\partial \xi} + \frac{\rho_0 C_d W_0}{\rho_0 H} \frac{W_0 \eta}{\sqrt{g \eta \eta}} \frac{\partial}{\partial \eta}
\]

(2.4.5b)

\[
\frac{\partial V}{\partial t} + \frac{U}{\sqrt{g \xi \xi}} \frac{\partial V}{\partial \xi} + \frac{V}{\sqrt{g \eta \eta}} \frac{\partial V}{\partial \eta} + \frac{UV}{\sqrt{g \xi \xi}} + \frac{U^2}{\sqrt{g \eta \eta}} \frac{\partial}{\partial \xi} \left( f + \frac{g}{\sqrt{g \eta \eta}} \right) - \frac{v}{\sqrt{g \xi \xi}} \frac{\partial}{\partial \eta}
\]

\[
+ g \frac{V}{C^2_{2\eta \xi}} \frac{U^2 + V^2}{H} = \frac{\rho_0 C_d W_0}{\rho_0 H} \frac{W_0 \xi + W_0 \eta}{\sqrt{g \eta \eta}} \frac{\partial}{\partial \xi} + \frac{\rho_0 C_d W_0}{\rho_0 H} \frac{W_0 \eta}{\sqrt{g \xi \xi}} \frac{\partial}{\partial \eta}
\]

(2.4.5c)

with

\[
F^1 = \frac{1}{\sqrt{g \cdot \xi}} \left[ \frac{\partial}{\partial \xi} (U \sqrt{g \eta \eta}) + \frac{\partial}{\partial \eta} (V \sqrt{g \xi \xi}) \right]
\]

(2.4.5d)

\[
F^2 = \frac{1}{\sqrt{g \cdot \eta}} \left[ \frac{\partial}{\partial \xi} (V \sqrt{g \eta \eta}) - \frac{\partial}{\partial \eta} (U \sqrt{g \xi \xi}) \right]
\]
For the depth-averaged transport equation in curvilinear co-ordinates we have following (Eq. (2.3.6)):

\[
\frac{\partial}{\partial t} (HC) + \frac{L}{\sqrt{g}} \frac{\partial}{\partial \xi} \left( HUC \sqrt{g_{\eta \eta}} \right) + \frac{L}{\sqrt{g}} \frac{\partial}{\partial \eta} \left( HVC \sqrt{g_{\eta \eta}} \right) =
\]

\[
\frac{L}{\sqrt{g}} \frac{\partial}{\partial \xi} \left( H(D_{h} + D_{\text{disp}}) \sqrt{g_{\eta \eta}} \frac{\partial C}{\partial \xi} \right)
\]

\[
+ \frac{L}{\sqrt{g}} \frac{\partial}{\partial \eta} \left( H(D_{h} + D_{\text{disp}}) \sqrt{g_{\eta \eta}} \frac{\partial C}{\partial \eta} \right) + S
\]

with $S$ the sum of the global source and sink terms as defined in (2.3.7).

### 2.5 Model Equations in Spherical Co-ordinates

When the area to be modelled covers a considerable part of the globe, the assumption of a flat (rectilinear or curvilinear) model is no longer valid. For such a model area WAQUA offers the possibility to apply a spherical co-ordinate system, see Figure 2.2.

The grid size is no longer defined in meters but in degrees. Users are advised to choose for spherical grids with an $n$-axes pointing North and an $m$-axes pointing East. Spherical grids with $m$- and $n$-axes not coinciding with longitude and latitude are possible but not convenient in use.

The governing equations written in spherical co-ordinates are given by:

\[
\frac{\partial \zeta}{\partial t} + \frac{1}{R \cos \phi} \frac{\partial}{\partial \lambda} (HU) + \frac{1}{R \cos \phi} \frac{\partial}{\partial \phi} (HV \cos \phi) = 0
\]

(2.5.1a)
Figure 2.2 Spherical co-ordinates grid

\[
\frac{\partial U}{\partial t} + \frac{U}{R \cos \phi} \frac{\partial U}{\partial \lambda} + \frac{V}{R} \frac{\partial U}{\partial \phi} - \frac{UV \tan \phi}{R} - 2\Omega V \sin \phi \frac{g}{R \cos \phi} \frac{\partial \zeta}{\partial \lambda}
+ gU \frac{\sqrt{U^2 + V^2}}{C_{2D}H} = \frac{\rho_{air} C_d W_k}{\rho_o H} \frac{\sqrt{W^2 + W^2_\phi}}{\rho_o R \cos \phi} \frac{1}{\frac{\partial P_{am}}{\partial \lambda}}
\]

(2.5.1b)

\[
\frac{\partial V}{\partial t} + \frac{U}{R \cos \phi} \frac{\partial V}{\partial \lambda} + \frac{V}{R} \frac{\partial V}{\partial \phi} + \frac{U^2 \tan \phi}{R} + 2\Omega U \sin \phi + \frac{g}{R} \frac{\partial \zeta}{\partial \phi}
+ gV \frac{\sqrt{U^2 + V^2}}{C_{2D}H} \frac{\rho_{air} C_d W_k}{\rho_o H} \frac{\sqrt{W^2 + W^2_\phi}}{\rho_o R \cos \phi} \frac{1}{\frac{\partial P_{am}}{\partial \phi}}
\]

(2.5.1c)

with \( R \) the radius of the earth.

The depth-averaged transport equation for dissolved constituents reads:

\[
\frac{\partial}{\partial t} (HC) + \frac{1}{R \cos \phi} \frac{\partial}{\partial \lambda} (HUC) + \frac{1}{R \cos \phi} \frac{\partial}{\partial \phi} (HVC \cos \phi) =
\]

\[
\frac{1}{R \cos \phi} \frac{\partial}{\partial \lambda} \left( H(D_h + D_{disp}) \frac{1}{R \cos \phi} \frac{\partial C}{\partial \lambda} \right)
+ \frac{1}{R \cos \phi} \frac{\partial}{\partial \phi} \left( H(D_h + D_{disp}) \frac{1}{R} \frac{\partial C}{\partial \phi} \cos \phi \right) + S
\]

(2.5.2)
The equations in spherical co-ordinates are a special case of the equations in orthogonal curvilinear co-ordinates. Define a fixed Cartesian frame through the origin of the earth, then the spherical co-ordinates of a point on the earth's surface are given by:

\[(x, y, z)^T = (\lambda, \phi, R)^T\] with

\[
x = R \cdot \cos \phi \cdot \cos \lambda \\
y = R \cdot \cos \phi \cdot \sin \lambda \\
z = R \cdot \sin \phi
\] (2.5.3)

Replacing in Eq. (2.4.1) \(\xi\) and \(\eta\) by:

\[\xi = \lambda, \; \eta = \phi, \; \sqrt{g_{\xi\xi}} = \sqrt{g_{\lambda\lambda}}, \; \sqrt{g_{\eta\eta}} = \sqrt{g_{\phi\phi}}\] (2.5.4)

yields Eq. (2.5.1).

### 2.6 Baroclinic Pressure Gradient

In Section 2.2 we have derived the pressure term in the depth-averaged equations using a constant density. For a constant density the pressure gradient is determined by the free surface slope, the so-called barotropic pressure gradient defined by Eq. (2.2.5). In this section we will derive a pressure gradient term for variable density. As has been stated in Section 2.3 a transport solver for salinity and heat is part of the WAQUA-system. At this moment the mathematical formulation for the heat exchange between air and water is not operational. Heat is treated as a conservative substance.

In a tidal river, salt water from the sea penetrates due to its greater density. The salt concentration is computed by the advection-diffusion equation. The influence of the salinity on the density is determined by the equation of state. WAQUA uses the empirical relation given by (Eckart, 1958):

\[\rho(S,T) = \frac{P_0}{\lambda + \alpha_o P_0} \] (2.6.1)

with

\[
\lambda = 1779.5 + 11.25T - 0.0745T^2 - (3.80 + 0.01T)S
\]

\[
\alpha_o = 0.6980
\] (2.6.1b)

\[P_o = 5890 + 38T - 0.375T^2 + 3S\]

Here \(T\) is the temperature in degrees Celsius and \(S\) is the salinity in parts per thousand. Because the density varies only weakly with the temperature, usually a constant temperature is applied. The default temperature in WAQUA is 14 °C.

Now we will derive the baroclinic pressure gradient. Therefore we recall Eq. (2.2.6).
\[ p(x, y, z, t) = \int_{z}^{\zeta} \rho(x, y, z', t) g dz' + P_{atm} \quad (2.6.2) \]

For the derivation we assume the atmospheric pressure to be constant. In WAQUA the user can only specify an atmospheric pressure field for a model area with spherical co-ordinates. Differentiation of Eq. (2.6.2) in the x-direction gives:

\[ \frac{\partial p(x, y, z, t)}{\partial x} = \frac{\partial}{\partial x} \int_{z}^{\zeta} \rho(x, t) g dz' \quad (2.6.3) \]

We integrate Eq. (2.6.3) over the water depth from the bed to the free surface:

\[ \int_{-d}^{\zeta} \frac{\partial p(x, y, z, t)}{\partial x} dz = \int_{-d}^{\zeta} \frac{\partial}{\partial x} \int_{z}^{\zeta} \rho(x, y, z, t) g dz' dz \quad (2.6.4) \]

WAQUA is a depth-averaged flow model and we assume that the water column is well-mixed in the vertical. The density is constant in the vertical direction, i.e. \( \rho(x, y, z', t) = \rho(x, y, t) \). Then we have:

\[ \int_{-d}^{\zeta} \frac{\partial}{\partial x} \int_{z}^{\zeta} \rho(x, y, t) dz' dz = \int_{-d}^{\zeta} \frac{\partial}{\partial x} ((\zeta' - z) \rho) g dz = \rho g H \frac{\partial \zeta}{\partial x} + \frac{1}{2} \frac{\partial \rho}{\partial x} g H^2 \quad (2.6.5) \]

The second term in the right-hand side is denoted as the baroclinic pressure gradient. In tidal areas it may be small compared to the barotropic gradient, but it may significantly influence the residual flow. Following the Boussinesq hypothesis the influence of variable density appears only in the baroclinic pressure term. In the other terms a constant reference density \( \rho_0 \) is assumed. Then, the pressure gradient in x-direction in the depth-averaged U-momentum equation is given by:

\[ \frac{1}{\rho_0} \frac{\partial p}{\partial x} = \frac{1}{\rho_0 H} \int_{-d}^{\zeta} \frac{\partial p}{\partial x} dz' + g \frac{\partial \zeta}{\partial x} + \frac{g H}{2 \rho_0} \frac{\partial \rho}{\partial x} \quad (2.6.6) \]

In the y-direction we obtain a similar expression. Notice that in the case of a constant density Eq. (2.6.6) reduces to Eq. (2.2.6).

Transformation of the gradient-operator to curvi-linear co-ordinates gives:

\[ \frac{1}{\rho_0 \sqrt{g_{\xi\xi}}} \frac{\partial p}{\partial \xi} = \frac{g}{\sqrt{g_{\xi\xi}}} \frac{\partial \zeta}{\partial \xi} + \frac{g H}{2 \sqrt{g_{\xi\xi}} \rho_0} \frac{\partial \rho}{\partial \xi} \quad (2.6.7a) \]

\[ \frac{1}{\rho_0 \sqrt{g_{\eta\eta}}} \frac{\partial p}{\partial \eta} = \frac{g}{\sqrt{g_{\eta\eta}}} \frac{\partial \zeta}{\partial \eta} + \frac{g H}{2 \sqrt{g_{\eta\eta}} \rho_0} \frac{\partial \rho}{\partial \eta} \quad (2.6.7b) \]
2.7 Structures

2.7.1 Barriers and sluices

In WAQUA the user may define in certain grid points hydraulic structures (sluices or barriers). The flow through the structure is not resolved on the grid. Upstream of a structure the flow is accelerated due to contraction and downstream the flow is decelerated due to expansion. The expansion introduces an important energy loss.

The mathematical formulation for barriers as used in WAQUA is based on the work of Leendertse. Leendertse situated a barrier, at a water level point. His approach was adapted, see (Langerak, 1988) and (Wybenga, 1989). In WAQUA barriers are situated at velocity points. The numerical implementation of barriers in WAQUA is described by (Lander, 1991).

In WAQUA, in a barrier point the wet cross-section may vary in time. In the vertical direction the wet cross section may vary both by the raising or lowering of a sill and by the lowering or raising of a gate. In the horizontal direction the effective wet width may also be increased or decreased. *U*-barriers are located at *U*-velocity points and *V*-barriers at *V*-velocity points. Diagonal barriers consist of a combination of a *U*- and a *V*-barrier. The length of a barrier is assumed to be smaller than one grid cell and is not taken into account (subgrid).

![Barrier Diagram](image)

**BARRIER**

Figure 2.3 Definitions for a barrier

The deceleration of the flow behind a hydraulic structure introduces an important energy loss. This energy loss is not resolved by the advection terms and is taken into account by adding an extra friction term to the momentum equation. This term has the same quadratic form as the bottom friction term, with a contraction coefficient (barrier coefficient) *M* that depends on the flow condition. The extra friction in the *U*-momentum equation is given by:

\[
\frac{UIU \sin \alpha + V \cos \alpha d}{2\Delta x} \left( \frac{1}{M^2} - 1 \right) \quad 0 < M \leq 1
\]  

(2.7.1)
with $\alpha$ the angle between the barrier and the $U$-direction. $\alpha$ is zero corresponds with a $U$-barrier. The contraction coefficient gives the ratio between the wet cross section of the barrier and the wet cross section upstream:

$$M = \frac{\mu H_0 B}{H_1 \Delta y}$$  \hspace{1cm} (2.7.2)

with (see also Figure 2.3)
- $B$ = relative width of opening
- $H_0$ = vertical distance from sill to free surface or bottom of gate at the barrier
- $H_1$ = vertical distance from the sill to the upstream water level
- $\mu$ = barrier flow coefficient for restricted flow

In WAQUA the appropriate contraction coefficient is determined from the flow condition at the barrier and the barrier coefficient specified by the user. In most cases the contraction coefficient is determined with $H_1$ being the vertical distance between the sill level and the upstream water level, but in some cases (conditions 2 and 3) the energy height is used and $E_1$ is determined by the Bernoulli equation:

$$E_1 = \zeta_1 + d_{sill} + \frac{U_1^2}{2g}$$  \hspace{1cm} (2.7.3)

where
- $E_1$ = upstream energy level
- $U_1$ = upstream velocity
- $d_{sill}$ = depth sill.

The barrier coefficient may be specified dependent on the flow direction and the flow condition, as the flow characteristics of the hydraulic structure may vary. The barrier coefficients are generally obtained from laboratory or field measurements.

At a hydraulic structure the flow may become supercritical. In the case of supercritical flow, the down-stream water level and velocity do not influence the discharge through the structure. In the continuity equation the flow-through height is determined by the upstream water level and in the discretized momentum equations a special treatment is required for the free surface gradient, and the advection and viscosity term, see (Lander, 1991). In the free surface gradient the downstream water level is determined with the theoretical value for critical flow,
\[ \zeta_2 = \frac{2}{3} \left( \zeta_1 + \frac{U_1^2}{2g} \right) \] \hspace{1cm} (2.7.4)

with

\[ \begin{align*}
\zeta_1 & = \text{upstream water level} \\
U_1 & = \text{upstream velocity} \\
\zeta_2 & = \text{downstream water level}
\end{align*} \]

For computation of the downstream advection term just behind the barrier, it is assumed that the discharge is steady. The downstream velocity at the barrier is determined from the discharge through the barrier and the downstream flow-through height.

In WAQUA, eight flow conditions are distinguished for the flow at the barrier. The flow condition is dependent on the upstream and downstream water level in relation to the sill depth and the height of the gate. We specify the discharge relation for the five basic conditions: 1, 3, 4, 7, 8. The other conditions 2, 5 and 6 are transition states. In Figure 3.10 of the User’s guide WAQUA a graphical overview is given of the five basic flow conditions 1, 3, 4, 7, 8.

**condition 1**

The flow is restricted by the gate, but not influenced by the downstream water level. This condition occurs when \( H_1 > 1.5 \ H_0 \) and when \( 0 < H_2 < H_0 \). For these conditions the flow is certainly supercritical and the discharge is given by:

\[ Q = \mu_{5,6} \ B \ H_0 \sqrt{2g(H_1 - H_0)} \] \hspace{1cm} (2.7.5)

where:

\[ \begin{align*}
Q & = \text{steady-state flow rate per unit width} \\
B & = \text{relative width of opening} \\
H_0 & = \text{vertical distance from sill to bottom of gate} \\
H_1 & = \text{vertical distance from the sill to the upstream water level} \\
H_2 & = \text{vertical distance from the sill to the downstream water level} \\
\mu_{5,6} & = \text{barrier flow coefficient for gate restricted flow}
\end{align*} \]

**condition 3**

The free surface does not touch the gate, and the sill is so high that the downstream water level has no influence on the flow rate. This condition occurs when \( H_1 < H_0 \) and when \( H_2 < 2/3 \ H_1 \). The flow is supercritical and the flow rate is given by:

\[ Q = \mu_{3,4} \ B \ \frac{2}{3} H_1 \sqrt{\frac{2}{3} g E_i} \] \hspace{1cm} (2.7.6)

where:
\[ \mu_{3,4} = \text{barrier coefficient for free surface supercritical flow} \]

**Condition 4**

In this case the free surface does not touch the gate, but the downstream water level is so high that it influences the flow rate. This condition occurs when \( H_I < H_0 \) and \( H_2 > \frac{2}{3} H_I \). The flow is subcritical and the discharge is given by:

\[ Q = \mu_{1,2} B \sqrt{2g(H_I - H_2)} \quad (2.7.7) \]

where:

\[ \mu_{1,2} = \text{barrier flow coefficient for free surface subcritical flow} \]

**Condition 7**

Both the upstream and downstream water levels are higher than the gate and the flow is subcritical, thus \( H_I > \frac{3}{2} H_0 \) and \( H_0 > 0 \). The discharge is given by:

\[ Q = \mu_{5,6} B H_0 \sqrt{2g(H_I - H_2)} \quad (2.7.8) \]

**Condition 8**

In this case the water flows through a slot which is situated above the downstream water level; thus \( H_I > H_0 \) and \( H_2 < 0 \).

The flow rate is given by:

\[ Q = \mu_{5,6} B H_0 \sqrt{2g(H_I - \frac{1}{2} H_0)} \quad (2.7.9) \]

The other conditions are transitions between the basic flow conditions or the special case of a closed barrier:

**Condition 0**

In the simulation the gate can be closed or the sill is above the highest water level and there is no discharge through the barrier. This occurs when \( H_0 = 0, B = 0 \), or \( H_I < 0 \), then
\[ Q = 0 \]  

\textit{condition 2}

This condition describes the transition between supercritical gate flow and supercritical free surface flow. This condition will be encountered when we are in condition 3 with free surface supercritical flow and we are lowering the gate. When the gate touches the water, the flow is suddenly much more restricted which will generate a flow discontinuity. This discontinuity requires a special numerical approach which has not been implemented. To prevent the occurrence of a discontinuity a gradual transition was implemented between condition 1 and 3.

\textit{conditions 5 and 6}

These conditions are for the gradual transition between the free surface subcritical flow (condition 1) and subcritical gate flow (condition 7).

\subsection*{2.7.2 Weirs}

In WAQUA the user may define in certain grid points weirs. Weirs are built to increase the water levels upstream of the weir for navigation or to protect an area behind a tidal weir for salt intrusion. The flow over a weir is not resolved on the computational grid. Upstream of a weir the flow is accelerated due to contraction and downstream the flow is decelerated due to expansion. The expansion introduces an important energy loss. The energy loss is dependent on the shape of the crest of the weir.

The mathematical formulation for weirs as used in WAQUA is based on the work in (Wybenga, 1990). Details of the numerical implementation of weirs in WAQUA are described in (Van Kester et al., 1997).

A weir is situated in a \textit{U}-point or in a \textit{V}-point. The length of a weir is always one grid space. It is also possible to define diagonal weirs, see Figure 2.4. A diagonal weir is a combination of a \textit{U}-weir and a \textit{V}-weir. The length of a diagonal weir is the square root of the length of the \textit{U}- and \textit{V}-weir. Let \( \alpha \) be the angle between the weir and the \textit{U}-direction. \( \alpha \) is zero corresponds to a \textit{U}-weir. A diagonal weir gives a better representation of the length of a skewed weir than the combination of a single \textit{U}- and a single \textit{V}-weir.

Weirs are commonly used in simulation models of rivers to model sudden changes in depths, the representation of summer dikes or the border of a sand pit. Also groynes are modelled as weirs. A WAQUA model of a dutch river can contain a lot of weirs.

The energy loss due to a weir is dependent on the shape of the crest. The extra energy loss in the direction perpendicular to the weir is denoted as \( \Delta E \). The energy loss is determined in the direction perpendicular to the weir with a one dimensional formulation dependent on the velocity at the weir: \( W_e \).
Figure 2.4 Definitions for a diagonal weir

The discharge through a skewed weir equals the sum of the discharges through the corresponding U- and V-weir:

\[ |W_i| \sqrt{(\Delta x)^2 + (\Delta y)^2} = |W_{\perp}| \Delta y \sin \alpha + \Delta x \cos \alpha \]  

(2.7.11)

For steady uniform flow, the energy gradient over the weir is parallel with the hydraulic gradient over the weir. The energy loss per unit of length is equal to the hydraulic gradient. The hydraulic gradient over the weir may be forced by a quadratic friction term.

For the x-direction we have:

\[ \frac{\Delta E}{\Delta x} = g \frac{W_i \sin \alpha |W_i|}{C_{ex}\left(\zeta + d\right)} \]  

(2.7.12a)

and

\[ C_{ex} = \sqrt{\frac{\Delta x (W_i)^2 \sin \alpha}{\Delta E(\zeta + d)}} \]  

(2.7.12b)

In WAQUA, in a weir point the momentum equation is solved. The height of the crest is taken into account in the drying and flooding control, see Chapter 8 but at a weir point, the flow-through height is determined independent of the weir crest. The energy loss due to the weir is added to the bottom friction term, which reduces the discharge:
\[ g \frac{\Delta \zeta}{\Delta x} + g \frac{U \sqrt{U^2 + V^2}}{C_{\text{tot},U} (\zeta + d)} = 0 \quad (2.7.13a) \]

with

\[ \frac{I}{C_{\text{tot},U}^2} = \frac{I}{C_{\text{field},U}^2} + \frac{W \sin(\alpha) W}{U \sqrt{U^2 + V^2} C_{\text{ex},U}} \quad (2.7.13b) \]

where:

- \( C_{\text{tot},U} \) = Chézy-coefficient total roughness in U-point
- \( C_{\text{field},U} \) = Chézy-coefficient field roughness in U-point
- \( C_{\text{ex},U} \) = Chézy-coefficient extra roughness caused by the weir

The energy loss and \( C_{\text{ex},U} \) are dependent on the flow velocities at the weir. They are determined outside the subroutines for the momentum equations and based on the velocities of the previous half timestep. This may lead to unstable behaviour at the moment the weir is flooded. Therefore the Chézy-coefficient of a dry weir is initialized at 0.1, yielding an almost infinite friction when a weir point is set wet. The user can specify a parameter \( \theta_c \) to reduce smoothly the friction coefficient during flooding:

\[ \left( \frac{I}{C_{\text{tot},U}^2} \right)^{1+y_2} = \theta_c \left( \frac{I}{C_{\text{tot},U}^2} \right)^{1+y_2} + (1-\theta_c) \left( \frac{I}{C_{\text{field},U}^2} + \frac{W \sin(\alpha) W}{U \sqrt{U^2 + V^2} C_{\text{ex},U}} \right)^{1+y_2} \quad (2.7.14) \]

subcritical flow

For subcritical flow over the crest of a weir (imperfect weir), the energy loss is based on the so-called 'Tabellenboek van Rijkswaterstaat' (Vermaas, 1987) and/or the Carnot equation. The relation for the energy loss depends on the flow velocity at the weir. An example of an imperfect weir is shown in Figure 2.5.

![Figure 2.5: Imperfect weir](image-url)
If the flow velocity at the weir is less than 0.25 m/s, the energy loss is calculated according to the Carnot equation for the energy loss in a sudden expansion. If the flow velocity above the weir is more than 0.50 m/s, the energy loss is determined by interpolation of measured data ('Tabellenboek', Vermaas, 1987). When the flow velocity is between 0.25 m/s and 0.50 m/s, a weighted average is taken between the energy loss following Carnot and the measurements.

**supercritical flow**

For supercritical flow the resulting upstream flow conditions are independent of the downstream water level, as defined for a perfect weir. The discharge depends on the energy head in relation to the sill depth of the weir. The energy head is computed by applying the Bernoulli equation:

\[ E_i = \xi + d_{sill} + \frac{U_i^2}{2g} \]  \hspace{1cm} (2.7.15)

The discharge formula for a perfect weir is given by:

\[ Q = \frac{2}{3} \sqrt{\frac{2g}{3}} E_{i,s} \]  \hspace{1cm} (2.7.16)

where:

- \( E_i \) = upstream energy head in relation to the sill depth
- \( E_s \) = downstream energy head in relation to the sill depth
- \( Q \) = supercritical discharge

The energy head downstream of the weir is calculated from the discharge and the downstream water level. The difference between the energy head at the weir and the energy head downstream of the weir is equal to the energy loss caused by the weir, see Figure 2.6.

![Perfect Weir Diagram](image-url)

Figure 2.6: Perfect weir
The energy level downstream is given by:

\[ E_2 = \zeta_2 + d_{ill} + \frac{1}{2g} \left( \frac{Q}{H_0} \right)^2 \]  

(2.7.18)

The energy loss due to a perfect weir is, see e.g. (Van Rijn, 1990), given by:

\[ \Delta E = \frac{E_1}{3} + \zeta_0 - E_2 \]  

(2.7.19)

with \( \zeta_0 \) the water level at weir and

\[ \zeta_0 = \frac{2E_1}{3} \]  

(2.7.20)
3 Considerations on numerical techniques used in WAQUA

3.1 Introduction

In Chapter 2 the depth-averaged shallow water equations were derived. The WAQUA system is a numerical flow model based on the solution of these equations. To discretize these equations in space, the model area is covered by a rectangular, curvilinear or spherical grid. WAQUA is based on finite differences and the grid must be orthogonal and well-structured. The grid is rectangular in the transformed space, see Figure 3.1. In case of a curvilinear grid, a file with curvilinear grid co-ordinates has to be provided. Such a file is generated with a grid generator, e.g. (RGFGRID, 1996). The numerical grid transformation is briefly described in Section 3.3. The transformation is implicitly known by the mapping of the co-ordinates of the grid vertices. The geometrical quantities \( \sqrt{g_{\xi\xi}}, \sqrt{g_{\eta\eta}} \) and \( g \), introduced in the transformed equations have to be discretized on the computational grid.

![Figure 3.1. Two-dimensional cell in physical domain \( \Omega \).](image)

The four basic variables water level, \( U \)-velocity, \( V \)-velocity and depth, describe the flow in WAQUA. The \( U \)-velocity and \( V \)-velocity are velocity components in the physical space. The velocity components are perpendicular to the grid cell faces. After a simulation, these velocity components must be transformed to Cartesian velocity components for output purposes.

To discretize the equations, the variables are arranged in a special way on the grid, see Figure 3.2. The pattern is called a staggered grid. This particular arrangement of the
variables is called the Arakawa C-grid (Vreugdenhil, 1994). The data structure is described in Section 3.3. In Chapter 4 the space discretizations of the separate terms are discussed. Chapter 5 is devoted to the time integration. The mathematical boundary conditions and the numerical boundary treatment are discussed in Chapter 6.

### 3.2 Introduction to the ADI method

The WAQUA system is applied for modelling a wide range of flow conditions. In all these cases the system should give a solution, so robustness has highest priority. Following (Stelling, 1984), the discretizations have to satisfy the following demands:

- unconditionally stable,
- at least second order consistency,
- suitable for both time-dependent and steady state problems,
- computationally efficient.

An explicit time integration of the 2D shallow water equations on a rectangular grid would lead to a time step condition based on the Courant number for wave propagation:

\[
C_{\text{wave}} = 2\Delta t \sqrt{gH\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)} \leq 1
\]  

(3.2.1)

with \(\Delta x\) and \(\Delta y\) the smallest grid spaces in the physical space. For many practical applications this requires a time step of a few seconds to simulate tidal propagation. Exceeding the time step would generate an instability and from the view of robustness this is not acceptable. Therefore an implicit method is needed. However, an implicit scheme can be uneconomic in computer time and storage if the inversion of a large matrix is required. A straightforward implicit finite difference approximation is the Crank Nicholson method. For the linearized 2D shallow water equations without advection, the Crank Nicholson method is defined in vector form reads:

\[
\frac{\bar{U}^{i+1} - \bar{U}^i}{\Delta t} + \frac{1}{2} A \bar{U}^i + \frac{1}{2} A \bar{U}^{i+1} = \bar{0}
\]

(3.2.2a)

with \(\bar{U} = (U, V, \zeta)^T\) and \(A = \begin{bmatrix} 0 & f & -g \partial_x \\ -f & 0 & -g \partial_y \\ -H \partial_x & -H \partial_y & 0 \end{bmatrix}\)

(3.2.2b)

The solution after one time step is given by

\[
\bar{U}^{i+1} = \left( I + \frac{1}{2} \Delta t A \right)^{-1} \times \left( I - \frac{1}{2} \Delta t A \right) \bar{U}^i
\]

(3.2.3)

The simultaneously taken spatial discretizations in both grid directions would after discretization generate a system of equations with a matrix with a band structure. In each
row there are at least five non zero entries, corresponding to the grid cells surrounding the water level point. The band width is large and all grid points are coupled. On the present-day computers it would be no problem to store and invert such a system of equations, but in the days of the first WAQUA-simulations (1970's) the core memory was too small to tackle these systems. Leendertse introduced an alternating direction implicit (ADI) method for the shallow water equations (Leendertse, 1967). The ADI-method splits one time step into two stages. Each stage consists of half a time step. In both stages the terms of the model equations are solved in a consistent way. In the first half time step, the \( x \) \((\xi)\)-derivatives are taken implicitly and in the second half time step the \( y \) \((\eta)\)-derivatives are taken implicitly. In vector form the ADI-method is given by:

**Step 1:**

\[
\frac{\bar{U}^{i+\frac{\Delta t}{2}} - \bar{U}^i}{\frac{\Delta t}{2}} + \frac{1}{2} A_x \bar{U}^{i+\frac{\Delta t}{2}} + \frac{1}{2} A_y \bar{U}^i = \tilde{0}
\]  

(3.2.4a)

**Step 2:**

\[
\frac{\bar{U}^{i+1} - \bar{U}^{i+\frac{\Delta t}{2}}}{\frac{\Delta t}{2}} + \frac{1}{2} A_x \bar{U}^{i+\frac{\Delta t}{2}} + \frac{1}{2} A_y \bar{U}^{i+1} = \tilde{0}
\]  

(3.2.4b)

\[
A_x = \begin{bmatrix} 0 & f & -g \partial_x \\ 0 & 0 & 0 \\ -H \partial_x & 0 & 0 \end{bmatrix} \quad \text{and} \quad A_y = \begin{bmatrix} 0 & 0 & 0 \\ -f & 0 & -g \partial_y \\ 0 & -H \partial_y & 0 \end{bmatrix} \]  

(3.2.4c)

The solution after one complete time step is given by

\[
\bar{U}^{i+1} = \left( I + \frac{1}{2} \Delta t A_x \right)^{-1} \times \left( I - \frac{1}{2} \Delta t A_x \right) \times \left( I + \frac{1}{2} \Delta t A_y \right)^{-1} \times \left( I - \frac{1}{2} \Delta t A_y \right) \bar{U}^i
\]  

(3.2.5)

In the first stage the time level proceeds from \( t \) to \( t + \frac{\Delta t}{2} \) and the simulation time from \( t = \Delta t \) to \( t = (t+\frac{\Delta t}{2}) \Delta t \). In this stage first the V-momentum equation (2.4.2c) is solved, followed by the U-momentum equation (2.4.2b) implicitly coupled with the continuity equation (2.4.2a). In the second stage the time level proceeds from \( t + \frac{\Delta t}{2} \) to \( t + 1 \). In this stage first the U-momentum equation is solved, followed by the V-momentum equation which is implicitly coupled with the continuity equation.

For a complete time step, each separate term of the equations is still a second-order consistent approximation to the differential equation. The advantage of the ADI-method is that the implicitly integrated water levels and velocities are coupled along grid lines. Substitution and elimination gives tridiagonal systems of equations, see Chapter 7, which can be solved efficiently by the Thomas algorithm.

Stelling (1984) extended the ADI method of Leendertse with a special approach for the cross advection terms, based on the dissipative reduced phase error scheme. The choice for
the spatial discretization is connected with the ADI time integration. In Chapter 4 we describe the spatial discretizations of the different terms. In Chapter 5 we give the ADI method for the complete system of the non-linear shallow water equations and the transport equation.

The second stage in the ADI-method is almost completely similar to the first stage. The grid quantities, direction dependent coefficients and the $U$-velocity and $V$-velocity are interchanged. The only principal difference between the $U$- and $V$-momentum equation is the sign of the Coriolis term. In the WAQUA system the symmetry is exploited, the same subroutine is used for the momentum equations in both stages, only the sign of the Coriolis term is dependent on the computational direction.

3.3 Computational grid and associated geometrical properties

The boundaries of a river, an estuary and a coastal sea are curved and not smoothly represented on a rectangular grid. The boundary becomes irregular (staircase) and in combination with the ADI scheme may introduce significant errors (Weare, 1979). To reduce these errors a boundary fitted orthogonal curvilinear co-ordinate transformation was introduced in the WAQUA system (Willemse et al., 1986). The velocities near the closed boundaries tend to be parallel to the boundary and therefore tend to be aligned along the grid lines for a boundary-fitted grid. The curvilinear grid allows local grid refinement in areas with strongly varying bottom topography. Grid refinement reduces the computational effort in areas far away from the area of interest.

The grid co-ordinates are generated with a numerical co-ordinate transformation. The co-ordinates are input for the WAQUA system. The grid generator is no part of the WAQUA-system but a separate program. For more details about grid generation we refer to (RGFGRID, 1996).

The curvilinear grid divides the domain in the physical space into cells of arbitrary shape and size. WAQUA assumes a structured grid, which means that each interior cell is surrounded by the same number of cells.

Let us consider a one-to-one boundary fitted co-ordinate mapping in two dimensions from a horizontal plane $G$ to a physical space $\Omega$. In $G$ a uniform grid $G_h$ is defined by

$$G_h = \{(\xi_{m+\frac{1}{2}l},\eta_{n+\frac{1}{2}l}) : \xi_{m+\frac{1}{2}l} = (m - 1)\Delta\xi, \eta_{n+\frac{1}{2}l} = (n - 1)\Delta\eta, m = 1,...,M, n = 1,...,N\}$$

(3.3.1)

These points are the vertices of cells. Figure 3.1 depicts a horizontal cell. The cell vertices are connected by segments of straight lines. These connections are called the faces of a cell. The cell with centre at $(\xi_m,\eta_n)$ is called $G_{mn}$ and its image in $\Omega$ is called $\Omega_{mn}$. The discrete mapping from the grid vertices $(\xi_{m+\frac{1}{2}l},\eta_{n+\frac{1}{2}l})$ in the transformed space to the original points $(x_{m+\frac{1}{2}l},y_{n+\frac{1}{2}l})$ in the physical space is extended to the continuous space by bilinear interpolation. In WAQUA the mapping is chosen such that $\Delta\xi = \Delta\eta = 1$. The discretization of the equations is carried out in the computational space $G_h$. Section 3.4 is devoted to the data representation.
All relevant geometrical quantities are calculated from the co-ordinates of the cell vertices. This involves the following geometrical quantities:

$$\sqrt{g_{xx}}, \sqrt{g_{\eta\eta}}, \text{ and } \sqrt{g}.$$  \hspace{1cm} (3.3.2)

The first two quantities are calculated on a staggered grid in the centre of the faces of a cell $G_{nn}$ according to

$$\sqrt{g_{xx}}_{mn+1/2} = \sqrt{(x_{m+1/2,n+1/2} - x_{m-1/2,n+1/2})^2 + (y_{m+1/2,n+1/2} - y_{m-1/2,n+1/2})^2}$$

$$\sqrt{g_{\eta\eta}}_{m+1/2,n} = \sqrt{(x_{m+1/2,n+1/2} - x_{m+1/2,n-1/2})^2 + (y_{m+1/2,n+1/2} - y_{m+1/2,n-1/2})^2}$$ \hspace{1cm} (3.3.3)

Thus, it is natural to define the location of $\sqrt{g_{xx}}$ at the $V$-velocity points $(m,n \pm 1/2)$ and $\sqrt{g_{\eta\eta}}$ at the $U$-velocity points $(m \pm 1/2,n)$, respectively. Note that $\sqrt{g_{xx}}$ and $\sqrt{g_{\eta\eta}}$ represent the length of the faces of cell $\Omega_{nn}$ in the physical space in $\xi$- and $\eta$-direction, respectively. We assumed that at the start of the program the quantities $\sqrt{g_{xx}}$ and $\sqrt{g_{\eta\eta}}$ are calculated and stored permanently. Furthermore, they are interpolated at points where they will be needed, using arithmetic averaging:

$$\sqrt{g_{xx}}_{mn} = \frac{1}{4}(\sqrt{g_{xx}}_{mn-1/2} + \sqrt{g_{xx}}_{mn+1/2})$$

$$\sqrt{g_{\eta\eta}}_{m+1/2,n} = \frac{1}{4}(\sqrt{g_{\eta\eta}}_{m-1/2,n} + \sqrt{g_{\eta\eta}}_{m+1/2,n} + \sqrt{g_{\eta\eta}}_{m,n+1/2} + \sqrt{g_{\eta\eta}}_{m,n-1/2})$$ \hspace{1cm} (3.3.4)

One can approximate the values of the Jacobian $\sqrt{g}$ in the required points. For example,

$$\sqrt{g}_{mn} = \frac{1}{4}(\sqrt{g_{xx}}_{mn-1/2} + \sqrt{g_{xx}}_{mn+1/2} + \sqrt{g_{\eta\eta}}_{m-1/2,n} + \sqrt{g_{\eta\eta}}_{m,n+1/2})$$ \hspace{1cm} (3.3.5)

The Jacobian (3.3.5) gives the area of cell $\Omega_{mn}$.

The averaging of the geometrical quantities introduces inaccuracy, especially if large grid size variations are applied. To keep the errors introduced by the averaging procedure restricted Wybenga (1985) derived an upper bound for the grid variations. For a steady uniform flow in a prismatic channel with a sinus shaped curvilinear grid he obtained an acceptable accuracy if the estimated error in the averaging procedure normalized by the grid size did not exceed 0.02. For $\sqrt{g_{xx}}$ this means that

$$\frac{(\Delta\xi)^2}{8} \frac{\partial^2}{\partial \xi^2} \sqrt{g_{xx}} + \frac{(\Delta\eta)^2}{8} \frac{\partial^2}{\partial \eta^2} \sqrt{g_{xx}} \leq 0.02$$ \hspace{1cm} (3.3.6)
A similar condition can be derived for $\sqrt{g_{\eta \eta}}$. For WAQUA we assume that the grid points are smoothly distributed in the physical space. This requires that the ratio between the grid size of two adjacent grid cells is bounded by a factor $C$:

$$\frac{\max(\sqrt{g_{\xi \xi}}_{m,n+1}, \sqrt{g_{\xi \xi}}_{m,n-1})}{\min(\sqrt{g_{\xi \xi}}_{m,n+1}, \sqrt{g_{\xi \xi}}_{m,n-1})} \leq C \quad \text{and} \quad \frac{\max(\sqrt{g_{\eta \eta}}_{m,n+1}, \sqrt{g_{\eta \eta}}_{m-1,n})}{\min(\sqrt{g_{\eta \eta}}_{m,n+1}, \sqrt{g_{\eta \eta}}_{m-1,n})} \leq C$$ \hspace{1cm} (3.3.7)

Eq. (3.3.6) will be satisfied if the mesh size along a grid line does not deviate more than 20% of the nearest mesh size in the same direction. Therefore $C$ must be smaller than 1.2. The smoothness of a WAQUA grid can be inspected with the grid generator (RGFGRID, 1996).

A second source of inaccuracy is the deviation of orthogonality. Before the introduction of orthogonality the free surface gradient in the $U$-momentum equation is of the following form:

$$\frac{1}{\sqrt{g}} \left[ \left( \frac{\partial x}{\partial \eta} \right)^2 + \left( \frac{\partial y}{\partial \eta} \right)^2 \right] \frac{\partial \xi}{\partial \xi} + \left( \frac{\partial y}{\partial \eta} \right) \left( \frac{\partial y}{\partial \xi} \right) + \left( \frac{\partial x}{\partial \eta} \right) \left( \frac{\partial x}{\partial \xi} \right) = 0$$ \hspace{1cm} (3.3.8)

For an orthogonal grid the second part in the surface free gradient is zero due to the orthogonality condition:

$$\left( \frac{\partial y}{\partial \eta} \right) \left( \frac{\partial x}{\partial \xi} \right) + \left( \frac{\partial x}{\partial \eta} \right) \left( \frac{\partial y}{\partial \xi} \right) = 0$$ \hspace{1cm} (3.3.9)

In WAQUA it is assumed that the second term is zero and therefore this term has not been implemented. For a grid which is not strictly orthogonal the inaccuracy is dependent on the ratio between the first and second term in Eq. (3.3.8). Wybenga (1985) derived for steady flow the following condition:

$$\frac{\left( \frac{\partial y}{\partial \eta} \right) \left( \frac{\partial x}{\partial \xi} \right) + \left( \frac{\partial x}{\partial \eta} \right) \left( \frac{\partial y}{\partial \xi} \right)}{\left( \frac{\partial x}{\partial \eta} \right)^2 + \left( \frac{\partial y}{\partial \eta} \right)^2} < 0.05$$ \hspace{1cm} (3.3.10)

Condition (3.3.10) may be inspected with the grid generator (RGFGRID, 1996). In general the inaccuracies introduced by the numerical approximation of the grid quantities in the pressure term, the advection terms and the curvature terms, are much larger than the inaccuracies introduced by neglecting the second term in the pressure term in Eq. (3.3.8) for almost orthogonal grids.


<table>
<thead>
<tr>
<th>Unknown or quantity</th>
<th>Name</th>
<th>Index set</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set-$\zeta$-points</td>
<td>water level</td>
<td>Set-$\zeta$-points $\subseteq {1,\ldots,M} \times {1,\ldots,N}$</td>
</tr>
<tr>
<td>Set-$U$-points</td>
<td>$U$-velocity</td>
<td>Set-$U$-points $\subseteq {1,\ldots,M} \times {1,\ldots,N}$</td>
</tr>
<tr>
<td>Set-$V$-point</td>
<td>$V$-velocity</td>
<td>Set-$V$-point $\subseteq {1,\ldots,M} \times {1,\ldots,N}$</td>
</tr>
<tr>
<td>Set-$d$-point</td>
<td>depth</td>
<td>Set-$d$-point $\subseteq {1,\ldots,M} \times {1,\ldots,N}$</td>
</tr>
<tr>
<td>$\mathbb{R}$</td>
<td>real numbers</td>
<td>Set of real numbers</td>
</tr>
<tr>
<td>$\mathbb{R}^+$</td>
<td>positive real numbers</td>
<td>Set of positive real numbers</td>
</tr>
</tbody>
</table>

Table 3.1: Basic sets

<table>
<thead>
<tr>
<th>Unknown or quantity</th>
<th>Name</th>
<th>Index set</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\zeta$</td>
<td>water elevation</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}$</td>
</tr>
<tr>
<td>$U$</td>
<td>$U$-velocity</td>
<td>Set-$U$-points $\rightarrow \mathbb{R}$</td>
</tr>
<tr>
<td>$V$</td>
<td>$V$-velocity</td>
<td>Set-$V$-points $\rightarrow \mathbb{R}$</td>
</tr>
<tr>
<td>$d$</td>
<td>depth</td>
<td>Set-$d$-points $\rightarrow \mathbb{R}$</td>
</tr>
<tr>
<td>$C$</td>
<td>concentration</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}^+$</td>
</tr>
<tr>
<td>$S$</td>
<td>salinity</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}^+$</td>
</tr>
<tr>
<td>$\rho$</td>
<td>density</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}^+$</td>
</tr>
</tbody>
</table>

Table 3.2: Representation of several unknowns in the computational grid by index sets
### 3.4 The data structure used in WAQUA

<table>
<thead>
<tr>
<th>Known quantity</th>
<th>Name</th>
<th>Index set</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu_H$</td>
<td>horizontal viscosity</td>
<td>constant</td>
</tr>
<tr>
<td>$C_{2D}^U$</td>
<td>Chézy coefficient at $U$-points</td>
<td>Set-$U$-points $\rightarrow \mathbb{R}^*$</td>
</tr>
<tr>
<td>$C_{2D}^V$</td>
<td>Chézy coefficient at $V$-points</td>
<td>Set-$V$-points $\rightarrow \mathbb{R}^*$</td>
</tr>
<tr>
<td>$D_H$</td>
<td>horizontal diffusivity</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}^*$</td>
</tr>
<tr>
<td>$S$</td>
<td>global sinks or sources</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}^*$</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>time step</td>
<td>constant</td>
</tr>
<tr>
<td>$f$</td>
<td>Coriolis parameter</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}^*$</td>
</tr>
<tr>
<td>$g$</td>
<td>acceleration of gravity</td>
<td>constant</td>
</tr>
<tr>
<td>$\rho_a$</td>
<td>density of air</td>
<td>constant</td>
</tr>
<tr>
<td>$\rho_0$</td>
<td>reference density</td>
<td>constant</td>
</tr>
<tr>
<td>$\sqrt{g_{55}}$</td>
<td>transformation coefficient</td>
<td>Set-$V$-points $\rightarrow \mathbb{R}^*$</td>
</tr>
<tr>
<td>$\sqrt{g_{\eta\eta}}$</td>
<td>transformation coefficient</td>
<td>Set-$U$-points $\rightarrow \mathbb{R}^*$</td>
</tr>
<tr>
<td>$P_{atm}$</td>
<td>atmospheric pressure</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}^*$</td>
</tr>
<tr>
<td>$H^U$</td>
<td>total water depth at $U$-points</td>
<td>Set-$U$-points $\rightarrow \mathbb{R}$</td>
</tr>
<tr>
<td>$\theta^U$</td>
<td>parameter for $H^U$ at $U$-points</td>
<td>Set-$U$-points $\rightarrow [0:1]$</td>
</tr>
<tr>
<td>$H^V$</td>
<td>total water depth at $V$-points</td>
<td>Set-$V$-points $\rightarrow \mathbb{R}$</td>
</tr>
<tr>
<td>$\theta^V$</td>
<td>parameter for $H^V$ at $V$-points</td>
<td>Set-$V$-points $\rightarrow [0:1]$</td>
</tr>
<tr>
<td>$W_\xi$</td>
<td>wind in $\xi$-direction</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}$</td>
</tr>
<tr>
<td>$W_\eta$</td>
<td>wind in $\eta$-direction</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}$</td>
</tr>
<tr>
<td>$W_\lambda$</td>
<td>wind in $\lambda$-direction</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}$</td>
</tr>
<tr>
<td>$W_\phi$</td>
<td>wind in $\phi$-direction</td>
<td>Set-$\zeta$-points $\rightarrow \mathbb{R}$</td>
</tr>
</tbody>
</table>

Table 3.3: Known quantities

WAQUA is based on finite differences. In WAQUA a staggered variable arrangement is used in which all scalar variables (density, water level, salinity and other substances) are located at the cell centre $(m,n)$ which is called the water level point, whereas the velocity component in a given direction is stored in the centre of a cell face orthogonal to that direction. These points are called the $U$- and $V$-velocity points, respectively. The depth data is defined at cell corners. It should be noted that the geometrical quantities $\sqrt{g_{55}}$ and $\sqrt{g_{\eta\eta}}$ are stored in $V$- and $U$-velocity points, respectively. For each unknown we define a finite number of non-overlapping cells that covers the whole domain $\Omega$. Because of the grid staggering, the four different grids (water level, $U$-, $V$- and depth points) shifted with respect to each other by one half mesh width. Using the staggered grid, the number of
computational values is decreased by a factor of four, whereas the accuracy is maintained in comparison with a collocated grid. Furthermore, the implementation of boundary conditions is simplified and spurious oscillations in the water levels are prevented. These advantages are illustrated in (Stelling, 1984).

To avoid the use of "mid-point" indices, we introduce the following convention. The water level point \((m,n)\), \(U\)-velocity point \((m+\frac{1}{2},n)\) and \(V\)-velocity point \((m,n+\frac{1}{2})\) within each 2D computational cell has the same group or cell index \((m,n)\), see Figure 3.1. With the exception of the Jacobian \(\sqrt{g}\), the geometrical quantities are properly represented on the staggered grid, using these indices. The Jacobian must be determined in \(U\)-, \(V\)- and water level points, all having the same \((m,n)\)-index. The Jacobian is not stored but computed. From now on, we shall employ these group indices in our description of the finite difference method.

Tables 3.2 and 3.3 summarize the representation of respectively all the unknowns and quantities to be used in WAQUA in the computational grid by means of the basic index sets as given in Table 3.1. The situation in the computational grid is now well defined.

### 3.4.1 Formal representation of unknowns in WAQUA

Tables 3.1-3 defines the unknowns and quantities to be used in WAQUA on the computational grid by means of index sets.

### 3.4.2 Indirect addressing

WAQUA was developed in the days when the core memory of the computers was relatively small. It was very important to store information in an economic way to save memory and to be able to run large models. Therefore in WAQUA so-called indirect addresses are used to store only the information of the active grid points. In WAQUA a cell is active if one of the velocity points lies within the computational domain or on the boundary. The table with addresses is the LGRID-table. The identification number of an active element is given by:

\[ nm = LGRID(n,m) \]

The indices of the neighbouring cells are given by:

\[ nm_d = LGRID(n,m-1) \]
\[ ndm = LGRID(n-1,m) \]
\[ nmu = LGRID(n,m+1) \]
\[ num = LGRID(n+1,m) \]

For the sake of simplicity, in the formulas of this technical documentation we do not use indirect addresses.
Figure 3.2 Default computational grid with arbitrary open boundary sections

When the tidal openings are not located along a grid line, a non-rectangular computational grid is fitted to the tidal openings. For limiting computations and storage, one or more polygons denoted as the grid enclosures have been introduced in the WAQUA system, see Figure 3.2. Each grid enclosure is a polygon through water level points, just outside the computational area of interest. The index set of the water level openings is a subset of the index set of enclosure points. Water level openings may be defined along rows or columns of the grid, but also along diagonals (45 degrees). For the other boundary types, diagonals are not allowed. Due to the staggered grid, the index set of the other type of openings is not a subset of the enclosure points. On the right of the computational grid the \( m \)-index of the velocity point is one lower than on the enclosure. On the top the \( n \)-index is one lower.

### 3.4.3 Averaging in WAQUA

Unknowns not defined at points where they are required, are obtained by averaging. For this purpose, it is convenient to introduce a short notation. The quantities \( \overline{\xi \phi}_{m,n} \) and \( \overline{\eta \phi}_{m,n} \) indicate arithmetic average values of \( \phi \) in \( \xi \)- and \( \eta \)-direction respectively, taken of two \( \phi \)-points that are nearest to grid point \( (m,n) \), where the values are required. In analogy, \( \overline{\xi \eta \phi}_{m,n} \)
gives the arithmetic average of $\varphi$ at $(m,n)$ resulting from four $\varphi$-points that surround the grid point $(m,n)$ where the value is required. So, we have, for example for the depth-averaged velocity $U$ in a water level point:

$$
\overline{U}^z_{m,n} = \frac{1}{2}(U_{m-1,n} + U_{m,n})
$$

(3.4.1)

and for the depth-averaged velocity $V$ in a $U$-velocity point:

$$
\overline{V}^\eta_{m,n} = \frac{1}{4}(V_{m,n} + V_{m+1,n} + V_{m,n-1} + V_{m+1,n+1})
$$

(3.4.2)

Both advective and diffusive fluxes involve quantities that do not coincide with their points of definition and they are obtained by averaging, interpolation or extrapolation. In these approximate values, the variation of the grid spaces and the curvature of the grid is not taken into account. This simplification will introduce a truncation error on non-smooth grids. Statements about order of consistency are therefore only valid for equidistant rectangular grids. The use of weighted bilinear interpolation would require the implementation of a number of additional terms to account for the variation of the grid.

In the next chapter we describe the space discretization of the depth-averaged continuity equation, the depth-averaged horizontal momentum equations and the depth-averaged transport equation. We use the notation introduced in the previous section.
4 Space Discretization

In the Sections 2.2 and 2.3 we derived the depth-averaged shallow water equations and the depth-averaged advection-diffusion equation in rectilinear coordinates. In Section 2.3 we transformed the equations to an orthogonal curvilinear grid and in Section 2.5 we showed that spherical coordinates are a special case of this transformation. In Chapter 3 we introduced the Alternating Direction Implicit time integration, which is used in WAQUA. The ADI-method splits one time step into two stages. Each stage is consistent with one half time step. In Chapter 3 we also introduced the staggered finite difference grid on which the equations are discretized and defined the unknowns and the grid quantities used in the WAQUA system. At this moment WAQUA has only subroutines for the curvilinear grid system. Rectilinear and sphericals grids are a special case of the curvilinear grid and computed with the same subroutines. This introduces some computational overhead.

In this chapter we specify the spatial discretizations used in WAQUA for orthogonal curvilinear coordinates for both stages of the ADI-scheme on the space staggered grid in the inner region. In Chapter 6 we discuss the implementation of the boundary conditions.

4.1 Discretization of the depth-averaged continuity equation

The discretization of the continuity equation is based on the finite-volume method in the physical space. We integrate the continuity equation over a control volume \( \Omega_{mn} \). To guarantee conservation of volume, the time derivative of the storage in a cell should equal the balance of the amount of water (volume fluxes) passing through the cell faces per unit of time. The discharge through a wet cell boundary is dependent on the normal velocity component which is defined in the centre of the cell boundary, the width of the cell boundary (grid size) and the flow through height (total water depth).

In WAQUA the Cartesian velocity components are replaced by components in the curvilinear system, which are perpendicular to the grid lines. Such components are convenient for a mass-conserving discretization of the continuity equation. In WAQUA, only the direction is transformed, the length of a vector is the same as in the physical space.

Due to the staggered grid the water level and bottom depth are not defined in the centre of the cell boundaries. In WAQUA the total water depth for the computation of the discharge through a cell boundary is normally determined by the arithmetic average of the depth in the corner points of the cell boundary plus the average of the water levels on each side of that boundary:

\[
H_{m,n}^U = \bar{d}^h + 0.5 \cdot (\zeta_{m+1,n}^h + \zeta_{m,n}^h) \quad (4.1.1)
\]

Around low water in shallow areas in the neighbourhood of a deep channel, or at high water near a summer dike, the application of the average water level may lead to a negative total water depth and drying of the velocity point. These cases are described in detail in Chapter 8. The velocity component across a dry cell boundary is set to zero. For the cases
described, the drying is physically not correct. Therefore WAQUA was extended (Van Kester et al., 1997) with an option to determine the water levels at the cell boundaries with a so-called upwind approach. This approach was already suggested by (Stelling, 1984) for shallow regions. The upwind flow through height in a \( U \)-velocity point based on an upwind water level is given by:

\[
H_{m,n}^{U} = \begin{cases} 
\bar{a}^q + \zeta_{m,n} & \text{if } U_{m,n} > 0 \\
\bar{a}^q + \zeta_{m+1,n} & \text{if } U_{m,n} < 0 \\
\bar{a}^q + \max(\zeta_{m,n}, \zeta_{m+1,n}) & \text{if } U_{m,n} = 0
\end{cases}
\]

(4.1.2)

The definition of the upwind total water depth \( H_{m,n}^{V} \) in a \( V \)-velocity point is similar. The upwind approach is physically more realistic for weir like situations between cells with different bottom depth at low water and falling tide. Upwinding the water level in the determination of the total water depth (flow through height) enhances the discharge because the upwind water level is generally higher than the average water level, resulting in a larger flow area, which allows the water level gradient to drive a larger amount of water into the neighbouring cell during the next time step. Taking the maximum of the two surrounding water levels at a dry cell boundary prevents that a cell boundary is artificially kept dry, see Chapter 8 (Figures 8.1 and 8.2).

The total water depth at a \( U \)-velocity point may be expressed with a parameter \( \theta_{m,n}^{U} \):

\[
H_{m,n}^{U} = \bar{a}^q + \theta_{m,n}^{U} \zeta_{m,n} + (1 - \theta_{m,n}^{U}) \zeta_{m+1,n}
\]

\[
\theta_{m,n}^{U} = \begin{cases} 
1.0 & \text{if } U_{m,n} > 0 \\
0.0 & \text{if } U_{m,n} < 0 \\
1.0 & \text{if } \zeta_{m,n} \geq \zeta_{m+1,n} \land U_{m,n} = 0 \\
0.0 & \text{if } \zeta_{m,n} < \zeta_{m+1,n} \land U_{m,n} = 0
\end{cases}
\]

(4.1.3)

The parameter \( \theta_{m,n}^{U} \) is dependent on the solution \((U_{m,n}, \zeta_{m,n})\) of the previous half time step. The average water level corresponds with taking \( \theta_{m,n}^{U} = \frac{1}{2} \). In WAQUA the choice between upwind and average for the water level in a \( U \)-point is controlled by the user-defined parameter DUPWND. The computational procedure is as follows:
\[ H_{m,n}^U = \overline{d}^n + 0.5 \ast (\zeta_{m,n} + \varepsilon_{m+1,n}) \]

*If* \((H_{m,n}^U > \text{DUPWND})\) *Then*

\[ \theta_{m,n}^U = 0.5 \]

*Else*

\[ \theta_{m,n}^U = \begin{cases} 
1.0 & \text{if } U_{m,n} > 0 \\
0.0 & \text{if } U_{m,n} \leq 0 \\
1.0 & \text{if } \zeta_{m,n} \geq \zeta_{m+1,n} \land U_{m,n} = 0 \\
0.0 & \text{if } \zeta_{m,n} < \zeta_{m+1,n} \land U_{m,n} = 0 
\end{cases} \] (4.1.4)

*Endif*

In barrier points always the upwind water level is always taken. For a detailed description of the discretizations at barrier points we refer to (Lander, 1991).

The discharge across a face is dependent on both water level and velocity. In the first half time step of the ADI-scheme, these variables are treated implicitly in a \(U\)-point and explicitly in a \(V\)-point. The non-linearity is removed by an iterative procedure which is described in Section 5.1. The depth-averaged continuity equation (2.4.5a) in a conservative form is discretized for the first half time step in water level point \((m,n)\) as follows:

\[
\frac{\left. \frac{\Box}{\Box} \right|_{m,n} - \left. \frac{\Box}{\Box} \right|_{m,n}^l}{\Delta t} + \frac{1}{(\sqrt{g} \cdot \eta)_{m,n}} \left( (H^U \sqrt{g \cdot \eta})_{m,n}^{l+1/2} - (H^U \sqrt{g \cdot \eta})_{m-1,n}^{l+1/2} \right) + \\
\left( (H^V \sqrt{g \cdot \eta})_{m,n}^{l} - (H^V \sqrt{g \cdot \eta})_{m,n-1}^{l} \right) = 0
\] (4.1.5)

with

\[
(\sqrt{g} \cdot \eta)_{m,n} = (\sqrt{g \cdot \eta})_{m,n}^{\eta} \cdot (\sqrt{g \cdot \eta})_{m,n}^{\xi} 
\] (4.1.6)

the determinant of the Jacobian of the transformation, corresponding with the area of the grid cell \(\Omega_{mn}\) in a water level point. The area is based on the average length of the faces of the grid cell. It would be more accurate to determine the area of the grid cell from the coordinates of the corners points.

### 4.2 Discretization of the \(U\)-momentum equation

Concerning the discretization of the depth-averaged \(U\)-momentum equation (2.4.5b) we discuss respectively the time-derivative, the horizontal advection terms including curvature terms, the barotropic pressure gradient which is due to the water level gradient, the baroclinic pressure gradient which is due to density gradients, the horizontal viscosity term, the Coriolis term and the bottom friction term. The depth-averaged \(U\)-momentum equation is discretized at the \(U\)-velocity points in a non-conservative form. In this chapter we only deal with the discretizations at the inner points, the treatment of the boundaries is discussed in Chapter 6.
4.2.1 Horizontal advective terms including curvature

The choice of the spatial discretization of the advective terms has great influence on the accuracy, monotonicity and efficiency of the computational method. Central differences are second order accurate, but may give rise to non-physical spurious oscillations, so-called "wiggles" (Gresho and Lee, 1979) in the solution. These wiggles arise in the vicinity of steep gradients of the quantity to be resolved. In shallow water flow these wiggles may be introduced near closed boundaries and thin dams. On the other hand, first order upwinding is unconditionally wiggle-free or monotone, thus promoting the stability of the solution process, but introduces a truncation error, which has the form of a second-order artificial viscosity term (see e.g. (Vreugdenhil, 1994)). In advection-dominated flows, this artificial viscosity dominates the physical viscosity and the computed solution is much more smooth than the correct one. Higher order upwinding is not free from numerical oscillations but introduces fourth-order artificial viscosity. This higher order viscosity suppresses the wiggles without smoothing the solution too much.

The discretization of the advection terms, applied in the WAQUA-system was introduced by (Stelling, 1984). The spatial discretization of the advection term $U \partial U / \partial \xi$ and the cross advection term $V \partial U / \partial \eta$ differ. For $U \partial U / \partial \xi$, a central difference operator is applied:

$$\frac{U}{\sqrt{g_{\xi \xi}}} \frac{\partial U}{\partial \xi}_{m,n} \approx \frac{U_{m,n} - U_{m+1,n}}{2\Delta \xi}$$

in both ADI stages while the discretization for the cross advection term $V \partial U / \partial \eta$ is based on the reduced phase error scheme (Stelling, 1984). It is a splitting of a third order upwind finite difference scheme for the first derivative into two second order consistent discretizations, which are successively used in both stages of the ADI-scheme. The scheme is denoted as a Cyclic Method (Stelling et al., 1991), (Vreugdenhil, 1991). To keep the numerical viscosity as small as possible only $V \partial U / \partial \eta$ is approximated by the Cyclic Method.

This third-order upwind discretization, given by:

$$\frac{V}{\sqrt{g_{\eta \eta}}} \frac{\partial U}{\partial \eta}_{m,n} \approx \begin{cases} \overline{V}_{m,n}^{\eta} \frac{U_{m,n+2} + 4U_{m,n+1} + 18U_{m,n} - 28U_{m,n-1} + 5U_{m,n-2}}{24\Delta \eta} & \text{for } \overline{V}_{m,n}^{\eta} \geq 0 \\ \overline{V}_{m,n}^{\eta} \frac{-5U_{m,n+2} + 28U_{m,n+1} - 18U_{m,n} - 4U_{m,n-1} - U_{m,n-2}}{24\Delta \eta} & \text{for } \overline{V}_{m,n}^{\eta} < 0 \end{cases}$$

(4.2.2a)

is the sum of the following two other second-order consistent approximations:
\[
\frac{V}{\sqrt{g_{\eta \eta}}} \frac{\partial U}{\partial \eta}_{m,n} = \frac{\bar{V}_{m,n}^{\eta \eta}}{(\sqrt{g_{\eta \eta}})_{m,n}} S_{\eta \eta} U_{m,n} = \frac{\bar{V}_{m,n}^{\eta \eta}}{(\sqrt{g_{\eta \eta}})_{m,n}} \frac{U_{m,n+1} - 4U_{m,n} + U_{m,n-1}}{12\Delta \eta}
\]

and

\[
\frac{V}{\sqrt{g_{\eta \eta}}} \frac{\partial U}{\partial \eta}_{m,n} = \frac{\bar{V}_{m,n}^{\eta \eta}}{\sqrt{g_{\eta \eta}} (\sqrt{g_{\eta \eta}})_{m,n}} S_{\eta \eta} U_{m,n} = \begin{cases} 
\frac{\bar{V}_{m,n}^{\eta \eta} - 3U_{m,n} - 4U_{m,n-1} + U_{m,n-2}}{2\Delta \eta} & \text{for } \bar{V}_{m,n}^{\eta \eta} \geq 0 \\
\frac{\bar{V}_{m,n}^{\eta \eta} + 3U_{m,n} + 4U_{m,n+1} - U_{m,n+2}}{2\Delta \eta} & \text{for } \bar{V}_{m,n}^{\eta \eta} < 0
\end{cases}
\]

where \( S_{\eta \eta} \) and \( S_{\eta \eta} \) are finite difference operators. Transformation of the advection terms to an orthogonal curvilinear grid introduces curvature terms:

\[
UV \frac{\partial \sqrt{g_{\xi \xi}}}{\partial \eta} \quad \text{and} \quad \frac{V^2}{\sqrt{g_{\eta \eta}}} \frac{\partial \sqrt{g_{\eta \eta}}}{\partial \xi}
\]

These terms are discretized straightforwardly:

\[
\frac{UV}{\sqrt{g_{\eta \eta}}} \frac{\partial \sqrt{g_{\xi \xi}}}{\partial \eta} = \frac{\sqrt{g_{\eta \eta}}}{\sqrt{g_{\eta \eta}}} \frac{\bar{V}^{\eta \eta}}{\bar{V}_{m,n}^{\eta \eta}} \left( \sqrt{g_{\eta \eta}} \right)_{m,n} = \frac{U_{m,n} \bar{V}_{m,n}^{\eta \eta} \left( \left( \sqrt{g_{\eta \eta}} \right)_{m,n} + \left( \sqrt{g_{\eta \eta}} \right)_{m+1,n} - \left( \sqrt{g_{\eta \eta}} \right)_{m-1,n} \right)}{2\Delta \eta}
\]

\[
\frac{V^2}{\sqrt{g_{\eta \eta}}} \frac{\partial \sqrt{g_{\eta \eta}}}{\partial \xi} = \frac{\sqrt{g_{\eta \eta}}}{\sqrt{g_{\eta \eta}}} \frac{\bar{V}^{\eta \eta}}{\bar{V}_{m,n}^{\eta \eta}} \left( \sqrt{g_{\eta \eta}} \right)_{m,n} = \frac{U_{m,n} \bar{V}_{m,n}^{\eta \eta} \left( \left( \sqrt{g_{\eta \eta}} \right)_{m,n} - \left( \sqrt{g_{\eta \eta}} \right)_{m+1,n} \right)}{2\Delta \xi}
\]

with

\[
(\sqrt{g_{\eta \eta}})_{m,n} = (\sqrt{g_{\eta \eta}})_{m,n} (\sqrt{g_{\eta \eta}})_{m,n}
\]

\( D_{\xi \xi} \) and \( D_{\eta \eta} \) are finite difference operators. The Jacobian is computed using averaging of the grid length \( \sqrt{g_{\xi \xi}} \). At solid walls the no-slip condition is enforced. Near the boundaries the higher order discretization stencils for the advection terms contain grid points on or across the boundary. To avoid an artificial boundary layer or instabilities, the discretizations have to be reduced to lower order discretizations with smaller stencils. Stelling (1984) introduced the numerical boundary treatment implemented in WAQUA. For more details we refer to Chapter 6.
4.2.2 Barotropic pressure gradient

The spatial discretization of the barotropic pressure gradient, the free surface slope, on the staggered WAQUA grid is given by:

\[
\frac{g}{\sqrt{g_{\xi\xi}}} \frac{\partial \xi}{\partial \xi} = \frac{g}{(\sqrt{g_{\xi\xi}})_{m,n}} \Delta \xi - \xi_{m+1,n} - \xi_{m,n}
\]

(4.2.5)

In the case of space-varying wind and pressure, the gradient of the atmospheric pressure is added:

\[
\frac{1}{\rho_0 \sqrt{g_{\xi\xi}}} \frac{\partial P_a}{\partial \xi} \approx \frac{1}{\rho_0 (\sqrt{g_{\xi\xi}})_{m,n}} \Delta \xi - (P_{a,m+1,n} - P_{a,m,n})
\]

(4.2.6)

This term is important for the simulation of storm surges.

4.2.3 Baroclinic pressure gradient

For accurate simulations of the tidal flow in stratified estuaries, the density must be a function of the salinity. WAQUA is a depth-averaged model and it assumes that the water column is well-mixed and that the salinity varies only in horizontal direction. The salinity is governed by the transport (advection-diffusion) equation. Density differences introduce a so-called baroclinic pressure gradient, see Section 2.6. In WAQUA the quantity \( \rho_{m,n} \) is defined as the relative density difference with the ambient density \( \rho_0 \). This increases the accuracy in the computation of the baroclinic pressure gradient, which is discretized as:

\[
\frac{g}{\rho_0 \sqrt{g_{\xi\xi}}} \frac{1}{2} H \frac{\partial \rho}{\partial \xi} = \frac{g}{\rho_0 (\sqrt{g_{\xi\xi}})_{m,n}} \frac{1}{2} H_{m,n}^{\nu} \frac{\rho_{m+1,n} - \rho_{m,n}}{\Delta \xi}
\]

(4.2.7)

4.2.4 Horizontal viscous terms

In WAQUA the horizontal viscosity coefficient is assumed to be constant and the stress terms simplify to the Laplace operator. In orthogonal curvilinear co-ordinates the Laplace operator is given by:

\[
\Delta U = \frac{\nu_H}{\sqrt{g_{\xi\xi}}} \frac{\partial F'}{\partial \xi} - \frac{\nu_H}{\sqrt{g_{\eta\eta}}} \frac{\partial F'}{\partial \eta}
\]

(4.2.8)

with

\[
F' = \frac{1}{\sqrt{g_{\xi\xi}}} \left( \frac{\partial}{\partial \xi} (U \sqrt{g_{\eta\eta}}) + \frac{\partial}{\partial \eta} (V \sqrt{g_{\xi\xi}}) \right)
\]

(4.2.9)
\[
F^2 = \frac{I}{\sqrt{g_*}} \left( \frac{\partial}{\partial \xi} \left( V \sqrt{g_{\eta \eta}} \right) - \frac{\partial}{\partial \eta} \left( U \sqrt{g_{\xi \xi}} \right) \right)
\]  
(4.2.10)

The first derivatives are approximated with central differences. Let the discretization of \( F^1 \) in the water level point with co-ordinates \((m,n)\) be given by \( F^1_{m,n} \):

\[
F^1_{m,n} = \frac{1}{\left( \sqrt{g_{\xi \xi}} \right)_{m,n} \left( \sqrt{g_{\eta \eta}} \right)_{m,n}} \left[ \frac{U_{m,n} \left( \sqrt{g_{\eta \eta}} \right)_{m,n} - U_{m-1,n} \left( \sqrt{g_{\eta \eta}} \right)_{m-1,n}}{\Delta \xi} + \frac{V_{m,n} \left( \sqrt{g_{\xi \xi}} \right)_{m,n} - V_{m,n-1} \left( \sqrt{g_{\xi \xi}} \right)_{m,n-1}}{\Delta \eta} \right]
\]
(4.2.11)

and the discretization of \( F^2 \) in the depth point with co-ordinates \((m,n)\) be given by \( F^2_{m,n} \):

\[
F^2_{m,n} = \frac{1}{\left( \sqrt{g_{\xi \xi}} \right)_{m,n} \left( \sqrt{g_{\eta \eta}} \right)_{m,n}} \left[ \frac{V_{m+1,n} \left( \sqrt{g_{\eta \eta}} \right)_{m+1,n} - V_{m,n} \left( \sqrt{g_{\eta \eta}} \right)_{m,n}}{\Delta \xi} - \frac{U_{m,n+1} \left( \sqrt{g_{\xi \xi}} \right)_{m,n+1} - U_{m,n} \left( \sqrt{g_{\xi \xi}} \right)_{m,n}}{\Delta \eta} \right]
\]
(4.2.12)

In a water level point (4.2.11) and a depth point (4.2.12), the determinant of the Jacobian, which equals the area of a grid cell, is determined from the horizontally-averaged grid sizes. This is only an accurate approximation for orthogonal grids.

The horizontal viscosity term is treated in a semi-implicit way. In Chapter 5 we give the time levels in the ADI-scheme. We will use the following representation of the spatial discretization:

\[
\nu_h \Delta U = \nu_h \frac{\partial F^1}{\partial \xi} - \nu_h \frac{\partial F^2}{\partial \eta} = \nu_h \Delta_{m,n} (U, V)
\]
(4.2.13)

### 4.2.5 Coriolis force term

The Coriolis parameter \( f \) is dependent on the geographical latitude, see Eq. (2.2.7).
For interior points the $V$-velocity in the Coriolis force is determined by an arithmetic average of the four surrounding $V$-velocity points

$$\frac{f}{V_{m,n}}$$ \hspace{1cm} (4.2.14)

The $V$-points on closed boundaries and thin dams are not excluded in the averaging. Near the open boundaries, the arithmetic averaging is based on the wet $V$-velocity points in the interior domain.

### 4.2.6 Bottom friction term

The bottom shear stress is proportional to the velocity squared. The direction of the shear stress is opposite to the flow. The Chézy values $C_{2D_x}$ and $C_{2D_y}$ defined at the velocity points. The $V$-velocity determined at a $U$-point using arithmetic averaging for the Coriolis term, is also used in the bottom friction term. The bottom friction term in the $U$-momentum equation is discretized as:

$$\frac{g U |\mathbf{U}|}{H C_{2D_x}^2} = \frac{g U |U| (U_{m,n})^2 + (\nabla V_{m,n})^2}{H_{m,n} C_{2D_x}^2}$$ \hspace{1cm} (4.2.15)

### 4.3 Discretization of the transport equation

The discretization of the depth-averaged transport equation (2.4.3) is carried out at a water level point, where the concentration (salinity) is defined. To guarantee conservation of mass the transport equation is written in integral form. It can be discretized in a natural manner by means of the finite volume method. The depth-averaged concentration is independent of the vertical co-ordinate and the control volume is a grid box defined by the grid lines around the water level point with corners in the four surrounding depth points. The velocity components used in WAQUA are perpendicular to the boundaries of the grid box.

The depth-averaged advection-diffusion equation is integrated over the control volume $\Omega_{mn}$. Using the Gauss divergence theorem, the volume integrals containing terms under the differential operators can be converted into surface integrals:

$$\frac{\partial}{\partial t} \int_{\Omega_{m,n}} C \, dv + \int_{\partial \Omega_{m,n}} \mathbf{F} \cdot \mathbf{n} \, ds = \int_{\Omega_{m,n}} S \, dv$$ \hspace{1cm} (4.3.1)

with $\mathbf{F}$ the flux vector and $\mathbf{n}$ the outer normal vector of the control volume. The flux vector contains advective and diffusive fluxes. The right-hand side contains the source and sink terms. The time derivative of the amount of mass in a cell should equal the balance of the mass fluxes across the cell faces per unit of time and the amount of mass discharged or withdrawn from the volume.

The surface integral over the advective flux is approximated by the following spatial discretization:
\[
\int_{\partial \Omega_{m,n}} \bar{U} \bar{C} \tilde{n} dS = \left( H^U \bar{U} C \sqrt{g_{\eta \eta}} \right)_{m,n} - \left( H^U \bar{U} C \sqrt{g_{\eta \eta}} \right)_{m-1,n} + \\
\left( H^V \bar{V} C \sqrt{g_{\xi \xi}} \right)_{m,n} - \left( H^V \bar{V} C \sqrt{g_{\xi \xi}} \right)_{m,n-1} 
\]

(4.3.2)

The concentration is not defined at the cell boundaries and should be approximated using the grid-point values. The approximation of the concentration in a velocity point, is discussed in Chapter 5.2. To conserve mass, the flow through-heights \( H_m^U \) and \( H_m^V \) should be equal to the values in the discretized continuity equation.

The surface integral over the diffusive flux contains derivatives of the concentration which are approximated by central discretizations:

\[
\int_{\partial \Omega_{m,n}} D_n \frac{\partial C}{\partial n} dS = \left( D_H H^U \frac{\partial C}{\partial \xi} \sqrt{g_{\eta \eta}} \right)_{m,n} - \left( D_H H^U \frac{\partial C}{\partial \xi} \sqrt{g_{\eta \eta}} \right)_{m-1,n} + \\
\left( D_H H^V \frac{\partial C}{\partial \eta} \sqrt{g_{\xi \xi}} \right)_{m,n} - \left( D_H H^V \frac{\partial C}{\partial \eta} \sqrt{g_{\xi \xi}} \right)_{m,n-1} 
\]

(4.3.3)

The time derivative of the concentration and the source term are approximated using the midpoint rule.

\[
\frac{\partial}{\partial t} \int_{\Omega_{m,n}} C d\Omega = (\bar{g}_*)_{m,n} \frac{\partial (H^C)}{\partial t} 
\]

(4.3.4)

with \( \sqrt{g} \) the area of cell \( \Omega_{mn} \) and

\[
(\bar{g}_*)_{m,n} = (\sqrt{g_{\xi \xi}})_{m,n} (\sqrt{g_{\eta \eta}})_{m,n}^{\xi} 
\]

The source term \( S \) is approximated as follows:

\[
\int_{\Omega_{mn}} S d\Omega = (\sqrt{g}_*)_{m,n} H^\xi S_{m,n} 
\]

(4.3.5)

The approximation of the concentrations and the concentration gradients at the cell faces is discussed in the next sections.
4.3.1 Advective fluxes

The horizontal advective flux requires an approximation of the concentrations at the velocity points. In WAQUA, at each velocity point the concentration is evaluated using an arithmetic average of the concentration in the two neighbouring cells:

\[
C^u_{m,n} = \frac{1}{2} (C_{m+1,n} + C_{m,n}) \tag{4.3.6a}
\]

\[
C^v_{m,n} = \frac{1}{2} (C_{m,n+1} + C_{m,n}) \tag{4.3.6b}
\]

This approximation substituted into Eq. (4.3.2) to a central difference scheme. On a completely smooth grid, the discretization is second order accurate but may generate odd-even decoupling (wiggles) in regions with steep gradients. The occurrence of wiggles is dependent on the grid Péclet number. Wiggles are avoided if

\[
P_{\Delta x} = \frac{|U| \sqrt{g z}}{D_H} \leq 2 \tag{4.3.7}
\]

This provides a restriction on the spatial resolution. In depth-averaged models the horizontal dispersion is relatively large to compensate for the vertical shear and the grid Péclet number may be small enough to prevent wiggles. Such wiggles do not necessarily arise if (4.3.7) is violated. Only steep gradients which are not sufficiently resolved trigger them. In the regions with coarse grid cells the condition (4.3.7) is not fulfilled, but there the solution should be smooth otherwise the grid has not been well-designed.

For the velocity points at the open boundary, the fluxes are determined with one-sided approximations of the concentrations:

\[
C^u_{m,n} = \begin{cases} 
C_{m,n} & \text{if } U_{m,n} \geq 0 \\
C_{m+1,n} & \text{if } U_{m,n} < 0 
\end{cases} \tag{4.3.8a}
\]

and

\[
C^v_{m,n} = \begin{cases} 
C_{m,n} & \text{if } V_{m,n} \geq 0 \\
C_{m,n+1} & \text{if } V_{m,n} < 0 
\end{cases} \tag{4.3.8b}
\]

For outflow the concentration at the open boundary is not taken into account to prevent wiggles.

For the approximation of the total water depth \(H^u\) and \(H^v\) at the velocity points we use the same approximation as in the discretized conservation equation of mass, see Section 4.1.
4.3.2 Diffusive fluxes

A central difference is used for the discretization of the first derivative in the horizontal
diffusive flux:

\[
D_H H_{m,n} \frac{\sqrt{g_{\eta \eta}}}{\sqrt{g_{\xi \xi}}} \frac{\partial C}{\partial \xi}_{m,n} = D_H H_{m,n} \frac{(\sqrt{g_{\eta \eta}})_{m,n}}{(\sqrt{g_{\xi \xi}})_{m,n}} \left( C_{m+1,n} - C_{m,n} \right) \Delta \xi
\]

(4.3.9a)

and

\[
D_H H_{m,n} \frac{\sqrt{g_{\eta \eta}}}{\sqrt{g_{\xi \xi}}} \frac{\partial C}{\partial \eta}_{m,n} = D_H H_{m,n} \frac{(\sqrt{g_{\eta \eta}})_{m,n}}{(\sqrt{g_{\xi \xi}})_{m,n}} \left( C_{m,n+1} - C_{m,n} \right) \Delta \eta
\]

(4.3.9b)

This leads to the familiar three point scheme. The diffusive flux through a closed boundary
is zero.

4.4 Space discretization figures

We will now illustrate the space discretization of all terms described in the previous
sections. A circle corresponds to the grid point of concern. A square denotes a grid point
that is involved in the space discretization. The horizontal and vertical arrows correspond to
grid distances in \( \xi \)- and \( \eta \)-direction, respectively.

Space discretization for \[ \frac{U}{\sqrt{g_{\xi \xi}}} \frac{\partial U}{\partial \xi} \] in Eq. (4.2.1)

Space discretization for \[ \frac{V}{\sqrt{g_{\eta \eta}}} \frac{\partial U}{\partial \eta} \] in Eq. (4.2.2b)
Space discretization for \( \frac{V}{\sqrt{g_{\eta \eta}}} \frac{\partial U}{\partial \eta_{m,n}} \) with \( V > 0 \)
in Eq. (4.2.2c)

Space discretization for \( \frac{V}{\sqrt{g_{\eta \eta}}} \frac{\partial U}{\partial \eta_{m,n}} \) with \( V < 0 \)
in Eq. (4.2.2c)

Space discretization for \( \frac{UV}{\sqrt{g}} \frac{\partial \sqrt{g_{\eta \eta}}}{\partial \eta} \)
in Eq. (4.2.3)

Space discretization for \( \frac{V^2}{\sqrt{g}} \frac{\partial \sqrt{g_{\eta \xi}}}{\partial \xi} \)
in Eq. (4.2.3)
Space discretization for \((\sqrt{g_s})_{m,n}\) in Eq. (4.2.4)

Space discretization for \(\frac{g}{\sqrt{g_{zz}}} \frac{\partial \zeta}{\partial z}\) in Eq. (4.2.5)

Space discretization for \(\frac{g}{\rho o \sqrt{g_z}} \frac{1}{2} H \frac{\partial p}{\partial z}\) in Eq. (4.2.7)

Space discretization for \(F_{m,n}^1\) in Eq. (4.2.11)
Space discretization for $F_{m,n}^2$ in Eq. (4.2.12)

Space discretization for $\nu_H \Delta U$ in Eq. (4.2.13)

Space discretization for $\int \bar{V}_{m,n}^{2n}$ in Eq. (4.2.14)

Space discretization for $\frac{gU|\bar{U}|}{HC_{2d}}$ in Eq. (4.2.15)
Space discretization for advective fluxes Eq. (4.3.6) and diffusive fluxes Eq. (4.3.9) in transport equation.
5 Time Discretization

This chapter deals with the finite difference framework for the time discretization of the governing equations in WAQUA and describes the iterative procedures to remove the non-linearities. Because WAQUA is applied to a wide range of flow conditions, basic requirements of the numerical method were:

- robustness (unconditionally stable)
- accuracy (at least second order)
- computational efficiency.

In WAQUA the system of ordinary differential equations, which is obtained by discretization in space of the governing conservation equations (see Chapter 4) is advanced in time with an Alternating Direction Implicit (ADI) scheme. The ADI-method was introduced for the shallow water equations by Leendertse (1967). Stelling (1984) stabilized the method by a special higher-order dissipative approximation of the cross advection term, see Section 4.2.1. The numerical method of WAQUA is unconditionally stable and lacks second order artificial viscosity. To improve stability, the bottom stress is taken partly implicit for each half time step and is not second order in time. When the baroclinic forcing is included, the transport equation of salt is coupled to the momentum equations. The rate of change with respect to time of salinity is small compared to the rate of change of flow. Therefore the baroclinic pressure lags one half time step in time without affecting the accuracy. As a result, the numerical method is subject to a weak stability condition based on the Courant number for internal waves.

An ADI-like method splits one time step into two stages. Each stage consists of half a time step. In both stages all the terms of the model equations are solved in a consistent way with at least second order accuracy in space. For each term the time levels are alternating. If in one stage a term is taken implicitly in time, this term will be taken explicitly in time in the other stage. The net result will be that each term of the equations is solved second-order accurate in time. The splitting in an implicit and explicit part is arranged in such a way that implicit coupling only occurs along grid lines without coupling in the other direction. The A.D.I. method requires the solution of a number of uncoupled systems of equations for each row or column of grid points, see Chapter 7. In each stage, only two time levels are needed. This requires less computer storage.

In the first stage the time level is proceeding from \( l \) to \( l+\frac{1}{2} \). The corresponding simulation time is proceeding from \( t = l\Delta t \) to \( t = (l+\frac{1}{2})\Delta t \). In the second stage the time level is proceeding from \( l+\frac{1}{2} \) to \( l+1 \). The time index is used as superscript in the difference equations.

For the staggered WAQUA grid the Courant number for wave propagation is defined as:
\[ C_{\text{wave}} = 2\Delta t \sqrt{g H \left( \frac{1}{\Delta \xi \sqrt{g_{\xi \xi}}} + \frac{1}{\Delta \eta \sqrt{g_{\eta \eta}}} \right)} \]  \hspace{1cm} (5.0.1)

Due to the implicit character of the ADI time integration, there is no Courant-Friederichs-Lewy (CFL) stability restriction on the time step, but Weare (1979), Benqué (1982), Stelling (1984) show that the ADI-method becomes inaccurate for large time steps in combination with a complex geometry or topography. Complex means closed boundaries or channels with more than one angle of 90°. This inaccuracy is introduced by the splitting of the spatial operator in two directions. A tidal wave cannot travel more than once through two 90° bends in a "zigzagging" channel in one complete ADI-time step (Stelling, 1984). For large time steps the numerical characteristic cone does not contain the analytical characteristic cone. This inaccuracy is called the ADI-effect. For Courant numbers defined by Eq. (5.0.1), the numerical solution becomes inaccurate if

\[ C_{\text{wave}} \geq 4\sqrt{2} \]

Furthermore, the Crank Nicolson time integration of the horizontal viscosity term may generate an oscillating solution. To prevent oscillations the time step must satisfy

\[ \Delta t \leq \frac{1}{V_h \left( \frac{1}{(\Delta \xi \sqrt{g_{\xi \xi}})^2} + \frac{1}{(\Delta \eta \sqrt{g_{\eta \eta}})^2} \right)^{-1}} \]  \hspace{1cm} (5.0.2)

In this chapter we present the time integration for the case of curvi-linear co-ordinates, see Section 2.4.

### 5.1 Time integration of the flow equations

In the first stage the depth-averaged momentum equation in \( V \)-direction (2.4.2c) is solved with the free surface gradient at the old time level while the advection terms are treated implicitly. The depth-averaged momentum equation in \( U \)-direction is solved with the free surface gradient at the new time level and the advection terms at the old time level. In the second stage, the discretizations the \( U \) and \( V \) are interchanged. WAQUA uses the same subroutines for the second stage as for the first stage, only the parameters in the subroutine calls are adapted.

In the first stage, the \( U \)-momentum equation is implicitly coupled with the non-linear term in the continuity equation (2.4.2a). The non-linear term requires an iterative procedure. An iterative procedure may cause instabilities near tidal flats. Recently (Van Kester et al., 1997) a new iterative procedure was implemented in WAQUA, which replaces the procedure described in Stelling (1984). The new procedure has as great advantage that after each iteration the numerical solution is mass conservative, while the old procedure requires convergence to preserve mass conservative. The new procedure was tested and turned out to be very robust. Usually, two iterations are enough both for accuracy and stability.
The non-linearity in the coupled system of depth-averaged continuity equation and $U$-momentum equation is removed by multiplying the free surface gradient by

$$r^n = \left( \frac{H'_{jj}}{H''_{jj}} \right)^{[q]} \frac{H'_{jj}}{H''_{jj}}^{[q-1]}$$

This factor converges to 1.

The advection terms in the $V$-momentum equation are solved implicitly. Together with the implicit treatment of the viscosity term this leads to a matrix with seven diagonals with non zero entries. The matrix is reduced to tridiagonal form by the introduction of a line Gauss Seidel iterative method, see Section 7.1. In the first stage the $V$-momentum equation is solved first so that the new $V$-velocities are available for the cross terms in the $U$-momentum equation. The finite difference equations of stage 1 can be written as:

First Stage:

$$\frac{V_{m,n}^{t+1/2} - V_{m,n}^t}{\Delta t / 2} + \frac{U_{m,n}^t - \frac{\eta}{2}}{\sqrt{\frac{g}{\xi}}} S_{m,n} \left[ V_{m,n}^{t+1/2} \right] + \frac{V_{m,n}^t}{\sqrt{\frac{g}{\eta}}} \frac{V_{m,n+1}^{t+1} - V_{m,n-1}^t}{2\Delta \eta}$$

$$\frac{U_{m,n}^t - \frac{\eta}{2}}{\sqrt{\frac{g}{\xi}}} \frac{U_{m,n}^{t+1/2}}{\sqrt{\frac{g}{\eta}}} D_{m,n} \left( \sqrt{\frac{g}{\xi}} + \sqrt{\frac{g}{\eta}} \right)$$

$$\frac{g}{\sqrt{\frac{g}{\eta}}} \frac{\zeta_{m,n+1}^t - \zeta_{m,n}^t}{\Delta \eta} - \frac{gH_{m,n}^t \rho_{m,n+1}^t - \rho_{m,n}^t}{2\rho_0 \sqrt{\frac{g}{\eta}}} \frac{\eta}{\Delta \eta}$$

$$\Delta_{m,n} \left( V_{m,n}^{t+1/2}, U_{m,n}^t \right) - \frac{gV_{m,n}^t \frac{\xi}{H_{m,n}^2} \left( U_{m,n}^t \right)^2 + \left( V_{m,n}^t \right)^2}{2C_{Dx}}$$
\[
\frac{U_{m,n}^{(q)} - U_{m,n}^i}{\Delta t / 2} + \frac{V_{m,n}^{i+1/2}}{\sqrt{g_{\eta \eta}}} S_{on}[U^i]_{m,n} + \frac{U_{m,n}^{(q)} - U_{m+1,n}^i - U_{m-1,n}^i}{2\Delta \xi} + \\
\frac{U_{m,n}^{i+1/2}}{\sqrt{g_{\eta \eta}}} V_{m,n}^{i+1/2} \frac{\xi_0^{i+1/2}}{\sqrt{g_{\eta \eta}}} D_{on} \sqrt{g_{\eta \eta}} + \frac{V_{m,n}^{i+1/2}}{\sqrt{g_{\eta \eta}}} V_{m,n}^{i+1/2} \frac{\xi_0^{i+1/2}}{\sqrt{g_{\eta \eta}}} D_{on} \sqrt{g_{\eta \eta}} = 0 
\]

(5.1.2)

\[
\frac{\xi_{m,n}^{(q)} - \xi_{m,n}^i}{\Delta t / 2} + \frac{1}{\sqrt{g_{\eta \eta}}} \left(\left(H_{m,n}^{U} \sqrt{g_{\eta \eta}}\right)^{i+1} - \left(H_{m,n}^{U} \sqrt{g_{\eta \eta}}\right)^{i-1}\right) \\
+ \frac{1}{\sqrt{g_{\eta \eta}}} \left(\left(H_{m,n}^{V} \sqrt{g_{\eta \eta}}\right)^i - \left(H_{m,n}^{V} \sqrt{g_{\eta \eta}}\right)^{i-1}\right) = 0 
\]

(5.1.3)

Substitution of the \( U \)-momentum equation in the continuity equation leads to a tridiagonal system of equations. The system is solved by a direct method (double sweep), see Section 7.4.
In the second stage the time is raised from \( t + \Delta t/2 \) to \( t + \Delta t \). The finite difference equations of stage 2 can be written as:

\[
\frac{U_{m,n}^{i+1} - U_{m,n}^{i-1}}{\Delta t/2} + \frac{V_{m,n}^{i+1/2}}{\sqrt{g_{\eta \eta}}} + S_{x,n}[U_{m,n}^{i+1}] + \frac{U_{m+1,n}^{i+1} - U_{m,n}^{i+1}}{2 \Delta x} + \frac{U_{m,n}^{i+1} V_{m,n}^{i+1/2}}{\sqrt{g_{\xi \xi}}} \frac{\xi_{m,n}^{i+1/2} - \xi_{m,n}^{i-1/2}}{\Delta \xi} - \frac{\xi_{m+1,n}^{i+1/2} - \xi_{m,n}^{i+1/2}}{\Delta \xi} - \frac{g H_u^{i+1/2} \rho_{m,n}^{i+1/2} - \rho_{m,n}^{i+1/2}}{2 \rho_0 \sqrt{g_{\xi \xi}}} + \frac{g U_{m,n}^{i+1}}{g_{\eta \eta}} \sqrt{\left(U_{m,n}^{i+1}\right)^2 + \left(V_{m,n}^{i+1/2}\right)^2} + \frac{g U_{m,n}^{i+1}}{g_{\eta \eta}} \sqrt{\left(U_{m,n}^{i+1}\right)^2 + \left(V_{m,n}^{i+1/2}\right)^2} \frac{C_d^2}{2D_x} = 0
\]

(5.1.4)

\[
\frac{V_{m,n}^{i+1} - V_{m,n}^{i-1}}{\Delta t/2} + \frac{U_{m,n}^{i+1/2}}{\sqrt{g_{\eta \eta}}} + S_{y,n}[V_{m,n}^{i+1}] + \frac{V_{m,n}^{i+1/2} - V_{m,n}^{i-1/2}}{2 \Delta \eta} + \frac{V_{m,n}^{i+1/2} U_{m,n}^{i+1/2}}{\sqrt{g_{\xi \xi}}} \frac{\xi_{m,n}^{i+1/2} - \xi_{m,n}^{i-1/2}}{\Delta \xi} - \frac{\xi_{m,n+1}^{i+1/2} - \xi_{m,n}^{i+1/2}}{\Delta \xi} - \frac{g H_v^{i+1/2} \rho_{m,n+1}^{i+1/2} - \rho_{m,n}^{i+1/2}}{2 \rho_0 \sqrt{g_{\xi \xi}}} + \frac{g V_{m,n}^{i+1}}{g_{\eta \eta}} \sqrt{\left(U_{m,n}^{i+1/2}\right)^2 + \left(V_{m,n}^{i+1/2}\right)^2} \frac{C_d^2}{2D_y} = 0
\]

(5.1.5)

\[
\frac{\zeta_{m,n}^{i+1} - \zeta_{m,n}^{i-1}}{\Delta t/2} + \frac{1}{\sqrt{g_{\eta \eta}}} \left( \left[H_u^{i+1/2} \sqrt{g_{\eta \eta}} \right]_{m,n}^{i+1/2} - \left[H_u^{i+1/2} \sqrt{g_{\eta \eta}} \right]_{m-1,n}^{i+1/2} \right) + \frac{1}{\sqrt{g_{\xi \xi}}} \left( \left[H_v^{i+1/2} \sqrt{g_{\xi \xi}} \right]_{m,n}^{i+1/2} - \left[H_v^{i+1/2} \sqrt{g_{\xi \xi}} \right]_{m,n-1}^{i+1/2} \right) = 0
\]

(5.1.6)
The difference equations are only valid in points with a positive total water depth. When the total water depth is negative, a point must be set dry. To guarantee stable and correct solutions when flooding and drying occurs, WAQUA has a number of checks on the total water depth at velocity points and at water level points. These checks are described in Chapter 8.

5.2 Time integration of the transport equation

The transport equation is coupled with the momentum equations by the baroclinic pressure term. The variations of the salinity are slow compared to the variations in the flow and therefore the baroclinic term in the momentum equations is treated explicitly. The coupling with the flow is weak and in WAQUA the transport equation is solved independently for each half time step. The time integration follows the ADI method for the continuity equation. In the first stage all space derivatives with respect to $\xi$ are taken implicitly and all derivatives in the $\eta$-direction are taken explicitly. In the second stage the directions for explicit and implicit integration are interchanged. In both stages we apply a second order central scheme for the approximation of the advection terms. The central scheme is very accurate but not monotinous and wiggles may arise in areas with steep concentration gradients when the transport is advection dominated.

The transport equation is discretized using finite volumes. Considering the first stage, application of the ADI factorization yields:

\[
\left( H^\xi C \sqrt{g_{\xi\eta}} \sqrt{g_{\xi\xi}} \right)_{m,n}^{i+1/2} \left( H^\eta C \sqrt{g_{\eta\eta}} \sqrt{g_{\eta\xi}} \right)_{m,n}^i \frac{\Delta t}{2} = \\
\left( H^U U \sqrt{g_{\eta\eta}} \right)_{m,n}^{i+1/2} \left( C_{m,n+1,n}^{i+1/2} + C_{m,n}^{i+1/2} \right) \frac{2}{2} - \left( H^U U \sqrt{g_{\eta\eta}} \right)_{m-1,n}^{i+1/2} \left( C_{m,n+1,n}^{i+1/2} + C_{m,n-1,n}^{i+1/2} \right) + \\
\left( H^V V \sqrt{g_{\xi\xi}} \right)_{m,n}^{i+1/2} \left( C_{m,n+1,n}^{i+1/2} + C_{m,n}^{i+1/2} \right) \frac{2}{2} - \left( H^V V \sqrt{g_{\xi\xi}} \right)_{m-1,n}^{i+1/2} \left( C_{m,n+1,n}^{i+1/2} + C_{m,n-1,n}^{i+1/2} \right) + \\
\left( D_H H^U \sqrt{g_{\eta\eta}} \sqrt{g_{\xi\eta}} \right)_{m,n}^{i+1/2} \left( C_{m,n+1,n}^{i+1/2} - C_{m,n,n}^{i+1/2} \right) \frac{\Delta \xi}{2} - \left( D_H H^U \sqrt{g_{\eta\eta}} \sqrt{g_{\xi\eta}} \right)_{m-1,n}^{i+1/2} \left( C_{m,n+1,n}^{i+1/2} - C_{m-1,n}^{i+1/2} \right) \frac{\Delta \xi}{2} + \\
\left( D_H H^V \sqrt{g_{\xi\xi}} \sqrt{g_{\eta\xi}} \right)_{m,n}^{i+1/2} \left( C_{m,n+1,n}^{i+1/2} - C_{m,n,n}^{i+1/2} \right) \frac{\Delta \eta}{2} - \left( D_H H^V \sqrt{g_{\xi\xi}} \sqrt{g_{\eta\xi}} \right)_{m-1,n}^{i+1/2} \left( C_{m,n+1,n}^{i+1/2} - C_{m-1,n}^{i+1/2} \right) \frac{\Delta \eta}{2} + \\
\left( H^\xi S_{IN} C_{IN} \sqrt{g_{\eta\eta}} \sqrt{g_{\xi\xi}} \right)_{m,n}^{i+1/2} - \left( H^\xi S_{OUT} C \sqrt{g_{\eta\eta}} \sqrt{g_{\xi\xi}} \right)_{m,n}^{i+1/2} (5.2.1)
\]
The difference equation represents a linear tridiagonal system of equations for the concentration (salinity). The system is solved with a direct method, see Section 7.4. The difference equation for the second stage can be written as:

\[
\begin{align*}
\left( H^e C \sqrt{g_{\eta \eta} \sqrt{g_{\xi \xi}}} \right)^{i+1}_{m,n} & - \left( H^e C \sqrt{g_{\eta \eta} \sqrt{g_{\xi \xi}}} \right)^{i+1/2}_{m,n} \\
\left( H^e U \sqrt{g_{\eta \eta}} \right)^{i+1/2}_{m,n} \left( \frac{C_{m+1,n}^{i+1} + C_{m,n}^{i+1}}{2} \right) & - \left( H^e U \sqrt{g_{\eta \eta}} \right)^{i+1/2}_{m-1,n} \left( \frac{C_{m,n}^{i+1} + C_{m-1,n}^{i+1}}{2} \right) \\
\left( H^e V \sqrt{g_{\xi \xi}} \right)^{i+1/2}_{m,n} \left( \frac{C_{m,n+1}^{i+1} + C_{m,n}^{i+1}}{2} \right) & - \left( H^e V \sqrt{g_{\xi \xi}} \right)^{i+1/2}_{m,n-1} \left( \frac{C_{m,n}^{i+1} + C_{m,n-1}^{i+1}}{2} \right) \\
\left( D_H H^u \sqrt{g_{\eta \eta}} \right)^{i+1/2}_{m,n} \left( \frac{C_{m,n+1}^{i+1} - C_{m,n}^{i+1}}{\Delta \xi} \right) & - \left( D_H H^u \sqrt{g_{\eta \eta}} \right)^{i+1/2}_{m-1,n} \left( \frac{C_{m,n}^{i+1} - C_{m-1,n}^{i+1}}{\Delta \xi} \right) \\
\left( D_H H^v \sqrt{g_{\xi \xi}} \right)^{i+1/2}_{m,n} \left( \frac{C_{m,n+1}^{i+1} - C_{m,n}^{i+1}}{\Delta \eta} \right) & - \left( D_H H^v \sqrt{g_{\xi \xi}} \right)^{i+1/2}_{m,n-1} \left( \frac{C_{m,n}^{i+1} - C_{m,n-1}^{i+1}}{\Delta \eta} \right) \\
\left( H^e S_{in} C_{in} \sqrt{g_{\eta \eta} \sqrt{g_{\xi \xi}}} \right)^{i+1/2}_{m,n} & - \left( H^e S_{out} C \sqrt{g_{\eta \eta} \sqrt{g_{\xi \xi}}} \right)^{i+1}_{m,n}
\end{align*}
\]

(5.2.2)

The ADI-method is unconditionally stable. The central scheme may introduce spurious oscillations (wiggles). To prevent wiggles the Peclet number must be restricted by:

\[
P_{\text{Pe}_\Delta} = \frac{\max(|U| \Delta \xi \sqrt{g_{\xi \xi}}, |V| \Delta \eta \sqrt{g_{\eta \eta}})}{D_H} \leq 2
\]

(5.2.3)

This numerical method for the advective terms in the transport equation is accurate but not very robust for coarse grids.

If the grid is fine enough, the Crank Nicolson time integration of the horizontal diffusivity term may still generate an oscillating solution. To prevent time step oscillations the time step must satisfy

\[
\Delta t \leq \frac{1}{D_H} \left( \frac{1}{(\Delta \xi \sqrt{g_{\xi \xi}})^2} + \frac{1}{(\Delta \eta \sqrt{g_{\eta \eta}})^2} \right)^{-1}
\]

(5.2.4)
6 Boundary Conditions

6.1 Introduction

In Chapter 2 we described the vertical integration over the water depth of the Reynolds-
averaged 3D Navier Stokes equations. At the bottom and free surface two stress terms were
introduced. The bottom stress takes into account the friction between the turbulent flow and
bottom, and the wind stress the velocity difference between the water surface and the air. In
Section 6.2 we give mathematical formulations for both stresses, which close the system of
governing equations.

The set of depth-averaged two-dimensional shallow water or long-wave equations solved in
the WAQUA system is a hyperbolic set of partial differential equations. The number of
specified boundary conditions at any particular point of the boundary should equal the
number of characteristics entering the region at that point, see (Courant and Hilbert, 1962)
or (Vreugdenhil, 1989) for a theoretical explanation. WAQUA assumes that the flow at the
open boundaries is subcritical, which means that the magnitude of the flow is smaller than the
velocity of wave propagation.

In this Chapter we assume that the boundary is parallel with a $\xi$ grid line, and that $U$ is the
velocity component normal to the open boundary and that $V$ is the component parallel to the
open boundary. Subcritical flow means that the Froude number is smaller than 1:

$$Fr = \frac{|U|}{\sqrt{gH}} < 1$$  \hspace{1cm} (6.1.1)

For subcritical flow, we discern two situations: inflow and outflow. At inflow we have to
specify two boundary conditions and at outflow we have to specify one boundary condition.
For tidal flow, the number of required boundary conditions varies between ebb and flood.

The first boundary condition in WAQUA is an external forcing by the water level, the
normal velocity, the discharge rate or the Riemann invariant specified by the user, see
Section 6.3. The second boundary condition is a built-in numerical boundary condition. In
WAQUA at inflow the advection of momentum in the tangential direction is neglected:

$$\frac{U}{\sqrt{g\xi}} \frac{\partial V}{\partial \xi} = 0.$$  \hspace{1cm} (6.1.2a)

On a curvilinear grid also the corresponding curvature term should be neglected:
\[
UV \frac{\partial \sqrt{g_z}}{\sqrt{g} \cdot \partial \eta} = 0
\]  

(6.1.2b)

The influence of these artificial boundary conditions is in most models restricted to only the grid cells near the boundary. For steady state simulations, the boundary condition (6.1.2) sometimes leads to an ill-posed problem. It would be better to specify the tangential velocity component. The tangential velocity may be determined from measurements, a coarser grid model or explicitly set to zero. At this moment the data structure of the open boundaries in WAQUA is not suitable to prescribe the tangential velocity component. Due to this limitation, it is a good modelling practice to put the model boundaries at locations where the grid lines of the boundary are perpendicular to the flow.

Open boundaries are necessary to restrict the computational area. They are boundaries in the mathematical model with no physical meaning. If we do not prescribe exactly the incoming characteristic at an open boundary, the outcoming characteristic will reflect at the boundary and propagate as a disturbance into the area. Usually we do not have information on both water level and velocity so we do not know the incoming characteristic. To reduce the reflections at the open boundary we use a so-called weakly reflecting boundary condition. This boundary condition is obtained using the characteristics of the linearised equations. (Verboom et al., 1983) derived a boundary condition which is non-reflective for waves, which pass normal to the boundary. The weakly reflected boundary conditions of the WAQUA system are discussed in Section 6.3.

For WAQUA applications the horizontal viscosity terms are in general less important. For the simulation of the flows in rivers, estuaries and seas the influence of the shear stresses along lateral boundaries can be neglected. In WAQUA a so-called free slip boundary condition is applied for all lateral boundaries, but on a curvilinear grid the implementation is more complicated. For flow along a closed boundary, in Eq. (4.2.9) and (4.2.10), the following boundary conditions are implemented:

\[
\frac{\partial \left( V \sqrt{g_Z} \right)}{\partial \eta} = 0
\]  

(6.1.3a)

\[
\frac{\partial \left( V \sqrt{g_{\eta \eta}} \right)}{\partial \xi} = 0
\]  

(6.1.3b)

After discretization it may no longer hold that:

\[
\frac{\partial}{\partial \eta} \left( \frac{\partial V}{\partial \xi} \right) = \frac{\partial}{\partial \xi} \left( \frac{\partial V}{\partial \eta} \right)
\]  

(6.1.4)

This generates a difference between the implementation of the difference equations in curvilinear coordinates on a rectangular grid and the implementation of the difference equations in Cartesian coordinates.
For the simulation of laboratory flumes, the effect of wall friction should be added to the system of equations.

Setting up a WAQUA model starts with covering the region of interest with a rectangular or curvilinear grid. The unknowns: water level, $U$-velocity and $V$-velocity, are staggered in space, see Section 3.1. The grid staggering leads to different locations of the boundary itself: a water level boundary in a water level point and a velocity or discharge boundary in a velocity point. The grid staggering, the higher order approximations of the advection terms and the horizontal viscosity terms give rise to numerical boundary conditions, which are not restricted to the boundary itself. These numerical boundary conditions are described in Section 6.4.

The transport of dissolved substances in rivers, estuaries and coastal seas is dominated by advection. The horizontal diffusion in flow direction is of secondary importance. The consequence is that the transport equation is advection dominated, has a wave character and from mathematical point of view is of hyperbolic type. The equation has only one characteristic, which is parallel to the flow. Without diffusion, an observer moving with the flow, observes a constant concentration. As meant before, open boundaries have to limit the computational area. At an open boundary during inflow a boundary condition is needed. During outflow the concentration must be free. At inflow we have to specify the concentration which may be determined by the concentration at outflow of the former ebb period. Because usually only the background concentration is known from measurements or from a coarse grid model, a special boundary condition based on the concentration in the interior area in combination with a return time is used, which does not completely fix the concentration. This so-called Thatcher-Harleman boundary condition is described in Section 6.4.

### 6.2 Bottom friction and wind stress

In WAQUA the shear stress of a turbulent flow over a rough bottom is assumed to be given by a quadratic friction law:

\[
|\tau_{\text{bottom}}| = \frac{\rho_0 g}{C_{2D}} |\bar{U}|^2
\]  

(6.2.1)

with components

\[
\tau_{\text{bottom}_x} = \frac{\rho_0 g U}{C_{2D_x}} \sqrt{U^2 + V^2} \quad \tau_{\text{bottom}_y} = \frac{\rho_0 g V}{C_{2D_y}} \sqrt{U^2 + V^2}
\]  

(6.2.1a)

$|\bar{U}|$ denotes the magnitude of the depth-averaged horizontal velocity. The momentum equations are discretized on a staggered grid. WAQUA computes the empirical 2D-Chézy coefficient both in $U$- and $V$-points, according to one of the following three formulations:

**Chézy :**

\[
C_{2D} = \text{Chézy coefficient (m}^2\text{/s)}
\]  

(6.2.2a)
Manning:  \[ C_{2D} = \frac{\sqrt[4]{H}}{n} \]  

where \( n \) is the Manning coefficient.

White Colebrook:

\[ C_{2D} = 18 \log_{10} \left( \max \left( \frac{12H}{k_s}, 1.0129 \right) \right) \]

where \( k_s \) is the Nikuradse roughness length. The upper boundary 1.0129 is used in the implementation to be sure that the argument of the logarithm remains positive.

To obtain a different Chézy coefficient for ebb and flood in a stratified tidal area WAQUA offers the possibility to introduce a correction factor. If \( C_{2D} \) stands for the not corrected Chézy coefficient and \( C^*_{2D} \) for the corrected one, then

\[ C^*_{2D} = \frac{C_{2D}}{\sqrt{\beta}} \]

with \( \beta \) equal to

\[ \beta = 1 - \alpha \frac{H}{\rho_0} \frac{U}{\sqrt{g \xi \frac{\partial \xi}{\partial x}}} + \frac{V}{\sqrt{\frac{g}{g \eta} \frac{\partial \eta}{\partial y}}} \]  

and \( \alpha \) a dimensionless coefficient given by the user. \( \beta \) must have a value between 1/3 and 3.

For Manning and White Colebrook the Chézy coefficients are dependent on the total water depth. In WAQUA the user has the possibility to specify the time interval to update these coefficients.

The bottom stress is integrated implicitly. For the discretization in space and time we refer to Section 4.2.6 and Chapter 5.

Without wind the stress at the free surface is zero. With wind the stress is given by:

\[ |\tau_{\text{wind}}| = \rho_a C_d (U_{10}) U_{10}^2 \]

where

\[ \rho_a \] the density of air
\[ U_{10} \] the wind speed 10 meter above the free surface
\[ C_d \] the wind drag coefficient

WAQUA offers the possibility to prescribe either local or global wind. Local wind corresponds to uniform in space and varying in time. Global winds vary both in space and time. Global wind is applied in combination with space and time varying atmospheric pressure.
The wind drag coefficient may be dependent on the wind velocity, reflecting increasing roughness of the sea surface with increasing wind speed. The user may specify an empirical relation following:

\[
C_d(U_{10}) = \begin{cases} 
C_d^0 & U_{10} \leq U_{10}^A \\
C_d^0 + \left( C_d^A - C_d^B \right) \frac{U_{10}^A - U_{10}}{U_{10}^B - U_{10}} & U_{10}^A \leq U_{10} \leq U_{10}^B \\
C_d^B & U_{10}^B \leq U_{10}
\end{cases}
\]

(6.2.6)

where

\[
\begin{align*}
C_d^{A,B} & \quad \text{user specified drag coefficients at respectively wind speed } U_d^{A,B} \\
U_{10}^{A,B} & \quad \text{user specified wind speed.}
\end{align*}
\]

### 6.3 Lateral boundary conditions

Usually open boundaries are introduced to obtain a limited computational area. In nature, waves can cross these boundaries unhindered and without reflections. In a numerical model this property must be included in the boundary conditions. If we do not prescribe exactly the incoming waves at an open boundary, the outgoing waves will reflect at the boundary and propagate as a disturbance into the area.

To reduce the reflections at the open boundary (Verboom and Slob, 1984) derived a so-called zero and first order weakly reflecting boundary condition based on the work of (Enquist and Majda, 1977). Assuming zero flow along the boundary, the zero order boundary condition may also be obtained using the characteristics of the linearised 1D equations normal to the open boundary.

\[
R = U \pm 2\sqrt{gH}
\]

(6.3.1)

The sign is dependent on the direction of the normal vector from the boundary into the model area. We restrict ourselves to the positive sign. The linearized Riemann invariant is given by:

\[
U + 2\sqrt{gH} = U + 2\sqrt{gd + \zeta} = U + 2\sqrt{gd} + \zeta \sqrt{g} \sqrt{d} , \text{ if } \frac{\zeta}{d} << 1
\]

(6.3.2)

The boundary condition specified by the user is: \( f(t) = U + \zeta \sqrt{g} \sqrt{d} \), the term \( 2\sqrt{gd} \) is computed from the known depth-field and added in the computational part of WAQUA.

The boundary condition based on the Riemann invariant is non-reflective for waves, which pass normal to the boundary and it reduces the reflection for waves which have an oblique incidence. Usually we do not have information on both water level and velocity so we do not know the incoming Riemann invariant.
A special type of open boundary for the simulations of flood waves in rivers with the WAQUA-system, is a discharge boundary with a spatial distribution of the total discharge through the opening, depending on the local water depth and the bottom friction. The local discharge $Q$ in a point at an opening is computed as:

$$Q = H_U \cdot \sqrt{g_{\eta\eta}} \cdot U$$  \hspace{1cm} (6.3.3)

where:

$U$ = velocity at the open boundary  
$H_U$ = total water depth at $U$-point  
$\sqrt{g_{\eta\eta}}$ = width of the open boundary cell

The local velocity $U$ in a boundary point is approximated by:

$$U = C_{2D} \sqrt{RT}$$  \hspace{1cm} (6.3.4)

where:

$C_{2D}$ = Chézy coefficient  
$R$ = hydraulic radius  
$I$ = hydraulic gradient

The hydraulic radius $R$ in a point of the open boundary is approximated by the local depth $H$. With the assumption of a constant hydraulic gradient $I$ along the open boundary the ratio between the local discharge $Q_i$ in a point $i$ and the total discharge $Q_{tot}$ through a opening can be expressed as follows:

$$\frac{Q_i^U}{Q_{tot}^U} = \frac{(Q_i^U)^{3/2} \cdot \sqrt{g_{\eta\eta}}}{\sum_n [(H_n^U)^{3/2} \cdot \sqrt{g_{\eta\eta}}_n \cdot (C_{2D})_n]}$$  \hspace{1cm} (6.3.5)

This expression is used for the computation of the spatial distribution of $Q_i$ along an open boundary section from a user specified total discharge $Q_{tot}$ through an open boundary section. The total water depth in (6.3.5) is taken from the previous time level.

Another type of open boundary for river simulations with the WAQUA system is the Q-H relation, specified by means of a table relating total (downstream) discharge and water level. With the computed total discharge through the open boundary the corresponding water level is computed from this table (using linear interpolation) and used as a water level boundary condition. For values of the computed total discharge outside the range specified in the Q-H table, the first or last value in the table is used. For smoothing in time, the computed water levels and user specified initial water levels are used.

At the start of the simulation the boundary conditions often do not match with the initial conditions. Therefore in WAQUA at the open boundaries a linear interpolation is applied between the initial condition and the boundary condition, to reduce the spin up time of the model. TLSMOOTH is the last time at which interpolation takes place. The interpolation for
water levels is between the given initial water level (interpolated across the opening using initial values at both ends) and the boundary condition. For velocity and discharge type of boundary conditions, smoothing is applied only for Fourier series. The interpolation is between A0 (which is interpolated in space along the boundary section, using phases at zero frequency for both ends) and the prescribed signal at the boundary.

In the computational part the following type of boundary conditions are discerned:

- water level: \( \zeta = F_\zeta(t) \)
- velocity (in normal direction): \( U = F_\nu(t) \)
- discharge: \( Q = F_\theta(t) \)
- Riemann invariant \( U \pm \zeta \sqrt{\frac{g}{d}} = F_R(t) \)

For the velocity, discharge and Riemann type of boundary condition, the flow is assumed to be perpendicular to the open boundary.

Stelling (1984) added the Riemann invariant to the water level and velocity boundary conditions, to make the boundaries less reflective for disturbances with the eigenfrequency of the model area. This reduces the spin-up time of a model from a cold start.

Water level boundary: \( \zeta + \alpha \frac{\partial}{\partial t} \left( U \pm 2 \sqrt{(gH)} \right) = F_\zeta(t) \) \hspace{1cm} (6.3.6a)

Velocity boundary: \( U + \alpha \frac{\partial}{\partial t} \left( U \pm 2 \sqrt{(gH)} \right) = F_\nu(t) \) \hspace{1cm} (6.3.6b)

The reflection coefficient \( \alpha \) is chosen sufficiently small to damp the short oscillations. The following values are advised:

Water level boundary: \( \alpha = T_d \sqrt{\frac{H}{g}} \) \hspace{1cm} (6.3.7a)

Velocity boundary: \( \alpha = T_d \) \hspace{1cm} (6.3.7b)

\( T_d \) is the time it takes for a free surface wave to travel from the left boundary to the right boundary of the model area. In ocean and sea models the period \( T_d \) is of the same order as the period of the tidal forcing. In that case \( \alpha \) must be set to zero, otherwise effectively the amplitude of one of the components in the boundary condition is reduced. These values can be derived with Fourier analysis for the 1D linear long wave equation without advection by substituting a wave with period \( T_d \).

### 6.4 Open boundary conditions for the transport model

The transport of dissolved substances such as salt, sediment and heat is described by the advection-diffusion equation. The transport is advection dominated and the equation is of hyperbolic type. At inflow one boundary condition is needed and the concentration is
specified. At outflow no boundary condition is allowed. The concentration is determined by pure advection from the interior area:

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = 0$$

(6.4.1)

At inflow there is also a dispersive flux through the open boundary.

If the concentration at outflow differs from the boundary condition at inflow, at the turn of the tide there is a discontinuity in the concentration. The transition of the concentration at the boundary from the outflow value to the inflow value may take some time. This depends on the refreshment of the water in the boundary region. The transition time is called the return time. The functional relationship describing the variation in concentration from the slack-water value to the present value is arbitrary. In WAQUA a half-cosine variation is used. After the return time, the boundary value remains constant until outward flow begins (Leendertse and Gritton, 1971), (Thatcher and Harleman, 1972). The mathematical formulation of this memory effect is given as follows:

$$C(t) = C_{\text{out}} + \frac{1}{2} (C_{\text{end}} - C_{\text{out}}) \left[ \cos \left( \frac{T_{\text{ret}} - t_{\text{out}}}{T_{\text{ret}}} \right) + 1 \right], \quad 0 \leq t_{\text{out}} \leq T_{\text{ret}}$$

(6.4.2)

$C_{\text{out}}$ is the computed concentration at the open boundary at the last time of outward flow, $C_{\text{end}}$ is the background concentration described by the user, $t_{\text{out}}$ is the elapsed time since the last outflow and $T_{\text{ret}}$ is the constituent return time, which is for each layer the same, as described by the user. When the flow turns inward ($t_{\text{out}} = 0$), the concentration is set equal to $C_{\text{out}}$. During the interval $0 \leq t_{\text{out}} \leq T_{\text{ret}}$, the concentration will return to the background concentration $C_{\text{end}}$. After that period, the concentration will remain $C_{\text{end}}$. The mechanism is illustrated in Figure 6.1.

![Figure 6.1. Illustration of memory effect for open boundary.](image)
6.5 Numerical treatment boundary conditions momentum and continuity equations

A curvilinear orthogonal grid which covers the computational region of a WAQUA model should be boundary-fitted. The closed boundaries should be co-ordinate lines. If the generation of such a grid is not possible, because the requirement of orthogonality is too strict, the boundary is approximated stepwise by co-ordinate lines. A stair case closed boundary may introduce an unphysical boundary layer, see (Weare, 1979).

WAQUA is based on a finite difference method, which makes use of space staggering (Arakawa C-grid). The system of difference equations for a computational row or computational column of the grid always starts with a water level point and ends with a water level point. The boundary condition for the water levels is prescribed in a water level point. It is assumed that the flow is normal to the boundary. The tangential velocity is set to zero for the velocity point at the boundary. The other types of boundary conditions: closed, velocity, discharge, Riemann invariant are specified at the velocity point normal to the boundary. For these types of boundary conditions the first and last water level point are virtual points.

When tide gauges to force the tidal openings are not located along a grid line, a non-rectangular computational grid is fitted to the tidal openings. For limiting computations and storage, one or more polygons denoted as the grid enclosures have been introduced in the WAQUA system, see Figure 3.2. Each grid enclosure is a polygon through water level points, just outside the computational area of interest. The index set of the water level openings is a subset of the index set of enclosure points. Water level openings may be defined along rows or columns of the grid, but also along diagonals (45 degrees). For the other boundary types, diagonals are not allowed. Due to the staggered grid, the index set of the other type of openings is not a subset of the enclosure points. On the right of the computational grid the $m$-index of the velocity point is one lower than on the enclosure. On the top the $n$-index is one lower.

For the time integration in WAQUA an alternating-direction implicit (ADI) method is applied. Alternatively the $U$- and $V$-direction are treated implicitly. WAQUA updates the boundary conditions following the ADI-directions only once in a complete time step. For a velocity, a discharge and a Riemann boundary the velocity is frozen at the previous half time step:

$$U^{j+1}_{m_f,n} = U^{j+1/2}_{m_f,n} \quad (6.5.1)$$

The staggered grid allows a simple treatment of the boundary conditions. At a boundary only one dependent variable (velocity or water level) is situated. We describe the implementation of the boundary conditions in the $U$-direction at the left side of the computational grid. A similar mathematical description is possible for the right boundary and for the boundaries at the top or bottom of the computational grid. Due to the staggered grid arrangement of the variables, the implementation of the right boundary is not symmetric with the left boundary.
The boundary conditions necessary to have a well-posed problem were discussed in Section 6.1. In this section we give the implementation of the boundary conditions. To have a well-determined system of difference equations, additional so-called numerical boundary conditions are needed.

The difference stencils for the advection terms involve a large number of grid points. Near boundaries and dam points, some of these grid points may lie at the boundary or outside the computational domain and the discretizations need to be adapted. The discretizations near the boundaries may be of lower order without influencing the order of convergence of the solution at the inner points. In WAQUA the discretizations near boundaries were generated following the principles suggested by Stelling (1984):

1. always avoid negative viscosity in the truncation error of the discretization,
2. if near a closed boundary, the discretization contains the boundary value zero, avoid this by using a discretization that needs fewer grid points or by the use of upwind differences,
3. the boundary scheme should be stable.

Without the special discretizations near the boundaries, the computational scheme may become unstable or generate spurious oscillations (wiggles) in the velocity field.

For the numerical implementation of the horizontal viscosity term near open and closed boundaries we refer to Van Kester (1989) and Stelling (1984). We assume free slip. The implementation of this boundary condition in curvilinear co-ordinates is complex and is not described in this document in full details.

### 6.5.1 Closed boundary

A closed boundary is situated at the transition between land and water. At a closed boundary, two boundary conditions have to be prescribed. One boundary condition has to do with the flow normal to the boundary and the other one with the shear stress along the boundary. We assume that the boundary is situated at m-index \( m_f \). At a closed boundary the following boundary conditions are prescribed:

No flow through the boundary:

\[
U_{m_f} = 0
\]  
(6.5.2)

and free slip along the boundary:

\[

\begin{align*}
\nu_H \frac{\partial \left( V \sqrt{g z} \right)}{\partial \eta} &= 0 \\
\nu_H \frac{\partial \left( V \sqrt{g \eta} \right)}{\partial \xi} &= 0
\end{align*}
\]  
(6.5.3a)  
(6.5.3b)
Near a closed boundary which is normal to the flow direction, the velocity point at the boundary is taken into account in the viscosity term:

$$\nu \frac{\partial}{\partial \xi} \left( \frac{U}{\sqrt{g \eta}} \right)$$

(6.5.4)

The staggered grid allows a simple discretization of the boundary conditions. No special boundary scheme is necessary at the boundary itself. An additional numerical boundary condition is implemented for the water level at the land side of the closed boundary:

$$\zeta_{m_f,n} = 0$$

(6.5.5)

to have a well-posed system of difference equations.

Near closed boundaries, the discretization of the advection terms is adapted. We use the notation of Chapter 3. The boundary schemes for the advection applied in WAQUA were carefully evaluated and tested by Stelling (1984). We describe the discretization for the velocity gradient in the direction of the flow.

The central approximation for the advection used for interior points is replaced by:

$$\frac{U}{\sqrt{g \zeta}} \frac{\partial U}{\partial \zeta} \bigg|_{m_f,n+1} = \begin{cases} \frac{U_{m_f,n+1,n} - U_{m_f,n+1,n}}{\Delta \zeta}\sqrt{g \zeta} & \text{if } U_{m_f,n+1,n} \leq 0 \\ 0 & \text{if } U_{m_f,n+1,n} > 0 \end{cases}$$

(6.5.6a)

The central discretization of the interior domain including the boundary point would introduce an artificial boundary layer, see (Stelling, 1984). The curvilinear transformation of the advection term introduces a curvature term, see Eq. (2.4.5). If the advection term is neglected also the curvature term should be neglected, so:

$$\frac{UV}{\sqrt{g}} \frac{\partial \sqrt{g \zeta}}{\partial \eta} \bigg|_{m_f,n} = \begin{cases} \frac{U_{m_f,n}}{\sqrt{g \eta}} \frac{\partial}{\partial \eta} \left( \frac{(\sqrt{g \zeta})_{m_f,n} + (\sqrt{g \zeta})_{m_f,n+1,n} - (\sqrt{g \zeta})_{m_f,n-1,n} - (\sqrt{g \zeta})_{m_f,n+1,n+1}}{2\Delta \eta} \right) & \text{if } U_{m_f,n} \leq 0 \\ 0 & \text{if } U_{m_f,n} > 0 \end{cases}$$

(6.5.6b)

For closed boundaries which are tangential with the U-direction the cross advection term should be adapted. In the computational stencil for the cross advection term a large number of grid points are involved. Near boundaries sixteen different conditions can be identified depending on the availability of the grid points. If one of the points is a boundary point, the computational stencil is reduced, by lowering the order of discretization. For the complete description of the discretization of the cross advection term near a closed boundary, we refer to Stelling (1984), page 149-151.
6.5.2 Water level boundary

Open boundaries are introduced to limit the number of grid points of the computational domain. The boundaries are artificial only existing in the mathematical model. The boundary conditions should be such that no unphysical reflection is introduced. In WAQUA the water level boundary is stabilized with a part of the Riemann-invariant (Stelling, 1984):

\[ \zeta \text{ boundary left : } \zeta + \alpha \frac{\partial}{\partial t} \left( U + 2\sqrt{gH} \right) = f(t) \]  
(6.5.7a)

\[ \zeta \text{ boundary right : } \zeta + \alpha \frac{\partial}{\partial t} \left( U - 2\sqrt{gH} \right) = f(t) \]  
(6.5.7b)

with \( H \) the total water depth, and \( U \) the depth-averaged velocity normal to the open boundary. This boundary condition is non-reflective for waves with short wave lengths generated inside the domain.

\[ \frac{\partial}{\partial t} \sqrt{H} = \frac{1}{2\sqrt{H}} \frac{\partial H}{\partial t} = \frac{1}{2\sqrt{H}} \frac{\partial \zeta}{\partial t} \]  
(6.5.8)

We describe the implementation of the weakly reflective \( \zeta \)-boundary at the left side of the computational domain, see Figure 6.2.

Figure 6.2. Open boundary normal to the \( U \)-direction

\[ \left( I + \frac{\alpha}{2\Delta t} \frac{\sqrt{g}}{\sqrt{(H_{m_r,n}^U)^l}} \right) \zeta_{m_r}^{l+\frac{1}{2}} + \left( \frac{\alpha}{\Delta t} \right) U_{m_r}^{l+\frac{1}{2}} + \left( \frac{\alpha}{2\Delta t} \frac{\sqrt{g}}{\sqrt{(H_{m_r,n}^U)^l}} \right) \zeta_{m_r+1}^{l+\frac{1}{2}} = \]  
(6.5.9)

\[ f(t^{l+\frac{1}{2}}) + \frac{\alpha}{\Delta t} U_{m_r}^l + \frac{\alpha}{2\Delta t} \frac{\sqrt{g}}{\sqrt{(H_{m_r,n}^U)^l}} \left( \zeta_{m_r}^l + \zeta_{m_r+1}^l \right) \]

At the explicit step the water level is not updated. The ADI-method introduces a splitting error. For steady state boundary conditions, the steady state numerical solution for the complete and intermediate time step may differ. The difference between the complete and intermediate time level
\[ U^{i+1}_{m_j,n} - U^{i+1/2}_{m_j,n} \] \hspace{1cm} (6.5.10)

may introduce a small forcing in the right hand side of Eq. (6.5.9).

The discretization of the advection terms in the momentum equation for the velocity point at m-index \( m_j \) requires lower order approximations. The discretization (6.5.11) is used in point \( m_j \):

\[
\left. \frac{U}{\sqrt{g_{\eta \xi}}} \frac{\partial U}{\partial \xi} \right|_{m_j,n} = \begin{cases} 
\frac{U_{m_j,n} - U_{m_j+1,n} - U_{m_j,n}}{\Delta \xi} & \text{if } U_{m_j,n} \leq 0 \\
0 & \text{if } U_{m_j,n} > 0
\end{cases} \hspace{1cm} (6.5.11)
\]

At inflow the advection term is neglected. If the advection term is neglected also the corresponding curvature term is be neglected.

The tangential velocity \( V \) at point \( m_j \) is set to zero:

\[ V_{m_j,n} = 0 \hspace{1cm} (6.5.12) \]

and in the \( U \)-momentum equation just inside the flow domain the cross advection term and the corresponding curvature term are neglected:

\[ V \frac{\partial U}{\partial y} \bigg|_{m_j,n} = 0 \hspace{1cm} (6.5.13a) \]

\[ \frac{V^2}{\sqrt{g \cdot \eta \xi}} \frac{\partial g_{\eta \xi}}{\partial \xi} \bigg|_{m_j,n} = 0 \hspace{1cm} (6.5.13b) \]

In the momentum equation at the boundary point \( m_j \) the wind stress, the atmospheric pressure gradient and the baroclinic pressure gradient are neglected. The \( V \)-velocity at \( U \)-point \( m_j \), used in the bottom friction and Coriolis force is based on the average over the active grid points:

\[ \left. \tau_{\eta} \right|_{m_j,n} = \frac{V_{n \eta}}{2} + \frac{V_{n+1 \eta}}{2} \hspace{1cm} (6.5.14) \]

The viscosity term for the boundary point \( m = m_j \) is simplified to:

\[ \Delta U_{m_j,n} = \nu \left. \frac{1}{\sqrt{g \cdot \eta \xi}} \frac{\partial (U \sqrt{g \cdot \eta \xi})}{\partial y} \right|_{m_j,n} \hspace{1cm} (6.5.15) \]
Figure 6.3. Open boundary parallel to the \( U \)-direction

For an open boundary which is parallel with the \( U \)-direction, at inflow the cross advection term in the first velocity point inside the flow domain is neglected, see also Figure 6.3:

\[
\frac{V}{\sqrt{g_{\eta \eta}}} \frac{\partial U}{\partial \eta} \bigg|_{m,n,r+1} = \frac{V_{m,n,r+1}}{\sqrt{g_{\eta \eta}}} \frac{U_{m,n,r+2} - U_{m,n,r+1}}{\Delta \eta} \quad \text{if} \quad \frac{V_{m,n,r+1}}{\sqrt{g_{\eta \eta}}} \leq 0 \\
0 \quad \text{if} \quad \frac{V_{m,n,r+1}}{\sqrt{g_{\eta \eta}}} > 0
\]

(6.5.16a)

\[
\frac{V^2}{\sqrt{g}} \frac{\partial \sqrt{g_{\eta \eta}}}{\partial \xi} \bigg|_{m,n,r+1} = \left( \frac{V_{m,n,r+1}}{\sqrt{g_{\eta \eta}}} \right)^2 \left( \sqrt{g_{\eta \eta}} \right)_{m+1,n,r+1} - \left( \sqrt{g_{\eta \eta}} \right)_{m,n,r+1} \frac{2 \Delta \xi}{\Delta \xi}
\]

(6.5.16b)

For a steady state simulation, neglecting the cross advection may lead to an ill-posed problem. The tangential velocity \( U \) along the open boundary is undetermined and may oscillate in time. In Chapter 9 we recommend to take the cross advection term into account at inflow.

For a water level boundary, the momentum equation is solved for the boundary point \( m_j \) at each half time step following the ADI-time integration for the water levels.

At the velocity point \( m_j + 1 \), the advection term is approximated by a first order upwind discretization:

\[
\frac{U}{\sqrt{g_{\xi \xi}}} \frac{\partial U}{\partial \xi} \bigg|_{m_j+1,n} = \begin{cases} 
\frac{U_{m_j+1,n} - U_{m_j+2,n}}{\Delta \xi} \quad & \text{if} \quad U_{m_j+1,n} \leq 0 \\
\frac{U_{m_j+1,n} - U_{m_j+1,n-1}}{\Delta \xi} \quad & \text{if} \quad U_{m_j+1,n} > 0 
\end{cases}
\]

(6.5.17)
6.5.3 Velocity boundary

Open boundaries are introduced to limit the number of grid points of the computational domain. The boundaries are artificial only existing in the mathematical model. The boundary conditions should be such that no unphysical reflection is introduced. In WAQUA the velocity boundary is stabilized with a part of the Riemann-invariant (Stelling, 1984):

\[
U\text{-boundary left : } U + \alpha \frac{\partial}{\partial t} \left( U + 2\sqrt{gH} \right) = f(t)
\]

\[
U\text{-boundary right : } U + \alpha \frac{\partial}{\partial t} \left( U - 2\sqrt{gH} \right) = f(t)
\]

We describe the implementation of the weakly reflective \textit{U}-boundary at the left side of the computational domain.

We introduce a virtual water level point for \( m = m_f \). An additional numerical boundary condition is implemented for the water level at the boundary, just outside the computational domain:

\[
\zeta_{m_f,n} = \zeta_{m_f+1,n}
\]

(6.5.18)

to have a well-posed system of difference equations.

For the implicit step, the weakly reflective \textit{U}-boundary is discretized at the velocity point \( m_f \).

\[
\left( \frac{\alpha}{2\Delta t} \frac{\sqrt{g}}{\left( H_{m_f,n}^U \right)^{\frac{1}{2}}} \right) \zeta_{m_f+1,n}^{i+\frac{1}{2}} + \left( 1 + \frac{\alpha}{\Delta t} \right) U_{m_f}^{i+\frac{1}{2}} + \left( \frac{\alpha}{2\Delta t} \frac{\sqrt{g}}{\left( H_{m_f,n}^U \right)^{\frac{1}{2}}} \right) \zeta_{m_f+1,n}^{i+\frac{1}{2}} = f(t) + \frac{\alpha}{\Delta t} U_{m_f}^{i} + \frac{\alpha}{2\Delta t} \frac{\sqrt{g}}{\left( H_{m_f,n}^U \right)^{\frac{1}{2}}} \left( \zeta_{m_f}^{i} + \zeta_{m_f+1,n}^{i} \right)
\]

(6.5.19)

For a velocity boundary, the boundary condition for the boundary point \( m_j \) is updated only once in each half time step. For the explicit step

\[
U_{m_f,n}^{i+\frac{1}{2}} = U_{m_f,n}^{i+\frac{1}{2}}
\]

(6.5.20)

The approximations for the advection terms near the velocity boundary are adapted following the same procedure as for the water level boundary. The discretization of the advection terms in the momentum equation for the velocity point at \( m_f + 1 \) requires lower order approximations. The advection term is approximated by an upwind discretization:
\[
\begin{align*}
\frac{U}{\sqrt{g_\xi}} \frac{\partial U}{\partial \xi} &= \begin{cases} 
\frac{U_{m_j+1,n} - U_{m_j+2,n}}{\sqrt{g_\xi}} & \text{If } U_{m_j+1,n} \leq 0 \\
\frac{U_{m_j+1,n}}{\sqrt{g_\xi}} & \text{If } U_{m_j+1,n} > 0
\end{cases}
\end{align*}
\] (6.5.21)

The tangential velocity \( V \) in point \( m_f \) along the open boundary is set to zero:

\[ V_{m_f,n} = 0 \] (6.5.22)

For an open boundary which is parallel with the \( U \)-direction, at inflow the cross advection term in the first velocity point inside the flow domain is neglected, Eq. (6.5.15).

### 6.5.4 Discharge boundary

In WAQUA, a discharge boundary condition is implemented as a special case of a velocity boundary condition. The value at the boundary depends on the discharge \( f(t^{+1/2}) \) specified by the user and the total water depth at the previous half time step. In the implicit step:

\[ U_{m_f,n}^{+1/2} = \frac{f(t^{+1/2})}{\left( H_{m_f,n}^U \right)^{1/2}} \] (6.5.23)

The boundary condition is specified outside the iteration for the continuity equation. This will introduce a mass closure error:

\[ \left( H_{m_f,n}^U \right)^{1+1/2} U_{m_f,n}^{+1/2} = \frac{f(t^{+1/2})}{\left( H_{m_f,n}^U \right)^{1/2}} - f(t^{+1/2}) \] (6.5.24)

For the other boundary conditions and implementations we refer to Section 6.5.3. For a discharge boundary, the boundary condition for the boundary point \( m_f \) is updated only once in each half time step. For the explicit step of the ADI-scheme:

\[ U_{m_f,n}^{+1} = U_{m_f,n}^{+1/2} \] (6.5.25)
6.5.5 Riemann invariant type of boundary

The incoming Riemann invariant at a left boundary is given by \( U + 2 \sqrt{gH} \), and the incoming Riemann invariant at a right boundary is given by \( U - 2 \sqrt{gH} \). We describe the implementation of a Riemann invariant boundary condition at the left side of the computational domain. The implementation at the right-hand side is similar.

The incoming Riemann invariant is prescribed at a velocity point. The Riemann invariant is non-linear and linearized around the old time level:

\[
[U + 2 \sqrt{gH}]^{t+\frac{1}{2}} = U^{t+\frac{1}{2}} + 2 \sqrt{gH^{t+\frac{1}{2}}} = U^{t+\frac{1}{2}} + 2 \sqrt{gH^t} + \sqrt{\frac{g}{H}} \left( H^{t+\frac{1}{2}} - H^t \right) = U^{t+\frac{1}{2}} + 2 \sqrt{gH^t} + \sqrt{\frac{g}{H}} \left( \zeta^{t+\frac{1}{2}} - \zeta^t \right)
\]

\[[6.5.26]\]

The boundary condition specified by the user is: \( f(t) = U + \zeta \sqrt{\frac{g}{d}} \), the term \( 2 \sqrt{gd} \) is computed from the known depth-field and added in the computational part of WAQA.

\[
U^{t+\frac{1}{2}} + 2 \sqrt{gH^t} + \sqrt{\frac{g}{H}} \left( \zeta^{t+\frac{1}{2}} - \zeta^t \right) = U + \zeta \sqrt{\frac{g}{d}} + 2 \sqrt{gd}
\]

\[[6.5.27]\]

Consequently:

\[
U_{n,t}^{t+\frac{1}{2}} + \frac{\sqrt{g}}{2 \sqrt{\left(H_{m,j,n}^{t} \right)^i}} \left( \zeta_{m,j,n}^{t+\frac{1}{2}} + \zeta_{m,j+1,n}^{t+\frac{1}{2}} \right) =
\]

\[[6.5.28]\]

\[
f(t^{t+\frac{1}{2}}) + 2 \sqrt{gd} - 2 \sqrt{g \left(H_{m,j,n}^{t} \right)^i} + \frac{\sqrt{g}}{2 \sqrt{\left(H_{m,j,n}^{t} \right)^i}} \left( \zeta_{m,j,n}^t + \zeta_{m,j+1,n}^t \right)
\]

For the other boundary conditions and implementations we refer to Section 6.5.3. For a discharge boundary, the boundary condition for the boundary point \( m_j \) is updated only once in each half time step. For the explicit step of the ADI-scheme:

\[
U_{m,j,n}^{t+1} = U_{m,j,n}^{t+\frac{1}{2}}
\]

\[[6.5.29]\]

The approximations for the advection terms near the Riemann type of boundary are adapted following the same procedure as for a velocity type of boundary, see Section 6.5.3.

6.6 Numerical treatment conditions for the transport equation

The depth-averaged transport equation of WAQA is discretized with finite differences on a staggered C-grid. The concentration is computed at the water level points. For a closed
boundary, the first concentration point lies outside the computational domain and is a virtual point. The concentration is set to zero.

At an open boundary the concentration at the boundary is prescribed at inflow and determined by pure advection from the interior area at outflow.

### 6.6.1 Closed boundary

The total flux through a closed boundary is zero

\[
UC + \left(D_H + D_{dop}\right) \frac{1}{\sqrt{g_{xx}}} \left. \frac{\partial C}{\partial \xi} \right|_{m_i,n} = 0
\]  

(6.6.1)

The concentration at the grid point at the land side of the closed boundary, with index \( m_i \) is set to zero.

### 6.6.2 Open boundary

At an open boundary, the boundary condition depends on the direction of the flow.

At inflow the concentration at the boundary is specified:

\[
C_{m_i,n}^{i+\frac{1}{2}} = f(t^{i+\frac{1}{2}})
\]  

(6.6.2)

The concentration specified at the boundary at inflow may be influenced by the concentrations at outflow. The mathematical formulation of this memory effect was given by (Leendertse and Gritton, 1971) and (Thatcher and Harleman, 1972), see Section 6.4.

The discretization of the advective and diffusive flux is not adapted at the open boundary.

At outflow the concentration at the open boundary is computed with a pure advection equation:

\[
\frac{\partial C}{\partial t} + \frac{U}{\sqrt{g_{xx}}} \frac{\partial C}{\partial \xi} = 0
\]  

(6.6.3)

The concentration at an open boundary point is updated once in a time step, following the ADI-directions. The time levels of the concentrations associated with open boundaries normal to the \( U \)-direction differ half a time step with the time levels of concentrations associated with open boundaries normal to the \( V \)-direction. The advection equation is discretized as:
\[
\frac{C^{i+\frac{1}{2}}_{m_j,n} - C^{i}_{m_j,n}}{\frac{1}{2} \Delta t} + \frac{U^{i+\frac{1}{2}}_{m_j,n}}{\left(\sqrt{g \zeta}\right)^\eta} \frac{C^{i+\frac{1}{2}}_{m_j+1,n} - C^{i+\frac{1}{2}}_{m_j,n}}{\Delta \xi} = 0
\] (6.6.4)

When water levels are prescribed, a WAQUA-model may have a diagonal open boundary. For the transport equation such a boundary is treated as a combination of a \(U\)- and \(V\)-boundary. The concentration is updated twice in a time step, following the ADI-directions.
7 Solution methods used in WAQUA

The spatial discretizations of Chapter 4, combined with the ADI-splitting and the iterative procedure to remove the non-linearity described in Chapter 5, results in a number of linear systems. In this chapter we describe how these systems are solved.

Discretization of the governing equations for depth-averaged flow on the staggered WAQUA-grid with the ADI-method introduces at each stage the two systems of equations, one along rows and one along columns of the computational grid. We start our description with the system of difference equations along columns, which results from the discretization of the momentum equation in $V$-direction at the first stage of the ADI-method, see (5.1.2) and Section 7.1. Next, we discuss the solution method for the coupled system of difference equations along rows for the water levels and $U$-velocities resulting from the discretization of the $U$-momentum equation (5.1.1) and the continuity equation (5.1.3), see Section 7.2. We restrict our description to the first stage of the ADI-method, because in the second stage the same numerical techniques are applied, see Eqs. (5.1.4-6). Only the directions are interchanged. Furthermore, in Section 7.3 we describe the system of equations resulting after discretization of the transport equation. The iterative solution procedure in WAQUA reduces all the linear systems of equations to tridiagonal form. These tridiagonal systems are solved with the so-called Thomas’ algorithm, which is given in Section 7.4.

7.1 System of equations for $V$-momentum equation

In the first half time step of the ADI-splitting the $V$-velocities are implicitly coupled by the advection terms. The advection term in $y(\eta)$-direction couples $V$-points along lines $m=$constant (columns), while the $U$ advection term couples along lines $n=$constant (rows). The higher order upwind discretization of the cross advection term (see Eq. (4.2.2)) leads to a matrix with a special form. The matrix has five non-zero entries. In each row the non-zero entries due to the cross advection are at one side of the main diagonal. If we assume that the $U$-velocity in grid point $(m,n)$ is in the direction of increasing $m$, the pentadiagonal system has the following form:

$$a_{m,n-1} V_{m,n-1} + b_{m,n} V_{m,n} + c_{m,n+1} V_{m,n+1} + e_{m-1,n} V_{m-1,n} + f_{m-2,n} V_{m-2,n} = d_{m,n} \quad (7.1)$$

The non-zero entries $e_{m-1,n}$ and $f_{m-2,n}$ correspond to $V$-points on grid lines in the upstream $\chi(\xi)$-direction.

If we add the implicit discretization of the horizontal viscosity term, a non-zero entry $g_{m+1,n}$ in the downstream direction is introduced:

$$a_{m,n-1} V_{m,n-1} + b_{m,n} V_{m,n} + c_{m,n+1} V_{m,n+1} + e_{m-1,n} V_{m-1,n} + f_{m-2,n} V_{m-2,n} + g_{m+1,n} V_{m+1,n} = d_{m,n} \quad (7.1a)$$
We remark that the coefficients in (7.1a) are different from the ones in (7.1) by the addition of the horizontal viscosity term. For the sake of simplicity we used the same symbols.

To solve the system of equations we introduce an iterative procedure. The supindex $p$ denotes the iteration counter. In WAQUA the system of equations for the $V$-velocities (7.1a) is solved iteratively along lines with fixed $m$ (column by column). The grid lines are coupled through the right-hand side. Along each grid line the system (7.1a) reduces to a tridiagonal system of equations. These equations are solved by the so-called Thomas algorithm, see Section 7.4. The grid lines are solved successively. The dominant flow direction, increasing or decreasing $m$, is determined by summation of all non-zero $U$-velocities:

$$\text{sign} = \text{sign} \left( \sum_{m,n} U_{m,n} \right)$$

The first sweep is in the dominant flow direction. If the sweep direction and the upwind direction are both in the direction of increasing $m$, the difference equation is given by:

$$a_{m,n-1} V_{m,n-1}^{[p]} + b_{m,n} V_{m,n}^{[p]} + c_{m,n+1} V_{m,n+1}^{[p]} =
\begin{align*}
d_{m,n} - e_{m-1,n} V_{m-1,n}^{[p]} & - f_{m-2,n} V_{m-2,n}^{[p]} - g_{m-1,n} V_{m-1,n}^{[p-1]} - h_{m+1,n} V_{m+1,n}^{[p-1]} 
\end{align*}$$

(7.1a')

The $V$-velocities in grid points upstream are known. The terms $V_{m-1,n}^{[p]}$ and $V_{m+1,n}^{[p-1]}$, which is part of the discretization of the horizontal viscosity is taken from the previous iteration. If $U$ has the same direction all over the grid and without horizontal viscosity, Eq. (7.1a') is solved in one $p$-iteration. In general more iterations are necessary. The next sweep always proceeds in the opposite direction of the preceding sweep. If the sweep direction is opposite to the dominant flow direction, then the upwind advection term is evaluated at the previous iteration level $p-1$, which gives

$$a_{m,n-1} V_{m,n-1}^{[p]} + b_{m,n} V_{m,n}^{[p]} + c_{m,n+1} V_{m,n+1}^{[p]} =
\begin{align*}
d_{m,n} - e_{m-1,n} V_{m-1,n}^{[p-1]} & - f_{m-2,n} V_{m-2,n}^{[p-1]} - h_{m+1,n} V_{m+1,n}^{[p-1]} 
\end{align*}$$

(7.1a'')

In WAQUA the maximum number of iterations is specified by the user. The default maximum number of iterations is two.

The system of equations for the $U$-velocities at the second stage is solved in a similar way. The only difference is that the system is solved row by row with the first sweep in the dominant direction of $V$.

7.2 The coupled system for $U$-momentum equation and continuity equation

The difference equations resulting from the discretized momentum equation (5.1.1) and the discretized continuity equation (5.1.3), are coupled by the implicit handling of the free surface gradient. The advection and viscosity terms are taken explicitly. To remove the non-
linear coupling between the $U$-momentum equation and the discretized continuity equation, the free surface gradient is multiplied by

$$r^{[q]} = \frac{H_{m,n}^{[q-1]}}{H_{m,n}^{[q]}}$$

with $q$ the iteration counter, and $H_{m,n}^{[q]}$ the total water depth in a $U$-point. This leads to a discretized $U$-momentum equation of the following form

$$\frac{H_{m,n}^{[q-1]}}{H_{m,n}^{[q]}} \cdot \frac{a_{m-1,n} r^{[q]}_{m-1,n}}{a_{m,n} r^{[q]}_{m,n}} + \frac{b_{m,n} U^{[q]}_{m,n}}{b_{m,n} U^{[q]}_{m,n}} + \frac{H_{m,n}^{[q-1]}}{H_{m,n}^{[q]}} cc_{m+1,n} r^{[q]}_{m,n} = d_{m,n}$$  \tag{7.2a}

The velocity unknowns $U^{[q]}$ can be expressed in the unknown water levels. The iterative procedure linearizes the system of difference equations at each cycle of the $q$-iteration, by substituting the $U$-momentum equation into the discrete continuity equation. This yields a tridiagonal system of equations to solve the water levels $r^{[q]}$:

$$a_{m-1,n} r^{[q]}_{m-1,n} + b_{m,n} r^{[q]}_{m,n} + c_{m+1,n} r^{[q]}_{m,n} = d_{m,n}$$  \tag{7.2b}

The velocities $U^{[q]}$ are computed by back substitution in Eq. (7.2a). The solution method for the tridiagonal system (7.2b) is described in Section 7.4.

### 7.3 System of equations for transport

The ADI-splitting applied to the advection and diffusion term of the transport equation couples the concentrations along grid lines (columns or rows) and yields tridiagonal systems of equations, see Eq. (5.2.1-2). The system of difference equations that corresponds to an implicit discretization in $x(\xi)$-direction, can be written in the form

$$a_{m-1,n} C_{m-1,n} + b_{m,n} C_{m,n} + c_{m+1,n} C_{m+1,n} = d_{m,n}$$  \tag{7.3a}

Similarly, in the other stage with an implicit discretization in $y(\eta)$-direction the system of equations reads

$$a_{m,n-1} C_{m,n-1} + b_{m,n} C_{m,n} + c_{m,n+1} C_{m,n+1} = d_{m,n}$$  \tag{7.3b}

The tridiagonal systems (7.3ab) are solved with a double sweep, see Section 7.4.

### 7.4 Thomas' algorithm for the solution of tridiagonal systems

The finite difference method of WAQUA is based on ADI-splitting and only requires the solution of tridiagonal systems of equations (7.1'), (7.2), (7.3a) and (7.3b). The well-known Thomas' algorithm is applied to solve these systems. In this section we describe this solution technique in detail. Let the tridiagonal matrix $A$ be given by
The tridiagonal system $Ax = d$ with $A$ as in (7.4) can be reduced to a bidiagonal system of the form

$$
\begin{pmatrix}
1 & \gamma_1 \\
\vdots & \ddots & \ddots \\
& \gamma_{k-1} & 1
\end{pmatrix}
\begin{pmatrix}
1 \\
\vdots \\
1
\end{pmatrix}
= \delta
$$

with

$$
\gamma_i = \frac{c_i}{b_i}, \quad \delta_i = \frac{d_i}{b_i}
$$

$$
\gamma_i = \frac{c_i}{b_i - a_i \gamma_{i-1}}, \quad i = 2, 3, \ldots, k
$$

$$
\delta_i = \frac{d_i - a_i \delta_{i-1}}{b_i - a_i \gamma_{i-1}}, \quad i = 2, 3, \ldots, k
$$

Next, the solution of $Ax = d$ is obtained by backward substitution:

$$
x_k = \delta_k, \quad x_i = \delta_i - \gamma_i x_{i+1}, \quad i = k-1, k-2, \ldots, 1
$$

This algorithm is also called the double sweep, because of the forward and backward sweeps needed to obtain the solution. This technique is very efficient since the computational work required for (7.6) and (7.7) is $8k - 7$ floating point operations, whereas the storage required for $\alpha_i$ and $\beta_i$ is $2k - 1$ reals. A disadvantage of the double sweep algorithm is that it is not suited for implementation on vector and parallel computers since it is a recursive algorithm.

To prevent the amplification of rounding off errors the matrix must be diagonal dominant. A sufficient condition is given by the following condition for the matrix elements:

$$
|b_i| > |a_i| + |c_i| \quad \text{for } i = 1, \ldots, k.
$$
For the systems solved in WAQUA (7.8) leads to a restriction on the time step, see (Stelling, 1984):

\[
\max \left( \frac{\Delta t |U_{m,n}'|}{\Delta \xi \sqrt{g_{xx}}}, \frac{\Delta t |V_{m,n}'|}{\Delta \eta \sqrt{g_{yy}}} \right) \leq 4. \tag{7.9}
\]
8 Drying and flooding procedure

8.1 Description of the general method

Estuaries and coastal embayments contain large, shallow and relatively flat areas separated and interleaved by deeper channels and creeks. When water levels are high the entire area is water covered but as tide falls, the shallow areas are exposed and ultimately the flow is confined only to the deeper channels. The dry tidal flats may occupy a substantial fraction of the total surface area. The accurate reproduction of covering or uncovering of the tidal flats is an important feature numerical tidal flow models based on the shallow water equations.

Many rivers have compound channels, consisting of a main channel which always carries flow (the summer-bed) and one or two flood plains which only carry flow during extreme river discharges (the winter-bed). The summer bed is surrounded by low dikes, which will overtop when the river discharge increases. The winter-bed is surrounded by much higher dikes which are designed to protect the polders against extreme river discharges. The flooding of the flood plains increases the drainage capacity of the river and reduces the local water level gradients.

In the numerical model WAQUA flooding and drying is represented by removing grid cells that become "dry" when tide falls and adding grid cells that become "wet" when tide rises. In this section we specify the rules which are used to determine the moment when a grid cell or cell boundary becomes wet or dry. In WAQUA drying and flooding is constrained to follow the sides of grid cells, so only velocity points are subject to drying and flooding. It is a discontinuous movement of the boundary and may generate small oscillations in water levels and velocities. The oscillations introduced by the drying and flooding algorithm are small if the grid sizes are small and the bottom has smooth gradients.

The number of grid cells that are set dry at low water, determines the storage capacity of an estuary during ebb tide and so the propagation of the tidal wave. The number of grid cells that are set wet at high water, determines the storage capacity of an estuary during flood tide or the capacity of a river during extreme river discharges.

The crucial items in a wetting and drying algorithm are:

1. the way in which the water level and bottom depth are defined at velocity points,
2. the criterion for setting a velocity point wet or dry,
3. the way in which the bottom depth is defined in a water level point (determines retention volume).

Since the treatment of the $\xi$- and $\eta$-direction are analogous in the ADI-method of WAQUA, only the flooding and drying procedure in the $\xi$-direction is explained.
WAQUA is based on a staggered grid with the depth defined at the corner points of a control volume (C-grid). A convex or concave bottom profile can be represented within two grid cells. The total water depth at the velocity points is usually computed by averaging the water levels and depths:

\[ H_{m,n}^U = \frac{1}{2} (d_{m,n} + d_{m,n+1}) + \frac{1}{2} (\zeta_{m,n} + \zeta_{m+1,n}) \]  

(8.1.1)

The total water depth should at least be positive to guarantee a realistic discharge across a cell face.

In WAQUA a \( U \)-velocity point \((m,n)\) is taken out of the computation if the total water depth drops below half of a given threshold \( \delta \):

\[ H_{m,n}^U < \frac{1}{2} \delta \]  

(8.1.2a)

and is re-admitted to the computation if the total water depth arises above the threshold:

\[ H_{m,n}^U > \delta. \]  

(8.1.2b)

The drying threshold is given half the value of the wetting threshold to inhibit changes of state in two consecutive time steps ("flip-flop"), due to oscillations introduced by the algorithm itself.

The control volume is closed for transport at the cell face where a dry velocity point is located. In WAQUA the status (dry or wet) of a velocity point is stored in mask arrays. The mask arrays for the \( U \)-velocity and \( V \)-velocity points are KHU and KHV respectively. If the status of a velocity point changes e.g. from wet to dry, then the mask array is updated. The mask array KHU is defined as follows:

- KHU(m,n) = 0, permanently dry \( U \)-point
- KHU(m,n) = -1, temporarily dry \( U \)-point
- KHU(m,n) = 1, temporarily wet \( U \)-point

A control volume is excluded when all the four sides are inactive. The retention volume is the cell area times the difference between water level and the bottom depth at the cell centre. Since the bottom is defined in the vertices of a grid cell, a set of methods is available to compute the bottom depth at a water level point. The user may select a method at input. The most straightforward approach is averaging:

\[ d_{m,n}^c = \frac{1}{4} (d_{m,n} + d_{m-1,n} + d_{m,n-1} + d_{m-1,n-1}) \]  

(8.1.3)

For the combination of flow computations with transport of dissolved substances, the control volume/retention volume should be positive. In Figure 8.1 an example is shown in which the bottom depth in a water level point \((dp)\), determined on the basis of the average depth, is below the bottom, while some of the adjacent velocity points still have a positive flow through height.
Therefore in the iterative procedure for the coupled system of continuity equation and momentum equation, see Chapter 5, there is a drying check applied to both the velocity points and the water level points after each iteration. If the total water depth in a water level point is below half the threshold value,

$$H_{m,n}^c = d_{m,n}^c + \zeta_{m,n} < \frac{1}{2} \delta$$  \hspace{1cm} (8.1.4)

both adjacent velocity points \((m,n)\) and \((m+1,n)\) in the direction of the ADI-step, are taken out of the computation and the iteration is restarted. The velocity points in the \(\eta\)-direction are still open, because the discharges (fluxes) are at the previous time level. The discharges in the \(\eta\)-direction may still suck the water level below the bottom. Hence negative volumes may still occur in WAQUA. Such negative volumes are not allowed in case of on-line coupling with transport (e.g. salt) or off-line coupling with water quality models. In order to guarantee positive control volumes it is necessary to redesign the computational part of WAQUA.

The drying and flooding control in the velocity points (8.1.2) and in the water level points (8.1.4) are incorporated in the ADI-computational procedure of WAQUA as follows:
Stage 1:

First the momentum equation in the V-direction is solved. Before the system of equations is built along the η-grid lines there is a flooding check (8.1.2b) for the open boundary points and a drying check for the interior points (8.1.2a) in the ADI-direction.

Next the coupled system of water levels and U-velocities is solved. Before the system of equations is built along grid lines, there is a drying check (8.1.2a) and a flooding check (8.1.2b) in the ζ-direction at the U-velocity points. The system of equations is solved iteratively. During the iteration process there is a drying check at the velocity points (8.1.2a) and a drying check at the water level points (8.1.4). When drying occurs, the coefficients in the system of equations are updated and the iterative process is restarted.

In the transport equation, for a dry computational cell, the values of the constituent are frozen at the previous time level.

In Stage 2 of the ADI-method the directions are interchanged.

8.2 Description of alternative methods available in WAQUA

Water level at cell sides

In the neighbourhood of steep bottom gradients, use of the average water level to compute the total water depth at a velocity point, may lead to an inaccurate determination of the flow-through height, see Fig. 8.2. The velocity point is set dry too early. A large volume of water is left on the tidal flat, increasing artificially the storage capacity of the wet area. The local surface elevations are not predicted very well.

Figure 8.3 shows the situation of a river which overtops its bank. If we take the average water level to determine the total water depth at the crest, the velocity point remains dry. The water level will rise too much in the main channel of the river, leading to unrealistic water levels downstream. When the river run off increases, suddenly the flood plains are filled with water, generating a shock wave.

Stelling (1984) and Van der Molen (1997) used an upwind approach to determine the flow-through height. The upwind water level is used at velocity points which are wet. At dry cell boundaries, the maximum of the two surrounding water levels is taken. Recently (Van Kester et al., 1997) implemented a similar method in WAQUA. The flow-through height is determined using the following algorithm, see also Section 4.1:
Figure 8.2: Drying of a tidal flat. Flow-through height based on the average water level, see Eq. (8.1.1). Depth in cell centre based on maximum depth, see Eq. (8.2.3a).

Figure 8.3: Overtopping of a river bank. Flow-through height based on the average water level, see Eq. (8.1.1). Depth in cell centre based on maximum depth, see Eq. (8.2.3a).
\[
H_{m,n}^U = \begin{cases} 
\bar{d}^\eta + \zeta_{m,n} & \text{if } U_{m,n} > 0 \\
\bar{d}^\eta + \zeta_{m+1,n} & \text{if } U_{m,n} < 0 \\
\bar{d}^\eta + \max(\zeta_{m,n}, \zeta_{m-1,n}) & \text{if } U_{m,n} = 0 
\end{cases}
\] (8.2.1)

Figure 8.4: Drying of a tidal flat.
Flow-through height determined by flow direction, see Eq. (8.2.1).
Depth in cell centre based on maximum depth, see Eq. (8.2.3a).

Figure 8.4 shows that in the case of ebb tide, the upwind approach to determine the flow-through height will keep the velocity point wet until the tidal flat becomes empty. Similarly, Figure 8.5 shows that by the new approach the river will overtop the dike at the correct moment.
Bottom depth at water level points

The initial water level at a dry cell is determined by the depth at the water level point:

\[ \zeta_{m,n} = -d^e_{m,n} + \delta \]  

(8.2.2)

In cases of steep bottom slopes, the average approach for the determination of the bottom depth in a water level point may lead to flooding of one of the velocity points (8.1.2) and afterwards drying in the first iteration by (8.1.4). This "flip-flop"-effect may deteriorate the speed of the computation. WAQUA offers two other ways to determine the depth in a water level point:

\[ d^e_{m,n} = \max(\bar{d}^e_{m,n}, \bar{d}^e_{m,n-1}, \bar{d}^n_{m,n}, \bar{d}^n_{m-1,n}) \]  

(8.2.3a)

\[ d^e_{m,n} = \min(\bar{d}^e_{m,n}, \bar{d}^e_{m,n-1}, \bar{d}^n_{m,n}, \bar{d}^n_{m-1,n}) \]  

(8.2.3b)

For method (8.2.3a) the check in the water level points is less restrictive. Method (8.2.3b) gives a more accurate tidal propagation.

Without coupling of transport, it is possible to leave out the extra check in the water level points, because negative retention volumes are allowed then. For the initialisation of the water levels, the average depth is used.
8.3 *Flooding and drying at weir point*

In WAQUA, the user may define in velocity points so-called weirs. Weirs are hydraulic structures causing energy losses. The height of the edge (HKRU) of the weir is taken into account in the drying and flooding algorithm. Drying:

\[
H_{m,n}^U < \frac{1}{2} \delta \wedge \max(\zeta_{m-1,n}, \zeta_{m,n}) + HKRU_{m,n} < \frac{1}{2} \delta \quad (8.3.1a)
\]

and flooding:

\[
H_{m,n}^U > \delta \wedge \max(\zeta_{m-1,n}, \zeta_{m,n}) + HKRU_{m,n} > \delta \quad (8.3.1b)
\]
9 Recommendations

In November 1997, Rijkswaterstaat/RIKZ commissioned WL | delft hydraulics to produce a technical documentation of the WAQUA system (contract RKZ-503) In order to achieve this goal, a thorough study of the present formulations and implementations used in WAQUA was required. During this inventory a number of shortcomings has been detected. This has led to recommendations to improve the WAQUA system. These recommendations involve numerical and maintenance aspects. In this chapter we will give an overview of the recommendations.

Improvement of drying and flooding procedure

The stage in which the continuity and the momentum equation are coupled and solved implicitly, does not start with a check on drying (see Chapter 8 and the subroutines WASSUC/WASSUV). In the first iteration of the solution process this may yield negative total water depths and consequently unrealistic coefficients in the system of equations. This may even lead to a division by zero for the computation of the bottom friction. After each iteration a check on drying is carried out. In case of drying, the coefficients will be set to zero and the iterative process will be restarted. We propose to implement a check on drying before the system of equations is built up, see also (Van Kester et al., 1997).

The drying check in WAQUA in the subroutine WASUXC/WASUXD is superfluous and can be removed.

The present implementation of the ADI method in WAQUA may generate negative control volumes. This is due to the fact that velocity points can be set dry in only one direction. The discharges in the other direction may still suck the water level below the bottom. Such negative volumes are not allowed in case of on-line coupling with transport (e.g. salt) or off-line coupling with water quality models.

In case of a negative control volume, a robust drying procedure should be able to take out of the computation a whole computational cell. This requires that also the flow in the direction perpendicular to the row or column that is computed, should be blocked. Then, the previous row (or column) has to be recomputed. Owing to the present recursion in the ADI method of WAQUA (computations are carried out row by row) this would require a redesign of the present WAQUA code.

Improvement of space discretization of the horizontal advective terms in the transport equation

For the advective terms in the transport equation a central difference scheme is applied, see Chapter 4. On a completely smooth grid, this discretization is second order accurate and may generate wiggles in regions with steep gradients. We therefore propose to implement in WAQUA the higher order scheme that is used in TRIWAQ. For a description of this scheme we refer to (Zijlema, 1998).
If this higher order scheme would be used in WAQUA, then the solution of a heptadiagonal system of equations is required. In WAQUA this can be performed by a direct method. We remark that in TRIWAQ the implicit treatment of the vertical transport terms prohibits a direct solver. Therefore an iterative method is applied in TRIWAQ.

To prevent wiggles upstream of a discharge point, the discretization of the advective terms near a discharge point should be lower order upstream.

**Maintenance of WAQUA**

From maintenance point of view we propose to restructure the WAQUA routines. WAQUA was developed in the days when the core memory of the computers was relatively small. It was very important to store information in an economic way. This has led to a very complex (but also very efficient) implementation. However, from the programmers point of view it is very difficult to update or to extend the routines. This was one of the reasons why the WAQUA subroutines that contain the integration of the ADI method have not been changed in the project in which the WAQUA system was redesigned according to SIMONA (in 1992). Thus, since the work of Stelling in 1984 the computational part of WAQUA has hardly changed.

With respect to maintenance, it will be worthwhile to separate the built up of the systems of equations from the applied solution methods. Such an approach has already been followed in TRIWAQ. We remark that such a reprogramming will decrease the performance of the WAQUA code.

Furthermore, we propose to introduce arrays that are able to identify hydraulic structures such as barriers and weirs. This allows a more elegant implementation of these special points. Moreover, identification arrays may be applied for other reasons as well. For example, these arrays may be used to distinguish different approximations for the advective or viscosity terms.

**Adaptation of boundary conditions**

At an open boundary, in the momentum equation for the tangential velocity the cross advection term is neglected at inflow. For a steady state simulation this may lead to an ill-posed problem. The tangential velocity $V$ along the open boundary is undetermined and may oscillate in time. Therefore, we recommend to prescribe at an open boundary the tangential velocity and to take the cross advection term into account at inflow.

The discharge boundary condition is specified outside the iteration for the continuity equation. This yields a mass closure error. The implementation of discharge boundaries can be improved in such a way that no mass closure error occurs.

For discharge boundaries in shallow areas the present implementation requires a local Courant number for advection smaller than one in order to guarantee flooding at the right moment.
The present implementation of incoming Riemann invariant is inconsistent. The Riemann invariant is non-linear and linearized around the old time level, whereas boundary condition (Riemann invariant) specified by the user is based on a different linearization. For a detailed description we refer to Chapter 6.

The implementation of the momentum equation in the first velocity point near a water level boundary can be improved by adding the wind stress, bottom stress, baroclinic pressure gradient and atmospheric pressure gradient.

**Hydraulic structures**

The implementation in WAQUA of hydraulic structures such as barriers and weirs is very complex and may be simplified (Van Kester et al, 1997).

If possible, the difference equations for structures should be computed in separate routines.

**Simplification of the viscosity term in case of curvilinear coordinates**

In the expressions for the viscosity term, in case of curvilinear coordinates, cross terms are introduced by the transformation, which are not present on a rectangular grid. It should be investigated whether the discretization of the viscosity term may be simplified by neglecting the curvature of the grid. In the latter case the cross terms will vanish.

**Introduction of a space varying horizontal viscosity coefficient**

The present implementation in WAQUA assumes a uniform viscosity coefficient. For a curvilinear model with larger differences in grid size this is an inaccurate way for modelling of subgrid processes. We suggest the implementation of a simple horizontal subgrid model, for example the Smagorinsky model (Smagorinsky, 1963).

**Model characteristics**

The performance of a numerical model is influenced by the choice of the numerical parameters time step and grid size. The choice of these parameters is determined by model characteristics such as Courant number for wave propagation, advection and dispersion. It is recommended that this information is computed by WAQUA and is made available to the user (both in preprocessor and processor).

**FORTRAN 90**

FORTRAN 90 is now generally available. If the WAQUA code will be rewritten, then it is recommended to use FORTRAN 90.
10 References


Lorentz H.A. (1926), "Verslag van de staatscommissie met als opdracht te onderzoeken in hoeverre, als gevolg van de afsluiting van de Zuiderzee (...) te verwachten is dat tijdens storm hoogere waterstanden en een grootere golfoploop (...) zullen voorkomen (...)", Algemeene Landsdrukkerij, The Hague (in Dutch).


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A Reference structures

In WAQUA the simulation within one time step is carried out by the subroutine WASSIM. This subroutine builds and solves the water movement and advection-diffusion equations for arbitrary consistuents. The structure of this subroutine and its main under subroutines is given in the following subsections. The subroutine is called at each time step.

A.0.1 Reference structure of WASSIM

wassim General WAQUA/TRIWAQ simulation
wasspu Compute flow (first stage)
wastru Compute constituents, if appropriate (first stage)
wasspv Compute flow (second stage)
wastrv Compute constituents, if appropriate (second stage)
wasmag Write flow-related data (map) to SDS

A.0.2 Reference structure of WASSPU and WASSPV

In each half time step the matrices and right-hand side vectors of the corresponding water movement equations are built. Subsequently, the resulting systems of equations are solved. For the building and solving of each half time step two subroutines WASSPU and WASSPV are used, which are similar. In WAQUA the structure of subroutine WASSPU for an application with rectangular co-ordinates reads:

dens Compute water density
wascsc Compute correction for Chézy coefficient, if appropriate
wasuxd Build and solve V-momentum equation
wasubr Compute barrier momentum equation, if appropriate
wassuv Compute water level and U-velocity
wassbr Compute barrier momentum equation, if appropriate
Similarly, in case of curvilinear co-ordinates we have

\begin{align*}
\text{dens} & \quad \text{Compute water density} \\
\text{wascsc} & \quad \text{Compute correction for Chézy coefficient, if appropriate} \\
\text{wasuxc} & \quad \text{Build and solve } V\text{-momentum equation} \\
\text{wasubc} & \quad \text{Compute barrier momentum equation, if appropriate} \\
\text{wassuc} & \quad \text{Compute water level and } U\text{-velocity} \\
\text{wassbc} & \quad \text{Compute barrier momentum equation, if appropriate}
\end{align*}

\subsection*{A.0.3 Reference structure of WASTRU and WASTRV}

In each half time step the matrix and right-hand side vector of the transport equation of an arbitrary constituent is built. Subsequently, the resulting system of equations is solved. For the building and solving of each half time step two subroutines WASTRU and WASTRV are used, which are similar. In WAQUA the structure of subroutine WASTRU is very simple:

\begin{align*}
\text{wasdfu/wasdfv} & \quad \text{Build and solve the transport equation}
\end{align*}

In case of rectangular co-ordinates subroutine WASDFU is applied, whereas WASDFV is used for curvilinear models.