MIKE Powered by DHI

MIKE 21 & MIKE 3 Flow Model

CWC Schemes

Scientific Documentation

DHI headquarters
Agern Allé 5
DK-2970 Hørsholm
Denmark

+45 4516 9200 Telephone
+45 4516 9333 Support
+45 4516 9292 Telefax

mike@dhigroup.com
www.mikepoweredbydhi.com

PLEASE NOTE

CONTENTS

MIKE 21 & MIKE 3 Flow Model
CWC Schemes
Scientific Documentation

1 Introduction

This document deals with some of the numerical aspects of the advection-dispersion (AD) schemes, implemented into the Flow Models of the MIKE 3 and MIKE 21 modelling systems.

For an in-depth description of the equations and numerical formulation used in the hydrodynamic (HD) modules of MIKE 3 and MIKE 21, the reader is referred to the respective Scientific Documentations which are assumed known in the following.

Aspects such as mass conservation, consistency with continuity, stability, source/sink terms, and diffusive terms for AD schemes are treated in the present document. For a description of the AD schemes used in MIKE 21 and MIKE 3 Flow Models such as the QUICKEST scheme, see e.g. the papers by Vested *et al.* (1992) and Ekebjærg and Justesen (1991).

The mass conservation property is widely recognised as being important in flow modelling. The concept of “consistency with continuity” (or CWC), on the other hand, is often neglected in the literature on advection modelling. CWC is a simple and very important concept. Putting details and mathematical rigor aside, a CWC scheme is one in which the discretised scalar transport equation is identical to the discretised continuity equation (i.e. the mass equation of the HD solver) when the scalar concentration is 1 everywhere. Thus, in a CWC scheme the mass flux through each flux face of a computational grid cell that occurs between two time steps is identical to the volume flux. The CWC property is clearly physically correct and of great practical importance. For more details on the CWC property, see e.g. the papers by Gross *et al.* listed in the References section.

Within the scope of the present document, the hydrostatic (HS) version of MIKE 3 is much similar to MIKE 21, the main difference being the absence of vertical terms in the continuity and AD transport equations in MIKE 21. Therefore, only the more general MIKE 3 HS is treated herein and the reader may easily reduce expressions to the MIKE 21 case.

As will be evident from the following, the classical, non-hydrostatic version of MIKE 3 cannot fully comply with the CWC concept within the framework of this document.

2 CWC Scheme for MIKE 3 HS

The layer-integrated advective transport equation for a substance *c* reads:

$$\frac{\partial hc}{\partial t}+\frac{\partial huc}{\partial x}+\frac{\partial hvc}{\partial y}+(wc)^{+}-(wc)^{-}=0 \tag{2.1}$$

neglecting source/sink terms. In Eq. (2.1), *h* is the local layer thickness. Introducing layer-averaged fluxes $u_f = hu$ and $v_f = hv$ and time-centring as in the HD at $n+1/2$, we get:

$$\begin{aligned}\frac{1}{\Delta t}\left[(hc)^{n+1}-(hc)^{n}\right]_{j,k,l} = & \\ & -\frac{1}{\Delta x}\left[c_E\left(u_f^{ADC}\right)_j - c_W\left(u_f^{ADC}\right)_{j-1}\right]_{k,l} \\ & -\frac{1}{\Delta y}\left[c_N\left(v_f^{ADC}\right)_k - c_S\left(v_f^{ADC}\right)_{k-1}\right]_{j,l} \\ & -\left[c_U\left(w^{ADC}\right)_l - c_D\left(w^{ADC}\right)_{l-1}\right]_{j,k}\end{aligned} \tag{2.2}$$

where c_E, c_W, c_N, c_S, c_U and c_D are the concentrations at the east, west, north, south, up and down faces, respectively, of the grid cell, and u_f^{ADC}, v_f^{ADC} and w^{ADC} are the AD-centred fluxes/velocities given as:

$$\begin{aligned} u_f^{ADC} &= \frac{1}{2}\left(u_f^{n}+u_f^{n+1}\right) \\ v_f^{ADC} &= \frac{1}{4}\left(v_f^{n-1/2}+2v_f^{n+1/2}+v_f^{n+3/2}\right) \\ w^{ADC} &= \frac{1}{2}\left(w^{n+1/4}+w^{n+3/4}\right)\end{aligned} \tag{2.3}$$

Eq. (2.2) is consistent with the continuity equation of MIKE 3 HS, i.e. it is a CWC scheme. This is easily seen by setting $c=1$ in Eq. (2.2) whereby the HS continuity equation is exactly obtained. Any reasonable scheme (e.g. QUICKEST or UPWIND) may be applied to obtain the face-centred concentrations.

3 Partial CWC Scheme for MIKE 3 ACM

The time staggering of the non-hydrostatic version of MIKE 3 (in which the artificial compressibility method, ACM, is applied) prescribes that pressure and elevation through the discretised continuity equation is advanced by two thirds of a time step during each of the three sweeps. For the x-sweep in the top layer this amounts to

$$\begin{aligned}
&\frac{3}{2\Delta t}\left[\eta^{n+1/2}-\frac{1}{3}\left(\eta^{n-1/2}+\eta^{n-1/6}+\eta^{n+1/6}\right)\right]_{j,k,l} \\
&+\frac{1}{\Delta x}\left[\frac{1}{2}\left(u_f^n+u_f^{n+1}\right)_j-\frac{1}{2}\left(u_f^n+u_f^{n+1}\right)_{j-1}\right]_{k,l} \\
&+\frac{1}{\Delta y}\left[\frac{1}{2}\left(v_f^{n-2/3}+v_f^{n+1/3}\right)_k-\frac{1}{2}\left(v_f^{n-2/3}+v_f^{n+1/3}\right)_{k-1}\right]_{j,l} \\
&+\left[-\frac{1}{2}\left(w^{n-1/3}+w^{n+2/3}\right)_{l-1}\right]_{j,k} \qquad = \qquad 0
\end{aligned} \tag{3.1}$$

neglecting source/sink terms, and where η is the surface elevation. Similar expressions can be obtained for the y- and the z-sweep. With H_0 denoting the thickness (with sign and constant in time) of the top layer grid cell up to the reference level, the actual layer thickness of the top layer is $h=\eta+H_0$, and the equation for the three sweeps, each weighted by 1/3, may be added to

$$\begin{aligned}
&\frac{1}{\Delta t}\left[\frac{1}{6}\left(h^{n+1/2}+2h^{n+5/6}+3h^{n+7/6}\right)-\frac{1}{6}\left(h^{n-1/2}+2h^{n-1/6}+3h^{n+1/6}\right)\right]_{j,k,l} \\
&+\frac{1}{\Delta x}\left[\frac{1}{2}\left(u_f^n+u_f^{n+1}\right)_j-\frac{1}{2}\left(u_f^n+u_f^{n+1}\right)_{j-1}\right]_{k,l} \\
&+\frac{1}{\Delta y}\left[\frac{1}{6}\left(v_f^{n-2/3}+3v_f^{n+1/3}+2v_f^{n+4/3}\right)_k-\frac{1}{6}\left(v_f^{n-2/3}+3v_f^{n+1/3}+2v_f^{n+4/3}\right)_{k-1}\right]_{j,l} \\
&+\left[-\frac{1}{6}\left(2w^{n-1/3}+3w^{n+2/3}+w^{n+5/3}\right)_{l-1}\right]_{j,k} \qquad = \qquad 0
\end{aligned} \tag{3.2}$$

Thus, with

$$\begin{aligned}
h^{n+17/18} &= \frac{1}{6}\left(h^{n+1/2}+2h^{n+5/6}+3h^{n+7/6}\right) \\
h^{n-1/18} &= \frac{1}{6}\left(h^{n-1/2}+2h^{n-1/6}+3h^{n+1/6}\right)
\end{aligned} \tag{3.3}$$

centred at n+17/18 and at n+1/18, respectively, and with

$$
\begin{aligned}
u_f^{ADC} &= \frac{1}{2}\left(u_f^{n} + u_f^{n+1}\right) \\
v_f^{ADC} &= \frac{1}{6}\left(v_f^{n-2/3} + 3v_f^{n+1/3} + 2v_f^{n+4/3}\right) \\
w^{ADC} &= \frac{1}{6}\left(2w^{n-1/3} + 3w^{n+2/3} + w^{n+5/3}\right)
\end{aligned}
\tag{3.4}
$$

which are all centred at n+1/2, the CWC scheme for the top layer of MIKE 3 ACM, written in a form corresponding to Eq. (2.2), becomes

$$
\begin{aligned}
\frac{1}{\Delta t}\left[(hc)^{n+17/18} - (hc)^{n-1/18}\right]_{j,k,l} = \\
-\frac{1}{\Delta x}\left[c_E\left(u_f^{ADC}\right)_j - c_W\left(u_f^{ADC}\right)_{j-1}\right]_{k,l} \\
-\frac{1}{\Delta y}\left[c_N\left(v_f^{ADC}\right)_k - c_S\left(v_f^{ADC}\right)_{k-1}\right]_{j,l} \\
-\left[c_U\left(w^{ADC}\right)_l - c_D\left(w^{ADC}\right)_{l-1}\right]_{j,k}
\end{aligned}
\tag{3.5}
$$

It is seen that the concentration *c* is centred backwards by 1/18 of a time step compared to Eq. (2.2). This holds generally for all layers of MIKE 3 ACM.

For non-surface layers of thickness Δz, the corresponding discrete continuity equation for the x-sweep reads

$$
\begin{aligned}
&\frac{3}{2\Delta t\,\rho_{j,k,l} C_S^2}\left[P^{n+1/2} - \frac{1}{3}\left(P^{n-1/2} + P^{n-1/6} + P^{n+1/6}\right)\right]_{j,k,l} \\
&+\frac{1}{\Delta x}\left[\frac{1}{2}\left(u^{n} + u^{n+1}\right)_j - \frac{1}{2}\left(u^{n} + u^{n+1}\right)_{j-1}\right]_{k,l} \\
&+\frac{1}{\Delta y}\left[\frac{1}{2}\left(v^{n-2/3} + v^{n+1/3}\right)_k - \frac{1}{2}\left(v^{n-2/3} + v^{n+1/3}\right)_{k-1}\right]_{j,l} \\
&+\frac{1}{\Delta z}\left[\frac{1}{2}\left(w^{n-1/3} + w^{n+2/3}\right)_l - \frac{1}{2}\left(w^{n-1/3} + w^{n+2/3}\right)_{l-1}\right]_{j,k} = 0
\end{aligned}
\tag{3.6}
$$

again neglecting source/sink terms. The variable *P* denotes pressure, and ρ and C_S are the local density and speed of sound in the water, respectively. (With spatially varying, but constant in time, layer thickness, i.e. for grid cells just above the seabed, the bottom fitted approach is used and the above equation is slightly modified). For the y- and the z-sweep similar expressions can be written, and if all three equations are weighted by a factor of 1/3 and added, the following is obtained

$$\frac{1}{\Delta t\,\rho_{j,k,l}\,C_S^2}\left[\frac{1}{6}\left(P^{n+1/2}+2P^{n+5/6}+3P^{n+7/6}\right)-\frac{1}{6}\left(P^{n-1/2}+2P^{n-1/6}+3P^{n+1/6}\right)\right]_{j,k,l}$$

$$+\quad \langle velocity\ terms\rangle \quad = \quad 0 \tag{3.7}$$

On the other hand, the layer-integrated, discrete advective transport scheme for the same layers is

$$\begin{aligned}\frac{1}{\Delta t}\left[h\left(c^{n+17/18}-c^{n-1/18}\right)\right]_{j,k,l} = &\\ & -\frac{1}{\Delta x}\left[c_E\left(u_f^{ADC}\right)_j - c_W\left(u_f^{ADC}\right)_{j-1}\right]_{k,l}\\ & -\frac{1}{\Delta y}\left[c_N\left(v_f^{ADC}\right)_k - c_S\left(v_f^{ADC}\right)_{k-1}\right]_{j,l}\\ & -\left[c_U\left(w^{ADC}\right)_l - c_D\left(w^{ADC}\right)_{l-1}\right]_{j,k}\end{aligned} \tag{3.8}$$

It is clear that in general this scheme is not fully CWC for MIKE 3 ACM, since with $c=1$ it does not reduce to the continuity equation applied in the HD solver: The pressure time derivative is absent. This can also be formulated as

$$\begin{aligned}&\frac{\Delta t}{\Delta x}\left[\left(u_f^{ADC}\right)_j - \left(u_f^{ADC}\right)_{j-1}\right]_{k,l}\\ +&\frac{\Delta t}{\Delta y}\left[\left(v_f^{ADC}\right)_k - \left(v_f^{ADC}\right)_{k-1}\right]_{j,l}\\ +&\Delta t\left[\left(w^{ADC}\right)_l - \left(w^{ADC}\right)_{l-1}\right]_{j,k} \quad \neq \quad 0\end{aligned} \tag{3.9}$$

i.e. that the layer-integrated, discrete divergence of the ADC does not vanish, which again means that the fluid is compressible.

Remarks:

To be able to use the same notation for all models in the following, superscript *“new”* will denote the new time step, which is *n+1* for MIKE 3 HS and for MIKE 21, while it is *n+17/18* for MIKE 3 ACM. In the same way, *“old”* denotes the old time step, i.e. *n* for MIKE 3 HS and for MIKE 21 and *n-1/18* for MIKE 3 ACM.

4 Stability of Advection Scheme

Stability of the simple scheme

$$\frac{1}{\Delta t}\left[S^{new} - S^{old}\right]_j = -\frac{u}{\Delta x}\left[S_j^{new} - S_{j-1}^{old}\right] \tag{4.1}$$

is obtained if the CFL criterion is fulfilled:

$$|u|\frac{\Delta t}{\Delta x} < 1 \tag{4.2}$$

Therefore, we expect that the stability criterion for Eq. (2.2) is like

$$|u_f|\frac{\Delta t}{\Delta x} + |v_f|\frac{\Delta t}{\Delta y} < h \tag{4.3}$$

where we have neglected the vertical velocity terms.

Note: Since we use a staggered grid, division by *h* in Eq. (4.3) is **not** in general identical to the more well-known restriction expressed in velocities

$$|u|\frac{\Delta t}{\Delta x} + |v|\frac{\Delta t}{\Delta y} < 1 \tag{4.4}$$

In models with large gradients in *h*, Eq. (4.3) is found to be much more restrictive than Eq. (4.4).

Tests have shown that Eq. (4.3) *may* occasionally be violated in a few isolated grid points and the model may still perform well as long as Eq. (4.4) is fulfilled everywhere.

5 Mass Correction

Even though Eq. (2.2) is a CWC scheme, practical cases can be found that do not fully preserve the mass through Eq. (2.2) as it is. These cases include applications with extensive flooding and drying.

We introduce a mass-correction term into the equation:

$$\frac{\partial hc}{\partial t} + \nabla \cdot \left(\bar{u}_f c \right) + (wc)^+ - (wc)^- = \varepsilon c^* \tag{5.1}$$

where c^* is a correction concentration to be determined below, and

$$\varepsilon = \frac{\partial h}{\partial t} + \nabla \cdot \bar{u}_f + w^+ - w^- \tag{5.2}$$

Usually $\varepsilon = 0$ due to the continuity equation, but the discrete version may differ from zero near e.g. flooded/dried points.

Different implementations of c^* have been analysed and tested. Best results are obtained if c^* is introduced as

$$c^* = \frac{1}{2}\left(c^{old} + c^{new} \right) \tag{5.3}$$

whereby Eq. (2.2) is replaced by

$$\left(h^{new} - \frac{1}{2}\nabla^{ADC} \right) c^{new} = \left(h^{old} + \frac{1}{2}\nabla^{ADC} \right) c^{old} + \Delta t \, RHS_{(2)} \tag{5.4}$$

where $RHS_{(2)}$ is short for the right-hand-side of Eq. (2.2)and

$$\begin{aligned} \nabla^{ADC} = \; & h^{new} - h^{old} \\ & + \frac{\Delta t}{\Delta x}\left[\left(u_f^{ADC} \right)_j - \left(u_f^{ADC} \right)_{j-1} \right]_{k,l} \\ & + \frac{\Delta t}{\Delta y}\left[\left(v_f^{ADC} \right)_k - \left(v_f^{ADC} \right)_{k-1} \right]_{j,l} \\ & + \Delta t\left[\left(w^{ADC} \right)_l - \left(w^{ADC} \right)_{l-1} \right]_{j,k} \end{aligned} \tag{5.5}$$

6 Source/Sink Terms

The layer-integrated advective transport equation for a substance *c* was stated in Eq. (2.1), and including source/sink terms it reads:

$$\frac{\partial hc}{\partial t} + \nabla \cdot \left(\bar{u}_f c\right) + \left(wc\right)^{+} - \left(wc\right)^{-} = S_{AD} \tag{6.1}$$

$$\begin{aligned} S_{AD} = & \, Pc_P - Ec_E + \frac{Q_H}{\rho C_{HW}} \\ & + \sum_{i_S=1}^{N_S} \delta\left(\bar{X} - \bar{X}_{s,i_S}\right) c_{s,i_S} \, Q_{s,i_S} \\ & + \sum_{i_D=1}^{N_D} \delta\left(\bar{X} - \bar{X}_{D,i_D}\right) D_{i_D} \end{aligned} \tag{6.2}$$

where

δ :	delta function of horizontal coordinates, m^{-2}
$\bar{X}_{s,i_S}$:	horizontal coordinate of point source/sink No. i_S
c_{s,i_S} :	concentration of point source/sink No. i_S , [c] e.g. mg/l
Q_{s,i_S} :	discharge at point source/sink No. i_S , m^3/s
P:	precipitation rate at surface, m/s
c_P:	concentration in rain at surface, [c]
E:	evaporation rate at surface, m/s
c_E:	evaporation concentration at surface, [c]
Q_H:	heat flux from heat exchange module (if *c* is temperature), W/m^2
ρ :	density of water, kg/m^3
C_{HW}:	specific heat of water, 4186 J/(kg ^oK)
D_{i_D} :	dry deposition rate, $[c]m^3/s$
$\bar{X}_{D,i_D}$:	horizontal coordinate of dry contributor No. i_D

At point sources:

c_S is source outlet concentration.

At point sinks:

c_S is sink concentration, numerically implemented as the concentration, c^{old}, of the ambient water at the sink point.

At connected point sources/sinks pairs:

$c_{Source} = c_{Sink} + c_{Excess}$ where c_{Excess} is the excess concentration and
$c_{Sink} = c^{old}(j_{Sink}, k_{Sink}, l_{Sink})$
$Q_{Sink} = - Q_{Source}$

Dry deposition:

Dry deposition is as a source term in the AD without a corresponding HD term. We distinguish between two different types of dry deposition

- Surface deposition, e.g. pollution from air
- Seabed deposition, e.g. leaching from highly contaminated soil

Evaporation/precipitation:

Specification c_P and c_E requires specification of what kind of component that is considered:

- If c is temperature, then often c_P is the air temperature and c_E is the temperature of the ambient water, but other formulations are possible, e.g. as obtained through the latent heat flux as calculated in the heat exchange module

- If c is salinity, c_P is zero and so is c_E

- For other concentrations, c_P should be user-specified (e.g. pollutant from rain) and while c_E is zero

Mass correction in presence of sources:

The layer-integrated continuity equation for MIKE 3 HS with source/sink terms reads:

$$\frac{\partial h}{\partial t} + \nabla \cdot \bar{u}_f + w^+ - w^- = S_{HD} \tag{6.3}$$

$$S_{HD} = P - E + \sum_{i_S=1}^{N_S} \delta\left(\overline{X} - \overline{X}_{s,i_S}\right) Q_{s,i_S} \tag{6.4}$$

Given Eqs. (6.1), (6.3) and (5.1), the mass-correction in presence of sources/sinks is defined as

$$\varepsilon = \frac{\partial h}{\partial t} + \nabla \cdot \bar{u}_f + w^+ - w^- - S_{HD} \tag{6.5}$$

and as in Eq.(5.4) we may write

$$\left(h^{new} - \frac{1}{2}\nabla^{ADC}\right)c^{new} = \left(h^{old} + \frac{1}{2}\nabla^{ADC}\right)c^{old} + \Delta t\left(RHS_{(2)} + \tilde{S}_{AD}\right) \tag{6.6}$$

with

$$\begin{aligned}\nabla^{ADC} = \quad & h^{new} - h^{old} \\ & + \frac{\Delta t}{\Delta x}\left[\left(u_f^{ADC}\right)_j - \left(u_f^{ADC}\right)_{j-1}\right]_{k,l} \\ & + \frac{\Delta t}{\Delta y}\left[\left(v_f^{ADC}\right)_k - \left(v_f^{ADC}\right)_{k-1}\right]_{j,l} \\ & + \Delta t\left[\left(w^{ADC}\right)_l - \left(w^{ADC}\right)_{l-1}\right]_{j,k} \\ & - \Delta t \tilde{S}_{HD}\end{aligned} \tag{6.7}$$

and where $\tilde{S}_{HD}$ and $\tilde{S}_{AD}$ denote the discrete versions of the source terms for the HD and the AD, respectively. $\tilde{S}_{HD}$ and $\tilde{S}_{AD}$ are expressed as

$$\tilde{S}_{HD} = \Delta t(P - E) + \frac{\Delta t}{\Delta x \Delta y}\sum_{i_S=1}^{N_S} Q_{s,i_S} \tag{6.8}$$

and

$$\tilde{S}_{AD} = \Delta t(Pc_P - Ec_E) + \frac{\Delta t Q_H}{\rho C_{HW}} + \frac{\Delta t}{\Delta x \Delta y}\sum_{i_S=1}^{N_S} c_{s,i_S} Q_{s,i_S} + \frac{\Delta t}{\Delta x \Delta y}\sum_{i_D=1}^{N_D} D_{i_D} \tag{6.9}$$

7 Diffusive Terms

The layer-integrated diffusive transport equation for a substance *c* reads:

$$\frac{\partial hc}{\partial t} = \int_{h^-}^{h^+} \left[\frac{\partial}{\partial x}\left(D_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial c}{\partial z} \right) \right] dz \tag{7.1}$$

with

$$h = h^+ - h^- \tag{7.2}$$

Formally, we have for the x-term

$$\int_{h^-}^{h^+} \frac{\partial}{\partial x}\left(D_x \frac{\partial c}{\partial x} \right) dz = \frac{\partial}{\partial x}\left(hD_x \frac{\partial c}{\partial x} \right) - \frac{\partial h^+}{\partial x}\left(D_x \frac{\partial c}{\partial x} \right)^+ + \frac{\partial h^-}{\partial x}\left(D_x \frac{\partial c}{\partial x} \right)^- \tag{7.3}$$

with a corresponding expression for the y-term, and for the z-term

$$\int_{h^-}^{h^+} \frac{\partial}{\partial z}\left(D_z \frac{\partial c}{\partial z} \right) dz = \left(D_z \frac{\partial c}{\partial z} \right)^+ - \left(D_z \frac{\partial c}{\partial z} \right)^- \tag{7.4}$$

For internal points, the last two terms in the x- and y-expressions are zero, but generally not at surface and bottom layers. We will ignore these terms anyway, thus assuming the layer-integrated diffusive transport equation to be

$$\frac{\partial hc}{\partial t} = \frac{\partial}{\partial x}\left(hD_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y}\left(hD_y \frac{\partial c}{\partial y} \right) + \left(D_z \frac{\partial c}{\partial z} \right)^+ - \left(D_z \frac{\partial c}{\partial z} \right)^- \tag{7.5}$$

In discrete form the horizontal diffusive transport is

$$hD_x \left. \frac{\partial c}{\partial x} \right|_j = \min(h_{j+1}, h_j)\, D_{xj} \frac{c_{j+1} - c_j}{\Delta x} \tag{7.6}$$

Different implementations have been analysed and tested, but the one described above with $h = \min(h_{j+1}, h_j)$ is the only one found satisfactory stable in situations with large layer gradients.

Stability considerations:

When implemented in an explicit scheme the stability criterion for the diffusive terms alone is

$$\Delta t \left(\frac{D_x}{\Delta x^2} + \frac{D_y}{\Delta y^2} + \frac{D_z}{\Delta z^2} \right) < \frac{1}{2} \tag{7.7}$$

This seldom imposes any severe restrictions on the horizontal terms, but often the above criterion is potentially violated due to the vertical term: Typically, Δz is relatively small implying that the time step size and/or the vertical diffusion coefficient should be unacceptably small. Cases where high vertical diffusion coefficients are essential include parameterisation of deep convection and heavy cooling/heating of the surface through heat exchange with the atmosphere, see e.g. Vested *et al*. (1998).

Therefore, the vertical diffusion terms may optionally be solved through an implicit scheme. With a combination of an explicit scheme for the horizontal terms and an implicit scheme for the vertical term, the above-mentioned stability criterion is replaced by

$$\Delta t\left(\frac{D_x}{\Delta x^2}+\frac{D_y}{\Delta y^2}\right) < \frac{1}{2}$$

$$\Delta t\frac{D_z}{\Delta z^2} < 10 \qquad (7.8)$$

The later is a recommendation for maintaining satisfactory accuracy; the implicit scheme is stable beyond that limit.

8 Comments on Implementation

To summarise, the flow of computations in the scheme laid out on the preceding pages, including CWC, mass-correction, source/sink terms and diffusive terms, goes like:

1. The ADC fluxes/velocities and layer thicknesses are obtained from the HD solver.

2. The correction term $\nabla^{ADC} = \Delta t\,\varepsilon$ with possible HD source/sink and evaporation/precipitation terms is calculated and stored.

3. AD source/sink terms $\Delta t\,S$ without evaporation/precipitation terms and heat exchange terms are calculated and stored.

4. The AD solver is applied and (hc) with correction term and possible evaporation/precipitation/deposition terms is updated and stored:

$$
\begin{aligned}
(hc)^{**} \quad &= \quad (hc)^{old} \\
&- \Delta t\left[\nabla\cdot\left(c^{old}\,\bar{u}_f^{ADC}\right) - \nabla\cdot\left(h^{old}\,\overline{\overline{D}}\,\nabla c^{old}\right) - Pc_P + Ec_E - \frac{\varepsilon c^{old}}{2}\right]
\end{aligned}
$$

where c^{old} in the advective term should be replaced by appropriate face-centred values obtained at the same time step, i.e. at *n* for MIKE 3 HS and MIKE 21 and at *n-1/18* for MIKE 3 ACM. The diffusive term includes only terms calculated by the explicit scheme.

5. Source/sink terms are added:

$$
(hc)^{***} = (hc)^{**} + \Delta t S
$$

6. The new concentration is then found from

$$
c^{new} = \frac{(hc)^{***}}{h^{new} - \varepsilon/2}
$$

7. If *c* is temperature, then possible heat exchange with the atmosphere is treated.

8. If implicit vertical diffusion scheme is selected, then it is applied as the last step (MIKE 3 only).

This scheme can be implemented directly as described above into MIKE 3 and MIKE 21 with any (reasonable) AD scheme:

- with different HD-engines, different ADC velocities/fluxes and elevations are required, and
- different advection schemes require different values for the face-centred concentrations.

For MIKE 3, both HS and ACM, the scheme has been implemented with 3D QUICKEST/SHARP, 3D UPWIND, directionally split ULTIMATE/QUICKEST, and simple directionally split UPWIND schemes. With MIKE 3 ACM, however, the resulting scheme is not fully CWC and concentrations are back-centred 1/18 of a time step compared to MIKE 3 HS.

For MIKE 21, the scheme has been implemented with 2D QUICKEST, 2D UPWIND, directionally split ULTIMATE, and simple directionally split UPWIND schemes.

When implemented with a time- and/or space-split AD scheme, it is important that the face-centred concentrations during all steps are obtained on basis of the concentration field at time step *n*. Otherwise, one or both of the properties, CWC and mass-conservation, is lost. Presently in MIKE 21 and MIKE 3, the directionally split schemes, ULTIMATE and simple UPWIND, have been designed with face-centred concentrations based on the intermediate concentration field (in order to save computer memory). Therefore, if the user has chosen one of these AD schemes, it is not guaranteed that a constant concentration field remains constant during e.g. extensive flooding and drying conditions.

9 References

/1/ Gross, E.S., L. Bonaventura, and G. Rosatti: Consistency with Continuity in Conservative Advective Schemes for Free Surface Models, International Journal for Numerical Methods in Fluids, 38, pp 307-327, 2002.

/2/ Gross, E.S., V. Casulli, L. Bonaventura, and J.R. Koseff: A Semi-Implicit Method for Vertical Transport in Multidimensional Models, International Journal for Numerical Methods in Fluids, 28, pp 157-186, 1998.

/3/ Gross, E.S., J.R. Koseff, and S.G. Monismith: Evaluation of Advective Schemes for Estuarine Salinity Simulations, Journal of Hydraulic Engineering, 125, No. 1, pp 32-46, 1999.

/4/ Gross, E.S., J.R. Koseff, and S.G. Monismith: Three-Dimensional Salinity Simulation of South San Fransco Bay, Journal of Hydraulic Engineering, 125, No. 11, pp 1199-1209, 1999.

/5/ Vested, H.J., P. Berg, and Th. Uhrenholdt: Dense Water Formation in the Northern Adriatic, Journal of Marine Systems, Elsevier, 18, pp 135-160, 1998.

/6/ Vested, H.J., P. Justesen, and L. Ekebjærg: Advection-Dispersion Modelling in Three Dimensions, Appl. Math. Modelling, 16, pp 506-519, 1992.

/7/ Ekebjærg, L. and P. Justesen: An Explicit Scheme for Advection-diffusion Modelling in Two Dimensions, Computer Methods in Applied Mechanics and Engineering, 88, No. 3, pp 287-297, 1991.