Numerical Model.

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We consider In non dimensional setting, a lake of maximal depth in the vertical z–direction equal to 1 (or less if immersed) and of horizontal extent a (in the horizontal $x-y$ plane).
Implicit diffusion in the vertical direction
explicit advection and horizontal diffusion

1 Time numerical scheme : generalities

1.1 Explicit method 1 (performed in the first code)

We have u_t and u_{t-1}
Predictor (explicit leapfrog)

$$u_* = u_{t-1} + 2\delta t[F(u_t)]$$

Corrector (of the type Adams-Moulton)

$$u_{t+1} = u_t + \frac{\delta t}{12}[5F(t+1, u_*) + 8F(t, u_t) - F(t-1, u_{t-1})]$$

1.2 semi-Implicit method 2

lmplicit Adams-Moulton

$$u_{t+1} = u_t + \frac{\delta t}{12}[5F(t+1, u_{n+1}) + 8F(t, u_t) - F(t-1, u_{t-1})]$$

1.3 semi-Implicit method 3

We split into two terms

$$F = F_0 + F_1$$

where F_0 is diffusion (implicit) and F_1 is advection (explicit)

Predictor : explicit leapfrog

$$u_* = u_{t-1} + 2\delta t[F(u_t)]$$

Corrector: implicit Adams-Moulton

$$u_{t+1} = u_t + \frac{\delta t}{12}[5F_0(t+1, u_{n+1}) + 5F_1(t+1, u_*) + 8F(t, u_t) - F(t-1, u_{t-1})]$$

To simplify the implicit method so that it becomes linear, we can write $F_0(t+1, u_{n+1})$ as

$$F_0(t+1, u_{n+1}) = \phi(u_*)G(u_{n+1})$$

with $G(u_{n+1})$ linear in u_{n+1}.

1.4 Implicit method 4

$$F = F_0 + F_1$$

where F_0 is diffusion (implicit) and F_1 is advection (explicit)

Predictor : explicit leapfrog for F_1 +implicit Adams-Moulton for F_0

$$u_* = u_{t-1} + 2\delta t[F_1(u_t)] + \frac{\delta t}{12}[5F_0(t+1, u_*) + 8F_0(t, u_t) - F_0(t-1, u_{t-1})]$$

Corrector: implicit (Adams-Moulton)

$$u_{t+1} = u_t + \frac{\delta t}{12}[5F_0(t+1, u_{n+1}) + 5F_1(t+1, u_*) + 8F(t, u_t) - F(t-1, u_{t-1})]$$

If we want to simplify the terms $F_0(t+1, u_*)$ and $F_0(t+1, u_{n+1})$. One can do the following

$$u_* = u_{t-1} + \frac{\delta t}{12}[5F_0^N(t+1, u_*) + 8F_0(t, u_t) - F_0(t-1, u_{t-1})] + 2\delta t[F_1(u_t)]$$

$$u_{t+1} = u_t + \frac{\delta t}{12}[5F_0^N(t+1, u_{n+1}) + 5F_1(t+1, u_*) + 8F(t, u_t) - F(t-1, u_{t-1})]$$

with

$$F_0^N(t+1, u_*) = [2\phi(u_t) - \phi(u_{t-1})]G(u_*)$$
$$F_0^N(t+1, u_{n+1}) = \phi(u_*)G(u_{n+1})$$

with $G(u_*)$ linear in u_* and $G(u_{n+1})$ linear in u_{n+1}.

1.5 Implicit method 5

$$F = F_0 + F_1$$

where F_0 is diffusion (implicit) and F_1 is advection (explicit)

Predictor: explicit leapfrog +implicit leapfrog

$u_* = u_{t-1} + 2\delta t[F_0(t+1, u_*) + F_1(t, u_t)] = 2\delta t[F_0(t+1, u_*) + F(t, u_t) - F_0(t, u_t)]$

Corrector: implicit (Adams-Moulton)

$$u_{t+1} = u_t + \frac{\delta t}{12}[5F_0(t+1, u_{n+1}) + 5F_1(t+1, u_*) + 8F(t, u_t) - F(t-1, u_{t-1})]$$

If we want to simplify the terms $F_0(t+1, u_*)$ and $F_0(t+1, u_{n+1})$. One can do the following

$$u_* - 2\delta t F_0^N(t+1, u_*) = u_{t-1} + 2\delta t F_1(t, u_t)$$

$$u_{t+1} - \frac{5\delta t}{12} F_0^N(t+1, u_{n+1}) = u_t + \frac{\delta t}{12}[5F_1(t+1, u_*) + 8F(t, u_t) - F(t-1, u_{t-1})]$$

with

$$F_0^N(t+1, u_*) = [2\phi(u_t) - \phi(u_{t-1})]G(u_*)$$

or (less precise)

$$F_0^N(t+1, u_*) = \phi(u_t)G(u_*)$$

with $G(u_*)$ linear in u_* and

$$F_0^N(t+1, u_{n+1}) = \phi(u_*)G(u_{n+1})$$

with $G(u_{n+1})$ linear in u_{n+1}.

1.6 Implicit method 5Bis

$$F = F_0 + F_1$$

where F_0 is diffusion (implicit) and F_1 is advection (explicit)

Predictor: explicit leapfrog +implicit leapfrog

$$u_* = u_{t-1} + 2\delta t[\frac{F_0(t+1, u_*) + F_0(t-1, u_{t-1})}{2} + F_1(t, u_t)]$$

Corrector: implicit (Adams-Moulton)

$$u_{t+1} = u_t + \frac{\delta t}{12}[5F_0(t+1, u_{n+1}) + 5F_1(t+1, u_*) + 8F(t, u_t) - F(t-1, u_{t-1})]$$

If we want to simplify the terms $F_0(t+1, u_*)$ and $F_0(t+1, u_{n+1})$. One can do the following

$$u_* - \delta t F_0^N(t+1, u_*) = u_{t-1} + 2\delta t[F_1(t, u_t) + \frac{F_0(t-1, u_{t-1})}{2}]$$

$$u_{t+1} - \frac{5\delta t}{12} F_0^N(t+1, u_{n+1}) = u_t + \frac{\delta t}{12}[5F_1(t+1, u_*) + 8F(t, u_t) - F(t-1, u_{t-1})]$$

with

$$F_0^N(t+1, u_*) = [2\phi(u_t) - \phi(u_{t-1})]G(u_*)$$

or (less precise)

$$F_0^N(t+1, u_*) = \phi(u_t)G(u_*)$$

with $G(u_*)$ linear in u_* and

$$F_0^N(t+1, u_{n+1}) = \phi(u_*)G(u_{n+1})$$

with $G(u_{n+1})$ linear in u_{n+1}.

1.7 Complete Implicit method in diffusion 6 (the one performed NOW)

We split into two terms

$$F = F_0 + F_1$$

where F_0 is diffusion (implicit) and F_1 is advection (explicit)

Predictor : explicit+implicit leapfrog

$$u_* = u_{t-1} + 2\delta t[F_0(t, u_*) + F_1(t, u_t)]$$

Corrector: implicit (Adams-Moulton)

$$u_{t+1} = u_t + \delta t F_0(t+1, u_{n+1}) + \frac{\delta t}{12}[5F_1(t+1, u_*) + 8F_1(t, u_t) - F_1(t-1, u_{t-1})]$$

If the term F_0 can be written as

$$F_0(u_t) = \phi(u_t)G(u_t)$$

where $G(u_t)$ is differential linear operator in u_t (like a second derivative) and $\phi(u_t)$ a local nonlinear function. We simplify the terms $F_0(t, u_*)$ and $F_0(t + 1, u_{n+1})$ as follows

$$u_* - 2\delta t F_0^N(t, u_*) = u_{t-1} + 2\delta t F_1(t, u_t)$$
$$u_{t+1} - \delta t F_0^N(t+1, u_{n+1}) = u_t + \frac{\delta t}{12}[5F_1(t, u_*) + 8F_1(t, u_t) - F_1(t-1, u_{t-1})]$$

with

$$F_0^N(t, u_*) = \phi(u_t)G(u_*)$$

with $G(u_*)$ linear in u_* and

$$F_0^N(t+1, u_{n+1}) = \phi(u_*)G(u_{n+1})$$

with $G(u_{n+1})$ linear in u_{n+1}.

2 Time numerical scheme : the equations

$$H(x,y,t) = \zeta_1(x,y) + h(x,y,t)$$

where $z = 0$ is the surface at rest, $h(x,y,t)$ the free surface perturbation amplitude (waves), $\zeta_1(x,y)$ is the layer depth at rest (with immersed boundaries it is the fictitious depth).

The "vertical" velocity ω is related to the true physical vertical velocity w by

$$\omega(x_\sigma, y_\sigma, \sigma, t_\sigma) = w - u((\sigma-1)\frac{\partial H}{\partial x_\sigma} + \frac{\partial h}{\partial x_\sigma}) - v((\sigma-1)\frac{\partial H}{\partial y_\sigma} + \frac{\partial h}{\partial y_\sigma}) - ((\sigma-1)\frac{\partial H}{\partial t_\sigma} + \frac{\partial h}{\partial t_\sigma}) \tag{1}$$

2.1 free surface

The evolution of the free surface is obtained by

$$\frac{\partial h}{\partial t_\sigma} + \frac{\partial}{\partial x_\sigma}\left(H\int_0^1 u d\sigma\right) + \frac{\partial}{\partial y_\sigma}\left(H\int_0^1 v d\sigma\right) = 0 \tag{2}$$

We obtain the "vertical" ω velocity in σ-coordinates by

$$\omega = -\int_0^\sigma \left(\frac{\partial h}{\partial t_\sigma} + \frac{\partial uH}{\partial x_\sigma} + \frac{\partial vH}{\partial y_\sigma}\right) d\sigma \tag{3}$$

METHOD : In the code this is obtained as follows: first we compute starting from the bottom $\sigma = 0$ the integral

$$\int_0^\sigma \left(\frac{\partial uH}{\partial x_\sigma} + \frac{\partial vH}{\partial y_\sigma}\right) d\sigma \tag{4}$$

then one computes $\frac{\partial h}{\partial t_\sigma}$ by changing the sign of the last integral. Finally one uses

$$\omega = -\frac{\partial h}{\partial t_\sigma}\sigma - \int_0^\sigma \left(\frac{\partial uH}{\partial x_\sigma} + \frac{\partial vH}{\partial y_\sigma}\right) d\sigma \tag{5}$$

2.2 Momentum equations

$$\frac{\partial u}{\partial t_\sigma}+u\frac{\partial u}{\partial x_\sigma}+v\frac{\partial u}{\partial y_\sigma}+\frac{\omega}{H}\frac{\partial u}{\partial \sigma} = -\frac{1}{\rho_0}\frac{\partial P}{\partial x}+\frac{1}{H}\frac{\partial}{\partial x_\sigma}\left(H\nu\frac{\partial u}{\partial x_\sigma}\right)+\frac{1}{H}\frac{\partial}{\partial y_\sigma}\left(H\nu\frac{\partial u}{\partial y}\right)+\frac{1}{H}\frac{\partial}{\partial \sigma}\left(\frac{K_v}{H}\frac{\partial u}{\partial \sigma}\right) \tag{6}$$

$$\frac{\partial v}{\partial t_\sigma}+u\frac{\partial v}{\partial x_\sigma}+v\frac{\partial v}{\partial y_\sigma}+\frac{\omega}{H}\frac{\partial v}{\partial \sigma} = -\frac{1}{\rho_0}\frac{\partial P}{\partial y}+\frac{1}{H}\frac{\partial}{\partial x_\sigma}\left(H\nu\frac{\partial v}{\partial x_\sigma}\right)+\frac{1}{H}\frac{\partial}{\partial y_\sigma}\left(H\nu\frac{\partial v}{\partial y_\sigma}\right)+\frac{1}{H}\frac{\partial}{\partial \sigma}\left(\frac{K_v}{H}\frac{\partial v}{\partial \sigma}\right) \tag{7}$$

with

$$-\frac{1}{\rho_0}\frac{\partial P}{\partial x} = -g\frac{\partial h}{\partial x_\sigma} + [(\sigma-1)\frac{\partial H}{\partial x_\sigma} + \frac{\partial h}{\partial x_\sigma}]b + \frac{\partial}{\partial x_\sigma}(H\int_\sigma^1 bd\sigma)$$

$$-\frac{1}{\rho_0}\frac{\partial P}{\partial y} = -g\frac{\partial h}{\partial y_\sigma} + [(\sigma-1)\frac{\partial H}{\partial y_\sigma} + \frac{\partial h}{\partial y_\sigma}]b + \frac{\partial}{\partial y_\sigma}(H\int_\sigma^1 bd\sigma)$$

where the buoyancy term b stands for

$$b \equiv -g\frac{\rho-\rho_0}{\rho_0}$$

2.3 Temperature equations

$$\frac{\partial T}{\partial t_\sigma}+u\frac{\partial T}{\partial x_\sigma}+v\frac{\partial T}{\partial y_\sigma}+\frac{\omega}{H}\frac{\partial T}{\partial \sigma}=-\frac{1}{H}\frac{\partial (HJ_x)}{\partial x_\sigma}-\frac{1}{H}\frac{\partial (HJ_y)}{\partial y_\sigma}-\frac{1}{H}\frac{\partial J_T}{\partial \sigma}+\frac{1}{H}\frac{\partial}{\partial \sigma}(I_{in}) \tag{8}$$

where the source term in I_{in} is due to the absorption of light by water. This term can be seen as a source term given by the equation

$$\frac{1}{H}\frac{\partial I_{in}}{\partial \sigma}=(k_{bg}+k_c c+....)\,I_{in}.$$

$$I_{in}(\sigma=1)=\frac{\Phi_{bulk}(\sigma=1)}{\rho C_w}.$$

and depends on the values of the temperature, biological tracers at that particular σ.

The fluxes for temperature are given by :

$$J_x=-\nu_T\frac{\partial T}{\partial x_\sigma} \tag{9}$$

$$J_y=-\nu_T\frac{\partial T}{\partial y_\sigma} \tag{10}$$

$$J_T=-\frac{K_T}{H}\frac{\partial T}{\partial \sigma} \tag{11}$$

2.4 Concentration equations

The concentration $c(x_\sigma, y_\sigma, \sigma, t)$ is the true density for an active tracer. We use the variable

$$\psi \equiv H\ c(x_\sigma, y_\sigma, \sigma, t)$$

Using the continuity equation, the evolution equation in a conservative way

$$\frac{\partial \psi}{\partial t_\sigma} = -\frac{\partial J_x^*}{\partial x_\sigma} - \frac{\partial J_y^*}{\partial y_\sigma} - \frac{\partial J_\psi^*}{\partial \sigma} + HR(c) \tag{12}$$

where $R(c)$ are the sources of the reaction terms of the biological tracer.
The fluxes due to diffusion or sedimentation are given by

$$J_x^* = HJ_x + uHc = -H\nu_c \frac{\partial c}{\partial x_\sigma} + u\psi \tag{13}$$

$$J_y^* = HJ_y + vHc = -H\nu_c \frac{\partial c}{\partial y_\sigma} + v\psi \tag{14}$$

$$J_\psi^* = J_\psi + \omega c = (\omega + \omega_s)c - \frac{K_c}{H}\frac{\partial c}{\partial \sigma} \tag{15}$$

with ω_s the "vertical" velocity of sedimentation when < 0, of buoyancy when > 0.

To avoid negative values of c we use flux corrected method. This is why these active scalars are written in conservative equations (12).

The reaction terms R_c can be written as

$$R_c = \hat{R}_c c + R_c^*$$

with $c = N_1, D, P_1, P_2, Z, S$
(Cf Patankar algorithm for R_c)

$$
\begin{aligned}
R^*_{N_1} &= D/\tau & (16)\\
R^*_D &= \sum_{i=1}^{2} m_{P_i}^{N_1} l_{P_i} P_i + m_Z^{N_1}\left(l_Z + (1-e)F_Z(P_1,P_2)\right) Z & (17)\\
R^*_{P_1} &= 0 & (18)\\
R^*_{P_2} &= 0 & (19)\\
R^*_Z &= 0 & (20)\\
R^*_S &= 0 & (21)
\end{aligned}
$$

We do not use an internal volume input $In_{Vol}(t)$ for the nutrient

$$
\begin{aligned}
\hat{R}_{N_1} &= \left(-\sum_{i=1}^{2} m_{P_i}^{N_1} \hat{F}_{P_i}(N_1,I) P_i\right) & (22)\\
\hat{R}_D &= -\frac{1}{\tau} & (23)\\
\hat{R}_{P_1} &= F_{P_1}(N_1,I) - l_{P_1} - F_Z(P_1,P_2)\frac{\alpha}{\alpha P_1 + (1-\alpha)P_2} Z & (24)\\
\hat{R}_{P_2} &= F_{P_2}(N_1,I) - l_{P_2} - F_Z(P_1,P_2)\frac{(1-\alpha)}{\alpha P_1 + (1-\alpha)P_2} Z & (25)\\
\hat{R}_Z &= eF_Z(P_1,P_2) - l_Z - \gamma\frac{Z}{Z_c^2 + Z^2} F & (26)\\
R_S &= 0 & (27)
\end{aligned}
$$

We do not use l_{N_1} here

$$
\hat{F}_{P_i}(N_1,I) = \frac{F_{P_i}(N_1,I)}{N_1} = \mu_{P_i} \min\left\{\frac{1}{N_{1,c}^i + N_1}, \frac{I}{(I_c^i + I)(N_1 + 10^{-9})}\right\}; \quad (28)
$$

since

$$
F_{P_i}(N_1,I) \quad = \quad \mu_{P_i} \min\left\{\frac{N_1}{N_{1,c}^i + N_1}, \frac{I}{I_c^i + I}\right\}; \quad (29)
$$

$$
F_Z(P_1,P_2) \quad = \quad \mu_Z \frac{(P_1 + P_2)}{P_c + (P_1 + P_2)}, \quad (30)
$$

$$
\mu_{P_1}(T) = C_{0,1} + C_{1,1}T + C_{2,1}T^2
$$

$$
\mu_{P_2}(T) = \frac{T^2}{C_{1,2}^2}\frac{(1 - \tanh(T - C_{1,2}))}{2} + C_{2,2}\exp(-(T - C_{1,2}))^2/C_{3,2})
$$

2.5 Light equation

$$\frac{\partial I}{\partial z} = \left(k_{bg} + k_D D/m_D^{N_1} + k_S S + k_{P_1} P_1 + k_{P_2} P_2\right) I. \tag{31}$$

hence

$$\frac{\partial ln(I)}{\partial \sigma} = H\left(k_{bg} + k_c c + ...\right) = H k_{bg} + k_c \psi + ... \tag{32}$$

$$\tag{33}$$

First Possibility: If radiation is computed it is given by Φ_{bulk}

$$I(\sigma = 1) = \frac{\Phi_{bulk}(\sigma = 1, t)}{\mu M}$$

Care !: I is used in the equation for the ecosystem and I_{in} used in the equation for temperature.

$$I_{in}(\sigma = 1) = \frac{\Phi_{bulk}(\sigma = 1)}{\rho C_w}.$$

They are not exactly the same quantities

$$I_{in}(\sigma = 1) = \frac{\mu M}{\rho C_w} I(\sigma = 1)$$

Second Possibility one assumes that the incident flux $I(\sigma = 1, t)$ is varying with time (see day and night forcing). It can be expressed simply by a simple law

$$I(\sigma = 1, t) = I_{top}(1 + \tanh[6 \sin(2\pi t - \pi/2)])/2. \tag{34}$$

$$I_{top} = \frac{\Phi_{top}}{\mu M}$$

where Φ_{top} is given and μM is a factor of MicroMole of photons with respect to Joules.

3 Spatial grid.

The w positions.
$zlw(k)$ are vertical levels defined in the rescaled vertical variable σ: $zlw(k=0)$ is the bottom ($\sigma = 0$) and $zlw(k = N_z)$ is the surface ($\sigma = 1$).

$$zlw(k) = \frac{1}{2}[\frac{tanh[\frac{\frac{k}{N_z}-0.5}{Tanpar}]}{tanh[\frac{0.5}{Tanpar}]} + 1], \quad k = 0, ...N_z$$

They are the locations where the vertical velocity w is defined. $w(k)$ is defined as w at location $zlw(k)$
One defines

$$zwdiff(k) = zlw(k+1) - zlw(k), \quad k = 0, ...N_z - 1$$

The u, v, c, T positions.

They are the vertical locations where c, u, v are defined (but u,v,c are defined in different horizontal points h is defined on the same horizontal point than z).

$$zlc(k) < zlw(k) < zlc(k+1) < zlw(k+1)$$

One defines

$$zcdiff(k) = zlc(k+1) - zlc(k), \quad k = 1, ..., N_z - 1$$

First possibility $zlc(k)$ are vertical levels defined in the rescaled vertical variable σ:

$$zlc(k) = \frac{1}{2}[\frac{tanh[\frac{\frac{k}{N_z}-1}{Tanpar}]}{tanh[\frac{0.5}{Tanpar}]} + 1]$$

Second possibility

$$zlc(k) = \frac{1}{2}[zlw(k) + zlw(k-1)], \quad k = 1, ...N_z$$

$$zlc(0) = -zlc(1)$$

$zlc(0)$ is under the bottom $zlc(N_Z)$ is under the surface

4 The fluxes (vertical diffusive terms) and their derivatives for u,v, T.

4.1 The F_1 for u,v, T.

Here F_1 are the horizontal diffusion terms and the advective nonlinear terms.

4.2 The fluxes and the F_0 term for u,v, T

The fluxes for T and v and derivatives of the fluxes for T and v. Their form is similar to those for u except that H should be evaluated at T or v points horizontally and K_V could be different from K_T.
In the following we define the true fluxes

$$J_u \equiv -\frac{K_v(U_*)}{H}\frac{\partial u}{\partial \sigma}$$

and the opposite flux (with a hat)

$$\hat{J}_u \equiv \frac{K_v(U_*)}{H}\frac{\partial u}{\partial \sigma}$$

Two vertical diffusive hat fluxes for u (CARE here these are hat fluxes)

$$\hat{J}_u \equiv \frac{K_v(U_*)}{H}\frac{\partial u}{\partial \sigma}$$

are defined **around** the point $zlc(k+1)$.

A first one is defined in the location $zlw(k+1)$

$$\hat{J}_u(zlw(k{+}1)) \equiv [\frac{K_v(U_*)}{H}\frac{\partial u}{\partial \sigma}]_{zlw(k+1)} = [\frac{K_v(U_*)}{H}](zlw(k{+}1))\ \ (\frac{u(k+2)-u(k+1)}{zlc(k+2)-zlc(k+1)})$$

$$\hat{J}_u(zlw(k+1)) = [\frac{K_v(U_*)}{H}](zlw(k+1))\ \ (\frac{u(k+2)-u(k+1)}{zcdiff(k+1)})$$

A second one is defined in the location $zlw(k)$

$$\hat{J}_u(zlw(k)) \equiv [\frac{K_v(U_*)}{H}\frac{\partial u}{\partial \sigma}]_{zlw(k)} = [\frac{K_v(U_*)}{H}](zlw(k))\ \ (\frac{u(k+1)-u(k)}{zlc(k+1)-zlc(k)})$$

$$\hat{J}_u(zlw(k)) = [\frac{K_v(U_*)}{H}](zlw(k))\ \ (\frac{u(k+1)-u(k)}{zcdiff(k)})$$

4.3 The derivative of the fluxes for u,v, T.

Here F_1 are the horizontal diffusion terms and the advective nonlinear terms. The derivative of the fluxes for u (the generalization of the second derivative of u) is defined in the location $zlc(k+1)$

$$\frac{1}{H}\frac{\partial \hat{J}_u}{\partial \sigma}[zlc(k+1)] = \frac{1}{H}\frac{\hat{J}_u(zlw(k+1)) - \hat{J}_u(zlw(k))}{zwdiff(k)}$$

For momentum in u at point $zlc(k+1)$, one needs the value of F_0 at point $zlc(k+1)$

$$F_0(u_{n+1}) = \frac{1}{H}\frac{\hat{J}_u(zlw(k+1)) - \hat{J}_u(zlw(k))}{zwdiff(k)}$$

$$\hat{J}_u(zlw(k+1)) = [\frac{K_v(U_*)}{H}]_{zlw(k+1)} \quad (\frac{u(k+2) - u(k+1)}{zcdiff(k+1)})$$

$$\hat{J}_u(zlw(k)) = [\frac{K_v(U_*)}{H}]_{zlw(k)} \quad (\frac{u(k+1) - u(k)}{zcdiff(k)})$$

$F_0(u_{n+1})$ at $zlc(k+1)$ is

$$\frac{1}{H^2}\frac{1}{zwdiff(k)}\left[\frac{K_v(U_*)_{zlw(k+1)}}{zcdiff(k+1)}u(k+2) + \frac{K_v(U_*)_{zlw(k)}}{zcdiff(k)}u(k)\right]$$
$$-\frac{1}{H^2}\frac{1}{zwdiff(k)}\left[[\frac{K_v(U_*)_{zlw(k+1)}}{zcdiff(k+1)} + \frac{K_v(U_*)_{zlw(k)}}{zcdiff(k)}]u(k+1)\right]$$

$F_0(u_{n+1})$ at $zlc(k)$ is

$$\frac{1}{H^2}\frac{1}{zwdiff(k-1)}\left[\frac{K_v(U_*)_{zlw(k)}}{zcdiff(k)}u(k+1) + \frac{K_v(U_*)_{zlw(k-1)}}{zcdiff(k-1)}u(k-1)\right]$$
$$-\frac{1}{H^2}\frac{1}{zwdiff(k-1)}\left[[\frac{K_v(U_*)_{zlw(k)}}{zcdiff(k)} + \frac{K_v(U_*)_{zlw(k-1)}}{zcdiff(k-1)}]u(k)\right]$$

OR IT IS EQUIVALENT one can define $F_0(u_{n+1})$ at $zlc(k)$ for $k = 2, ..., (N-1)$

$$-C_f F_0(u_{n+1}) = a(k)u(k-1) + b(k)u(k) + c(k)u(k+1)$$

For $k = 2, ..., (N-1)$

$$a(k) = -C_f \left(\frac{1}{H^2} \frac{1}{zwdiff(k-1)} \left[\frac{K_v(U_*)_{zlw(k-1)}}{zcdiff(k-1)} \right] \right)$$

$$b(k) = -C_f \left(-\frac{1}{H^2} \frac{1}{zwdiff(k-1)} \left[[\frac{K_v(U_*)_{zlw(k)}}{zcdiff(k)} + \frac{K_v(U_*)_{zlw(k-1)}}{zcdiff(k-1)}] \right] \right)$$

$$c(k) = -C_f \left(\frac{1}{H^2} \frac{1}{zwdiff(k-1)} \left[\frac{K_v(U_*)_{zlw(k)}}{zcdiff(k)} \right] \right)$$

OR

$$a(k) = -\frac{C_f}{H} \frac{1}{zwdiff(k-1)} \left(\frac{1}{H} \left[\frac{K_v(U_*)_{zlw(k-1)}}{zcdiff(k-1)} \right] \right)$$

$$b(k) = -\frac{C_f}{H} \frac{1}{zwdiff(k-1)} \left(-\frac{1}{H} \left[[\frac{K_v(U_*)_{zlw(k)}}{zcdiff(k)} + \frac{K_v(U_*)_{zlw(k-1)}}{zcdiff(k-1)}] \right] \right)$$

$$c(k) = -\frac{C_f}{H} \frac{1}{zwdiff(k-1)} \left(\frac{1}{H} \left[\frac{K_v(U_*)_{zlw(k)}}{zcdiff(k)} \right] \right)$$

CARE : $a(k)$, $b(k)$ and $c(k)$ depend on time.

5 The fluxes (vertical diffusive terms) and their derivatives for $\psi \equiv Hc$.

5.1 The F_1 term for ψ.

For ψ, F_1 are the horizontal diffusion terms, the advective nonlinear terms **and part of the reaction terms** The value of $F_1^{react}(u_{n+1})$ for ψ are:

$$F_{1,\psi}^{react} = HR_c^* \tag{35}$$

5.2 The fluxes and the F_0 term for ψ.

The fluxes for $\psi \equiv Hc$ and derivatives of the fluxes for ψ are not similar to those for u .

FOR CONCENTRATIONS, we use TRUE FLUXES

$$J_x^* = HJ_x + uHc = -H\nu_c \frac{\partial c}{\partial x_\sigma} + uHc \tag{36}$$

$$J_y^* = HJ_y + vHc = -H\nu_c \frac{\partial c}{\partial y_\sigma} + vHc \tag{37}$$

we define the true vertical flux

$$J_\psi^* = J_\psi + \omega c = (\omega + \omega_s)c - \frac{K_c(U_*)}{H}\frac{\partial c}{\partial \sigma} \tag{38}$$

with ω_s the "vertical" velocity of sedimentation when < 0, of buoyancy when > 0.
We define the opposite flux (with a hat)

$$\hat{J}_\psi \equiv -J_\psi^* = -(\omega + \omega_s)c + \frac{K_c(U_*)}{H}\frac{\partial c}{\partial \sigma}$$

Two vertical diffusive hat fluxes for ψ (CARE here these are hat fluxes) $\hat{J}_\psi$ are defined **around** the point $zlc(k+1)$.
A first one is defined in the location $zlw(k+1)$

$$\hat{J}_\psi(zlw(k+1)) \equiv -(\omega + \omega_s)c + [\frac{K_c(U_*)}{H}\frac{\partial u}{\partial \sigma}]_{zlw(k+1)}$$

$$\hat{J}_\psi(zlw(k+1)) = -(\omega+\omega_s)c(zlw(k+1)) + [\frac{K_c(U_*)}{H}]_{(zlw(k+1))} \; (\frac{c(k+2) - c(k+1)}{zlc(k+2) - zlc(k+1)})$$

$$\hat{J}_\psi(zlw(k{+}1)) = -(\omega{+}\omega_s)c(zlw(k{+}1)){+}[\frac{K_c(U_*)}{H}]_{(zlw(k+1))} \ (\frac{c(k+2)-c(k+1)}{zcdiff(k+1)})$$

A second one is defined in the location $zlw(k)$

$$\hat{J}_\psi(zlw(k)) \equiv -(\omega+\omega_s)c(zlw(k)) + [\frac{K_c(U_*)}{H}\frac{\partial u}{\partial \sigma}]_{zlw(k)}$$

$$\hat{J}_\psi(zlw(k)) \equiv -(\omega+\omega_s)c(zlw(k)) + [\frac{K_c(U_*)}{H}]_{zlw(k)} \ (\frac{c(k+1)-c(k)}{zlc(k+1)-zlc(k)})$$

$$\hat{J}_\psi(zlw(k)) = -(\omega+\omega_s)c(zlw(k)) + [\frac{K_c(U_*)}{H}]_{zlw(k)} \ (\frac{c(k+1)-c(k)}{zcdiff(k)})$$

5.3 The derivative of the fluxes for ψ

For the equation for ψ at point $zlc(k{+}1)$, one needs the value at point $zlc(k{+}1)$ of

$$\frac{\partial \hat{J}_\psi}{\partial \sigma}[zlc(k+1)] = \frac{\hat{J}_\psi(zlw(k+1)) - \hat{J}_\psi(zlw(k))}{zwdiff(k)}$$

$$\hat{J}_\psi(zlw(k{+}1)) = -(\omega{+}\omega_s)c(zlw(k{+}1)){+}[\frac{K_c(U_*)}{H}]_{(zlw(k+1))} \ (\frac{c(k+2)-c(k+1)}{zcdiff(k+1)})$$

$$\hat{J}_\psi(zlw(k)) = -(\omega+\omega_s)c(zlw(k)) + [\frac{K_c(U_*)}{H}]_{zlw(k)} \ (\frac{c(k+1)-c(k)}{zcdiff(k)})$$

5.4 The value of $F_0^{diff}(u_{n+1})$ for ψ

One has

$$F_0(u_{n+1}) = F_0^{diff}(u_{n+1}) + F_0^{react}(u_{n+1}).$$

The value of $F_0^{diff}(u_{n+1})$ at $zlc(k+1)$ is

$$\frac{1}{H^2}\frac{1}{zwdiff(k)}\left[\frac{K_c(U_*)_{zlw(k+1)}}{zcdiff(k+1)}\psi(k+2)+\frac{K_c(U_*)_{zlw(k)}}{zcdiff(k)}\psi(k)\right]$$
$$-\frac{1}{H^2}\frac{1}{zwdiff(k)}\left[\left[\frac{K_c(U_*)_{zlw(k+1)}}{zcdiff(k+1)}+\frac{K_c(U_*)_{zlw(k)}}{zcdiff(k)}\right]\psi(k+1)\right]$$
$$-\frac{\omega_s}{H}\frac{1}{zwdiff(k)}\left[\psi(zlw(k+1))-\psi(zlw(k))\right]+$$
$$-\frac{1}{H}\frac{1}{zwdiff(k)}\left[\omega\psi(zlw(k+1))-\omega\psi(zlw(k))\right]$$

Let us define

$$f_0(k)\equiv\frac{[zlc(k+1)-zlw(k)]}{[zlc(k+1)-zlc(k)]}$$
$$f_1(k)\equiv\frac{[zlw(k)-zlc(k)]}{[zlc(k+1)-zlc(k)]}$$
$$\psi(zlw(k))=f_0(k)\psi(k)+f_1(k)\psi(k+1)$$
$$\psi(zlw(k+1))=f_0(k+1)\psi(k+1)+f_1(k+1)\psi(k+2)$$

Possibility 1 (USED IN THE CODE)

$$\psi(zlw(k+1))-\psi(zlw(k))=g_1(k+1)\psi(k)+g_2(k+1)\psi(k+1)+g_3(k+1)\psi(k+2)$$

$$\psi(zlw(k+1))-\psi(zlw(k))=-f_0(k)\psi(k)+[f_0(k+1)-f_1(k)]\psi(k+1)+f_1(k+1)\psi(k+2)$$

$$g_1(k+1)=-f_0(k)$$
$$g_2(k+1)=[f_0(k+1)-f_1(k)]$$
$$g_3(k+1)=f_1(k+1)$$

$$\omega\psi(zlw(k{+}1)){-}\omega\psi(zlw(k)) = \omega(k{+}1)[f_0(k{+}1)\psi(k{+}1){+}f_1(k{+}1)\psi(k{+}2)]{-}\omega(k)[f_0(k)\psi(k){+}f_1(k)\psi(k{+}1)]$$

$$\omega\psi(zlw(k{+}1)){-}\omega\psi(zlw(k)) = -[\omega(k)f_0(k)]\psi(k){+}[\omega(k{+}1)f_0(k{+}1){-}\omega(k)f_1(k)]\psi(k{+}1) + \omega(k+1)f_1(k+1)\psi(k+2)$$

Possibility 2 (NOT USED IN THE CODE)

$$\psi(zlw(k+1)) - \psi(zlw(k)) = \frac{[zlw(k+1) - zlw(k)]}{[zlc(k+2) - zlc(k)]}[\psi(k+2) - \psi(k)]$$

then

$$g_1(k+1) = -\frac{[zlw(k+1) - zlw(k)]}{[zlc(k+2) - zlc(k)]}$$

$$g_2(k+1) = 0$$

$$g_3(k+1) = \frac{[zlw(k+1) - zlw(k)]}{[zlc(k+2) - zlc(k)]}$$

Possibility 3 (NOT USED IN THE CODE)

$$g_1(k{+}1) = \frac{[zlc(k+2) - zlc(k+1)]}{g_4(k+1)}[zlw^2(k{+}1){-}zlw^2(k)]{+}\frac{[zlc^2(k+2) - zlc^2(k+1)]}{g_5(k+1)}[zlw(k{+}1){-}zlw(k)]$$

$$g_2(k{+}1) = -\frac{[zlc(k+2) - zlc(k)]}{g_4(k+1)}[zlw^2(k{+}1){-}zlw^2(k)]{-}\frac{[zlc^2(k+2) - zlc^2(k)]}{g_5(k+1)}[zlw(k{+}1){-}zlw(k)]$$

$$g_3(k{+}1) = \frac{[zlc(k+1) - zlc(k)]}{g_4(k+1)}[zlw^2(k{+}1){-}zlw^2(k)]{+}\frac{zlc^2(k+1) - zlc^2(k)}{g_5(k+1)}[zlw(k{+}1){-}zlw(k)]$$

$$g_4(k{+}1) = [zlc^2(k{+}2)){-}zlc^2(k{+}1)][zlc(k{+}2){-}zlc(k)]{-}[zlc^2(k{+}2)){-}zlc^2(k)][zlc(k{+}2){-}zlc(k{+}1)]$$

$$g_5(k{+}1) = [zlc(k{+}2)){-}zlc(k{+}1)][zlc^2(k{+}2){-}zlc^2(k)]{-}[zlc(k{+}2)){-}zlc(k)][zlc^2(k{+}2){-}zlc^2(k{+}1)]$$

5.5 The value of $F_0^{react}(u_{n+1})$ for ψ

$$F_{0,\psi}^{react} = \hat{R}_c(k)\psi(k) \tag{39}$$

5.6 The value of $F_0(u_{n+1})$ for ψ

one can define $F_0(u_{n+1})$ at $zlc(k)$ for $k = 2, ..., (N-1)$

$$-C_f F_0(u_{n+1}) = a_\psi(k)\psi(k-1) + b_\psi(k)\psi(k) + c_\psi(k)\psi(k+1)$$

For $k = 2, ..., (N-1)$

$$a_\psi(k) = -C_f\left(\frac{1}{Hzwdiff(k-1)}[\omega_s f_0(k-1) + \omega(k-1)f_0(k-1)]\right) - \frac{C_f}{H}\frac{1}{zwdiff(k-1)}\left(\frac{1}{H}\left[\frac{K_v(U_*)_{zlw(k-1)}}{zcdiff(k-1)}\right]\right)$$

$$b_\psi(k) = -C_f\left(\hat{R}_c(k) - \frac{1}{Hzwdiff(k-1)}[\omega_s f_0(k) - \omega_s f_1(k-1) + \omega(k)f_0(k) - \omega(k-1)f_1(k-1)]\right) - \frac{C_f}{H}\frac{1}{zwdiff(k-1)}\left(-\frac{1}{H}\left[[\frac{K_v(U_*)_{zlw(k)}}{zcdiff(k)} + \frac{K_v(U_*)_{zlw(k-1)}}{zcdiff(k-1)}]\right]\right)$$

$$c_\psi(k) = -C_f\left(\frac{1}{Hzwdiff(k-1)}[-\omega_s f_1(k) - \omega(k)f_1(k)]\right) - \frac{C_f}{H}\frac{1}{zwdiff(k-1)}\left(\frac{1}{H}\left[\frac{K_v(U_*)_{zlw(k)}}{zcdiff(k)}\right]\right)$$

6 Bottom Boundary conditions for u and v : No-slip without immersed boundaries

$$u(x_\sigma, y_\sigma, \sigma = 0) = v(x_\sigma, y_\sigma, \sigma = 0) = 0$$

discretized as

$$u(k = 1) = -u(k = 0)$$

The derivative of the fluxes for u (the generalization of the second derivative of u) is defined in the location $zlc(1)$

$$\frac{1}{H}\frac{\partial \hat{J}_u}{\partial \sigma}[zlc(1)] = \frac{1}{H}\frac{\hat{J}_u(zlw(1)) - \hat{J}_u(zlw(0))}{zwdiff(0)}$$

with

$$\hat{J}_u(zlw(k)) \equiv [\frac{K_v(U_*)}{H}\frac{\partial u}{\partial \sigma}]_{zlw(k)} = [\frac{K_v(U_*)}{H}](zlw(k)) \quad (\frac{u(k+1) - u(k)}{zlc(k+1) - zlc(k)})$$

For momentum in u at point $zlc(1)$, one needs the value of F_0 at point $zlc(1)$

$$F_0(u_{n+1}) = \frac{1}{H}\frac{\hat{J}_u(zlw(1)) - \hat{J}_u(zlw(0))}{zwdiff(0)}$$

$$\hat{J}_u(zlw(1)) = [\frac{K_v(U_*)}{H}]_{zlw(1)} \quad (\frac{u(2) - u(1)}{zcdiff(1)})$$

The value of

$$\hat{J}_u(zlw(0)) \equiv [\frac{K_v(U_*)}{H}\frac{\partial u}{\partial \sigma}]_{zlw(0)}$$

can be computed in two ways

First choice for $\hat{J}_u(zlw(0))$

This quantity can be computed using

$$\hat{J}_u(zlw(0)) = [\frac{K_v(U_*)}{H}]_{zlw(0)} \quad (\frac{u(1) - u(0)}{zcdiff(0)}) = [\frac{K_v(U_*)}{H}]_{zlw(0)} \quad (\frac{2u(1)}{zcdiff(0)})$$

Hence

$F_0(u_{n+1})$ at $zlc(1)$ is

$$\frac{1}{H^2}\frac{1}{zwdiff(0)}\left[\frac{K_v(U_*)_{zlw(1)}}{zcdiff(1)}u(2) - [\frac{K_v(U_*)_{zlw(1)}}{zcdiff(1)} + 2\frac{K_v(U_*)_{zlw(0)}}{zcdiff(0)}]u(1)\right]$$

$$-C_f F_0(u_{n+1}) = b_u(1)u(1) + c_u(1)u(2)$$

$$a_u(1) = 0$$

$$b_u(1) = C_f \left(\frac{1}{H^2} \frac{1}{zwdiff(0)} \left[[\frac{K_v(U_*)_{zlw(1)}}{zcdiff(1)} + 2\frac{K_v(U_*)_{zlw(0)}}{zcdiff(0)}] \right] \right)$$

$$c_u(1) = -C_f \left(\frac{1}{H^2} \frac{1}{zwdiff(0)} \left[\frac{K_v(U_*)_{zlw(1)}}{zcdiff(1)} \right] \right)$$

Second choice for $\hat{J}_u(zlw(0))$

This quantity can be computed using

$$\hat{J}_u(zlw(0)) = [\frac{K_v(U_*)}{H}]_{zlw(0)} \frac{\partial u}{\partial \sigma}]_{zlw(0)} = [\frac{K_v(U_*)}{H}]_{zlw(0)} \frac{\partial u}{\partial \sigma}|_{\sigma=0}$$

$$\frac{\partial u}{\partial \sigma}]_{zlw(0)} = -\frac{zlc(1)}{zlc(2)(zlc(2)-zlc(1))}u(2) + \frac{zlc(2)}{zlc(1)(zlc(2)-zlc(1))}u(1)$$

$$-[\frac{zlc(2)}{zlc(1)(zlc(2)-zlc(1))} - \frac{zlc(1)}{zlc(1)(zlc(2)-zlc(1))}]u(zlw(0))$$

since $u(zlw(0)) = 0$

$$\frac{\partial u}{\partial \sigma}]_{zlw(0)} = -\frac{zlc(1)}{zlc(2)zcdiff(1)}u(2) + \frac{zlc(2)}{zlc(1)zcdiff(1)}u(1)$$

$F_0(u_{n+1})$ at $zlc(1)$ is

$$\frac{1}{H^2} \frac{1}{zwdiff(0)} \left[\frac{K_v(U_*)_{zlw(1)}}{zcdiff(1)}u(2) - [\frac{K_v(U_*)_{zlw(1)}}{zcdiff(1)}]u(1)] \right] +$$

$$\frac{1}{H^2} \frac{1}{zwdiff(0)} \left[-K_v(U_*)_{zlw(0)}[-\frac{zlc(1)}{zlc(2)zcdiff(1)}u(2) + \frac{zlc(2)}{zlc(1)zcdiff(1)}u(1)] \right]$$

$$-C_f F_0(u_{n+1}) = b_u(1)u(1) + c_u(1)u(2)$$

$$a_u(1) = 0$$

$$b_u(1) = -C_f \left(\frac{1}{H^2} \frac{1}{zwdiff(0)} \left[-\frac{K_v(U_*)_{zlw(1)}}{zcdiff(1)} - K_v(U_*)_{zlw(0)} \frac{zlc(2)}{zlc(1)zcdiff(1)} \right] \right)$$

$$c_u(1) = -C_f \left(\frac{1}{H^2} \frac{1}{zwdiff(0)} \left[\frac{K_v(U_*)_{zlw(1)}}{zcdiff(1)} + K_v(U_*)_{zlw(0)} \frac{zlc(1)}{zlc(2)zcdiff(1)} \right] \right)$$

7 Bottom Boundary conditions for u and v : No-slip with immersed boundaries

Suppose that we impose a no-slip at wall located at $zww(i,j)$ such that

$$zlc(k_{thres} - 1) < zww < zlc(k_{thres})$$

with $k_{thres}(i,j) \leq 1$. In order to avoid complicated useless computations, we slightly modify the lake bottom so that we set

$$zww(i,j) = zlw(k_{thres} - 1)$$

For $k < k_{thres}$ we impose
For $k = 1, ..., k_{thres}$

$$a_u(k) = 0.$$

$$b_u(k) = 1$$

$$c_u(k) = 0$$

For momentum in u at point $zlc(k_{thres})$, one needs the value of F_0 at point $zlc(k_{thres})$

$$F_0(u_{n+1}) = \frac{1}{H} \frac{\hat{J}_u(zlw(k_{thres})) - \hat{J}_u(zlw(k_{thres} - 1))}{zwdiff(k_{thres} - 1)}$$

$$\hat{J}_u(zlw(k_{thres})) = [\frac{K_v(U_*)}{H}]_{zlw(k_{thres})} \quad (\frac{u(k_{thres}+1) - u(k_{thres})}{zcdiff(k_{thres})})$$

First choice for $\hat{J}_u(zlw(k_{thres}-1))$ (USED IN THE CODE)

Quantity $\hat{J}_u(zlw(k_{thres}-1))$ can be computed using

$$\hat{J}_u(zlw(k_{thres}-1)) = [\frac{K_v(U_*)}{H}]_{zlw(k_{thres}-1)} \frac{\partial u}{\partial \sigma}]_{zlw(k_{thres}-1)}$$

$$\frac{\partial u}{\partial \sigma}]_{zlw(k_{thres}-1)} = u(k_{thres}) \frac{1}{zlc(k_{thres}) - zlw(k_{thres}-1)}$$

$$\hat{J}_u(zlw(k_{thres}-1)) = [\frac{K_v(U_*)}{H}]_{zlw(k_{thres}-1)} \frac{1}{zlc(k_{thres}) - zlw(k_{thres}-1)} u(k_{thres})$$

For momentum in u at point $zlc(k_{thres})$, one needs the value of F_0 at point $zlc(k_{thres})$

$$F_0(u_{n+1}) = \frac{1}{H^2 zwdiff(k_{thres}-1)} \frac{[K_v(U_*)]_{zlw(k_{thres})}}{zcdiff(k_{thres})} \; u(k_{thres}+1)$$
$$-\frac{1}{H^2 zwdiff(k_{thres}-1)} \left(\frac{[K_v(U_*)]_{zlw(k_{thres})}}{zcdiff(k_{thres})} + \frac{[K_v(U_*)]_{zlw(k_{thres}-1)}}{zlc(k_{thres}) - zlw(k_{thres}-1)} \right) u(k_{thres})$$

$$-C_f F_0(u_{n+1}) = b_u(k_{thres}) u(k_{thres}) + c_u(k_{thres}) u(k_{thres}+1)$$

$$a_u(k_{thres}) = 0$$

$$b_u(k_{thres})) = -C_f \left(-\frac{1}{H^2 zwdiff(k_{thres}-1)} \left(\frac{[K_v(U_*)]_{zlw(k_{thres})}}{zcdiff(k_{thres})} + \frac{[K_v(U_*)]_{zlw(k_{thres}-1)}}{zlc(k_{thres}) - zlw(k_{thres}-1)} \right) \right)$$

$$c_u(k_{thres})) = -C_f \left(\frac{1}{H^2 zwdiff(k_{thres}-1)} \frac{[K_v(U_*)]_{zlw(k_{thres})}}{zcdiff(k_{thres})} \right)$$

Second choice for $\hat{J}_u(zlw(k_{thres}-1))$(NOT USED IN THE CODE)

We use the Second choice for $\hat{J}_u(zlw(k_{thres}-1))$. This quantity can be computed using

$$\hat{J}_u(zlw(k_{thres}-1)) = [\frac{K_v(U_*)}{H}]_{zlw(k_{thres}-1)} \frac{\partial u}{\partial \sigma}]_{zlw(k_{thres}-1)}$$

$$\frac{\partial u}{\partial \sigma}]_{zlw(k_{thres}-1)} = u(k_{thres}+1)\frac{g_{13}}{g_{12}} + u(k_{thres})\frac{g_{14}}{g_{12}}$$

$$g_{12} = [zlc^2(k_{thres}+1) - zlw^2(k_{thres}-1)][zlc(k_{thres}) - zlw(k_{thres}-1)]$$
$$-[zlc^2(k_{thres}) - zlw^2(k_{thres}-1)][zlc(k_{thres}+1) - zlw(k_{thres}-1)]$$

$$g_{13} = 2\ \ zlw(k_{thres}-1)\ [zlc(k_{thres})-zlw(k_{thres}-1)]-[zlc^2(k_{thres})-zlw^2(k_{thres}-1)]$$

$$g_{14} = -2\ \ zlw(k_{thres}-1)\ [zlc(k_{thres}+1)-zlw(k_{thres}-1)]+[zlc^2(k_{thres}+1)-zlw^2(k_{thres}-1)]$$

$F_0(u_{n+1})$ at $zlc(k_{thres})$ is

$$\frac{1}{H^2 zwdiff(k_{thres}-1)}[\frac{K_v(U_*)_{zlw(k_{thres})}}{zcdiff(k_{thres})} - \frac{g_{13}}{g_{12}}[K_v(U_*)]_{zlw(k_{thres}-1)}]\ \ u(k_{thres}+1)$$
$$-\frac{1}{H^2 zwdiff(k_{thres}-1)}[\frac{K_v(U_*)_{zlw(k_{thres})}}{zcdiff(k_{thres})} + \frac{g_{14}}{g_{12}}[K_v(U_*)]_{zlw(k_{thres}-1)}]\ \ u(k_{thres})$$

$F_0(u_{n+1})$ at $zlc(k_{thres})$ is

$$-C_f F_0(u_{n+1}) = b_u(k_{thres})u(k_{thres}) + c_u(k_{thres})u(k_{thres}+1)$$

$$a_u(k_{thres}) = 0$$

$$b_u(k_{thres})) = -C_f \left(-\frac{1}{H^2 zwdiff(k_{thres}-1)} [\frac{K_v(U_*)_{zlw(k_{thres})}}{zcdiff(k_{thres})} + \frac{g_{14}}{g_{12}} [K_v(U_*)]_{zlw(k_{thres}-1)}] \right)$$

$$c_u(k_{thres})) = -C_f \left(\frac{1}{H^2 zwdiff(k_{thres}-1)} [\frac{K_v(U_*)_{zlw(k_{thres})}}{zcdiff(k_{thres})} - \frac{g_{13}}{g_{12}} [K_v(U_*)]_{zlw(k_{thres}-1)}] \right)$$

8 Bottom Boundary conditions Temperature : adiabatic condition and without immersed boundaries

$$\frac{\partial T}{\partial \sigma}(x_\sigma, y_\sigma, \sigma = 0, t) = 0$$

The derivative of the fluxes for T is defined in the location $zlc(1)$

$$\frac{1}{H}\frac{\partial \hat{J}_T}{\partial \sigma}[zlc(1)] = \frac{1}{H}\frac{\hat{J}_T(zlw(1)) - \hat{J}_T(zlw(0))}{zwdiff(0)}$$

For T at point $zlc(1)$, one needs the value of F_0 at point $zlc(1)$

$$F_0(u_{n+1}) = \frac{1}{H}\frac{\hat{J}_T(zlw(1)) - \hat{J}_T(zlw(0))}{zwdiff(0)}$$

$$\hat{J}_T(zlw(1)) = [\frac{K_T(U_*)}{H}]_{zlw(1)} \quad (\frac{T(2) - T(1)}{zcdiff(1)})$$

$$\hat{J}_T(zlw(0)) = 0$$

$F_0(u_{n+1})$ at $zlc(1)$ is

$$\frac{1}{H^2}\frac{1}{zwdiff(0)}\left[\frac{K_T(U_*)_{zlw(1)}}{zcdiff(1)}T(2) - [\frac{K_T(U_*)_{zlw(1)}}{zcdiff(1)}]T(1)\right]$$

$$-C_f F_0(u_{n+1}) = b_T(1)T(1) + c_T(1)T(2)$$

$$a_T(1) = 0$$

$$b_T(1) = C_f\left(\frac{1}{H^2}\frac{1}{zwdiff(0)}[\frac{K_T(U_*)_{zlw(1)}}{zcdiff(1)}]\right)$$

$$c_T(1) = -C_f\left(\frac{1}{H^2}\frac{1}{zwdiff(0)}[\frac{K_T(U_*)_{zlw(1)}}{zcdiff(1)}]\right)$$

9 Bottom Boundary conditions Temperature : adiabatic condition and with immersed boundaries

Suppose that we impose a no-slip at wall located at $zww(i,j)$ such that

$$zlc(k_{thres}-1) < zww < zlc(k_{thres})$$

with $k_{thres}(i,j) \leq 1$. In order to avoid complicated useless computations, we slightly modify the lake bottom so that we set

$$zww(i,j) = zlw(k_{thres}-1)$$

For $k < k_{thres}$ we impose
For $k = 1, ..., k_{thres}$

$$a_T(k) = 0.$$

$$b_T(k) = 1$$

$$c_T(k) = 0$$

For T at point $zlc(k_{thres})$, one needs the value of F_0 at point $zlc(k_{thres})$

$$F_0(u_{n+1}) = \frac{1}{H}\frac{\hat{J}_T(zlw(k_{thres})) - \hat{J}_T(zlw(k_{thres}-1))}{zwdiff(k_{thres}-1)}$$

$$\hat{J}_T(zlw(k_{thres})) = [\frac{K_T(U_*)}{H}]_{zlw(k_{thres})} \quad (\frac{T(k_{thres}+1) - T(k_{thres})}{zcdiff(k_{thres})})$$

Adiabatic implies

$$\hat{J}_T(zlw(k_{thres}-1)) = 0$$

$F_0(u_{n+1})$ at $zlc(k_{thres})$ is

$$-C_f F_0(u_{n+1}) = b_T(k_{thres})u(k_{thres}) + c_T(k_{thres})u(k_{thres}+1)$$

IMPORTANT :

$$a_T(k_{thres}) = 0$$

$$b_T(k_{thres})) = -C_f \left(-\frac{1}{H^2 zwdiff(k_{thres}-1)} [\frac{K_v(U_*)_{zlw(k_{thres})}}{zcdiff(k_{thres})} \right)$$

$$c_T(k_{thres})) = -C_f \left(\frac{1}{H^2 zwdiff(k_{thres}-1)} [\frac{K_v(U_*)_{zlw(k_{thres})}}{zcdiff(k_{thres})}] \right)$$

10 Concentration : flux via stress or permeability without immersed boundaries

10.1 The value of $F_0^{react}(u_{n+1})$ for ψ

$$F_{0,\psi}^{react}(zlc(1)) \quad = \quad \hat{R}_c(1)\psi(1) \tag{40}$$

10.2 The value of $F_0^{diff}(u_{n+1})$ for ψ

FOR CONCENTRATIONS, we use the FLUXES

$$J_x^* = HJ_x + uHc = -H\nu_c \frac{\partial c}{\partial x_\sigma} + uHc \tag{41}$$

$$J_y^* = HJ_y + vHc = -H\nu_c \frac{\partial c}{\partial y_\sigma} + vHc \tag{42}$$

we define the true vertical flux

$$J_\psi^* = J_\psi + \omega c = (\omega + \omega_s)c - \frac{K_c(U_*)}{H}\frac{\partial c}{\partial \sigma} \tag{43}$$

with ω_s the "vertical" velocity of sedimentation when < 0, of buoyancy when > 0.
The opposite flux (with a hat) is defined as

$$\hat{J}_\psi \equiv -(\omega + \omega_s)c + \frac{K_c(U_*)}{H}\frac{\partial c}{\partial \sigma}$$

The derivative of the fluxes for ψ is defined in the location $zlc(1)$

$$F_0^{diff}(u_{n+1}) = \frac{\partial \hat{J}_\psi}{\partial \sigma}[zlc(1)] = \frac{\hat{J}_\psi(zlw(1)) - \hat{J}_\psi(zlw(0))}{zwdiff(0)}$$

The value of $\hat{J}_\psi(zlw(1))$

$$\hat{J}_\psi(zlw(1)) = -(\omega(1) + \omega_s)c(zlw(1)) + [\frac{K_c(U_*)}{H}]_{zlw(1)} \quad (\frac{c(2) - c(1)}{zcdiff(1)})$$

We need to compute $c(zlw(1))$

$$c(zlw(1)) = f_0(1)c(1) + f_1(1)c(2)$$

The value of $\hat{J}_\psi(zlw(0))$

The value of $\hat{J}_\psi(zlw(0))$ is computed as follows. Let us first remind that

$$J_\psi = \omega_s c - \frac{K_c}{H}\frac{\partial c}{\partial \sigma} \tag{44}$$

At at $\sigma = 0$, $\omega = 0$ then

$$\hat{J}_\psi(\sigma = 0) = -J_\psi(\sigma = 0, t) = -[\hat{E}_b + \hat{D}_b c(\sigma = 0)] \tag{45}$$

We need to compute $c(\sigma = 0)$ as a function of $c(1)$

$$c(\sigma = 0) = g_6 c(1) + g_7$$

$$g_6 = \frac{1}{[1 + [zlc(1) - zlw(0)]\frac{[\omega_s - \hat{D}_b]}{K_c(\sigma=0)}H]}$$

$$g_7 = [zlc(1) - zlw(0)]\frac{H\hat{E}_b}{[K_c(\sigma = 0) + [zlc(1) - zlw(0)][\omega_s - \hat{D}_b]H]}$$

$$\hat{J}_\psi(\sigma = 0) = -[\hat{E}_b + \hat{D}_b g_7] - \frac{\hat{D}_b g_6}{H}\psi(1). \tag{46}$$

$F_0^{diff}(u_{n+1})$ at $zlc(1)$ is

$$F_0^{diff}(u_{n+1}) = \frac{1}{zwdiff(0)}\hat{J}_\psi(zlw(1)) - \frac{1}{zwdiff(0)}\hat{J}_\psi(zlw(0))$$

$$F_0^{diff}(u_{n+1}) = \frac{1}{zwdiff(0)}[-(\omega+\omega_s)c(zlw(1)) + [\frac{K_c(U_*)}{H}]_{zlw(1)}\ (\frac{c(2)-c(1)}{zcdiff(1)})] - \frac{1}{zwdiff(0)}\hat{J}_\psi(\sigma = 0)$$

10.3 computations of $\tau_b(t)$ bottom shear stress at $\sigma = 0$

$\tau_b(t)$ denotes the bottom shear stress at $\sigma = 0$

$$\tau_b(t) = \frac{\rho_{wat} K_v(U=0,\sigma=0)}{H}\sqrt{[|\frac{\partial u}{\partial\sigma}(x_\sigma, y_\sigma, \sigma=0)|^2 + |\frac{\partial v}{\partial\sigma}(x_\sigma, y_\sigma, \sigma=0)|^2]}$$

where

$$\frac{\partial u}{\partial\sigma}]_{zlw(0)} = (\frac{u(1)-u(0)}{zcdiff(0)}) = \frac{2u(1)}{zcdiff(0)}$$

$$\frac{\partial v}{\partial\sigma}]_{zlw(0)} = (\frac{v(1)-v(0)}{zcdiff(0)}) = \frac{2v(1)}{zcdiff(0)}$$

10.4 computations of $\hat{D}_b$, $\hat{E}_b$

$$\hat{E}_b = J_{in} + E_b$$

where $J_{in}(t)$ is an unsteady uniform input and

$$E_b = \begin{cases} 0 & |\tau_b(t)| < \tau_{ce} \\ \beta_c M\left(\frac{|\tau_b(t)|}{\tau_{ce}} - 1\right) & |\tau_b(t)| \geq \tau_{ce} \end{cases} \tag{47}$$

where τ_{ce} is the critical shear stress for erosion, β_c is the percentage of c in the eroded sediment and M is the erodibility coefficient related to the sediment properties.

D_b the deposition rate (only meaningful when $\omega_s < 0$)

$$\hat{D}_b = \begin{cases} 0 & |\tau_b(t)| > \tau_{cd} \\ \omega_s\left(1 - \frac{|\tau_b(t)|}{\tau_{cd}}\right) & |\tau_b(t)| \leq \tau_{cd} \end{cases} \tag{48}$$

where the quantity τ_{cd} is the critical shear stress.

10.5 The value of $F_0(u_{n+1})$ for ψ

$$-C_f F_0(u_{n+1}) = b_\psi(1)\psi(1) + c_\psi(1)\psi(2) - C_f \frac{1}{zwdiff(0)}[\hat{E}_b + \hat{D}_b g_7]$$

with

$$a_\psi(1) = 0$$

$$b_\psi(1) = -C_f \left(\hat{R}_c(1) - \frac{1}{Hzwdiff(0)}(\omega(1) + \omega_s) f_0(1) + \frac{1}{zwdiff(0)} \frac{\hat{D}_b g_6}{H} \right)$$
$$-C_f \left(-\frac{1}{Hzwdiff(0)} [\frac{K_c(U_*)}{H}]_{zlw(1)} \quad (\frac{1}{zcdiff(1)}) \right)$$

$$c_\psi(1) = -C_f \left(-\frac{1}{Hzwdiff(0)}(\omega(1) f_1(1) + \omega_s f_1(1)) + \frac{1}{Hzwdiff(0)} [\frac{K_c(U_*)}{H}]_{zlw(1)} \quad (\frac{1}{zcdiff(1)}) \right)$$

11 Concentration : flux via stress or permeability with immersed boundaries

Suppose that we impose a no-slip at wall located at $zww(i,j)$ such that

$$zlc(k_{thres}-1) < zww < zlc(k_{thres})$$

with $k_{thres}(i,j) \leq 1$. In order to avoid complicated useless computations, we slightly modify the lake bottom so that we set

$$zww(i,j) = zlw(k_{thres}-1)$$

For $k < k_{thres}$ we impose
For $k = 1, ..., k_{thres}$

$$a_\psi(k) = 0.$$

$$b_\psi(k) = 1$$

$$c_\psi(k) = 0$$

11.1 The value of $F_0^{react}(u_{n+1})$ for ψ

$$F_{0,\psi}^{react}(zlc(k_{thres})) \quad = \quad \hat{R}_c(k_{thres})\psi(k_{thres}) \tag{49}$$

11.2 The value of $F_0^{diff}(u_{n+1})$ for ψ

FOR CONCENTRATIONS, we use the FLUXES

$$J_x^* = HJ_x + uHc = -H\nu_c \frac{\partial c}{\partial x_\sigma} + uHc \tag{50}$$

$$J_y^* = HJ_y + vHc = -H\nu_c \frac{\partial c}{\partial y_\sigma} + vHc \tag{51}$$

we define the true vertical flux

$$J_\psi^* = J_\psi + \omega c = (\omega + \omega_s)c - \frac{K_c(U_*)}{H}\frac{\partial c}{\partial \sigma} \tag{52}$$

with ω_s the "vertical" velocity of sedimentation when < 0, of buoyancy when > 0.
The opposite flux (with a hat) is defined as

$$\hat{J}_\psi \equiv -(\omega + \omega_s)c + \frac{K_c(U_*)}{H}\frac{\partial c}{\partial \sigma}$$

The derivative of the fluxes for ψ is defined in the location $zlc(k_{thres})$

$$F_0^{diff}(u_{n+1}) = \frac{\partial \hat{J}_\psi}{\partial \sigma}[zlc(k_{thres})] = \frac{\hat{J}_\psi(zlw(k_{thres})) - \hat{J}_\psi(zlw(k_{thres}-1))}{zwdiff(k_{thres}-1)}$$

The value of $\hat{J}_\psi(zlw(k_{thres}))$

$$\hat{J}_\psi(zlw(k_{thres})) = -(\omega(k_{thres})+\omega_s)c(zlw(k_{thres}))+[\frac{K_c(U_*)}{H}]_{zlw(k_{thres})}\;(\frac{c(k_{thres}+1) - c(k_{thres})}{zcdiff(k_{thres})})$$

We need to compute $c(zlw(k_{thres}))$

$$c(zlw(k_{thres})) = f_0(k_{thres})c(k_{thres}) + f_1(k_{thres})c(k_{thres}+1)$$

$$\hat{J}_\psi(zlw(k_{thres})) = [-(\omega(k_{thres})+\omega_s)f_1(k_{thres})+[\frac{K_c(U_*)}{H}]_{zlw(k_{thres})}\;\frac{1}{zcdiff(k_{thres})}]c(k_{thres}+1)$$

$$-[(\omega(k_{thres}) + \omega_s)f_0(k_{thres}) + [\frac{K_c(U_*)}{H}]_{zlw(k_{thres})}\quad\frac{1}{zcdiff(k_{thres})}]c(k_{thres})$$

The value of $\hat{J}_\psi(zlw(k_{thres}-1))$

The value of $\hat{J}_\psi(zlw(k_{thres}-1))$ is computed as follows. Let us first remind that

$$J_\psi = \omega_s c - \frac{K_c}{H}\frac{\partial c}{\partial \sigma} \tag{53}$$

At at $\sigma = zlw(k_{thres}-1)$, $\omega = 0$ then

$$\hat{J}_\psi(\sigma = zlw(k_{thres}-1)) = -J_\psi(zlw(k_{thres}-1), t) = -[\hat{E}_b + \hat{D}_b c(zlw(k_{thres}-1))] \tag{54}$$

$$\hat{J}_\psi(zlw(k_{thres}-1)) = -J_\psi(zlw(k_{thres}-1),t) = -[\hat{E}_b + \hat{D}_b c(zlw(k_{thres}-1))] \quad (55)$$

We need to compute $c(zlw(k_{thres}-1))$ as a function of $c(k_{thres})$

$$c(zlw(k_{thres}-1)) = g_{17}c(k_{thres}) + g_{18}$$

$$g_{17} = \frac{1}{[1 + [zlc(k_{thres}) - zlw(k_{thres}-1)]\frac{[\omega_s - \hat{D}_b]}{K_c(zlw(k_{thres}-1))}H]}$$

$$g_{18} = [zlc(k_{thres}) - zlw(k_{thres}-1)]\frac{H\hat{E}_b}{[K_c(zlw(k_{thres}-1)) + [zlc(k_{thres}) - zlw(k_{thres}-1)][\omega_s - \hat{D}_b]H]}$$

$$\hat{J}_\psi(zlw(k_{thres}-1))) = -[\hat{E}_b + \hat{D}_b g_{18}] - \frac{\hat{D}_b g_{17}}{H}\psi(k_{thres}). \quad (56)$$

The derivative of the fluxes for ψ is defined in the location $zlc(k_{thres})$

$$F_0^{diff}(u_{n+1}) = \frac{\partial \hat{J}_\psi}{\partial \sigma}[zlc(k_{thres})] = \frac{\hat{J}_\psi(zlw(k_{thres})) - \hat{J}_\psi(zlw(k_{thres}-1))}{zwdiff(k_{thres}-1)}$$

$$F_0^{diff}(u_{n+1}) = \frac{\hat{J}_\psi(zlw(k_{thres}))}{zwdiff(k_{thres}-1)} - \frac{\hat{J}_\psi(zlw(k_{thres}-1))}{zwdiff(k_{thres}-1)}$$

$$F_0^{diff}(u_{n+1}) = \frac{1}{zwdiff(k_{thres}-1)}[-(\omega(k_{thres})+\omega_s)f_1(k_{thres}) + [\frac{K_c(U_*)}{H}]_{zlw(k_{thres})}\frac{1}{zcdiff(k_{thres})}]c(k_{thres}$$

$$-\frac{1}{zwdiff(k_{thres}-1)}[(\omega(k_{thres})+\omega_s)f_0(k_{thres}) + [\frac{K_c(U_*)}{H}]_{zlw(k_{thres})}\frac{1}{zcdiff(k_{thres})}]c(k_{thres})$$

$$+\frac{1}{zwdiff(k_{thres}-1)}([\hat{E}_b + \hat{D}_b g_{18}] + \frac{\hat{D}_b g_{17}}{H}\psi(k_{thres})).$$

11.3 computations of $\tau_b(t)$ bottom shear stress at $\sigma = zlw(k_{thres} - 1)$

$\tau_b(t)$ denotes the bottom shear stress at $\sigma = zlw(k_{thres} - 1)$

$$\tau_b(t) = \frac{\rho_{wat} K_v(U = 0, \sigma = zlw(k_{thres} - 1))}{H} \sqrt{[|\frac{\partial u}{\partial \sigma}(x_\sigma, y_\sigma, \sigma = 0)|^2 + |\frac{\partial v}{\partial \sigma}(x_\sigma, y_\sigma, \sigma = 0)|^2]}$$

where

$$\frac{\partial u}{\partial \sigma}]_{zlw(k_{thres}-1)} = \frac{u(k_{thres})}{zlc(k_{thres}) - zlw(k_{thres} - 1)}$$

$$\frac{\partial v}{\partial \sigma}]_{zlw(k_{thres}-1)} = \frac{v(k_{thres})}{zlc(k_{thres}) - zlw(k_{thres} - 1)}$$

11.4 computations of $\hat{D}_b$, $\hat{E}_b$

$$\hat{E}_b = J_{in} + E_b$$

where $J_{in}(t)$ is an unsteady uniform input and

$$E_b = \begin{cases} 0 & |\tau_b(t)| < \tau_{ce} \\ \beta_c M \left(\frac{|\tau_b(t)|}{\tau_{ce}} - 1 \right) & |\tau_b(t)| \geq \tau_{ce} \end{cases} \tag{57}$$

where τ_{ce} is the critical shear stress for erosion, β_c is the percentage of c in the eroded sediment and M is the erodibility coefficient related to the sediment properties.

D_b the deposition rate (only meaningful when $\omega_s < 0$)

$$\hat{D}_b = \begin{cases} 0 & |\tau_b(t)| > \tau_{cd} \\ \omega_s \left(1 - \frac{|\tau_b(t)|}{\tau_{cd}} \right) & |\tau_b(t)| \leq \tau_{cd} \end{cases} \tag{58}$$

where the quantity τ_{cd} is the critical shear stress.

11.5 The value of $F_0(u_{n+1})$ for ψ

$$-C_f F_0(u_{n+1}) = b_\psi(k_{thres})\psi(k_{thres}) + c_\psi(k_{thres})\psi(k_{thres}+1)$$
$$-C_f[\frac{1}{zwdiff(k_{thres}-1)}[\hat{E}_b + \hat{D}_b g_{18}]]$$

with

$$a_\psi(k_{thres}) = 0$$

$$b_\psi(k_{thres}) = -C_f\left(\hat{R}_c(k_{thres}) + \frac{1}{zwdiff(k_{thres}-1)}\frac{\hat{D}_b g_{17}}{H}\right)$$
$$-C_f\left(-\frac{1}{zwdiff(k_{thres}-1)}[(\omega(k_{thres})+\omega_s)f_0(k_{thres}) + [\frac{K_c(U_*)}{H}]_{zlw(k_{thres})}\quad\frac{1}{zcdiff(k_{thres})}]\right)$$

$$c_\psi(k_{thres}) = -C_f\left(\frac{1}{zwdiff(k_{thres}-1)}[-(\omega(k_{thres})+\omega_s)f_1(k_{thres}) + [\frac{K_c(U_*)}{H}]_{zlw(k_{thres})}\ \ \frac{1}{zcdiff(k_{thres})}]\right)$$

12 Top Boundary conditions: u and v stress

momentum is transferred from the wind in the x and y direction by

$$\frac{\partial u}{\partial \sigma}(x_\sigma, y_\sigma, \sigma = 1) = H\frac{\tau_s}{\rho_{wat} K_v(\sigma = 1)} \cos(\theta_W)$$

$$\frac{\partial v}{\partial \sigma}(x_\sigma, y_\sigma, \sigma = 1) = H\frac{\tau_s}{\rho_{wat} K_v(\sigma = 1)} \sin(\theta_W)$$

with

$$\tau_s = C_D \rho_{air} W^2.$$

and θ_W the angle of the wind

$$\hat{J}_u(zlw(N)) = \frac{K_v(U_*, \sigma = 1)}{H} \frac{\partial u}{\partial \sigma} = \frac{\tau_s}{\rho_{wat}} \cos(\theta_W)$$

For momentum in u at point $zlc(N)$, one needs the value of F_0 at point $zlc(N)$ where

$$F_0(u_{n+1}) = \frac{1}{H}\frac{\partial \hat{J}_u}{\partial \sigma}[zlc(N)] = \frac{1}{H}\frac{\hat{J}_u(zlw(N)) - \hat{J}_u(zlw(N-1))}{zwdiff(N-1)}$$

which is the derivative of the fluxes for u defined in the location $zlc(N)$.

$$\hat{J}_u(zlw(N-1)) = [\frac{K_v(U_*)}{H}]_{zlw(N-1)} \quad (\frac{u(N) - u(N-1)}{zcdiff(N-1)})$$

$-C_f F_0(u_{n+1})$ at $zlc(N)$ is

$$-C_f F_0(u_{n+1}) = a_u(N)u(N-1) + b_u(N)u(N) - C_f\frac{\hat{J}_u(zlw(N))}{Hzwdiff(N-1)}$$

$$a_u(N) = -C_f\left(\frac{1}{Hzwdiff(N-1)}\frac{1}{zcdiff(N-1)}[\frac{K_v(U_*)}{H}]_{zlw(N-1)}\right)$$

$$b_u(N) = C_f\left(\frac{1}{Hzwdiff(N-1)}\frac{1}{zcdiff(N-1)}[\frac{K_v(U_*)}{H}]_{zlw(N-1)}\right)$$

$$c_u(N) = 0$$

13 Top Boundary conditions: Temperature : time dependent flux

On the top free surface condition for temperature $T(x_\sigma, y_\sigma, \sigma = 1, t)$ We impose the condition on the flux $J_T(zlw(N))$

$$J_T(zlw(N)) = -K_T \frac{\partial T}{\partial z} = \frac{1}{\rho C_w} [\Phi_{convec} + \Phi_{lat} + \Phi_{wat} - 0.55(1-A)\Phi_{sol} - \Phi_{atm}] \tag{59}$$

Let us define

$$\hat{J}_T(zlw(N)) \equiv -J_T(zlw(N)) = K_T \frac{\partial T}{\partial z} \tag{60}$$

For T at point $zlc(N)$, one needs the value of F_0 at point $zlc(N)$

$$F_0(T_{n+1}) = -\frac{1}{H}\frac{\partial J_T}{\partial \sigma}[zlc(N)] = \frac{1}{H}\frac{\partial \hat{J}_T}{\partial \sigma}[zlc(N)]$$

$$F_0(T_{n+1}) = \frac{1}{H}\frac{\hat{J}_T(zlw(N)) - \hat{J}_T(zlw(N-1))}{zwdiff(N-1)}$$

which is the derivative of the fluxes for T defined in the location $zlc(N)$.

$$\hat{J}_T(zlw(N-1)) = [\frac{K_v(U_*)}{H}]_{zlw(N-1)} \quad (\frac{T(N) - T(N-1)}{zcdiff(N-1)})$$

$-C_f F_0(u_{n+1})$ at $zlc(N)$ is

$$-C_f F_0(u_{n+1}) = a_T(N)T(N-1) + b_T(N)T(N) - C_f \frac{\hat{J}_T(zlw(N))}{Hzwdiff(N-1)}$$

$$a_T(N) = -C_f \left(\frac{1}{Hzwdiff(N-1)}\frac{1}{zcdiff(N-1)}[\frac{K_T(U_*)}{H}]_{zlw(N-1)}\right)$$

$$b_T(N) = C_f \left(\frac{1}{Hzwdiff(N-1)}\frac{1}{zcdiff(N-1)}[\frac{K_T(U_*)}{H}]_{zlw(N-1)}\right)$$

$$c_T(N) = 0$$

14 Top Boundary conditions: Concentration : imposed unsteady flux or no flux

14.1 The value of $F_0^{diff}(u_{n+1})$ for ψ

For the equation for ψ at point $zlc(N)$, one needs the value of F_0^{diff} at point $zlc(N)$

$$F_0^{diff} = \frac{\partial \hat{J}_\psi}{\partial \sigma}[zlc(N)] = \frac{\hat{J}_\psi(zlw(N)) - \hat{J}_\psi(zlw(N-1))}{zwdiff(N-1)}$$

The flux at $\hat{J}_\psi(zlw(N))$

$$J_\psi \equiv \omega_s c - \frac{K_c(U_*)}{H}\frac{\partial c}{\partial \sigma} \tag{61}$$

and

$$\hat{J}_\psi \equiv -(\omega + \omega_s)c + \frac{K_c(U_*)}{H}\frac{\partial c}{\partial \sigma}$$

At $zlw(N) = \sigma = 1$, $\omega = 0$ then

$$\hat{J}_\psi(zlw(N)) = -J_\psi(zlw(N)) = -J_{top}(t).$$

Since we assume a direct input at the fluid surface, (at $\sigma = 1$) :

$$J_\psi(\sigma = 1) = J_{top}(t). \tag{62}$$

The flux at $\hat{J}_\psi(zlw(N-1))$
A second one is defined in the location $zlw(N-1)$

$$\hat{J}_\psi(zlw(N-1)) \equiv -(\omega(zlw(N-1)) + \omega_s)c(zlw(N-1)) + [\frac{K_c(U_*)}{H}\frac{\partial u}{\partial \sigma}]_{zlw(N-1)}$$

$$\hat{J}_\psi(zlw(N-1)) \equiv -(\omega(zlw(N-1)) + \omega_s)c(zlw(N-1)) + [\frac{K_c(U_*)}{H}]_{zlw(N-1)}\ (\frac{c(N) - c(N-1)}{zcdiff(N-1)})$$

$F_0^{diff}(u_{n+1})$ at $zlc(N)$ is

$$F_0^{diff} = -\frac{\hat{J}_\psi(zlw(N-1))}{zwdiff(N-1)} + \frac{\hat{J}_\psi(zlw(N))}{zwdiff(N-1)}$$

$$F_0^{diff} = \frac{1}{zwdiff(N-1)}[\frac{1}{H}(\omega(N-1)+\omega_s)\psi(zlw(N-1))]$$
$$-\frac{1}{zwdiff(N-1)}[\frac{K_c(U_*)}{H^2}]_{zlw(N-1)}\ \ (\frac{\psi(N)-\psi(N-1)}{zcdiff(N-1)})$$
$$+\frac{1}{zwdiff(N-1)}\hat{J}_\psi(zlw(N))$$

We need to compute $c(zlw(N-1))$

$$\psi(zlw(N-1)) = f_0(N-1)\psi(N-1) + f_1(N-1)\psi(N)$$

14.2 The value of $F_0^{react}(u_{n+1})$ for ψ

$$F_{0,\psi}^{react}(zlc(N)) \quad = \quad \hat{R}_c(N)\psi(N) \tag{63}$$

14.3 The value of $F_0(u_{n+1})$ for ψ

$-C_f F_0(u_{n+1})$ at $zlc(N)$ is

$$-C_f F_0(u_{n+1}) = a_\psi(N)\psi(N-1) + b_\psi((N)\psi(N) + C_f\frac{1}{zwdiff(N-1)}J_{top}(t)$$

$$a_\psi(N) = -C_f\frac{1}{zwdiff(N-1)}[\frac{f_0(N-1)}{H}[\omega(N-1)+\omega_s]+[\frac{K_c(U_*)}{H^2}]_{zlw(N-1)}\ \ (\frac{1}{zcdiff(N-1)})]$$

$$b_\psi(N) = -C_f\frac{1}{zwdiff(N-1)}[\hat{R}_c(N)+[\frac{f_1(N-1)}{H}(\omega(N-1)+\omega_s)]-[\frac{K_c(U_*)}{H^2}]_{zlw(N-1)}\ \ (\frac{1}{zcdiff(N-1)})]$$

$$c_\psi((N) = 0$$

15 Appendix: parabolic approximation for the derivative of u, v or T.

If one does a parabolic approximation $u(z) = az^2 + bz + c$ around the region

$$zlw(k_{thres} - 1) < zlc(k_{thres}) < zlc(k_{thres} + 1)$$

one gets (using $u(zlw(k_{thres} - 1)) = 0$)

$$u(k_{thres}+1) = [zlc^2(k_{thres}+1) - zlw^2(k_{thres}-1)]a + [zlc(k_{thres}+1) - zlw(k_{thres}-1)]b$$

$$u(k_{thres}) = [zlc^2(k_{thres}) - zlw^2(k_{thres} - 1)]a + [zlc(k_{thres}) - zlw(k_{thres} - 1)]b$$

$$\frac{\partial u}{\partial \sigma}]_{zlw(k_{thres}-1)} = 2azlw(k_{thres} - 1) + b$$

$$\frac{\partial u}{\partial \sigma}]_{zlw(k_{thres}-1)} = u(k_{thres} + 1)\frac{g_{13}}{g_{12}} + u(k_{thres})\frac{g_{14}}{g_{12}}$$

$$g_{12} = [zlc^2(k_{thres} + 1) - zlw^2(k_{thres} - 1)][zlc(k_{thres}) - zlw(k_{thres} - 1)]$$
$$-[zlc^2(k_{thres}) - zlw^2(k_{thres} - 1)][zlc(k_{thres} + 1) - zlw(k_{thres} - 1)]$$

$$g_{13} = 2\ zlw(k_{thres}-1)\ [zlc(k_{thres}) - zlw(k_{thres}-1)] - [zlc^2(k_{thres}) - zlw^2(k_{thres}-1)]$$

$$g_{14} = -2\ zlw(k_{thres}-1)\ [zlc(k_{thres}+1) - zlw(k_{thres}-1)] + [zlc^2(k_{thres}+1) - zlw^2(k_{thres}-1)]$$

16 Appendix: linear approximation for ψ

If one does a linear approximation $\psi(z) = bz + c$ around the region $zlc(k) < zlw(k) < zlc(k + 1) < zlw(k + 1) < zlc(k + 2)$ one may use

$$\psi(zlw(k+1)) - \psi(zlw(k)) = g_1(k+1)\psi(k) + g_2(k+1)\psi(k+1) + g_3(k+1)\psi(k+2)$$

with
Possibility 1 (USED IN THE CODE)

$$\psi(zlw(k)) = f_0(k)\psi(k) + f_1(k)\psi(k+1)$$

$$\psi(zlw(k+1)) = f_0(k+1)\psi(k+1) + f_1(k+1)\psi(k+2)$$

with

$$f_0(k) \equiv \frac{[zlw(k) - zlc(k)]}{[zlc(k+1) - zlc(k)]}$$

$$f_1(k) \equiv \frac{[zlc(k+1) - zlw(k)]}{[zlc(k+1) - zlc(k)]}$$

$$\psi(zlw(k+1)) - \psi(zlw(k)) = -f_0(k)\psi(k) + [f_0(k+1) - f_1(k)]\psi(k+1) + f_1(k+1)\psi(k+2)$$

$$g_1(k+1) = -f_0(k)$$

$$g_2(k+1) = [f_0(k+1) - f_1(k)]$$

$$g_3(k+1) = f_1(k+1)$$

or one may use (NOT USED IN THE CODE)

$$\psi(zlw(k+1)) - \psi(zlw(k)) = \frac{[zlw(k+1) - zlw(k)]}{[zlc(k+1) - zlc(k)]}[\psi(k+1) - \psi(k)]$$

then

$$g_1(k+1) = -\frac{[zlw(k+1) - zlw(k)]}{[zlc(k+1) - zlc(k)]}$$

$$g_2(k+1) = \frac{[zlw(k+1) - zlw(k)]}{[zlc(k+1) - zlc(k)]}$$

$$g_3(k+1) = 0$$

or one may use (NOT USED IN THE CODE)

$$\psi(zlw(k+1)) - \psi(zlw(k)) = \frac{[zlw(k+1) - zlw(k)]}{[zlc(k+2) - zlc(k)]}[\psi(k+2) - \psi(k)]$$

then

$$\psi(zlw(k+1)) - \psi(zlw(k)) = g_1(k+1)\psi(k) + g_2(k+1)\psi(k+1) + g_3(k+1)\psi(k+2)$$

$$g_1(k+1) = -\frac{[zlw(k+1) - zlw(k)]}{[zlc(k+2) - zlc(k)]}$$

$$g_2(k+1) = 0$$

$$g_3(k+1) = \frac{[zlw(k+1) - zlw(k)]}{[zlc(k+2) - zlc(k)]}$$

17 Appendix: parabolic approximation for ψ

If one does a parabolic approximation $\psi(z) = az^2 + bz + c$ around the region $zlc(k) < zlw(k) < zlc(k+1) < zlw(k+1) < zlc(k+2)$ one gets

$$\psi(zlw(k+1)) - \psi(zlw(k)) = [zlw^2(k+1) - zlw^2(k)]a + [zlw(k+1) - zlw(k)]b$$

with

$$a = \frac{a_1}{g_4(k+1)}$$

$$b = \frac{b_1}{g_5(k+1)}$$

$$a_1 = [\psi(k+2) - \psi(k+1)][zlc(k+2) - zlc(k)] - [\psi(k+2) - \psi(k)][zlc(k+2) - zlc(k+1)]$$

$$g_4(k+1) = [zlc^2(k+2)) - zlc^2(k+1)][zlc(k+2) - zlc(k)] - [zlc^2(k+2)) - zlc^2(k)][zlc(k+2) - zlc(k+1)]$$

$$b_1 = [\psi(k+2) - \psi(k+1)][zlc^2(k+2) - zlc^2(k)] - [\psi(k+2) - \psi(k)][zlc^2(k+2) - zlc^2(k+1)]$$

$$g_5(k+1) = [zlc(k+2)) - zlc(k+1)][zlc^2(k+2) - zlc^2(k)] - [zlc(k+2)) - zlc(k)][zlc^2(k+2) - zlc^2(k+1)]$$

OR ELSE

$$a = \frac{[zlc(k+1) - zlc(k)]}{g_4(k+1)}\psi(k+2) - \frac{[zlc(k+2) - zlc(k)]}{g_4(k+1)}\psi(k+1) + \frac{[zlc(k+2) - zlc(k+1)]}{g_4(k+1)}\psi(k)$$

$$g_4(k+1) = [zlc^2(k+2)) - zlc^2(k+1)][zlc(k+2) - zlc(k)] - [zlc^2(k+2)) - zlc^2(k)][zlc(k+2) - zlc(k+1)]$$

$$b = \frac{zlc^2(k+1) - zlc^2(k)}{g_5(k+1)}\psi(k+2) - \frac{[zlc^2(k+2) - zlc^2(k)]}{g_5(k+1)}\psi(k+1) + \frac{[zlc^2(k+2) - zlc^2(k+1)]}{g_5(k+1)}\psi(k)$$

$$g_5(k+1) = [zlc(k+2)) - zlc(k+1)][zlc^2(k+2) - zlc^2(k)] - [zlc(k+2)) - zlc(k)][zlc^2(k+2) - zlc^2(k+1)]$$

OR ELSE

$$\psi(zlw(k+1)) - \psi(zlw(k)) = g_1(k+1)\psi(k) + g_2(k+1)\psi(k+1) + g_3(k+1)\psi(k+2)$$

$$g_1(k+1) = \frac{[zlc(k+2) - zlc(k+1)]}{g_4(k+1)}[zlw^2(k+1) - zlw^2(k)] + \frac{[zlc^2(k+2) - zlc^2(k+1)]}{g_5(k+1)}[zlw(k+1) - zlw(k)]$$

$$g_2(k+1) = -\frac{[zlc(k+2) - zlc(k)]}{g_4(k+1)}[zlw^2(k+1) - zlw^2(k)] - \frac{[zlc^2(k+2) - zlc^2(k)]}{g_5(k+1)}[zlw(k+1) - zlw(k)]$$

$$g_3(k+1) = \frac{[zlc(k+1) - zlc(k)]}{g_4(k+1)}[zlw^2(k+1) - zlw^2(k)] + \frac{zlc^2(k+1) - zlc^2(k)}{g_5(k+1)}[zlw(k+1) - zlw(k)]$$