1

Fluid Dynamics - Numerical Techniques 1.

1). Simplify the system for $b(z,t)$; We have

$$\partial_t b + \partial_z (ub) = 0 \,, \quad u = \alpha b^2 - \beta b^2 \partial_z b \,, \quad z \in [0, H] \quad (1)$$

Subbing in u into the PDE yields.

$$\partial_t b + \partial_z (\alpha b^3 - \beta b^3 \partial_z b) = 0 . \quad \square .$$

Linearising around D_0. We do this by subbing in $b = D_0 + b'$, which yields

$$\partial_t (b' + D_0) + \partial_z (\alpha (b' + D_0)^3 - \beta (b' + D_0)^3 \partial_z (b' + D_0)) = 0$$

$$\Rightarrow \partial_t b' + 3\alpha D_0^2 \partial_z b' - \beta D_0^3 \partial_{zz} b' + O(b'^2) = 0 \text{ (Assuming } b' \text{ Small).}$$

$\therefore$ We have

$$\partial_t b' + 3\alpha D_0^2 \partial_z b' - \beta D_0^3 \partial_z b' = 0 \quad \square .$$

These PDEs are called the non-liner & liner convective diffusion equations respectively because they describe both describe diffusion & convection simultaneously.

This is because the PDE in eqn (1) is the mass balance. Hence, it describes all the ways mass can be transported in the system. When subbing in velocity we can see that the mass can be transported via convection, ~~which is the ∂_z~~ and diffusion which are represented by the $\partial_z(\alpha b^3)$ and $\partial_z(\beta b^3 \partial_z b)$ terms respectively.

(2)

And eq^n (6) in the HW Sheet is simply the linearised form of eq^n (5) ~~about~~ about D_0.

b). The upwind scheme states that we use a backwards difference in space if ~~α is positive~~ α is positive and a forward differencing α is negative.

∴ As $\alpha \geq 0$ by def^n we use a backwards difference in space for the convective term.

Additionally, for the adjoint form of the convective term by Morton & Mayers (2005) we construct a difference approximation to the eq^n in its original form we can ~~write~~ write.

$$\left[b^3 \frac{\partial b}{\partial t} \right]^n_{j+\frac{1}{2}} = \left(b^n_{j+\frac{1}{2}} \right)^3 \left(\frac{b^n_{j+1} - b^n_j}{\Delta Z} \right) = F^n_{j+\frac{1}{2}}$$

Similarly, ~~with~~

$$\left[b^3 \frac{\partial b}{\partial Z} \right]^n_{j-\frac{1}{2}} = \left(b^n_{j-\frac{1}{2}} \right)^3 \left(\frac{b^n_j - b^n_{j-1}}{\Delta Z} \right) = F^n_{j-\frac{1}{2}}$$

Notice: We used a central difference scheme for the $\frac{\partial b}{\partial Z}$ term

∴ By these considerations we get the following discretization for the non-linear convective diffusion eq^n.

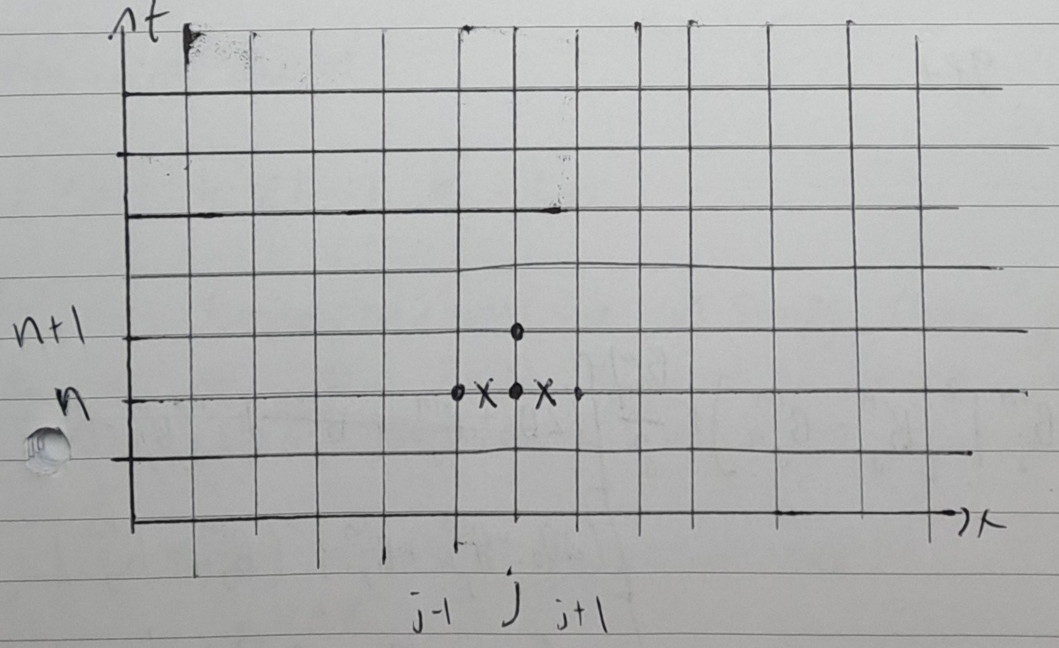
(3)

$$\frac{B_j^{n+1}-B_j^n}{\Delta t}+3\alpha\left(B_j^n\right)^2\left[\frac{B_j^n-B_{j-1}^n}{\Delta Z}\right]-\beta\left[\frac{F_{j+\frac{1}{2}}^n-F_{j-\frac{1}{2}}^n}{\Delta Z}\right]=0.$$

$$\Rightarrow B_j^{n+1}=B_j^n-3\alpha r\left(B_j^n\right)^2\left[B_j^n-B_{j-1}^n\right]+\beta\eta\left[\left(B_{j+\frac{1}{2}}^n\right)^3\left(B_{j+1}^n-B_j^n\right)-\left(B_{j-\frac{1}{2}}^n\right)^3\left(B_j^n-B_{j-1}^n\right)\right]$$

Where $r=\frac{\Delta t}{\Delta Z}$, $\eta=\frac{\Delta t}{(\Delta Z)^2}$

We first make a sketch of our grid.



Now note that $j\pm\frac{1}{2}$ is not in our grid $\therefore$ to overcome this we define the halfstep as the mean of the points between it

$B_{j+\frac{1}{2}}^n=\frac{B_{j+1}^n+B_j^n}{2}$ and similar for $B_{j-\frac{1}{2}}^n$ subbing this in

yields.

4

$$B_j^{n+1} = B_j^n - 3\alpha\sqrt{}(B_j^n)^2\left[B_j^n - B_{j-1}^n\right) + \frac{\beta m}{8}\left[(B_{j+1}^n + B_j^n)^3(B_{j+1}^n - B_j^n) - (B_j^n + B_{j-1}^n)^3(B_j^n - B_{j-1}^n)\right].$$

Discretising the linear eq^n is easier. Using the same upwind scheme as before for the convective term & using second-order central difference for the diffusive term yields.

$$B_j^{'n+1} = B_j^{'n} - 3\alpha D_0^2 \sqrt{}\left[B_j^{'n} - B_{j-1}^{'n}\right] + \beta D_0^3 m\left[B_{j+1}^{'n} - 2B_j^{'n} + B_{j-1}^{'n}\right).$$

Linearising the discretization of the non-linear eq^n by subbing in

$B_j^n = D_0 + B_j^{'n}$ we get

$$B_j^{'n+1} = B_j^{'n} - 3\alpha\sqrt{}\left(D_0 + B_j^{'n}\right)^2\left[B_j^{'n} - B_{j-1}^{'n}\right] + \frac{\beta m}{8}\left\{\left[(2D_0 + B_{j+1}^{'n} + B_j^{'n})^3(B_{j+1}^{'n} - B_j^{'n}) - (2D_0 + B_j^{'n} + B_{j-1}^{'n})^3(B_j^{'n} - B_{j-1}^{'n})\right]\right\}$$

Now assuming $B_j^{'n+1}$ is small we get

$$B_j^{'n+1} = B_j^{'n} - 3\alpha D_0^2\sqrt{}\left[B_j^{'n} - B_{j-1}^{'n}\right] + \beta m D_0^3\left[B_{j+1}^{'n} - 2B_j^{'n} + B_{j-1}^{'n}\right]. \text{ ✓}$$

∴ They match

5

I believe the advantage of the adjoint form is that it preserves ~~the~~ conservation and makes the scheme more stable.

~~Finally, we simply define the boundary conditions~~

If ~~we~~ the interior grid points run from $j=1, \dots, J-1$ we simply define the Dirichlet boundary condition as

$$b(0,t) = b_B = 1 \quad B_0^n = b_B \quad \forall n.$$

$$b(H,t) = b_T = 1 \quad B_J^n = b_T, \quad \forall n$$

with initial condition

$$b(z,0) = b_i(z) \Rightarrow b_j^0 = b_{j+1}^0$$

For the boundary conditions we can simply create 'ghost' points outside our grid points so that the ~~initial~~ first and last grid points are able to 'obtain' ~~the~~ relevant information

(). To perform a Fourier analysis we sub in

$$B_j'^n = \lambda^n e^{ijk\Delta z},$$

doing so ~~first~~ and dividing through by $e^{ijk\Delta z}$ yields

~~$\lambda = 1 - 3\alpha D_0^2 v \left[B_j'^n - B'^n \right.$~~

$$\lambda = 1 - 3\alpha D_0^2 v \left[1 - e^{-ik\Delta z} \right] + \beta D_0^3 \eta \left[e^{ik\Delta z} - 2 + e^{-ik\Delta z} \right].$$

(6)

$$\Rightarrow \lambda = 1 - 3\alpha D_0^2 v\left[1 - e^{-ik\Delta z}\right] + \beta D_0^3 \eta\left[2\cos(k\Delta z) - 2\right]$$

For the case when $\alpha = 0, \beta \neq 0$ we have.

$$\lambda = 1 + \beta D_0^3 \eta\left[2\cos(k\Delta z) - 2\right]$$

$$\Rightarrow \lambda = 1 + 2\beta D_0^3 \eta\left[\cos(k\Delta z) - 1\right].$$

~~Cos~~ Double angle formula $\cos(2x) = 2\cos^2(x) - 1$

$$\Rightarrow \lambda = 1 + 4\beta D_0^3 \eta\left[\cos^2\left(\frac{k\Delta z}{2}\right) - 1\right]$$

$$\Rightarrow \lambda = 1 - 4\beta D_0^3 \eta \sin^2\left(\frac{k\Delta z}{2}\right).$$

Now for stability we require.

$$|\lambda| < 1$$

$\Rightarrow$ we need.

$$\left|1 - 4\beta D_0^3 \eta \sin^2\left(\frac{k\Delta z}{2}\right)\right| < 1$$

$$\Rightarrow 0 < \beta D_0^3 \eta \sin^2\left(\frac{k\Delta z}{2}\right) < \frac{1}{2}$$

Clearly $\beta D_0^3 \eta \sin^2\left(\frac{k\Delta z}{2}\right) > 0$. $\therefore$ we need

(7)

$$\beta D_0^3 M < \frac{1}{2}$$

$$\Rightarrow \Delta t < \frac{(\Delta z)^2}{2\beta D_0^3}$$

To ensure stability in ~~ex~~ diffusion scheme.

Similarly for $\beta = 0$ & $\alpha \neq 0$ we have

$$\lambda = 1 - 3\alpha D_0^2 \nu \left[1 - e^{-ik\Delta z}\right]$$

We need $|\lambda| < 1$ for stability

$$\Rightarrow \left|1 - 3\alpha D_0^2 \nu \left[1 - e^{-ik\Delta z}\right]\right| < 1$$

$$\Rightarrow -1 < 1 - 3\alpha D_0^2 \nu \left[1 - e^{-ik\Delta z}\right] < 1$$

$$\Rightarrow -2 < -3\alpha D_0^2 \nu \left[1 - e^{-ik\Delta z}\right] < 0$$

$$\Rightarrow 0 < \alpha D_0^2 \nu \left[1 - e^{-ik\Delta z}\right] < \frac{2}{3}$$

Clearly $Re\left(\alpha D_0^2 \left[1 - e^{-ik\Delta z}\right]\right) > 0$

$\therefore$ To ensure stability we need.

$$\alpha D_0^2 \nu < \frac{1}{3}$$

$$\Rightarrow \Delta t = \frac{\Delta z}{3\alpha D_0^2}$$

8

Hence, to ensure a stable time step & we choose Δt is sm

$$\Delta t < \min\left(\frac{\Delta z}{3\alpha D_0^2}, \frac{(\Delta z)^2}{2\beta D_0^3}\right).$$

d). Re-writing the discretisation of the linear convective diffusion eqn yields

$$B_j'^{n+1} = \left(1 - 3\alpha D_0^2 \nu - 2\beta D_0^3 m\right) B_j'^{n} + \beta m D_0^3 B_{j+1}'^{n} + \left[3\alpha D_0^2 \nu + \beta m D_0^3\right] B_{j-1}'^{n}$$

$\therefore$ Assuming $B_j'^n > 0$ to ensure $B_j'^{n+1} > 0$ ~~we need~~. (which is the maximum principle) we need.

$$1 - 3\alpha D_0^2 \nu - 2\beta D_0^3 m > 0.$$

$$\Rightarrow 3\alpha D_0^2 \frac{\Delta t}{\Delta z} + 2\beta D_0^3 \frac{\Delta t}{(\Delta z)^2} < 1$$

$$\Rightarrow \Delta t < \frac{1}{\frac{3\alpha D_0^2}{\Delta z} + \frac{2\beta D_0^3}{(\Delta z)^2}}$$

$$\Rightarrow \Delta t < \frac{(\Delta z)^2}{3\alpha D_0^2 \Delta z + 2\beta D_0^3}.$$

(9)

e). We do this by using the maximum principle, the discretisation is given by

$$B_j^{n+1} = \left[1 - 3\alpha r (B_j^n)^2 - \frac{\beta m}{8}\left[(B_{j+1}^n + B_j^n)^3 + (B_j^n + B_{j-1}^n)^3\right]\right] B_j^n$$

$$+ \frac{\beta m}{8}(B_{j+1}^n + B_j^n)^3 B_{j+1}^n + \left[\frac{\beta m}{8}(B_j^n + B_{j-1}^n)^3 + 3\alpha r (B_j^n)^2\right] B_{j-1}^n$$

$\therefore$ Assuming $B_j^n > 0$ for $B_j^{n+1} > 0$ we require

$$1 - 3\alpha r (B_j^n)^2 - \frac{\beta m}{8}\left[(B_{j+1}^n + B_j^n)^3 + (B_j^n + B_{j-1}^n)^3\right] > 0.$$

$$\Delta t \left[\frac{3\alpha (B_j^n)^2}{\Delta z} + \frac{\beta\left[(B_{j+1}^n + B_j^n)^3 + (B_j^n + B_{j-1}^n)^3\right]}{8(\Delta z)^2}\right] < 1.$$

$$\therefore \Delta t < \frac{8(\Delta z)^2}{24\alpha (B_j^n)^2 \Delta z + \beta\left[(B_{j+1}^n + B_j^n)^3 + (B_j^n + B_{j-1}^n)^3\right]}$$

$\therefore$ To guarantee stability we require.

$$\Delta t < \frac{(\Delta z)^2}{3\alpha B_m^2 \Delta z + 2\beta B_m^3}$$, where ~~$B_m = \max(B_j^n)$~~.

$B_m = \max(B_j^n) \; \forall n, j.$

f). By Morton and Mayers (2005) we get Second-order spatial discretisation if we take a double interval central difference for the first difference in space, which yields.

$$B_j^{n+1} = B_j^n - \frac{3\alpha\sqrt{\ }(B_j^n)^2}{2}\left[B_{j+1}^n - B_{j-1}^n\right] + \frac{\beta m}{8}\left[(B_{j+1}^n + B_j^n)^3(B_{j+1}^n - B_j^n) - (B_j^n + B_{j-1}^n)^3(B_j^n - B_{j-1}^n)\right]$$

∴ Re-writing we get

$$B_j^{n+1} = \left[1 - \frac{\beta m}{8}\left[(B_{j+1}^n + B_j^n)^3 + (B_j^n + B_{j-1}^n)^3\right]\right] B_j^n$$

$$+ \left(\frac{\beta m}{8}(B_{j+1}^n + B_j^n)^3 - \frac{3\alpha\sqrt{\ }}{2}(B_j^n)^2\right] B_{j+1}^n$$

$$+ \left[\frac{\beta m}{8}(B_j^n + B_{j-1}^n)^3 + \frac{3\alpha\sqrt{\ }}{2}(B_j^n)^2\right) B_{j-1}^n .$$

∴ For stability we require the following constraint on the time step:

$$1 - \frac{\beta m}{8}\left[(B_{j+1}^n + B_j^n)^3 + (B_j^n + B_{j-1}^n)^3\right] \geq 0$$

$$\Delta t\left[\frac{\beta\left[(B_{j+1}^n + B_j^n)^3 + (B_j^n + B_{j-1}^n)^3\right]}{\cancel{8(\Delta z)^2}\ 8(\Delta z)^2}\right) < 1.$$

(11)

$$\therefore \Delta t < \frac{\cancel{\phi}\ 8(\Delta z)^2}{\beta\left[(B_{j+1}^n + B_j^n)^3 + (B_j^n + B_{j-1}^n)^3\right]}$$

Furthermore, to ensure we need.

$$\Delta t < \frac{(\Delta z)^2}{2\beta B_M^3}$$

we also need the following constraint on the Δz. given by B_{j+1}^n coefficient, ~~which~~

$$\frac{\beta}{8}\left(B_{j+1}^n + B_j^n\right)^3 - \frac{3\alpha v}{2}(B_j^n)^2 > 0 .$$

$$\therefore \frac{\beta}{8(\Delta z)^2}\left(B_{j+1}^n + B_j^n\right)^3 > \frac{3\alpha}{2\Delta z}(B_j^n)^2$$

$$\frac{\beta\left(B_{j+1}^n + B_j^n\right)^3}{8} > \frac{3\alpha\Delta z}{2}(B_j^n)^2$$

(12)

$$\Rightarrow \Delta z < \frac{2\beta(2B_m)^3}{3\alpha B_m^2 \cdot 8}$$

∴ To ensure stability we need.

$$\Rightarrow \Delta z < \frac{2\beta B_m}{3\alpha}$$

∴ To ensure stability we need

$$\Delta t < \frac{(\Delta z)^2}{2\beta B_m^3} \quad \& \quad \Delta z < \frac{2\beta B_m}{3\alpha}$$

$$\Rightarrow \Delta t < \frac{\left(\frac{2\beta B_m}{3\alpha}\right)^2}{2\beta B_m^3}$$

$$= \frac{\frac{4\beta^2 B_m^2}{9\alpha^2}}{2\beta B_m^3}$$

$$= \frac{4\beta^2 B_m^2}{18\alpha^2\beta B_m^3}$$

$$= \frac{\cancel{2\beta B}\ 2\beta}{9\alpha^2 B_m}$$

∴ we need $\Delta t < \frac{2\beta}{9\alpha^2 B_m}$