

Firstly, I hope I have not erred, but here is the derivation. Starting with Tessum et al., eqn. 3 (simplifying to one direction, letting $f_{w,e}=1$), and dividing by Δt :

$$\frac{\Delta C_i}{\Delta t} = \frac{F_A(U_{pos}C_w - U_{neg}C_i)}{\Delta x} + \frac{F_A(U_{neg}C_e - U_{pos}C_i)}{\Delta x}$$

First, let the west cell be the $i-1$ cell and the east cell be the $i+1$ cell. Then put the U_{pos} and U_{neg} terms together:

$$\frac{\Delta C_i}{\Delta t} = \frac{F_A U_{pos}(C_{i-1} - C_i)}{\Delta x} + \frac{F_A U_{neg}(C_{i+1} - C_i)}{\Delta x}$$

Now add and subtract $\frac{F_A U_{pos}(C_{i+1} - C_i)}{\Delta x}$ (the two middle terms):

$$\frac{\Delta C_i}{\Delta t} = \frac{F_A U_{pos}(C_{i-1} - C_i)}{\Delta x} + \frac{F_A U_{pos}(C_{i+1} - C_i)}{\Delta x} - \frac{F_A U_{pos}(C_{i+1} - C_i)}{\Delta x} + \frac{F_A U_{neg}(C_{i+1} - C_i)}{\Delta x}$$

Rearranging gives:

$$\frac{\Delta C}{\Delta t} = \frac{F_A(U_{pos})}{\Delta x} \left[\frac{C_{i-1} - 2C_i + C_{i+1}}{\Delta x} \right] + F_A(U_{pos} - U_{neg}) \left(\frac{C_i - C_{i+1}}{\Delta x} \right)$$

Multiply the numerator and denominator of the first term by Δx :

$$\frac{\Delta C}{\Delta t} = \frac{F_A(\Delta x U_{pos})}{\Delta x^2} \left[\frac{C_{i-1} - 2C_i + C_{i+1}}{\Delta x^2} \right] + F_A(U_{pos} - U_{neg}) \left(\frac{C_i - C_{i+1}}{\Delta x} \right)$$

The authors may wish to consider if the last term may have some numerical/physical issues in some cases.

I do believe that if you have the first term using $(U_{pos}+U_{neg})/2$, you get:

$$\frac{\Delta C}{\Delta t} = \frac{F_A \Delta x (U_{pos} + U_{neg})}{2} \left[\frac{C_{i-1} - 2C_i + C_{i+1}}{\Delta x^2} \right] + F_A (U_{neg} - U_{pos}) \left(\frac{C_{i+1} - C_{i-1}}{2\Delta x} \right)$$

This leads to a central difference form for both advection and diffusion. Both the first order advection and central difference advection adds increased numerical diffusion, on top of the diffusion from the first term, and the advection term is not dependent upon the concentration in the i cell. The authors might consider dividing their solution to four periods, and during each period use the different

combinations of U_{pos} , U_{neg} , V_{pos} and V_{neg} . This would remove the large diffusion term introduced in the current method, though the advection approach used is still diffusive. They might consider using a higher order advection scheme that is less diffusive. They should also consider making F_A equal to 1 to maintain concordance with the original equation and have the correct asymptotic behaviour. Whichever approach is chosen, it should be tested against cases with a known solutions.