Centered finite difference in space and forward finite difference in time

Equilibrium dispersive model with linear isotherm:

$$\left(\frac{1}{D_{ax,i}}+\frac{(1+\varepsilon)K_{H,i}}{\varepsilon D_{ax,i}}\right)\frac{\partial c_{i,l}(t,x)}{\partial t}=\frac{\partial^2 c_{i,l}(t,x)}{\partial x^2}-\frac{u_m}{D_{ax,i}}\frac{\partial c_{l,i}(t,x)}{\partial x}$$

$$C_1=\left(\frac{1}{D_{ax,i}}+\frac{(1+\varepsilon)K_{H,i}}{\varepsilon D_{ax,i}}\right)$$

$$C_2=\frac{u_m}{D_{ax,i}}$$

$$C_1\frac{\partial c_{i,l}(t,x)}{\partial t}=\frac{\partial^2 c_{i,l}(t,x)}{\partial x^2}-C_2\frac{\partial c_{l,i}(t,x)}{\partial x}$$

Forward finite difference:

$$\frac{\partial c_{i,l}(t,x)}{\partial t}\approx\frac{c_{i,l}(t+\Delta t,x)-c_{i,l}(t,x)}{\Delta t}$$

Second-order finite difference:

$$\frac{\partial^2 c_{i,l}(t,x)}{\partial x^2}\approx\frac{c_{i,l}(t,x+\Delta x)-2c_{i,l}(t,x)+c_{i,l}(t,x-\Delta x)}{\Delta x^2}$$

Centered finite difference:

$$\frac{\partial c_{l,i}(t,x)}{\partial x}\approx\frac{c_{i,l}(t,x+\Delta x)-c_{i,l}(t,x-\Delta x)}{2\Delta x}$$

$$c_{i,l}(t+\Delta t,x)=c_{i,l}(t,x)+\frac{\Delta t(c_{i,l}(t,x+\Delta x)-2c_{i,l}(t,x)+c_{i,l}(t,x-\Delta x))}{C_1\Delta x^2}-\frac{C_2\Delta t(c_{i,l}(t,x+\Delta x)-c_{i,l}(t,x-\Delta x))}{2C_1\Delta x}$$

Left boundary:

$$\left(\frac{\partial c_{l,i}(t,x)}{\partial x}\right)\bigg|_{x=0}\approx\frac{c_{i,l}(t,0+\Delta x)-c_{i,l}(t,0-\Delta x)}{2\Delta x}=\frac{u_m}{D_{ax,i}}\left(c_{l,i}(t,x)-c_{l,i}^{in}\right)$$

Fictitious point $L+\Delta x$ outside the domain. Elimination of $c_{i,l}(t,0-\Delta x)$ by usage of discrete boundary condition:

$$c_{i,l}(t,0-\Delta x)=c_{i,l}(t,L+\Delta x)$$

$$\frac{\partial^2 c_{i,l}(t,x)}{\partial x^2}\approx\frac{2c_{i,l}(t,0+\Delta x)-2c_{i,l}(t,x)}{\Delta x^2}$$

$$c_{i,l}(t+\Delta t,0)=\frac{\Delta t(2c_{i,l}(t,0+\Delta x)-2c_{i,l}(t,0))}{C_1\Delta x^2}-\frac{\Delta t C_2^2\left(c_{l,i}(t,0)-c_{l,i}^{in}\right)}{C_1}+c_{i,l}(t,0)$$

Right boundary:

$$\left(\frac{\partial c_{l,i}}{\partial x}\right)\bigg|_{x=L}\approx\frac{c_{i,l}(t,L+\Delta x)-c_{i,l}(t,L-\Delta x)}{2\Delta x}=0$$

Fictitious point $L+\Delta x$ outside the domain. Elimination of $c_{i,l}(t,L+\Delta x)$ by usage of discrete boundary condition:

$$c_{i,l}(t,L+\Delta x)=c_{i,l}(t,L-\Delta x)$$

$$\frac{\partial^2 c_{i,l}(t,x)}{\partial x^2}\approx\frac{2c_{i,l}(t,L-\Delta x)-2c_{i,l}(t,x)}{\Delta x^2}$$

$$c_{i,l}(t+\Delta t, L) = c_{i,l}(t, L) + \frac{\Delta t(2c_{i,l}(t, L-\Delta x) - 2c_{i,l}(t, x)}{C_1 \Delta x^2}$$

Initial conditions:

$$c_{l,i}|_{t=0} = 0$$