Discretización ecuación reacción difusión: | Fecha / Date:

Queremos resolver el siguiente sistema de forma numérica

$$\frac{\partial C_+}{\partial t} = -D_+\left(\nabla^2 C_+ - \nabla(C_+\nabla\psi)\right) \quad (1)$$

$$\frac{\partial C_-}{\partial t} = -D_{\pm}\left(\nabla^2 C_- + \nabla(C_-\nabla\psi)\right) \quad (2)$$

$$\nabla^2\psi = -\kappa^2(C_+ - C_-) \quad (3)$$

aproximando

$$\frac{\partial C_+(x_k)}{\partial t} \simeq \frac{C_+^{n+1,k} - C_+^{n,k}}{\Delta t}$$

y $$\frac{\partial^2\psi}{\partial x^2} = \frac{\psi^{n,k+1} - 2\psi^{n,k} + \psi^{n,k-1}}{\Delta x^2}$$

~~tenemos~~

y $$\frac{\partial^2 C_s}{\partial x^2} = C_s^{n,k+1} - 2C_s^{n,k} + C_s^{n,k-1}$$

Reemplazando en la ecuación (1) tenemos

Notas / Notes:

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$$C_+^{n+1,k} - C_+^{n,k} = -D_+ \Delta t \left(\frac{C_+^{n,k+1} - 2C_+^{n,k} + C_+^{n,k-1}}{\Delta x^2} - \left(\frac{C_+^{n,k+1} - C_+^{n,k}}{\Delta x}\right)\left(\frac{\psi^{n,k+1} - \psi^{n,k}}{\Delta x}\right) - C_+^{n,k}\left(\frac{\psi^{n,k+1} - 2\psi^{n,k} + \psi^{n,k-1}}{\Delta x^2}\right)\right)$$

$$= -D_+ \frac{\Delta t}{\Delta x^2}\Big(C_+^{n,k+1} - 2C_+^{n,k} + C_+^{n,k-1} - C_+^{n,k+1}\left(\psi^{n,k+1} - \psi^{n,k}\right) + C_+^{n,k}\left(\psi^{n,k+1} - \psi^{n,k}\right) - C_+^{n,k}\left(\psi^{n,k+1} - 2\psi^{n,k} + \psi^{n,k-1}\right)\Big)$$

$$\cancel{= -D_+ \frac{\Delta t}{\Delta x^2}\Big(}$$

Sea $\rho_s = D_s \frac{\Delta t}{\Delta x^2}$; $s = \pm$.

Tenemos

$$\cancel{C_+^{n+1,k} = C_+^{n,k}\left(1 - \rho_+\left(-2 + \left(\psi^{n,k+1} - \psi^{n,k} - \psi^{n,k+1} + 2\psi^{n,k} - \psi^{n,k-1}\right.\right.\right.}$$

$$= C_+^{n,k}\left(1 + \rho_+\left(2 - \left(2\psi^{n,k+1} - \psi^{n,k} - \psi^{n,k-1}\right)\right)\right)$$

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$$C_+^{n+1,k} = C_+^{n,k} - \rho_+\Big(C_+^{n,k}\big(-2+\psi^{n,k}-\psi^{n,k-1}\big)$$
$$+ C_+^{n,k+1}\big(1+\psi^{n,k}-\psi^{n,k+1}\big)$$
$$+ C_+^{n,k-1}\Big)$$

$$\boxed{C_+^{n+1,k} = \Big(C_+^{n,k}\big(1-\rho_+\big(-2+\psi^{n,k}-\psi^{n,k-1}\big)\big) - \rho_+\big(1+\psi^{n,k}-\psi^{n,k+1}\big) - \rho_+ C_+^{n,k-1}\Big)}$$

En la ecuación (2) tenemos

$$C_-^{n,k+1} - C_-^{n,k} = -D_-\frac{\Delta t}{\Delta x^2}\Big(C_-^{n,k+1} - 2C_-^{n,k} + C_-^{n,k-1}$$
$$+ \big(C_-^{n,k+1} - C_-^{n,k}\big)\big(\psi^{n,k+1}-\psi^{n,k}\big)$$
$$+ C_-^{n,k}\big(\psi^{n,k+1} - 2\psi^{n,k} + \psi^{n,k-1}\big)\Big)$$

$$C_+^{n,k+1} = C_-^{n,k} - \rho_-\Big(C_-^{n,k+1}\big(1+\psi^{n,k+1}-\psi^{n,k}\big)$$
$$+ C_-^{n,k-1}$$
$$+ C_-^{n,k}\big(-2+\cancel{\psi^{n,k}}-\cancel{\psi^{n,k+1}}\big)$$
$$+ C_-^{n,k}\big(\cancel{\psi^{n,k+1}} - \underset{1}{\cancel{2}}\psi^{n,k} + \psi^{n,k-1}\big)\Big)$$

$$C_-^{n,k+1} = C_-^{n,k}\big(1-\rho_-\big(-2-\psi^{n,k}+\psi^{n,k-1}\big)\big)$$
$$-\rho_- C_-^{n,k+1}\big(1+\psi^{n,k+1}-\psi^{n,k}\big)$$
$$-\rho_- C_-^{n,k-1}$$

Notas / Notes:

Finalmente en la ecuación (3) tenemos:

$$\psi^{n,k+1} - 2\psi^{n,k} + \psi^{n,k-1} = -K^2 \Delta x^2 \left(C_+^{n,k} - C_-^{n,k} \right)$$

$$\boxed{\psi^{n,k+1} - 2\psi^{n,k} + \psi^{n,k-1} = -\bar{K}^2 \left(C_+^{n,k} - C_-^{n,k} \right)}$$