Caso transporte difusivo y decaimiento de contaminantes

Tips para formulación General

Descripción general del caso

En este caso se deben determinar los perfiles de concentración de dos contaminantes en un río. Uno de los contaminantes (P) decae gradualmente hacia un contaminante más estable (Q). Ambas sustancias obedecen a una evolución de advección-difusión. Ambos contaminantes son transportados advectivamente a una velocidad constante u, aunque también presentan difusión espacial dada por un coeficiente de difusión $D(x)$ NO contante en el espacio. El sistema se puede describir con el siguiente conjunto de ecuaciones de advección, difusión, reacción:

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x}\left[D(x)\,\frac{\partial P}{\partial x}\right] - u\,\frac{\partial P}{\partial x} - \tau P + S \tag{2}$$

$$\frac{\partial Q}{\partial t} = \frac{\partial}{\partial x}\left[D(x)\,\frac{\partial Q}{\partial x}\right] - u\,\frac{\partial Q}{\partial x} + \tau P \tag{3}$$

Formulacion adimensional

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Utilizando tres propiedades para adimensionalizar: longitud (L_c), tiempo (t_c), y cantidad de reactivo de referencia (c), las expresiones anteriores se pueden expresar de forma adimensional como:

$$\frac{\partial P^*}{\partial t^*} = \frac{t_c}{L_c^2}\frac{\partial}{\partial x^*}\left[D(x)\,\frac{\partial P^*}{\partial x^*}\right] - \frac{u\,t_c}{L_c}\,\frac{\partial P*}{\partial x*} - \tau\,t_c\,P^* + \frac{t_c}{c}S$$

$$\frac{\partial Q^*}{\partial t^*} = \frac{t_c}{L_c^2}\frac{\partial}{\partial x}\left[D(x)\,\frac{\partial Q^*}{\partial x^*}\right] - \frac{u\,t_c}{L_c}\,\frac{\partial Q^*}{\partial x^*} + \tau\,t_c\,P^*$$

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$$\frac{\partial Q^*}{\partial t^*} = \frac{t_c}{L_c^2}\frac{\partial}{\partial x}\left[D(x)\frac{\partial Q^*}{\partial x^*}\right] - \frac{u\,t_c}{L_c}\frac{\partial Q^*}{\partial x^*} + \tau\, t_c\, P^*$$

la cual puede simplificarse si se selecciona como tiempo caracteristico la relación $t_c = L_c/u$, lo que resulta en:

$$\frac{\partial P^*}{\partial t^*} = \frac{1}{u\,L_c}\frac{\partial}{\partial x^*}\left[D(x)\frac{\partial P^*}{\partial x^*}\right] - \frac{\partial P*}{\partial x*} - \frac{\tau\, L_c}{u}P^* + \frac{L_c}{u\,c}S$$

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y con condiciones de frontera ahora expresadas como:

$$\left.\left(\frac{\partial P^*}{\partial x^*} - \frac{u\,L_c}{D}P^*\right)\right|_{x=0} = \left.\left(\frac{\partial Q^*}{\partial x^*} - \frac{u\,L_c}{D}\,Q^*\right)\right|_{x=0} = 0$$

definamos : $K_1 = \frac{1}{uL_c}$; $K_2 = \frac{G L_c}{u}$; $K_3 = \frac{L_c}{u \cdot C}$; $K_4 = \frac{u \cdot L_c}{D}$

$D(x)_{x=0}$

$$\frac{\partial P}{\partial t} = K_1 \cdot \frac{\partial}{\partial x}\left[D(x)\frac{\partial P}{\partial x}\right] - \frac{\partial P}{\partial x} - K_2\, P + K_3 \cdot S$$

$$\frac{P_i^{n+1} - P_i^{n}}{\Delta t} = \boxed{\frac{K_1}{2}\frac{\partial}{\partial x}\left[D(x)\cdot \frac{P_{i+1}^{n+1} - P_{i-1}^{n+1}}{x_{i+1} - x_{i-1}}\right]} - \frac{1}{2}\frac{P_{i+1}^{n+1} - P_{i-1}^{n+1}}{x_{i+1} - x_{i-1}} - \frac{K_2}{2}P_i^{n+1}$$

$$+ \frac{K_3}{2} S_i^{n+1} + \frac{K_1}{2}\frac{\partial}{\partial x}\left[D(x)\cdot \frac{P_{i+1}^{n} - P_{i-1}^{n}}{x_{i+1} - x_{i-1}}\right] - \frac{1}{2}\frac{P_{i+1}^{n} - P_{i-1}^{n}}{x_{i+1} - x_{i-1}} - \frac{K_2}{2}P_i^{n}$$

$$+ \frac{K_3}{2} S_i^{n} +$$

OJO: Expresiones SON Adimensionales

$$\frac{P_i^{n+1}-P_i^{n}}{\Delta t} = \frac{k_1}{2}\left[\frac{D_{i+1/2}\dfrac{P_{i+1}^{n+1}-P_i^{n+1}}{x_{i+1}-x_i} - D_{i-1/2}\dfrac{P_i^{n+1}-P_{i-1}^{n+1}}{x_i-x_{i-1}}}{1/2\,(x_{i+1}-x_{i-1})}\right] - \frac{1}{2}\left(\frac{P_{i+1}^{n+1}-P_{i-1}^{n+1}}{x_{i+1}-x_{i-1}}\right)$$

$$-\frac{k_2}{2}P_i^{n+1} + \frac{k_3}{2}\cdot S_i^{n+1} +$$

$$\frac{k_1}{2}\left[\frac{D_{i+1/2}\dfrac{P_{i+1}^{n}-P_i^{n}}{x_{i+1}-x_i} - D_{i-1/2}\dfrac{P_i^{n}-P_{i-1}^{n}}{x_i-x_{i-1}}}{1/2\,(x_{i+1}-x_{i-1})}\right] - \frac{1}{2}\left(\frac{P_{i+1}^{n}-P_{i-1}^{n}}{x_{i+1}-x_{i-1}}\right)$$

$$-\frac{k_2}{2}P_i^{n} + \frac{k_3}{2}\cdot S_i^{n}$$

$$
\begin{aligned}
P_i^{n+1} = P_i^n &+ \frac{K_1 \Delta t}{2}\left[\frac{D_{i+1/2}\left(P_{i+1}^{n+1} - P_i^{n+1}\right)(x_i - x_{i-1}) - D_{i-1/2}\left(P_i^{n+1} - P_{i-1}^{n+1}\right)(x_{i+1} - x_i)}{1/2\,(x_{i+1} - x_{i-1})(x_{i+1} - x_i)(x_i - x_{i-1})}\right] \\
&- \frac{\Delta t}{2(x_{i+1} - x_{i-1})}\left(P_{i+1}^{n+1} - P_{i-1}^{n+1}\right) - \frac{K_2 \Delta t}{2} P_i^{n+1} + \frac{K_3 \Delta t}{2} S_i^{n+1} \\
&+ \frac{K_1 \Delta t}{2}\left[\frac{D_{i+1/2}\left(P_{i+1}^{n} - P_i^{n}\right)(x_i - x_{i-1}) - D_{i-1/2}\left(P_i^{n} - P_{i-1}^{n}\right)(x_{i+1} - x_i)}{1/2\,(x_{i+1} - x_{i-1})(x_{i+1} - x_i)(x_i - x_{i-1})}\right] \\
&- \frac{\Delta t}{2(x_{i+1} - x_{i-1})}\left(P_{i+1}^{n} - P_{i-1}^{n}\right) - \frac{K_2 \Delta t}{2} P_i^{n} + \frac{K_3 \Delta t}{2} S_i^{n}
\end{aligned}
$$

$$P_i^{n+1} = P_i^{n} + \boxed{\frac{\Delta t\, D_{i+1/2}\, K_1\,(x_i - x_{i-1})}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)(x_i - x_{i-1})}}\,\alpha\,\left(P_{i+1}^{n+1} - P_i^{n+1}\right)$$

$$- \boxed{\frac{\Delta t\, D_{i-1/2}\, K_1\,(x_{i+1} - x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)(x_i - x_{i-1})}}\,\beta\,\left(P_i^{n+1} - P_{i-1}^{n+1}\right)$$

$$- \boxed{\frac{\Delta t}{2\,(x_{i+1}-x_{i-1})}\ \gamma}\cdot\left(P_{i+1}^{n+1} - P_{i-1}^{n+1}\right) - \overset{\delta}{\boxed{\frac{K_2\,\Delta t}{2}}}\,P_i^{n+1} + \overset{\eta}{\boxed{\frac{K_3\,\Delta t}{2}}}\,S_i^{n+1}$$

$$+ \boxed{\frac{\Delta t\, D_{i+1/2}\, K_1\,(x_i - x_{i-1})}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)(x_i - x_{i-1})}}\,\alpha\,\left(P_{i+1}^{n} - P_i^{n}\right)$$

$$- \boxed{\frac{\Delta t\, D_{i-1/2}\, K_1\,(x_{i+1} - x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)(x_i - x_{i-1})}}\left(P_i^{n} - P_{i-1}^{n}\right)$$

$$- \frac{\Delta t}{2\,(x_{i+1}-x_{i-1})}\cdot\left(P_{i+1}^{n} - P_{i-1}^{n}\right) - \frac{K_2\,\Delta t}{2}\,P_i^{n} + \frac{K_3\,\Delta t}{2}\,S_i^{n}$$

$$P_i^{n+1} = P_i^n + \alpha P_{i+1}^{n+1} - \alpha P_i^{n+1} - \beta P_i^{n+1} + \beta P_{i-1}^{n+1} - \gamma P_{i+1}^{n+1} + \gamma P_{i-1}^{n+1} - \delta P_i^{n+1} + \eta S_i^{n+1}$$

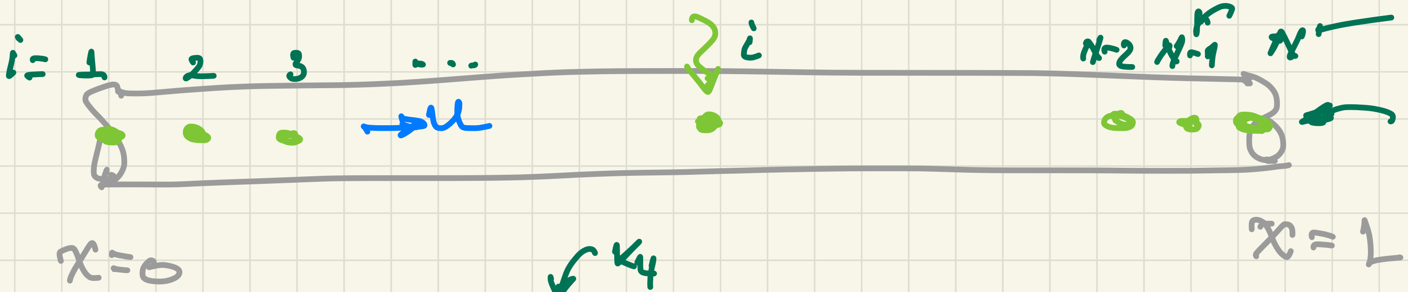
$$+ \alpha P_{i+1}^{n} - \alpha P_i^{n} - \beta P_i^{n} + \beta P_{i-1}^{n} - \gamma P_{i+1}^{n} + \gamma P_{i-1}^{n} - \delta P_i^{n} + \eta S_i^{n}$$

$$-\underbrace{(\beta+\gamma)}_{a} P_{i-1}^{n+1} + \underbrace{(1+\alpha+\beta+\delta)}_{b_1} P_i^{n+1} - \underbrace{(\alpha-\gamma)}_{c} P_{i+1}^{n+1} =$$

$$\underbrace{(\beta+\gamma)}_{a} P_{i-1}^{n} + \underbrace{(1-\alpha-\beta-\delta)}_{b2} P_i^{n} + \underbrace{(\alpha-\gamma)}_{c} P_{i+1}^{n} + \eta(\underbrace{S_i^{n+1} + S_i^{n}}_{\text{No hay variación temporal}})$$

$$-aP_{i-1}^{n+1} + b_1 P_i^{n+1} - c\,P_{i+1}^{n+1} = a P_{i-1}^{n} + b_2 P_i^{n} + c\,P_{i+1}^{n} + 2\eta S_i$$

$\boxed{\text{i-ésimo nodo.}}$ (N-2 nodos)



en $x=L$

$P=C$

$Q=C$

$P^*=1$

$Q^*=1$

En $x=0$

$$\frac{\partial P}{\partial x} - \frac{u L_c}{D}\cdot P = 0 \qquad \left(\frac{u L_c}{D} = K_4\right)$$

$$\frac{\partial P}{\partial x} = K_4 P \quad \therefore \quad \frac{P^{o}_{i+1} - P^{o}_{i-1}}{x_{i+1} - x_{i-1}} = K_4 P^{o}_i$$

$$P_{i-1} = P_{i+1} - K_4\,(x_{i+1} - x_{i-1})\,P_i$$

En $x=0$

En $i=1$ $\quad \boxed{P_0 = P_2 - K_4\,(x_2 - x_0)\,P_1}$

$$-a\left(P_{i+1}^{n+1}-K_4(x_{i+1}-x_{i-1})P_i^{n+1}\right)+b_1P_i^{n+1}-c\,P_{i+1}^{n+1}=$$

$$a\left(P_{i+1}^{n}-K_4(x_{i+1}-x_{i-1})P_i^{n}\right)+b_2P_i^{n}+cP_{i+1}^{n}+2\eta S_i$$

$$\underbrace{\left(aK_4(x_{i+1}-x_{i-1})+b_1\right)}_{d_1}P_i^{n+1}-(a+c)P_{i+1}^{n+1}=$$

$$\underbrace{\left(b_2-aK_4(x_{i+1}-x_{i-1})\right)}_{d_2}P_i^{n}+(a+c)P_{i+1}^{n}+2\eta S_i$$

En $i=1$

$$-aP_{i-1}^{n+1}+b_1P_i^{n+1}-cP_{i+1}^{n+1}=aP_{i-1}^{n}+b_2P_i^{n}+cP_{i+1}^{n}+2\eta S_i$$

Para $i=2,\dots,N-1$

$$
\begin{bmatrix}
d_1 & -(a+c) & & & & \\
-a & b_1 & -c & & & \\
 & -a & b_1 & -c & & \\
 & & & \ddots & & \\
 & & & -a & b_1 & -c \\
 & & & & -a & b_1
\end{bmatrix}
\begin{bmatrix}
P_1 \\ P_2 \\ P_3 \\ \vdots \\ P_{N-2} \\ P_{N-1}
\end{bmatrix}^{n+1}
=
$$

$$
\underline{\underline{A}}\,\underline{P}^{n+1} =
$$

$$
\begin{bmatrix}
d_2 & (a+c) & & & & & \\
a & b_2 & c & & & & \\
 & a & b_2 & c & & & \\
 & & a & b_2 & c & & \\
 & & & & \ddots & & \\
 & & & & a & b_2 & c \\
 & & & & & a & b_2
\end{bmatrix}
\begin{bmatrix}
P_1 \\ P_2 \\ P_3 \\ \vdots \\ \\ P_{N-2} \\ P_{N-1}
\end{bmatrix}^n
+
\begin{bmatrix}
2\eta S_1 \\ 2\eta S_2 \\ 2\eta S_3 \\ \vdots \\ \\ 2\eta S_{N-2} \\ 2\eta S_{N-1} + c\hat{P}_N^n + c\hat{P}_N^{n+1}
\end{bmatrix}
$$

$$\underline{\underline{B}}\ \underline{P}^n$$