Equilibrium Dispersive Model with Linear isotherm

Equilibrium dispersive model with linear isotherm:

$$\left(\frac{1}{D_{ax}} + \frac{(1+\varepsilon)K_H}{\varepsilon D_{ax}}\right)\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} - \frac{u_m}{D_{ax}}\frac{\partial c}{\partial x}$$

$$C_1 = \frac{1}{D_{ax}}\left(1 + \frac{(1+\varepsilon)K_H}{\varepsilon}\right)$$

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

$$C_1\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} - C_2\frac{\partial c}{\partial x}$$

Feed injection piecewise function:

$$c_{in} = \begin{cases} c^{feed} & pro\ t \leq t^{feed} \\ 0 & pro\ t\ >\ t^{feed} \end{cases}$$

Left boundary:

$$\left.\left(\frac{\partial c}{\partial x}\right)\right|_{x=0} = u_m[c - c_{in}]$$

Right boundary:

$$\left.\left(\frac{\partial c}{\partial x}\right)\right|_{x=L} = 0$$

Initial Conditions:

$$c|_{t=0} = 0$$

Implicit Crank-Nicolson scheme

Average of Centered Differencing formulas in space:

$$\frac{\partial c}{\partial x} \approx \frac{1}{2}\left[\frac{c_{i+1}^{j} - c_{i-1}^{j}}{2\Delta x} + \frac{c_{i+1}^{j+1} - c_{i-1}^{j+1}}{2\Delta x}\right]$$

Average of Second-order centered differencing formulas in space:

$$\frac{\partial^2 c}{\partial x^2} \approx \frac{1}{2}\left[\frac{c_{i+1}^{j} - 2c_i^{j} + c_{i-1}^{j}}{\Delta x^2} + \frac{c_{i+1}^{j+1} - 2c_i^{j+1} + c_{i-1}^{j+1}}{\Delta x^2}\right]$$

Forward differencing in time:

$$\frac{\partial c}{\partial t} \approx \frac{c_i^{j+1} - c_i^{j}}{\Delta t}$$

Full approximation:

$$c_i^{j+1} = c_i^{j} + \frac{\Delta t}{2C_1\Delta x^2}\left[c_{i+1}^{j} - 2c_i^{j} + c_{i-1}^{j} + c_{i+1}^{j+1} - 2c_i^{j+1} + c_{i-1}^{j+1}\right] - \frac{C_2\Delta t}{4C_1\Delta x}\left[c_{i+1}^{j} - c_{i-1}^{j} + c_{i+1}^{j+1} - c_{i+1}^{j-1}\right]$$

Left boundary

Left boundary uses averages of previous and calculated values:

$$\left.\left(\frac{\partial c}{\partial x}\right)\right|_{x=0} = u_m\left[c_0^{j} - c_{in}\right]$$

Substitution of derivation by linear approximation arises:

$$\frac{\partial c}{\partial x} \approx \frac{c_1^{j+1} - c_{-1}^{j+1}}{2\Delta x}$$

$$\frac{c_1^{j+1} - \boldsymbol{c_{-1}^{j+1}}}{2\Delta x} = u_m\left[c_0^j - c_{in}\right]$$

Second derivative by linear approximation is expressed as:

$$\frac{\partial^2 c}{\partial x^2} \approx \frac{c_1^{j+1} - 2c_0^{j+1} + c_{-1}^{j+1}}{\Delta x^2}$$

Centered scheme average with fictious point substitution:

Fictitious point c_{-1}^j is being introduced. It has negative axial coordinate $-\Delta x$.

Expressing c_{-1}^{j+1} as function of c_0^j, c_1^{j+1} and c_0^{j+1} from initial PDE:

$$C_1 \frac{c_0^{j+1} - c_0^j}{\Delta t} = \frac{c_1^{j+1} - 2c_0^{j+1} + c_{-1}^{j+1}}{\Delta x^2} - C_2 \frac{c_1^{j+1} - c_{-1}^{j+1}}{2\Delta x}$$

$$\frac{C_1}{\Delta t} c_0^{j+1} - \frac{C_1}{\Delta t} c_0^j = \frac{1}{\Delta x^2} c_1^{j+1} - \frac{2}{\Delta x^2} c_0^{j+1} + \frac{1}{\Delta x^2} \boldsymbol{c_{-1}^{j+1}} - \frac{C_2}{2\Delta x} c_1^{j+1} + \frac{C_2}{2\Delta x} \boldsymbol{c_{-1}^{j+1}}$$

$$-\left(\frac{1}{\Delta x^2} + \frac{C_2}{2\Delta x}\right) \boldsymbol{c_{-1}^{j+1}} = \left(\frac{1}{\Delta x^2} - \frac{C_2}{2\Delta x}\right) c_1^{j+1} - \left(\frac{2}{\Delta x^2} + \frac{C_1}{\Delta t}\right) c_0^{j+1} + \frac{C_1}{\Delta t} c_0^j$$

$$\boldsymbol{c_{-1}^{j+1}} = \frac{\left(\frac{1}{\Delta x^2} - \frac{C_2}{2\Delta x}\right)}{-\left(\frac{1}{\Delta x^2} + \frac{C_2}{2\Delta x}\right)} c_1^{j+1} - \frac{\left(\frac{2}{\Delta x^2} + \frac{C_1}{\Delta t}\right)}{-\left(\frac{1}{\Delta x^2} + \frac{C_2}{2\Delta x}\right)} c_0^{j+1} + \frac{\frac{C_1}{\Delta t}}{-\left(\frac{1}{\Delta x^2} + \frac{C_2}{2\Delta x}\right)} c_0^j$$

Substituting expression into equation for left boundary:

$$\frac{c_1^{j+1} - \left[\frac{\left(\frac{1}{\Delta x^2} - \frac{C_2}{2\Delta x}\right)}{-\left(\frac{1}{\Delta x^2} + \frac{C_2}{2\Delta x}\right)} c_1^{j+1} - \frac{\left(\frac{2}{\Delta x^2} + \frac{C_1}{\Delta t}\right)}{-\left(\frac{1}{\Delta x^2} + \frac{C_2}{2\Delta x}\right)} c_0^{j+1} + \frac{\frac{C_1}{\Delta t}}{-\left(\frac{1}{\Delta x^2} + \frac{C_2}{2\Delta x}\right)} c_0^j\right]}{2\Delta x} = u_m\left[c_0^j - c_{in}\right]$$

$$\left(1 - \frac{\left(\frac{1}{\Delta x^2} - \frac{C_2}{2\Delta x}\right)}{-\left(\frac{1}{\Delta x^2} + \frac{C_2}{2\Delta x}\right)}\right) c_1^{j+1} + \frac{\left(\frac{2}{\Delta x^2} + \frac{C_1}{\Delta t}\right)}{-\left(\frac{1}{\Delta x^2} + \frac{C_2}{2\Delta x}\right)} c_0^{j+1} = \left(2\Delta x u_m + \frac{\frac{C_1}{\Delta t}}{-\left(\frac{1}{\Delta x^2} + \frac{C_2}{2\Delta x}\right)}\right) c_0^j - 2\Delta x u_m c_{in}$$

Right boundary

$$\left.\left(\frac{\partial c}{\partial x}\right)\right|_{x=L} = 0$$

Substitution of derivation by linear approximation arises:

$$\frac{\partial c}{\partial x} \approx \frac{c_1^{j+1} - c_{-1}^{j+1}}{2\Delta x}$$

$$\frac{\boldsymbol{c_1^{j+1}} - c_{-1}^{j+1}}{2\Delta x} = 0$$

Expressing c_1^{j+1} as function of c_0^j, c_{-1}^{j+1} and c_0^{j+1} from initial PDE:

$$\frac{c_i^{j+1} - c_i^j}{\Delta t} = \frac{c_1^{j+1} - 2c_0^{j+1} + c_{-1}^{j+1}}{\Delta x^2} - C_2 \frac{c_1^{j+1} - c_{-1}^{j+1}}{2\Delta x}$$

$$-\left(\frac{1}{\Delta x^2} - \frac{C_2}{2\Delta x}\right) \boldsymbol{c_1^{j+1}} = \left(\frac{1}{\Delta x^2} + \frac{C_2}{2\Delta x}\right) c_{-1}^{j+1} - \left(\frac{2}{\Delta x^2} + \frac{C_1}{\Delta t}\right) c_0^{j+1} + \frac{C_1}{\Delta t} c_0^j$$

$$\boldsymbol{c_1^{j+1}} = \frac{\left(\frac{1}{\Delta x^2}+\frac{C_2}{2\Delta x}\right)}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} c_{-1}^{j+1} - \frac{\left(\frac{2}{\Delta x^2}+\frac{C_1}{\Delta t}\right)}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} c_0^{j+1} + \frac{\frac{C_1}{\Delta t}}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} c_0^j$$

Substituting expression into equation for Right boundary:

$$\frac{\left(\frac{\left(\frac{1}{\Delta x^2}+\frac{C_2}{2\Delta x}\right)}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} - \right) 1 c_{-1}^{j+1} - \frac{\left(\frac{2}{\Delta x^2}+\frac{C_1}{\Delta t}\right)}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} c_0^{j+1} + \frac{\frac{C_1}{\Delta t}}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} c_0^j}{2\Delta x} = 0$$

$$\left(\frac{\left(\frac{1}{\Delta x^2}+\frac{C_2}{2\Delta x}\right)}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} - 1\right) c_{-1}^{j+1} - \frac{\left(\frac{2}{\Delta x^2}+\frac{C_1}{\Delta t}\right)}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} c_0^{j+1} = -\frac{\frac{C_1}{\Delta t}}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} c_0^j$$

Final Cranck-Nicolson expression

Leading to system of algebraic equations:

$$A \cdot \vec{c}^{\,j+1} = B \cdot \vec{c}^{\,j} + \vec{c}_{in}$$

Where $A,\ B,\ \vec{c}^{\,j}\ and\ \vec{c}_{in}$ are known and $\vec{c}^{\,j+1}$is solution vector of next time step which needs to be find by Seidl-Gauss iterative method.

$$\left(\frac{\left(\frac{1}{\Delta x^2}+\frac{C_2}{2\Delta x}\right)}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} - 1\right) c_{-1}^{j+1} - \frac{\left(\frac{2}{\Delta x^2}+\frac{C_1}{\Delta t}\right)}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} c_0^{j+1} = -\frac{\frac{C_1}{\Delta t}}{-\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)} c_0^j$$

$$A = \begin{bmatrix}
\frac{\left(\frac{2}{\Delta x^2}+\frac{C_1}{\Delta t}\right)}{-\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}} & 1-\frac{\left(\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}\right)}{-\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}} & 0 & 0 & \dots & 0 \\
-\frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}+\frac{C_2}{2}\right) & 1+\frac{\Delta t}{C_1\Delta x^2} & -\frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}-\frac{C_2}{2}\right) & 0 & \dots & 0 \\
0 & -\frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}+\frac{C_2}{2}\right) & 1+\frac{\Delta t}{C_1\Delta x^2} & -\frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}-\frac{C_2}{2}\right) & \dots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \dots & 0 & -\frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}+\frac{C_2}{2}\right) & 1+\frac{\Delta t}{C_1\Delta x^2} & -\frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}-\frac{C_2}{2}\right) \\
0 & \dots & 0 & 0 & \frac{\left(\frac{1}{\Delta x^2}+\frac{C_2}{2\Delta x}\right)}{-\frac{1}{\Delta x^2}+\frac{C_2}{2\Delta x}} - 1 & -\frac{\left(\frac{2}{\Delta x^2}+\frac{C_1}{\Delta t}\right)}{-\frac{1}{\Delta x^2}+\frac{C_2}{2\Delta x}}
\end{bmatrix}$$

$$B = \begin{bmatrix}
2\Delta x u_m + \frac{\frac{C_1}{\Delta t}}{-\frac{1}{\Delta x^2}-\frac{C_2}{2\Delta x}} & 0 & 0 & 0 & \dots & 0 \\
\frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}+\frac{C_2}{2}\right) & 1-\frac{\Delta t}{C_1\Delta x^2} & \frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}-\frac{C_2}{2}\right) & 0 & \dots & 0 \\
0 & \frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}+\frac{C_2}{2}\right) & 1-\frac{\Delta t}{C_1\Delta x^2} & \frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}-\frac{C_2}{2}\right) & \dots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \dots & 0 & \frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}+\frac{C_2}{2}\right) & 1-\frac{\Delta t}{C_1\Delta x^2} & \frac{\Delta t}{2\Delta x}\left(\frac{1}{C_1\Delta x}-\frac{C_2}{2}\right) \\
0 & \dots & 0 & 0 & 0 & -\frac{\frac{C_1}{\Delta t}}{-\frac{1}{\Delta x^2}+\frac{C_2}{2\Delta x}}
\end{bmatrix}$$

$$\vec{c}^{\,j+1} = \begin{bmatrix} c_0^{j+1} \\ c_1^{j+1} \\ \vdots \\ c_i^{j+1} \\ \vdots \\ c_N^{j+1} \end{bmatrix}$$

$$\vec{c}^{\,j} = \begin{bmatrix} c_0^{j} \\ c_1^{j} \\ \vdots \\ c_i^{j} \\ \vdots \\ c_N^{j} \end{bmatrix}$$

$$\vec{c}_{in} = \begin{bmatrix} -2\Delta x u_m c_{in} \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$