Finite Difference Schemes for the numerical solution of heterogeneous diffusion equation in 2D

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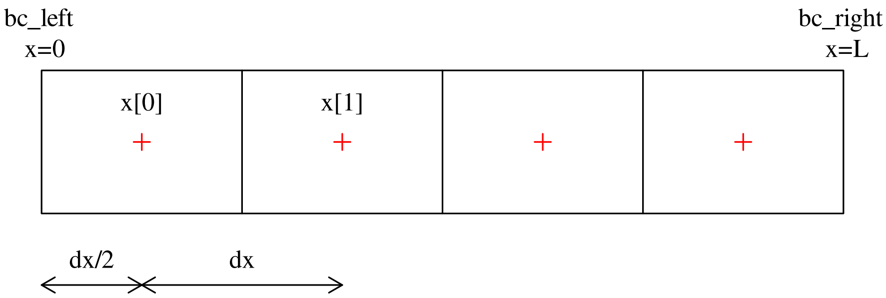
1 Homogeneous diffusion in 1D

1.1 Finite differences with nodes as cells' centres

The 1D diffusion equation for spatially constant diffusion coefficients α is:

$$\begin{aligned}\frac{\partial C}{\partial t} &= \frac{\partial}{\partial x}\left(\alpha \frac{\partial C}{\partial x}\right) \\ &= \alpha \frac{\partial^2 C}{\partial x^2}\end{aligned} \quad (1)$$

We aim at numerically solving 1 on a spatial grid such as:



The left boundary is defined on $x = 0$ while the center of the first cell - which are the points constituting the finite difference nodes - is in $x = dx/2$, with $dx = L/n$.

1.2 The explicit FTCS scheme (as in PHREEQC)

We start by discretizing 1 following an explicit Euler scheme and specifically a Forward Time, Centered Space finite difference.

For each cell index $i \in 1, \ldots, n-1$ and assuming constant α, we can write:

$$\frac{C_i^{t+1} - C_i^t}{\Delta t} = \alpha \frac{\frac{C_{i+1}^t - C_i^t}{\Delta x} - \frac{C_i^t - C_{i-1}^t}{\Delta x}}{\Delta x} \quad (2)$$

In practice, we evaluate the first derivatives of C w.r.t. x on the boundaries of each cell (i.e., $(C_{i+1} - C_i)/\Delta x$ on the right boundary of the i-th cell and $(C_i - C_{i-1})/\Delta x$ on its left cell boundary) and then repeat the differentiation to get the second derivative of C on the the cell centre i.

This discretization works for all internal cells, but not for the domain boundaries ($i = 0$ and $i = n$). To properly treat them, we need to account for the discrepancy in the discretization.

For the first (left) cell, whose center is at $x = dx/2$, we can evaluate the left gradient with the left boundary using such distance, calling l the numerical value of a constant boundary condition:

$$\frac{C_0^{t+1} - C_0^t}{\Delta t} = \alpha \frac{\frac{C_1^t - C_0^t}{\Delta x} - \frac{C_0^t - l}{\frac{\Delta x}{2}}}{\Delta x} \tag{3}$$

This expression, once developed, yields:

$$\begin{aligned} C_0^{t+1} &= C_0^t + \frac{\alpha \cdot \Delta t}{\Delta x^2} \cdot \left(C_1^t - C_0^t - 2C_0^t + 2l\right) \\ &= C_0^t + \frac{\alpha \cdot \Delta t}{\Delta x^2} \cdot \left(C_1^t - 3C_0^t + 2l\right) \end{aligned} \tag{4}$$

In case of constant right boundary, the finite difference of point C_n - calling r the right boundary value - is:

$$\frac{C_n^{t+1} - C_n^t}{\Delta t} = \alpha \frac{\frac{r - C_n^t}{\frac{\Delta x}{2}} - \frac{C_n^t - C_{n-1}^t}{\Delta x}}{\Delta x} \tag{5}$$

Which, developed, gives

$$\begin{aligned} C_n^{t+1} &= C_n^t + \frac{\alpha \cdot \Delta t}{\Delta x^2} \cdot \left(2r - 2C_n^t - C_n^t + C_{n-1}^t\right) \\ &= C_n^t + \frac{\alpha \cdot \Delta t}{\Delta x^2} \cdot \left(2r - 3C_n^t + C_{n-1}^t\right) \end{aligned} \tag{6}$$

If on the right boundary we have closed or Neumann condition, the left derivative in eq. 5 becomes zero and we are left with:

$$C_n^{t+1} = C_n^t + \frac{\alpha \cdot \Delta t}{\Delta x^2} \cdot (C_{n-1}^t - C_n^t) \tag{7}$$

A similar treatment can be applied to the BTCS implicit scheme.

1.3 Implicit BTCS scheme

First, we define the Backward Time difference:

$$\frac{\partial C^{t+1}}{\partial t} = \frac{C_i^{t+1} - C_i^t}{\Delta t} \tag{8}$$

Second the spatial derivative approximation, evaluated at time level $t + 1$:

$$\frac{\partial^2 C^{t+1}}{\partial x^2} = \frac{\frac{C_{i+1}^{t+1} - C_i^{t+1}}{\Delta x} - \frac{C_i^{t+1} - C_{i-1}^{t+1}}{\Delta x}}{\Delta x} \tag{9}$$

Taking the 1D diffusion equation from 1 and substituting each term by the equations given above leads to the following equation:

$$\begin{aligned} \frac{C_i^{t+1} - C_i^t}{\Delta t} &= \alpha \frac{\frac{C_{i+1}^{t+1} - C_i^{t+1}}{\Delta x} - \frac{C_i^{t+1} - C_{i-1}^{t+1}}{\Delta x}}{\Delta x} \\ &= \alpha \frac{C_{i-1}^{t+1} - 2C_i^{t+1} + C_{i+1}^{t+1}}{\Delta x^2} \end{aligned} \tag{10}$$

This only applies to inlet cells with no ghost node as neighbor. For the left cell with its center at $\frac{dx}{2}$ and the constant concentration on the left ghost node called l the equation goes as followed:

$$\frac{C_0^{t+1} - C_0^t}{\Delta t} = \alpha \frac{\frac{C_1^{t+1} - C_0^{t+1}}{\Delta x} - \frac{C_0^{t+1} - l}{\frac{\Delta x}{2}}}{\Delta x} \tag{11}$$

This expression, once developed, yields:

$$\begin{aligned} C_0^{t+1} &= C_0^t + \frac{\alpha \cdot \Delta t}{\Delta x^2} \cdot \left(C_1^{t+1} - C_0^{t+1} - 2C_0^{t+1} + 2l\right) \\ &= C_0^t + \frac{\alpha \cdot \Delta t}{\Delta x^2} \cdot \left(C_1^{t+1} - 3C_0^{t+1} + 2l\right) \end{aligned} \tag{12}$$

Now we define variable s_x as followed:

$$s_x = \frac{\alpha \cdot \Delta t}{\Delta x^2} \tag{13}$$

Substituting with the new variable s_x and reordering of terms leads to the equation applicable to our model:

$$-C_0^t = (2s_x) \cdot l + (-1 - 3s_x) \cdot C_0^{t+1} + s_x \cdot C_1^{t+1} \tag{14}$$

The right boundary follows the same scheme. We now want to show the equation for the rightmost inlet cell C_n with right boundary value r:

$$\frac{C_n^{t+1} - C_n^t}{\Delta t} = \alpha \frac{\frac{r - C_n^{t+1}}{\frac{\Delta x}{2}} - \frac{C_n^{t+1} - C_{n-1}^{t+1}}{\Delta x}}{\Delta x} \tag{15}$$

This expression, once developed, yields:

$$\begin{aligned} C_n^{t+1} &= C_n^t + \frac{\alpha \cdot \Delta t}{\Delta x^2} \cdot \left(2r - 2C_n^{t+1} - C_n^{t+1} + C_{n-1}^{t+1}\right) \\ &= C_0^t + \frac{\alpha \cdot \Delta t}{\Delta x^2} \cdot \left(2r - 3C_n^{t+1} + C_{n-1}^{t+1}\right) \end{aligned} \tag{16}$$

Now rearrange terms and substituting with s_x leads to:

$$-C_n^t = s_x \cdot C_{n-1}^{t+1} + (-1 - 3s_x) \cdot C_n^{t+1} + (2s_x) \cdot r \tag{17}$$

TODO

- Tridiagonal matrix filling

2 Diffusion in 2D: the Alternating Direction Implicit scheme

In 2D, the diffusion equation (in absence of source terms) and assuming homogeneous but anisotropic diffusion coefficient $\alpha = (\alpha_x, \alpha_y)$ becomes:

$$\frac{\partial C}{\partial t} = \alpha_x \frac{\partial^2 C}{\partial x^2} + \alpha_y \frac{\partial^2 C}{\partial y^2} \tag{18}$$

2.1 2D ADI using BTCS scheme

The Alternating Direction Implicit method consists in splitting the integration of eq. 18 in two half-steps, each of which represents implicitly the derivatives in one direction, and explicitly in the other. Therefore we make use of second derivative operator defined in equation 9 in both x and y direction for half the time step Δt.

Denoting i the grid cell index along x direction, j the index in y direction and t as the time level, the spatially centered second derivatives can be written as:

$$\frac{\partial^2 C^t_{i,j}}{\partial x^2} = \frac{C^t_{i-1,j} - 2C^t_{i,j} + C^t_{i+1,j}}{\Delta x^2} \tag{19}$$

$$\frac{\partial^2 C^t_{i,j}}{\partial y^2} = \frac{C^t_{i,j-1} - 2C^t_{i,j} + C^t_{i,j+1}}{\Delta y^2} \tag{20}$$

The ADI scheme is formally defined by the equations:

$$\begin{cases} \dfrac{C^{t+1/2}_{i,j} - C^t_{i,j}}{\Delta t/2} = \alpha_x \dfrac{\partial^2 C^{t+1/2}_{i,j}}{\partial x^2} + \alpha_y \dfrac{\partial^2 C^t_{i,j}}{\partial y^2} \\ \dfrac{C^{t+1}_{i,j} - C^{t+1/2}_{i,j}}{\Delta t/2} = \alpha_x \dfrac{\partial^2 C^{t+1/2}_{i,j}}{\partial x^2} + \alpha_y \dfrac{\partial^2 C^{t+1}_{i,j}}{\partial y^2} \end{cases} \tag{21}$$

The first of equations 21, which writes implicitly the spatial derivatives in x direction, after bringing the $\Delta t/2$ terms on the right hand side and substituting $s_x = \frac{\alpha_x \cdot \Delta t}{2\Delta x^2}$ and $s_y = \frac{\alpha_y \cdot \Delta t}{2\Delta y^2}$ reads:

$$C^{t+1/2}_{i,j} - C^t_{i,j} = s_x(C^{t+1/2}_{i-1,j} - 2C^{t+1/2}_{i,j} + C^{t+1/2}_{i+1,j}) + s_y(C^t_{i,j-1} - 2C^t_{i,j} + C^t_{i,j+1}) \tag{22}$$

Separating the known terms (at time level t) on the left hand side and the implicit terms (at time level $t + 1/2$) on the right hand side, we get:

$$-C^t_{i,j} - s_y(C^t_{i,j-1} - 2C^t_{i,j} + C^t_{i,j+1}) = -C^{t+1/2}_{i,j} + s_x(C^{t+1/2}_{i-1,j} - 2C^{t+1/2}_{i,j} + C^{t+1/2}_{i+1,j}) \tag{23}$$

Equation 23 can be solved with a BTCS scheme since it corresponds to a tridiagonal system of equations, and resolves the $C^{t+1/2}$ at each inner grid cell.

The second of equations 21 can be treated the same way and yields:

$$-C^{t+1/2}_{i,j} - s_x(C^{t+1/2}_{i-1,j} - 2C^{t+1/2}_{i,j} + C^{t+1/2}_{i+1,j}) = -C^{t+1}_{i,j} + s_y(C^{t+1}_{i,j-1} - 2C^{t+1}_{i,j} + C^{t+1}_{i,j+1}) \tag{24}$$

This scheme only applies to inner cells, or else $\forall i, j \in [1, n-1] \times [1, n-1]$. Following an analogous treatment as for the 1D case, and noting l_x and l_y the constant left boundary values and r_x and r_y the right ones for each direction x and y, we can modify equations 23 for $i = 0, j \in [1, n-1]$

$$-C^t_{0,j} - s_y(C^t_{0,j-1} - 2C^t_{0,j} + C^t_{0,j+1}) = -C^{t+1/2}_{0,j} + s_x(C^{t+1/2}_{1,j} - 3C^{t+1/2}_{0,j} + 2l_x) \tag{25}$$

Similarly for $i = n, j \in [1, n-1]$:

$$-C^t_{n,j} - s_y(C^t_{n,j-1} - 2C^t_{n,j} + C^t_{n,j+1}) = -C^{t+1/2}_{n,j} + s_x(C^{t+1/2}_{n-1,j} - 3C^{t+1/2}_{n,j} + 2r_x) \tag{26}$$

For $i = j = 0$:

$$-C^t_{0,0} - s_y(C^t_{0,1} - 3C^t_{0,0} + 2l_y) = -C^{t+1/2}_{0,0} + s_x(C^{t+1/2}_{1,0} - 3C^{t+1/2}_{0,0} + 2l_x) \tag{27}$$

Analogous expressions are readily derived for all possible combinations of $i, j \in 0 \times n$. In practice, wherever an index i or j is 0 or n, the centered spatial derivatives in x or y directions must be substituted in relevant parts of the sweeping equations **in both the implicit or the explicit sides** of equations 23 and 24 by a term

$$s(C_{forw} - 3C + 2bc) \tag{28}$$

where bc is the boundary condition in the given direction, s is either s_x or s_y, and C_{forw} indicates the contiguous cell opposite to the boundary. Alternatively, noting the second derivative operator as ∂^2_{dir}, we can write in compact form:

$$\begin{cases} \partial^2_x C_{0,j} & = 2l_x - 3C_{0,j} + C_{1,j} \\ \partial^2_x C_{n,j} & = 2r_x - 3C_{n,j} + C_{n-1,j} \\ \partial^2_y C_{i,0} & = 2l_y - 3C_{i,0} + C_{i,1} \\ \partial^2_y C_{i,n} & = 2r_y - 3C_{i,n} + C_{i,n-1} \end{cases} \tag{29}$$

3 Heterogeneous diffusion

If the diffusion coefficient α is spatially variable, equation 1 can be rewritten as:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial C}{\partial x}\right) \tag{30}$$

3.1 Discretization of the equation using chain rule

From the product rule for derivatives we obtain:

$$\frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial C}{\partial x}\right) = \frac{\partial \alpha}{\partial x}\cdot\frac{\partial C}{\partial x} + \alpha\frac{\partial^2 C}{\partial x^2} \tag{31}$$

Using a spatially centred second order finite difference approximation at $x = x_i$ for both α and C, we have

$$\begin{aligned}\frac{\partial \alpha}{\partial x}\cdot\frac{\partial C}{\partial x} + \alpha\frac{\partial^2 C}{\partial x^2} &\simeq \frac{\alpha_{i+1}-\alpha_{i-1}}{2\Delta x}\cdot\frac{C_{i+1}-C_{i-1}}{2\Delta x} + \alpha_i\frac{C_{i+1}-2C_i+C_{i-1}}{\Delta x^2} \\ &= \frac{1}{\Delta x^2}\frac{\alpha_{i+1}-\alpha_{i-1}}{4}(C_{i+1}-C_{i-1}) + \frac{\alpha_i}{\Delta x^2}(C_{i+1}-2C_i+C_{i-1}) \\ &= \frac{1}{\Delta x^2}\left\{AC_{i+1} - 2\alpha_i C_i + AC_{i-1})\right\}\end{aligned} \tag{32}$$

having set

$$A = \frac{\alpha_{i+1}-\alpha_{i-1}}{4} + \alpha_i$$

In 2D the ADI scheme 21 with heterogeneous diffusion coefficients can thus be written:

$$\begin{cases}\dfrac{C_{i,j}^{t+1/2}-C_{i,j}^{t}}{\Delta t/2} = \dfrac{\partial}{\partial x}\left(\alpha_{i,j}^{x}\dfrac{\partial C_{i,j}^{t+1/2}}{\partial x}\right) + \dfrac{\partial}{\partial y}\left(\alpha_{i,j}^{y}\dfrac{\partial C_{i,j}^{t}}{\partial y}\right) \\ \dfrac{C_{i,j}^{t+1}-C_{i,j}^{t+1/2}}{\Delta t/2} = \dfrac{\partial}{\partial x}\left(\alpha_{i,j}^{x}\dfrac{\partial C_{i,j}^{t+1/2}}{\partial x}\right) + \dfrac{\partial}{\partial y}\left(\alpha_{i,j}^{y}\dfrac{\partial C_{i,j}^{t+1}}{\partial y}\right)\end{cases} \tag{33}$$

We define for compactness $S_x = \frac{\Delta t}{2\Delta x^2}$ and $S_y = \frac{\Delta t}{2\Delta y^2}$ and

$$\begin{cases}A_{i,j} = \dfrac{\alpha_{i+1,j}^{x}-\alpha_{i-1,j}^{x}}{4} + \alpha_{i,j}^{x} \\ B_{i,j} = \dfrac{\alpha_{i,j+1}^{y}-\alpha_{i,j-1}^{y}}{4} + \alpha_{i,j}^{y}\end{cases} \tag{34}$$

Plugging eq. (32) into the first of equations (33) - so called "sweep by x" - and putting all implicit terms (at time level $t + 1/2$) on the left hand side we obtain:

$$\begin{aligned}-S_x A_{i,j}C_{i+1,j}^{t+1/2} + (1+2S_x\alpha_{i,j}^{x})C_{i,j}^{t+1/2} - S_x A_{i,j}C_{i-1,j}^{t+1/2} &= \\ S_y B_{i,j}C_{i,j+1}^{t} + (1-2S_y\alpha_{i,j}^{y})C_{i,j}^{t} + S_y B_{i,j}C_{i,j-1}^{t}&\end{aligned} \tag{35}$$

In the same way for the second of eq. 33 we have:

$$\begin{aligned}-S_y B_{i,j}C_{i,j+1}^{t+1} + (1+2S_y\alpha_{i,j}^{y})C_{i,j}^{t+1} - S_y B_{i,j}C_{i,j-1}^{t+1} &= \\ S_x A_{i,j}C_{i+1,j}^{t+1/2} + (1-2S_x\alpha_{i,j}^{x})C_{i,j}^{t+1/2} + S_x A_{i,j}C_{i-1,j}^{t+1/2}&\end{aligned} \tag{36}$$

If the diffusion coefficients are constant, $A_{i,j} = B_{i,j} = \alpha$ and the scheme reverts to the homogeneous case. Problem with this discretization is that the terms in A_{ij} and B_{ij} can be negative depending on the derivative of the diffusion coefficient, resulting in unphysical values for the concentrations.

3.2 Direct discretization

As noted in literature (LeVeque and Numerical Recipes) a better way is to discretize directly the physical problem (eq. 30) at points halfway between grid points:

$$\begin{cases} \alpha(x_{i+1/2})\dfrac{\partial C}{\partial x}(x_{i+1/2}) & = \alpha_{i+1/2}\left(\dfrac{C_{i+1}-C_i}{\Delta x}\right) \\ \alpha(x_{i-1/2})\dfrac{\partial C}{\partial x}(x_{i-1/2}) & = \alpha_{i-1/2}\left(\dfrac{C_{i}-C_{i-1}}{\Delta x}\right) \end{cases}$$

A further differentiation gives us the spatially centered approximation of $\frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial C}{\partial x}\right)$:

$$\begin{aligned} \frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial C}{\partial x}\right)(x_i) &\simeq \frac{1}{\Delta x}\left[\alpha_{i+1/2}\left(\frac{C_{i+1}-C_i}{\Delta x}\right) - \alpha_{i-1/2}\left(\frac{C_i - C_{i-1}}{\Delta x}\right)\right] \\ &= \frac{1}{\Delta x^2}\left[\alpha_{i+1/2}C_{i+1} - (\alpha_{i+1/2}+\alpha_{i-1/2})C_i + \alpha_{i-1/2}C_{i-1}\right] \end{aligned} \tag{37}$$

The ADI scheme with this approach becomes:

$$\begin{cases} \dfrac{C_{i,j}^{t+1/2}-C_{i,j}^{t}}{\Delta t/2} = \dfrac{1}{\Delta x^2}\left[\alpha_{i+1/2,j}C_{i+1,j}^{t+1/2} - (\alpha_{i+1/2,j}+\alpha_{i-1/2,j})C_{i,j}^{t+1/2} + \alpha_{i-1/2,j}C_{i-1,j}^{t+1/2}\right] + \\ \qquad \dfrac{1}{\Delta y^2}\left[\alpha_{i,j+1/2}C_{i,j+1}^{t} - (\alpha_{i,j+1/2}+\alpha_{i,j-1/2})C_{i,j}^{t} + \alpha_{i,j-1/2}C_{i,j-1}^{t}\right] \\ \dfrac{C_{i,j}^{t+1}-C_{i,j}^{t+1/2}}{\Delta t/2} = \dfrac{1}{\Delta y^2}\left[\alpha_{i+1/2,j}C_{i+1,j}^{t+1/2} - (\alpha_{i+1/2,j}+\alpha_{i-1/2,j})C_{i,j}^{t} + \alpha_{i-1/2,j}C_{i-1,j}^{t+1/2}\right] + \\ \qquad \dfrac{1}{\Delta x^2}\left[\alpha_{i,j+1/2}C_{i,j+1}^{t+1} - (\alpha_{i,j+1/2}+\alpha_{i,j-1/2})C_{i,j}^{t+1} + \alpha_{i,j-1/2}C_{i,j-1}^{t+1}\right] \end{cases} \tag{38}$$

Doing the usual algebra and separating implicit from explicit terms, the two sweeps become:

$$\begin{cases} -S_x\alpha^x_{i+1/2,j}C_{i+1,j}^{t+1/2} + (1+S_x(\alpha^x_{i+1/2,j}+\alpha^x_{i-1/2,j}))C_{i,j}^{t+1/2} - S_x\alpha^x_{i-1/2,j}C_{i-1,j}^{t+1/2} = \\ \qquad S_y\alpha^y_{i,j+1/2}C_{i,j+1}^{t} + (1-S_y(\alpha^y_{i,j+1/2}+\alpha^y_{i,j-1/2}))C_{i,j}^{t} + S_y\alpha^y_{i,j-1/2}C_{i,j-1}^{t} \\ \\ -S_y\alpha^y_{i,j+1/2}C_{i,j+1}^{t+1} + (1+S_y(\alpha^y_{i,j+1/2}+\alpha^y_{i,j-1/2}))C_{i,j}^{t+1} - S_y\alpha^y_{i,j-1/2}C_{i,j-1}^{t+1} = \\ \qquad S_x\alpha^x_{i+1/2,j}C_{i+1,j}^{t+1/2} + (1-S_x(\alpha^x_{i+1/2,j}+\alpha^x_{i-1/2,j}))C_{i,j}^{t+1/2} + S_x\alpha^x_{i-1/2,j}C_{i-1,j}^{t+1/2} \end{cases} \tag{39}$$

The "interblock" diffusion coefficients $\alpha_{i+1/2,j}$ can be arithmetic mean:

$$\alpha_{i+1/2,j} = \frac{\alpha_{i+1,j}+\alpha_{i,j}}{2}$$

or the harmonic mean:

$$\alpha_{i+1/2,j} = \frac{2}{\frac{1}{\alpha_{i+1,j}}+\frac{1}{\alpha_{i,j}}}$$

4 Explicit scheme for 2D heterogeneous diffusion

A classical explicit FTCS scheme (forward in time, central in space) for 2D heterogeneous diffusion can be expressed simply leveraging the discretization of equation 37:

$$
\begin{aligned}
\frac{C_{i,j}^{t+1} - C_{i,j}^{t}}{\Delta t} = & \frac{1}{\Delta x^2}\left[\alpha^x_{i+1/2,j}C^t_{i+1,j} - (\alpha^x_{i+1/2,j} + \alpha^x_{i-1/2,j})C^t_{i,j} + \alpha^x_{i-1/2,j}C^t_{i-1,j}\right] + \\
& \frac{1}{\Delta y^2}\left[\alpha^y_{i,j+1/2}C^t_{i,j+1} - (\alpha^y_{i,j+1/2} + \alpha^y_{i,j-1/2})C^t_{i,j} + \alpha^y_{i,j-1/2}C^t_{i,j-1}\right]
\end{aligned}
\tag{40}
$$

where in the RHS only the known concentrations at time t appear. Rearranging the terms, we get:

$$
\begin{aligned}
C^{t+1}_{i,j} = & C^t_{i,j} + \\
& \frac{\Delta t}{\Delta x^2}\left[\alpha^x_{i+1/2,j}C^t_{i+1,j} - (\alpha^x_{i+1/2,j} + \alpha^x_{i-1/2,j})C^t_{i,j} + \alpha^x_{i-1/2,j}C^t_{i-1,j}\right] + \\
& \frac{\Delta t}{\Delta y^2}\left[\alpha^y_{i,j+1/2}C^t_{i,j+1} - (\alpha^y_{i,j+1/2} + \alpha^y_{i,j-1/2})C^t_{i,j} + \alpha^y_{i,j-1/2}C^t_{i,j-1}\right]
\end{aligned}
\tag{41}
$$

The Courant-Friedrichs-Lewy stability criterion (cfr Lee, 2017) for this scheme reads:

$$
\Delta t \leq \frac{1}{2\max(\alpha_{i,j})} \cdot \frac{1}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}} \tag{42}
$$

Note that other derivations for the CFL condition are found in literature. For example, the sources cited by Wikipedia solution give:

$$
\Delta t \leq \frac{1}{4\max(\alpha)\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)} \tag{43}
$$

We can produce a more restrictive condition than equation 42 by considering the min of the Δx and Δy:

$$
\Delta t \leq \frac{\min(\Delta x, \Delta y)^2}{4\max(\alpha_{i,j})} \tag{44}
$$

In practice for the implementation it is advantageous to specify an optional parameter C, $C \in [0, 1]$ so that the user can restrict the "inner time stepping":

$$
\Delta t \leq C \cdot \frac{\min(\Delta x, \Delta y)^2}{4\max(\alpha_{i,j})} \tag{45}
$$

4.1 Boundary conditions

In analogy to the treatment of the 1D homogeneous FTCS scheme (cfr section 1), we need to differentiate the domain boundaries ($i = 0$ and $i = n_x$; the same applies to j of course) accounting for the discrepancy in the discretization.

For the zero-th (left) cell, whose center is at $x = dx/2$, we can evaluate the left gradient with the left boundary using such distance, calling l the numerical value of a constant boundary condition, equation 37 becomes:

$$
\begin{aligned}
\frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial C}{\partial x}\right)(x_0) & \simeq \frac{1}{\Delta x}\left[\alpha_{i+1/2}\left(\frac{C_{i+1} - C_i}{\Delta x}\right) - \alpha_i\left(\frac{C_i - l}{\frac{\Delta x}{2}}\right)\right] \\
& = \frac{1}{\Delta x^2}\left[\alpha_{i+1/2}C_{i+1} - (\alpha_{i+1/2} + 2\alpha_i)C_i + 2\alpha_i \cdot l\right]
\end{aligned}
\tag{46}
$$

Similarly, for $i = n_x$,

$$\frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial C}{\partial x}\right)(x_n) \simeq \frac{1}{\Delta x}\left[\alpha_i\left(\frac{r - C_i}{\frac{\Delta x}{2}}\right) - \alpha_{i-1/2}\left(\frac{C_i - C_{i-1}}{\Delta x}\right)\right]$$
$$= \frac{1}{\Delta x^2}\left[2\alpha_i r - (\alpha_{i+1/2} + 2\alpha_i)C_i + \alpha_{i-1/2}\cdot C_{i-1}\right] \tag{47}$$

If on the right boundary we have **closed** or Neumann condition, the left derivative becomes zero and we are left with:

$$\frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial C}{\partial x}\right)(x_n) \simeq \frac{1}{\Delta x}\left[\cancel{\alpha_{i+1/2}\left(\frac{C_{i+1} - C_i}{\Delta x}\right)} - \alpha_{i-1/2}\left(\frac{C_i - C_{i-1}}{\Delta x}\right)\right]$$
$$= \frac{\alpha_{i-1/2}}{\Delta x^2}(C_{i-1} - C_i) \tag{48}$$