

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

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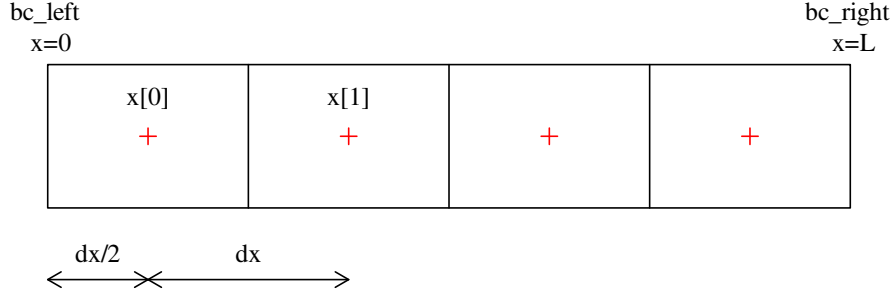
1 Homogeneous diffusion in 1D

1.1 Finite differences with nodes as cells' centres

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

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

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 $i \in 1, \dots, n-1$ and assuming constant α , we can write:

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

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:

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

This expression, once developed, yields:

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

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

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

Which, developed, gives

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

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

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

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

1.3 Implicit BTCS scheme

First, we define the Backward Time difference:

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

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

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

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

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

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:

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

This expression, once developed, yields:

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

Now we define variable s_x as followed:

$$s_x = \frac{\alpha \cdot \Delta t}{\Delta x^2} \quad (13)$$

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

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

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 :

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

This expression, once developed, yields:

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

Now rearrange terms and substituting with s_x leads to:

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

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:

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

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:

$$\frac{\partial^2 C_{i,j}^t}{\partial x^2} = \frac{C_{i-1,j}^t - 2C_{i,j}^t + C_{i+1,j}^t}{\Delta x^2} \quad (19)$$

$$\frac{\partial^2 C_{i,j}^t}{\partial y^2} = \frac{C_{i,j-1}^t - 2C_{i,j}^t + C_{i,j+1}^t}{\Delta y^2} \quad (20)$$

The ADI scheme is formally defined by the equations:

$$\begin{cases} \frac{C_{i,j}^{t+1/2} - C_{i,j}^t}{\Delta t/2} = \alpha_x \frac{\partial^2 C_{i,j}^{t+1/2}}{\partial x^2} + \alpha_y \frac{\partial^2 C_{i,j}^t}{\partial y^2} \\ \frac{C_{i,j}^{t+1} - C_{i,j}^{t+1/2}}{\Delta t/2} = \alpha_x \frac{\partial^2 C_{i,j}^{t+1/2}}{\partial x^2} + \alpha_y \frac{\partial^2 C_{i,j}^{t+1/2}}{\partial y^2} \end{cases} \quad (21)$$

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 $s_x = \frac{\alpha_x \Delta t}{2\Delta x^2}$ and $s_y = \frac{\alpha_y \Delta t}{2\Delta y^2}$ reads:

$$C_{i,j}^{t+1/2} - C_{i,j}^t = s_x(C_{i-1,j}^{t+1/2} - 2C_{i,j}^{t+1/2} + C_{i+1,j}^{t+1/2}) + s_y(C_{i,j-1}^t - 2C_{i,j}^t + C_{i,j+1}^t) \quad (22)$$

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:

$$-C_{i,j}^t - s_y(C_{i,j-1}^t - 2C_{i,j}^t + C_{i,j+1}^t) = -C_{i,j}^{t+1/2} + s_x(C_{i-1,j}^{t+1/2} - 2C_{i,j}^{t+1/2} + C_{i+1,j}^{t+1/2}) \quad (23)$$

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:

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

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 $i = 0, j \in [1, n-1]$

$$-C_{0,j}^t - s_y(C_{0,j-1}^t - 2C_{0,j}^t + C_{0,j+1}^t) = -C_{0,j}^{t+1/2} + s_x(C_{1,j}^{t+1/2} - 3C_{0,j}^{t+1/2} + 2l_x) \quad (25)$$

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

$$-C_{n,j}^t - s_y(C_{n,j-1}^t - 2C_{n,j}^t + C_{n,j+1}^t) = -C_{n,j}^{t+1/2} + s_x(C_{n-1,j}^{t+1/2} - 3C_{n,j}^{t+1/2} + 2r_x) \quad (26)$$

For $i = j = 0$:

$$-C_{0,0}^t - s_y(C_{0,1}^t - 3C_{0,0}^t + 2l_y) = -C_{0,0}^{t+1/2} + s_x(C_{1,0}^{t+1/2} - 3C_{0,0}^{t+1/2} + 2l_x) \quad (27)$$

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

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

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 ∂_{dir}^2 , we can write in compact form:

$$\left\{ \begin{array}{ll} \partial_x^2 C_{0,j} & = 2l_x - 3C_{0,j} + C_{1,j} \\ \partial_x^2 C_{n,j} & = 2r_x - 3C_{n,j} + C_{n-1,j} \\ \partial_y^2 C_{i,0} & = 2l_y - 3C_{i,0} + C_{i,1} \\ \partial_y^2 C_{i,n} & = 2r_y - 3C_{i,n} + C_{i,n-1} \end{array} \right. \quad (29)$$

3 Heterogeneous diffusion

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

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

3.1 Discretization of the equation using chain rule

From the product rule for derivatives we obtain:

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

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

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

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:

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

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

$$\begin{cases} A_{i,j} = \frac{\alpha_{i+1,j}^x - \alpha_{i-1,j}^x}{4} + \alpha_{i,j}^x \\ B_{i,j} = \frac{\alpha_{i,j+1}^y - \alpha_{i,j-1}^y}{4} + \alpha_{i,j}^y \end{cases} \quad (34)$$

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:

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

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

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

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 $A_{i,j}$ and $B_{i,j}$ 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:

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

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

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

The ADI scheme with this approach becomes:

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

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

$$\begin{cases} -S_x \alpha_{i+1/2,j}^x C_{i+1,j}^{t+1/2} + (1 + S_x (\alpha_{i+1/2,j}^x + \alpha_{i-1/2,j}^x)) C_{i,j}^{t+1/2} - S_x \alpha_{i-1/2,j}^x C_{i-1,j}^{t+1/2} = \\ \quad S_y \alpha_{i,j+1/2}^y C_{i,j+1}^t + (1 - S_y (\alpha_{i,j+1/2}^y + \alpha_{i,j-1/2}^y)) C_{i,j}^t + S_y \alpha_{i,j-1/2}^y C_{i,j-1}^t \\ -S_y \alpha_{i,j+1/2}^y C_{i,j+1}^{t+1} + (1 + S_y (\alpha_{i,j+1/2}^y + \alpha_{i,j-1/2}^y)) C_{i,j}^{t+1} - S_y \alpha_{i,j-1/2}^y C_{i,j-1}^{t+1} = \\ \quad S_x \alpha_{i+1/2,j}^x C_{i+1,j}^{t+1/2} + (1 - S_x (\alpha_{i+1/2,j}^x + \alpha_{i-1/2,j}^x)) C_{i,j}^{t+1/2} + S_x \alpha_{i-1/2,j}^x C_{i-1,j}^{t+1/2} \end{cases} \quad (39)$$

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:

$$\begin{aligned} \frac{C_{i,j}^{t+1} - C_{i,j}^t}{\Delta t} = & \frac{1}{\Delta x^2} \left[\alpha_{i+1/2,j}^x C_{i+1,j}^t - (\alpha_{i+1/2,j}^x + \alpha_{i-1/2,j}^x) C_{i,j}^t + \alpha_{i-1/2,j}^x C_{i-1,j}^t \right] + \\ & \frac{1}{\Delta y^2} \left[\alpha_{i,j+1/2}^y C_{i,j+1}^t - (\alpha_{i,j+1/2}^y + \alpha_{i,j-1/2}^y) C_{i,j}^t + \alpha_{i,j-1/2}^y C_{i,j-1}^t \right] \end{aligned} \quad (40)$$

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

$$\begin{aligned} C_{i,j}^{t+1} = & C_{i,j}^t + \\ & \frac{\Delta t}{\Delta x^2} \left[\alpha_{i+1/2,j}^x C_{i+1,j}^t - (\alpha_{i+1/2,j}^x + \alpha_{i-1/2,j}^x) C_{i,j}^t + \alpha_{i-1/2,j}^x C_{i-1,j}^t \right] + \\ & \frac{\Delta t}{\Delta y^2} \left[\alpha_{i,j+1/2}^y C_{i,j+1}^t - (\alpha_{i,j+1/2}^y + \alpha_{i,j-1/2}^y) C_{i,j}^t + \alpha_{i,j-1/2}^y C_{i,j-1}^t \right] \end{aligned} \quad (41)$$

The Courant-Friedrichs-Lewy stability criterion for this scheme reads:

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

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:

$$\begin{aligned} \frac{\partial}{\partial x} \left(\alpha(x) \frac{\partial C}{\partial x} \right) (x_0) & \simeq \frac{1}{\Delta x} \left[\alpha_{i+1/2} \left(\frac{C_{i+1} - C_i}{\Delta x} \right) - \alpha_i \left(\frac{C_i - l}{\frac{\Delta x}{2}} \right) \right] \\ & = \frac{1}{\Delta x^2} \left[\alpha_{i+1/2} C_{i+1} - (\alpha_{i+1/2} + 2\alpha_i) C_i + 2\alpha_i \cdot l \right] \end{aligned} \quad (43)$$

Similarly, for $i = n_x$,

$$\begin{aligned} \frac{\partial}{\partial x} \left(\alpha(x) \frac{\partial C}{\partial x} \right) (x_n) & \simeq \frac{1}{\Delta x} \left[\alpha_i \left(\frac{r - C_i}{\frac{\Delta x}{2}} \right) - \alpha_{i-1/2} \left(\frac{C_i - C_{i-1}}{\Delta x} \right) \right] \\ & = \frac{1}{\Delta x^2} \left[2\alpha_i r - (\alpha_{i+1/2} + 2\alpha_i) C_i + \alpha_{i-1/2} \cdot C_{i-1} \right] \end{aligned} \quad (44)$$

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

$$\begin{aligned} \frac{\partial}{\partial x} \left(\alpha(x) \frac{\partial C}{\partial x} \right) (x_n) & \simeq \frac{1}{\Delta x} \left[\cancel{\alpha_{i+1/2} \left(\frac{C_{i+1} - C_i}{\Delta x} \right)} - \alpha_{i-1/2} \left(\frac{C_i - C_{i-1}}{\Delta x} \right) \right] \\ & = \frac{\alpha_{i-1/2}}{\Delta x^2} (C_{i-1} - C_i) \end{aligned} \quad (45)$$