D – Solution to the model

The following rescaled system of partial differential equations with initial and boundary conditions describing problem of interdiffusion (obtained after rescaling - see section C):

$$\begin{cases} \dfrac{\partial \overline{c}_i}{\partial \overline{t}} = -\dfrac{\partial \overline{J}_i}{\partial \overline{x}}, \\ \overline{J}_i = -\sum_{k=1}^{r} \overline{D}_{i,k}(\overline{c}_1,\ldots,\overline{c}_r)\dfrac{\partial \overline{c}_k}{\partial \overline{x}} + \overline{c}_i \overline{K}(\overline{t}) + \dfrac{c_s}{c}\overline{c}_i \sum_{k,l=1}^{r} \overline{D}_{k,l}(\overline{c}_1,\ldots,\overline{c}_r)\dfrac{\partial \overline{c}_l}{\partial \overline{x}}, \\ \overline{c}_i(\overline{x},0) = \overline{c}_i^{\,0}(\overline{x}), \quad for \ \ \overline{x} \in [0,1] \\ \overline{J}_i(0,\overline{t}) = \overline{j}_i^{\,0}(\overline{t}), \\ \overline{J}_i(d,\overline{t}) = \overline{j}_i^{\,d}(\overline{t}) \quad for\ i = 1,\ldots r-1 \\ \overline{J}_r(1,\overline{t}) = \overline{J}_r(0,\overline{t}) - \sum_{j=1}^{r-1}\left(\overline{J}_j(0,\overline{t}) - \overline{J}_j(1,\overline{t})\right) \end{cases} \tag{1}$$

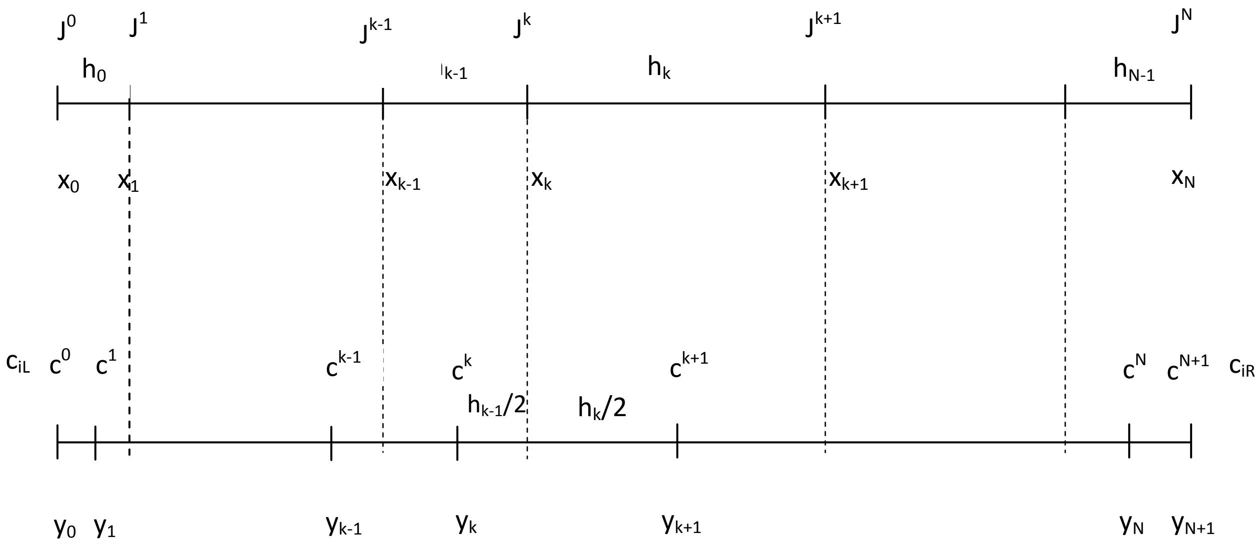
where

$$\overline{j}_i^{\,0}(\overline{t}) = \frac{t_s}{x_s} j_i^0(t_s\overline{t}), \ \overline{j}_i^{\,d}(\overline{t}) = \frac{t_s}{x_s} j_i^d(t_s\overline{t}), \tag{2}$$

$$\overline{c}_i^{\,0}(\overline{x}) = c(x_s\overline{x})/c_s$$

The problem given by eqns. (1)-(2) will be solved numerically using method of lines (variant of finite difference method – see Category: Numerical methods.

Below we display the general arrangement of the nodes. It can be viewed as two intertwined grids: one, with nodes denoted by x_k, for computing the values of $J = J(x,t)$, second, with nodes denoted by y_k, for computing the values of $c_i = c_i(y,t)$. In both cases $x, y \in [0,d]$. The space step is not assumed to be uniform and we have $h_k = x_{k+1} - x_k$



We start from the basic equations

$$\frac{\partial c_i}{\partial t} = -\frac{\partial J_i}{\partial x} \quad (i = 1, \ldots, r) \tag{3}$$

which subsequently will be discretized at the nodes $x = y_k$ for eq. (3)

$$\left.\frac{\partial c_i}{\partial t}\right|_{x=y_k} = -\left.\frac{\partial J_i}{\partial x}\right|_{x=y_k} \tag{4}$$

Recalling that $J_i^k = J_i\big|_{x=x_k} = J_i(x_k, t)$ and $c_i^k = c_i(y_k, t)$ we use the central finite difference for the approximation of the flux space derivative for the inner nods

$$\left.\frac{\partial J_i}{\partial x}\right|_{x=y_k} \simeq \frac{J_i^k - J_i^{k-1}}{h_{k-1}} \quad (k=1,\dots,N) \tag{5}$$

At the left and right boundary the fluxes are approximated using the following right and left finite difference respectively

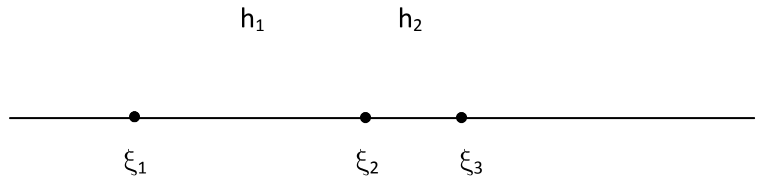
$$\left.\frac{\partial J_i}{\partial x}\right|_{x=y_0} \simeq \frac{-h_1(2h_0+h_1)J_i^0 + (h_0+h_1)^2 J_i^1 - h_0^2 J_i^2}{h_0 h_1 (h_0+h_1)} \tag{6}$$

$$\left.\frac{\partial J_i}{\partial x}\right|_{x=y_{N+1}} \simeq \frac{h_{N-1}^2 J_i^{N-2} - (h_{N-2}+h_{N-1})^2 J_i^{N-1} + h_{N-1}(h_{N-1}+2h_{N-2})J_i^N}{h_0 h_1 (h_0+h_1)} \tag{7}$$

Because $\left.\frac{\partial c_i}{\partial t}\right|_{x=y_k} = \frac{dc_i^k}{dt}$ we can write a discretized form of eqs. (3) as

$$\begin{aligned}
\frac{dc_i^0}{dt} &= -\frac{-h_1(2h_0+h_1)J_i^0 + (h_0+h_1)^2 J_i^1 - h_0^2 J_i^2}{h_0 h_1 (h_0+h_1)} \\
\frac{dc_i^k}{dt} &= -\frac{J_i^k - J_i^{k-1}}{h_{k-1}} \quad (k=1,\dots,N,\ i=1,\dots,r) \\
\frac{dc_i^{N+1}}{dt} &= -\frac{h_{N-1}^2 J_i^{N-2} - (h_{N-2}+h_{N-1})^2 J_i^{N-1} + h_{N-1}(h_{N-1}+2h_{N-2})J_i^N}{h_0 h_1 (h_0+h_1)}
\end{aligned}$$

To get the value $J_i^k = J_i(x_k,t)$, we have to compute $\frac{\partial c_i}{\partial x}(x_k,t)$. This is done by the formula, presented below, that is valid for any sufficiently regular function $f = f(x)$. Suppose that we have tree points $\xi_1 < \xi_2 < \xi_3$ on the real line



Then the first derivative at $\xi = \xi_2$ may be expressed as follow

$$f'(\xi_2) = \frac{h_1^2 f(\xi_3) - h_2^2 f(\xi_1) + (h_2^2 - h_1^2) f(\xi_2)}{h_1 h_2 (h_1 + h_2)} + r \tag{8}$$
$$\text{where } \; r = O(h_1 h_2)$$

After applying this formula to $\frac{\partial c_i}{\partial x}(x_k, t)$ with the nodes $x = y_{k-1}$, $x = x_k$, $x = y_k$ we must get rid of the value $c_i(x_k, t)$, because the final form of ODEs must contain only functions $c_i^k(t) = c_i(y_k, t)$. One of the possibility is to express it in terms of $c_i(y_k, t)$, $c_i(y_{k+1}, t)$ only, by taking a weighted linear approximation

$$c(x_k, t) \simeq \frac{h_k c_i(y_k, t) + h_{k-1} c(y_{k+1}, t)}{h_{k-1} + h_k} = \frac{h_k c_i^k + h_{k-1} c_i^{k+1}}{h_{k-1} + h_k} \tag{9}$$

Combining (8) (applied to c_i) together with (9) yields the final approximation of the concentration gradient

$$\left.\frac{\partial c_i}{\partial x}\right|_{x=x_k} = 2\,\frac{h_{k-1}^2 c_i^{k+1} - h_k^2 c_i^k + (h_k - h_{k-1})(h_k c_i^k + h_{k-1} c_i^{k+1})}{h_{k-1} h_k (h_{k-1} + h_k)} \tag{10}$$

Now, the whole flux may be discretized and written as

$$J_i^k = -2a_i \frac{h_{k-1}^2 c_i^{k+1} - h_k^2 c_i^k + (h_k - h_{k-1})(h_k c_i^k + h_{k-1} c_i^{k+1})}{h_{k-1} h_k (h_{k-1} + h_k)} + \\ + \frac{h_k c_i^k + h_{k-1} c_i^{k+1}}{h_{k-1} + h_k} \left(\beta + 2 \sum_{j=1}^{r} g_j \frac{h_{k-1}^2 c_j^{k+1} - h_k^2 c_j^k + (h_k - h_{k-1})(h_k c_j^k + h_{k-1} c_j^{k+1})}{h_{k-1} h_k (h_{k-1} + h_k)} + \right. \tag{11}$$

The ODEs in the single-index notation

This part deals with expressing the above discretised system by using only one index instead two indices. This may be useful when one applies a numerical subroutine which usually assumes ODEs written with one index notation as follows

$$\begin{cases} y_1' = f_1(t, y_1, \ldots, y_n), \\ \vdots \\ y_n' = f_n(t, y_n, \ldots, y_n), \end{cases}$$

czyli $y_l' = f_l(t, y_1, \ldots, y_l)$ dla $l = 1, \ldots, n.$

In order to rewrite the above system in one-index form we apply the translation $l(i,k) = l = (i-1)(N+2) + k + 1$ and use the simple relations

$$l = (i-1)(N+2) + k + 1 \Leftrightarrow \begin{cases} k = (l-1) \bmod (N+2), \\ i = 1 + (l-1) \operatorname{div} (N+2). \end{cases} \tag{12}$$

where $i = 1, \ldots, r+1, \; k = 0, \ldots, N+2.$

The single index $l = 1, \ldots, (N+2)r$ is connected with concentrations and electric field as follows

$$l = 1, 2, \ldots, (N+2)r. \tag{13}$$

Further we will write

$$k_l = k(l) = (l-1) \bmod (N+2) \text{ and } i_l = i(l) = 1 + (l-1) \operatorname{div} (N+2). \tag{14}$$

For the whole system the single index l of the components which are adjacent to the boundary has the property:

- next to the left boundary: $(l-1) \bmod (N+2) = 0$,
- before the right boundary: $l \bmod (N+2) = 0$.

Now the ODEs system may be written as follows.

The index l runs over the range $1, 2, \ldots, (N+2)r$.

(1) For nodes $x_1, \ldots x_N$, i.e. $(l-1) \bmod N-1 \neq 0$ and $l \bmod N-1 \neq 0$.

$$\frac{dc_l}{dt} = \sum_{j=1}^{r} \Big(C_{l,j} (w_{2,k(l)-1} c_{l(j,k(l)-1)} + w_{2,k} c_{l(j,k(l))} + w_{2,k(l)+1} c_{l(j,k(l)+1)}) -$$
$$-\frac{D_j}{c_{mix}} (w_{1,k(l)-1} c_{l-1} + w_{1,k(l)} c_l + w_{1,k(l)+1} c_{l+1})(w_{1,k(l)-1} c_{l(j,k(l)-1)} + w_{1,k(l)} c_{l(j,k(l))} + w_{1,k(l)+1} c_{l(j,k(l)+1)}) -$$
$$+\frac{1}{c_{mix}} (w_{1,k(l)-1} c_{l-1} + w_{1,k(l)} c_l + w_{1,k(l)+1} c_{l+1}) k_{j,L} (c_j^0 - c_{j,L}) \Big)$$

where $C_{l,j} = (\delta_{i(l),j} - \frac{c_l}{c_{mix}}) D_j$.

(2) For the node x_1, i.e. $(l-1) \bmod (N-1) = 0$.

$$\frac{dc_l}{dt} = \sum_{j=1}^{r} \Big(C_{l,j} (w_{2,0} c_j^0 + w_{2,1} c_{l(j,k(l))} + w_{2,2} c_{l(j,k(l)+1)}) -$$
$$-\frac{D_j}{c_{mix}} (w_{1,0} c_{l(i,0)}^0 + w_{1,1} c_l + w_{1,2} c_{l+1})(w_{1,0} c_{l(j,0)}^0 + w_{1,1} c_{l(j,k(l))} + w_{1,2} c_{l(j,k(l)+1)}) -$$
$$+\frac{1}{c_{mix}} (w_{1,0} c_{i(l)}^0 + w_{1,1} c_l + w_{1,2} c_{l+1}) k_{j,L} (c_j^0 - c_{j,L}) \Big)$$

where $c_i^0 = bv(left, i)$.

(3) For the node x_{N-1}, i.e. $l \bmod N-1 = 0$.

$$\frac{dc_l}{dt} = \sum_{j=1}^{r} \Big(C_{l,j} (w_{2,N-2} c_{l(j,k(l)-1)} + w_{2,N-1} c_{l(j,k(l))} + w_{2,N} c_j^N) -$$
$$- \frac{D_j}{c_{mix}} (w_{1,N-2} c_{l-1} + w_{1,N-1} c_l + w_{1,N} c_{i(l)}^N)(w_{1,N-2} c_{l(j,k(l)-1)} + w_{1,N-1} c_{l(j,k(l))} + w_{1,N} c_j^N) -$$
$$+ \frac{1}{c_{mix}} (w_{1,N-2} c_{l-1} + w_{1,N-1} c_l + w_{1,N} c_{i(l)}^N) k_{j,L} (c_j^0 - c_{j,L}) \Big)$$

where $c_i^N = bv(right, i)$.