2D Polyelectrolyte Gel Discretization

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Dissolved Ions

We would like to discretize the following equation:

$$\partial_t C_i + \nabla \cdot (\vec{u}_s C_l) = \frac{1}{\theta_s}\Big[\nabla \cdot (D_l \theta_s (\nabla C_l + z_l C_l \nabla \Phi))\Big] + f_l \tag{1}$$

Note that l= H, B, Na, C, Ca. Also, we are going to use $\nabla \Phi = \begin{pmatrix} \phi \\ \varphi \end{pmatrix}$

Since we have already corrected any ionic imbalances that the volume fraction advection step may have created (I still have to type up this part), we can take a time step of the electrodiffusive equations. Therefore, there is no need to explicitly calculate the advective terms when we form the discrete form of the equation above.

2D discretization

Here i, j denote the location in the x and y-direction respectively.

$$\begin{aligned}\frac{C_{i,j}^{k+1} - C_{i,j}^{*}}{\Delta t} = {} & \frac{D_l}{h^2 \theta_{i,j}}\Big[\overline{\theta}_{i+\frac{1}{2},j}^{k+1}(C_{i+1,j}^{k+1} - C_{i,j}^{k+1}) - \overline{\theta}_{i-\frac{1}{2},j}^{k+1}(C_{i,j}^{k+1} - C_{i-1,j}^{k+1})\Big] + \\ & \frac{D_l}{h^2 \theta_{i,j}}\Big[\overline{\theta}_{i,j+\frac{1}{2}}^{k+1}(C_{i,j+1}^{k+1} - C_{i,j}^{k+1}) - \overline{\theta}_{i,j-\frac{1}{2}}^{k+1}(C_{i,j}^{k+1} - C_{i,j-1}^{k+1})\Big] + \\ & \frac{D_l z_l}{\theta_{i,j} h}\Big[\overline{\theta}_{i+\frac{1}{2},j}^{k+1}\frac{(\widetilde{C}_{i+1,j}^{k+1} + \widetilde{C}_{i,j}^{k+1})}{2}\phi_{i+\frac{1}{2},j} - \overline{\theta}_{i-\frac{1}{2},j}^{k+1}\frac{(\widetilde{C}_{i,j}^{k+1} + \widetilde{C}_{i-1,j}^{k+1})}{2}\phi_{i-\frac{1}{2},j}\Big] + \\ & \frac{D_l z_l}{\theta_{i,j} h}\Big[\overline{\theta}_{i,j+\frac{1}{2}}^{k+1}\frac{(\widetilde{C}_{i,j+1}^{k+1} + \widetilde{C}_{i,j}^{k+1})}{2}\varphi_{i,j+\frac{1}{2}} - \overline{\theta}_{i,j-\frac{1}{2}}^{k+1}\frac{(\widetilde{C}_{i,j}^{k+1} + \widetilde{C}_{i,j-1}^{k+1})}{2}\varphi_{i,j-\frac{1}{2}}\Big] + f_l\end{aligned} \tag{2}$$

If l is for Hydrogen then:

$$f_H = -k_H^{On}(\tilde{z}\theta_{n_{i,j}}^{k+1} - B_{H_{i,j}}^{k+1} - B_{Na_{i,j}}^{k+1} - B_{Ca_{i,j}}^{k+1} - 2B_{C2_{i,j}}^{k+1}) + k_H^{off}\theta_{s_{i,j}}^{k+1} B_{H_{i,j}}^{k+1} - k(C_{H_{i,j}}^{k+1}\widetilde{C}_{B_{i,j}}^{k+1}) \tag{3}$$

In order to make equation 2 look similar to the discretized equations in the 1D polyelectrolyte gel notes, I am going to expand out the first two lines of equation 2 by using the definition of $\overline{\theta}$ and then grouping the volume fractions together as coefficients of the concentration. Therefore, I get:

$$\begin{aligned}&\frac{C_{i,j}^{k+1} - C_{i,j}^{*}}{\Delta t} = \\ &\frac{D_l}{h^2\theta_{i,j}}\Big[\Big(\frac{\theta_{i,j}^{k+1} + \theta_{i-1,j}^{k+1}}{2}\Big)C_{i-1,j}^{k+1} - \Big(\frac{\theta_{i+1,j}^{k+1} + 2\theta_{i,j}^{k+1} + \theta_{i-1,j}^{k+1}}{2}\Big)C_{i,j}^{k+1} + \Big(\frac{\theta_{i+1,j}^{k+1} + \theta_{i,j}^{k+1}}{2}\Big)C_{i+1,j}^{k+1}\Big] + \\ &\frac{D_l}{h^2\theta_{i,j}}\Big[\Big(\frac{\theta_{i,j}^{k+1} + \theta_{i,j-1}^{k+1}}{2}\Big)C_{i,j-1}^{k+1} - \Big(\frac{\theta_{i,j+1}^{k+1} + 2\theta_{i,j}^{k+1} + \theta_{i,j-1}^{k+1}}{2}\Big)C_{i,j}^{k+1} + \Big(\frac{\theta_{i,j+1}^{k+1} + \theta_{i,j}^{k+1}}{2}\Big)C_{i,j+1}^{k+1}\Big] + \\ &\frac{D_l z_l}{\theta_{i,j} h}\Big[\Big(\frac{\theta_{i+1,j}^{k+1} + \theta_{i,j}^{k+1}}{2}\Big)\Big(\frac{\widetilde{C}_{i+1,j}^{k+1} + \widetilde{C}_{i,j}^{k+1}}{2}\Big)\phi_{i+\frac{1}{2},j} - \Big(\frac{\theta_{i,j}^{k+1} + \theta_{i-1,j}^{k+1}}{2}\Big)\Big(\frac{\widetilde{C}_{i,j}^{k+1} + \widetilde{C}_{i-1,j}^{k+1}}{2}\Big)\phi_{i-\frac{1}{2},j}\Big] + \\ &\frac{D_l z_l}{\theta_{i,j} h}\Big[\Big(\frac{\theta_{i,j+1}^{k+1} + \theta_{i,j}^{k+1}}{2}\Big)\Big(\frac{\widetilde{C}_{i,j+1}^{k+1} + \widetilde{C}_{i,j}^{k+1}}{2}\Big)\varphi_{i,j+\frac{1}{2}} - \Big(\frac{\theta_{i,j}^{k+1} + \theta_{i,j-1}^{k+1}}{2}\Big)\Big(\frac{\widetilde{C}_{i,j}^{k+1} + \widetilde{C}_{i,j-1}^{k+1}}{2}\Big)\varphi_{i,j-\frac{1}{2}}\Big] + f_l\end{aligned} \tag{4}$$

By observing 4 we can define the following linear operators:

$$\mathcal{L}_i^l = \frac{D_l}{h^2} \times$$

$$\begin{bmatrix} -\frac{\theta_{i+1,1}+2\theta_{i,1}+\theta_{i-1,1}}{2\theta_{i,1}} - \frac{\theta_{i,2}+2\theta_{i,1}}{2\theta_{i,1}} & \frac{\theta_{i,2}+\theta_{i,1}}{2\theta_{i,1}} & 0 & \cdots & 0 \\ \frac{\theta_{i,2}+\theta_{i,1}}{2\theta_{i,2}} & -\frac{\theta_{i+1,2}+2\theta_{i,2}+\theta_{i-1,2}}{2\theta_{i,2}} - \frac{\theta_{i,3}+2\theta_{i,2}+\theta_{i,1}}{2\theta_{i,2}} & \frac{\theta_{i,3}+\theta_{i,2}}{2\theta_{i,2}} & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \frac{\theta_{i,J-1}+\theta_{i,J-2}}{2\theta_{i,J-1}} & -\frac{\theta_{i+1,J-1}+2\theta_{i,J-1}+\theta_{i-1,J-1}}{2\theta_{i,J-1}} - \frac{\theta_{i,J}+2\theta_{i,J-1}+\theta_{i,J-2}}{2\theta_{i,J-1}} & \frac{\theta_{i,J+1}+\theta_{i,J-1}}{2\theta_{i,J-1}} \\ 0 & \cdots & 0 & \frac{\theta_{i,J}+\theta_{i,J-1}}{2\theta_{i,J}} & -\frac{\theta_{i+1,J}+2\theta_{i,J}+\theta_{i-1,J}}{2\theta_{i,J}} - \frac{2\theta_{i,J}+\theta_{i,J-1}}{2\theta_{i,J}} \end{bmatrix} \quad (5)$$

In order to write matrix 5 in a more compact form, let us denote the terms along the diagonal as follows:

$$-\frac{\theta_{i+1,1}+2\theta_{i,1}+\theta_{i-1,1}}{2\theta_{i,1}} - \frac{\theta_{i,2}+2\theta_{i,1}}{2\theta_{i,1}} = -M_1 - N_1$$

$$\vdots$$

$$\vdots$$

$$-\frac{\theta_{i+1,J}+2\theta_{i,J}+\theta_{i-1,J}}{2\theta_{i,J}} - \frac{\theta_{i,J+1}+2\theta_{i,J}+\theta_{i,J-1}}{2\theta_{i,J}} = -M_J - N_J$$

Therefore, this linear operator can be written as:

$$\mathcal{L}_i^l = \frac{D_l}{h^2} \times \begin{bmatrix} -M_1 - N_1 & \frac{\theta_{i,2}+\theta_{i,1}}{2\theta_{i,1}} & 0 & \cdots & 0 \\ \frac{\theta_{i,2}+\theta_{i,1}}{2\theta_{i,2}} & -M_2 - N_2 & \frac{\theta_{i,3}+\theta_{i,2}}{2\theta_{i,2}} & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \frac{\theta_{i,J-1}+\theta_{i,J-2}}{2\theta_{i,J-1}} & -M_{J-1} - N_{J-1} & \frac{\theta_{i,J+1}+\theta_{i,J-1}}{2\theta_{i,J-1}} \\ 0 & \cdots & 0 & \frac{\theta_{i,J}+\theta_{i,J-1}}{2\theta_{i,J}} & -M_J - N_J \end{bmatrix} \tag{6}$$

The above operator is of size $J \times J$. This operator acts on the vector:

$$\mathcal{C}_{J\times 1}^l = \begin{bmatrix} C_{i,1}^l \\ C_{i,2}^l \\ \vdots \\ C_{i,J}^l \end{bmatrix}$$

Now define the following diagonal operators:

$$\mathcal{D}\ominus_i^l = \frac{D_l}{h^2} \begin{bmatrix} \frac{\theta_{i,1}+\theta_{i-1,1}}{2\theta_{i,1}} & 0 & \cdots & \cdots & 0 \\ 0 & \frac{\theta_{i,2}+\theta_{i-1,2}}{2\theta_{i,2}} & \ddots & \cdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \frac{\theta_{i,J-1}+\theta_{i-1,J-1}}{2\theta_{i,J-1}} & 0 \\ 0 & \cdots & \cdots & 0 & \frac{\theta_{i,J}+\theta_{i-1,J}}{2\theta_{i,J}} \end{bmatrix} \tag{7}$$

$$\mathcal{D}\oplus_i^l = \frac{D_l}{h^2} \begin{bmatrix} \frac{\theta_{i,1}+\theta_{i+1,1}}{2\theta_{i,1}} & 0 & \cdots & \cdots & 0 \\ 0 & \frac{\theta_{i,2}+\theta_{i+1,2}}{2\theta_{i,2}} & \ddots & \cdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \frac{\theta_{i,J-1}+\theta_{i+1,J-1}}{2\theta_{i,J-1}} & 0 \\ 0 & \cdots & \cdots & 0 & \frac{\theta_{i,J}+\theta_{i+1,J}}{2\theta_{i,J}} \end{bmatrix} \tag{8}$$

Finally, we can define the operator:

$$\mathcal{A}^l = \frac{D_l}{h^2} \begin{bmatrix} \mathcal{L}_1^l & \mathcal{D}\oplus_1^l & \cdots & \cdots & 0 \\ \mathcal{D}\ominus_2^l & \mathcal{L}_2^l & \mathcal{D}\oplus_2^l & \cdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \mathcal{D}\ominus_{I-1}^l & \mathcal{L}_{I-1} & \mathcal{D}\oplus_{I-1}^l \\ 0 & \cdots & \cdots & \mathcal{D}\ominus_I^l & \mathcal{L}_I^l \end{bmatrix} \tag{9}$$

Operator 9 acts on the vector:

$$\mathcal{C}^l_{(IJ)\times 1} = \begin{bmatrix} C^l_{1,1} \\ C^l_{1,2} \\ \vdots \\ C^l_{1,J} \\ C^l_{2,1} \\ C^l_{2,2} \\ \vdots \\ C^l_{2,J} \\ \vdots \\ C^l_{I,1} \\ C^l_{I,2} \\ \vdots \\ C^l_{I,J} \end{bmatrix}$$

$$\mathcal{D}^l_{I\times I} = \frac{D_l z_l}{h} \times$$
$$\begin{bmatrix} \left(\frac{\theta_{2,j}+\theta_{1,j}}{2\theta_{1,j}}\right)\left(\frac{\widetilde{C}_{2,j}+\widetilde{C}_{1,j}}{2}\right) & 0 & \cdots & 0 \\ -\left(\frac{\theta_{2,j}+\theta_{1,j}}{2\theta_{2,j}}\right)\left(\frac{\widetilde{C}_{2,j}+\widetilde{C}_{1,j}}{2}\right) & \left(\frac{\theta_{3,j}+\theta_{2,j}}{2\theta_{2,j}}\right)\left(\frac{\widetilde{C}_{3,j}+\widetilde{C}_{2,j}}{2}\right) & 0 & \vdots \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & -\left(\frac{\theta_{I-1,j}+\theta_{I-2,j}}{2\theta_{I-1,j}}\right)\left(\frac{\widetilde{C}_{I-1,j}+\widetilde{C}_{I-2,j}}{2}\right) & \left(\frac{\theta_{I,j}+\theta_{I-1,j}}{2\theta_{I-1,j}}\right)\left(\frac{\widetilde{C}_{I,j}+\widetilde{C}_{I-1,j}}{2}\right) \\ 0 & \cdots & 0 & -\left(\frac{\theta_{I,j}+\theta_{I-1,j}}{2\theta_{I,j}}\right)\left(\frac{\widetilde{C}_{I,j}+\widetilde{C}_{I-1,j}}{2}\right) \end{bmatrix} \tag{10}$$

This operator acts on the vector: $\phi = \begin{bmatrix} \phi_{\frac{3}{2},j} & \phi_{\frac{5}{2},j} & \cdots & \phi_{I-\frac{1}{2},j} \end{bmatrix}^T$

$$\mathcal{E}^l_{I\times I} = \frac{D_l z_l}{h} \times$$
$$\begin{bmatrix} \left(\frac{\theta_{i,2}+\theta_{i,1}}{2\theta_{i,1}}\right)\left(\frac{\widetilde{C}_{i,2}+\widetilde{C}_{i,1}}{2}\right) & 0 & \cdots & 0 \\ -\left(\frac{\theta_{i,2}+\theta_{i,1}}{2\theta_{i,2}}\right)\left(\frac{\widetilde{C}_{i,2}+\widetilde{C}_{i,1}}{2}\right) & \left(\frac{\theta_{i,3}+\theta_{i,2}}{2\theta_{i,2}}\right)\left(\frac{\widetilde{C}_{i,3}+\widetilde{C}_{i,2}}{2}\right) & 0 & \vdots \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & -\left(\frac{\theta_{i,J-1}+\theta_{i,J-2}}{2\theta_{i,J-1}}\right)\left(\frac{\widetilde{C}_{i,J-1}+\widetilde{C}_{i,J-2}}{2}\right) & \left(\frac{\theta_{i,J}+\theta_{i,J-1}}{2\theta_{i,J-1}}\right)\left(\frac{\widetilde{C}_{i,J}+\widetilde{C}_{i,J-1}}{2}\right) \\ 0 & \cdots & 0 & -\left(\frac{\theta_{i,J}+\theta_{i,J-1}}{2\theta_{i,J}}\right)\left(\frac{\widetilde{C}_{i,J}+\widetilde{C}_{i,J-1}}{2}\right) \end{bmatrix} \tag{11}$$

This operator acts on the vector: $\varphi = \begin{bmatrix} \varphi_{i,\frac{3}{2}} & \varphi_{i,\frac{5}{2}} & \cdots & \varphi_{i,J-\frac{1}{2}} \end{bmatrix}^T$

Some New Notation

For convenience, we will define some new notation. We will denote the Hadamard product between two matrices as:

$$A \bigotimes B$$

The operator $\bigotimes$ refers to the element-wise multiplication of two matrices. For example, the matrix multiplaction in the last term of equation 3 can be performed as follows:

$$\begin{bmatrix} C_{H_{11}} & C_{H_{12}} & C_{H_{13}} & \cdots & C_{H_{1n}} \\ C_{H_{21}} & C_{H_{22}} & C_{H_{23}} & \cdots & C_{H_{2n}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ C_{H_{n1}} & C_{H_{n2}} & C_{H_{n3}} & \cdots & C_{H_{nn}} \end{bmatrix} \bigotimes \begin{bmatrix} \widetilde{C}_{B_{11}} & \widetilde{C}_{B_{12}} & \widetilde{C}_{B_{13}} & \cdots & \widetilde{C}_{B_{1n}} \\ \widetilde{C}_{B_{21}} & \widetilde{C}_{B_{22}} & \widetilde{C}_{B_{23}} & \cdots & \widetilde{C}_{B_{2n}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \widetilde{C}_{B_{n1}} & \widetilde{C}_{B_{n2}} & \widetilde{C}_{B_{n3}} & \cdots & \widetilde{C}_{B_{nn}} \end{bmatrix} \tag{12}$$