HOMOGENIZATION OF ELECTROKINETIC FLOWS IN POROUS MEDIA: THE ROLE OF NON-IDEALITY.

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1. Introduction

2. Partial linearization of the model

3. Homogenization and macroscopic Onsager properties

4. Numerical results on the effective coefficients

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We consider ion transport in a charged porous medium.

Coupled model:
- Poisson equation for the electrostatic potential $\Psi^e$,
- Stokes equations for the fluid velocity and pressure $(u^e, p^e)$,
- Nernst-Planck (convection-diffusion) equations for the $N$ species concentrations $n_j^e$.

Non-ideal model for the ion diffusion: activity coefficients given by the MSA model.

Our goal is to homogenize this model and compare the effective properties in the ideal and MSA cases.

Small pores: Debye length of the order of the pore size.

We choose a scaling of the model for which all unknowns are varying at the pore scale (similar to Looker and Carnie 2006).
Assumptions and notations

- Rigid solid part of the porous medium.
- Saturated incompressible single phase flow containing $N$ dilute charged species with valence $z_j$ and same ion radius $\sigma$.
- For each species: diffusion coefficient $D_j^0$, Péclet number $\text{Pe}_j$, diffusive flux $\mathbf{j}_j^\epsilon$.
- Surface charge $-\Sigma^*$ on the pore walls.
- Small hydrostatic force $\mathbf{f}^*$ and external potential $\Psi^{\text{ext},*}$.
Small parameter $\epsilon = \text{ratio between the period and a macroscopic lengthscale}$.

Periodic porous medium $\Omega$: fluid part $\Omega^\epsilon$, solid part $\Omega \setminus \Omega^\epsilon$. 
Adimensionalized equations (Poisson + Stokes + Nernst-Planck):

\[-\epsilon^2 \Delta \Psi^e = \beta \sum_{j=1}^{N} z_j n_j^e \quad \text{in} \quad \Omega^e,\]

\[\epsilon^2 \Delta u^e - \nabla p^e = f^* + \sum_{j=1}^{N} z_j n_j^e \nabla \Psi^e \quad \text{in} \quad \Omega^e,\]

\[\text{div} u^e = 0 \quad \text{in} \quad \Omega^e,\]

\[\text{div} \left( j_i^e + \text{Pe}_i n_i^e u^e \right) = 0 \quad \text{in} \quad \Omega^e, \quad i = 1, \ldots, N,\]

\[j_i^e = - \sum_{j=1}^{N} L_{ij}^e \nabla M_j^e \quad \text{and} \quad M_j^e = \ln \left( n_j^e \gamma_j^e \epsilon_j^e \Psi^e \right),\]

\[L_{ij}^e = n_i^e \left( \delta_{ij} + \frac{k_B T}{D_i^0} \Omega_{ij} \right) \left( 1 + R_{ij} \right) \quad i, j = 1, \ldots, N,\]

Boundary conditions on the pore walls:

\[\epsilon \nabla \Psi^e \cdot \nu = -\Sigma^*, \quad u^e = 0, \quad j_i^e \cdot \nu = 0 \quad \text{on} \quad \partial \Omega^e, \quad i = 1, \ldots, N.\]
Non-ideality: MSA model

\( \gamma_j^\varepsilon = \) activity coefficient

**Ideal case:** \( \gamma_j^\varepsilon = 1, \Omega_{ij} = 0 \) and \( \mathcal{R}_{ij} = 0 \) \( \Rightarrow L_{ij}^\varepsilon = n_i^\varepsilon \delta_{ij} \).

**Non-ideal case:**

\[
\gamma_j^\varepsilon = \gamma^{HS} \exp\left\{- \frac{L_B \Gamma_c^\varepsilon z_j^2}{(1 + \Gamma_c^\varepsilon \sigma)} \right\} \quad \text{and} \quad (\Gamma^\varepsilon)^2 = \sum_{k=1}^{N} \frac{n_k^\varepsilon z_k^2}{(1 + \Gamma_c^\varepsilon \sigma)^2}
\]

where \( \Gamma^\varepsilon \) is the screening parameter and \( \gamma^{HS} \) is the hard-sphere term

\[
\gamma^{HS} = \exp\{p(\xi)\} \quad \text{with} \quad p(\xi) = \xi \frac{8 - 9\xi + 3\xi^2}{(1 - \xi)^3} \quad \text{and} \quad \xi = \frac{\pi n_c}{6} \sum_{k=1}^{N} n_k^\varepsilon \sigma^3
\]

Complicated formulas for \( \Omega_{ij} \) and \( \mathcal{R}_{ij} \) (but the Onsager tensor \( L_{ij}^\varepsilon \) is symmetric).
External boundary conditions

For simplicity we choose a cube domain $\Omega = (0, L)^d$ with $d = 2, 3$.

On the outer boundary $\partial \Omega^\epsilon \cap \partial \Omega$ we can thus impose periodic boundary conditions.

- The fluid velocity and pressure $(u^\epsilon, p^\epsilon)$ and the concentrations $n^\epsilon_j$ are $L$-periodic.

- Given an external potential $\Psi_{ext,*}(x)$, the total electrokinetic potential $\Psi^\epsilon + \Psi_{ext,*}$ is $L$-periodic.

The forcing is caused by $\Psi_{ext,*}$, the surface charge density $-\Sigma^*$ and the hydrodynamic force $f^*$.
Strategy for the homogenization process

✧ Find so-called \textit{equilibrium solutions} in the absence of exterior forcing. In the ideal case it yields the (non-linear) Poisson-Boltzmann equation.

✧ For small exterior forcing $\mathbf{f}^*$ and $\Psi^{ext,*}$ (but large surface charge $\Sigma^*$), \textit{linearize} the transport model.

✧ \textbf{Homogenize} the linear model on a non-linear electrostatic background.
Bibliography


❉ Many numerical works on the upscaling: Adler, Coelho, Marino, Shapiro, Smith...


❉ Homogenization: Schmuck (2010), Ray (2011)...

Following the lead of O’Brien and White (1978) we perform a (partial) linearization.

In the ideal case, this is the same as in Looker and Carnie (2006).

We assume that the forcing terms $\Psi_{\text{ext},*}$ and $f^*$ are small, but not the surface charge density $\Sigma^*$ which can still be large.

We denote by $n_i^{0,\epsilon}, \Psi^{0,\epsilon}, u^{0,\epsilon}, p^{0,\epsilon}$ the equilibrium quantities for $f^* = 0$ and $\Psi_{\text{ext},*} = 0$.

At equilibrium we look for a solution with vanishing fluxes

$$u^{0,\epsilon} = 0 \quad \text{and} \quad j_i^{0,\epsilon} = 0$$

and an $\epsilon$-periodic electrostatic potential

$$\Psi^{0,\epsilon}(x) = \Psi^0\left(\frac{x}{\epsilon}\right)$$
Equilibrium solution

Consequence of the zero ionic flux $\mathbf{j}_i^{0,\epsilon} = 0$:

$$\nabla M_j^\epsilon = 0 \quad \text{with} \quad M_j^\epsilon = \ln \left( n_j^\epsilon \gamma_j^\epsilon e^{z_j \Psi_j^\epsilon} \right)$$

Thus

$$n_j^{0,\epsilon}(x) = n_j^0(\infty) \gamma_j^0(\infty) \frac{\exp \left\{-z_j \Psi_j^{0,\epsilon}(x)\right\}}{\gamma_j^{0,\epsilon}(x)}$$

where $n_j^0(\infty)$ are constants (called infinite dilution concentrations) and $\gamma_j^0(\infty)$ are the constant activity coefficients for zero potential.
\[ -\Delta_y \Psi^0(y) = \beta \sum_{j=1}^{N} z_j n_j^0(y) \quad \text{in } Y_F, \]
\[ \nabla_y \Psi^0 \cdot \nu = -\Sigma^* \quad \text{on } \partial Y_F \setminus \partial Y, \]
\[ y \to \Psi^0(y) \text{ is } 1 \text{- periodic}, \]
\[ n_j^0(y) = n_j^0(\infty) \gamma_j^0(\infty) \frac{\exp \{-z_j \Psi^0(y)\}}{\gamma_j^0(y)}, \]

with the activity coefficient defined by
\[ \gamma_j^0(y) = \gamma^{HS}(y) \exp\{-\frac{L_B \Gamma^0(y) \Gamma_c z_j^2}{(1 + \Gamma^0(y) \Gamma_c \sigma)}\} \quad \text{and} \quad (\Gamma^0(y))^2 = \sum_{k=1}^{N} \frac{n_k^0(y) z_k^2}{(1 + \Gamma_c \Gamma^0(y) \sigma)^2}, \]
\[ \gamma^{HS} = \exp\{p(\xi)\} \quad \text{with} \quad p(\xi) = \xi \frac{8 - 9\xi + 3\xi^2}{(1 - \xi)^3} \quad \text{and} \quad \xi(y) = \frac{\pi n_c}{6} \sum_{k=1}^{N} n_k^0(y) \sigma^3. \]
We impose the **bulk electroneutrality condition**, i.e., for $\Psi^0 = 0$,

$$\sum_{j=1}^{N} z_j n_j^0(\infty) = 0.$$ 

**Theorem.** Assuming that the ion radius $\sigma$ is not too small and that the characteristic concentration $n_c$ is not too large, there exists a solution $\Psi^0$ of the Poisson-Boltzmann equation.

**Remark.** In the ideal case, $\gamma_j^0(y) = 1$, the Poisson-Boltzmann equation has always a unique solution since it corresponds to the minimization of a convex energy. The MSA model destroys this convexity property.
Linearization

\[ n_i^\varepsilon(x) = n_i^{0,\varepsilon}(x) + \delta n_i^\varepsilon(x), \quad \Psi^\varepsilon(x) = \Psi^{0,\varepsilon}(x) + \delta \Psi^\varepsilon(x), \]
\[ u^\varepsilon(x) = u^{0,\varepsilon}(x) + \delta u^\varepsilon(x), \quad p^\varepsilon(x) = p^{0,\varepsilon}(x) + \delta p^\varepsilon(x), \]

Trick (O’Brien and White): introduce the ionic potential \( \Phi_i^\varepsilon \) defined by

\[ n_i^\varepsilon(x) \gamma_i^\varepsilon(x) = n_i^{0}(\infty) \exp\{-z_i(\Psi^\varepsilon(x) + \Phi_i^\varepsilon(x) + \Psi^{ext,*}(x))\}. \]

In the ideal case, this trick is useful because it yields the following change of variables

\[ \delta n_i^\varepsilon(x) = -z_i n_i^{0,\varepsilon}(x) \left( \delta \Psi^\varepsilon(x) + \Phi_i^\varepsilon(x) + \Psi^{ext,*}(x) \right) \]

However, in the non-ideal case the algebra is much more complex!

In particular, each \( \delta n_i^\varepsilon \) involves all \( \Phi_k^\varepsilon \).
After linearization (and some algebra!) we obtain the problem we want to homogenize:

\[
\begin{aligned}
\epsilon^2 \Delta u^\epsilon - \nabla P^\epsilon &= f^* - \sum_{j=1}^{N} z_j n^{0,\epsilon}_j \nabla \left( \Phi_j^\epsilon + \Psi^{ext,*} \right) \quad \text{in } \Omega^\epsilon, \\
\text{div} u^\epsilon &= 0 \quad \text{in } \Omega^\epsilon, \quad u^\epsilon = 0 \quad \text{on } \partial \Omega^\epsilon \setminus \partial \Omega, \\
\text{div} n^{0,\epsilon}_i \left( \sum_{j=1}^{N} K^\epsilon_{ij} z_j \nabla \left( \Phi_j^\epsilon + \Psi^{ext,*} \right) + P e_i u^\epsilon \right) &= 0 \quad \text{in } \Omega^\epsilon, \quad i = 1, \ldots, N, \\
K^\epsilon_{ij} &= \left( \delta_{ij} + \frac{k_B T}{D_0^i} \Omega_{ij} \right) \left( 1 + R_{ij} \right), \quad i, j = 1, \ldots, N, \\
\sum_{j=1}^{N} K^\epsilon_{ij} z_j \nabla \left( \Phi_j^\epsilon + \Psi^{ext,*} \right) \cdot \nu &= 0 \quad \text{on } \partial \Omega^\epsilon \setminus \partial \Omega, \\
\end{aligned}
\]

\( u^\epsilon, \ P^\epsilon, \ \Phi_j^\epsilon \) are L–periodic.
In the previous equations, $n_{j,\epsilon}^0$ and $K_{ij,\epsilon}$ are $\epsilon$-periodic coefficients evaluated at equilibrium (by solving the non-linear Poisson-Boltzmann equation).

$$\Psi_{0,\epsilon}(x) = \Psi^0\left(\frac{x}{\epsilon}\right), \quad n_{j,\epsilon}^0(x) = n_j^0\left(\frac{x}{\epsilon}\right), \quad K_{ij,\epsilon}(x) = K_{ij}\left(\frac{x}{\epsilon}\right).$$

The linearization is thus partial because $\Psi^0$ is solution of a (highly) non-linear equation.

**Lemma.** The linearized problem admits a unique solution.

**Remark.** It is a crucial assumption that all ions have the same diameter.
-III- HOMOGENIZATION AND TWO-SCALE LIMIT

✗ We assume that the porous medium is periodic.

✗ Periodic unit cell \( Y = (0, 1)^n = Y_F \cup \Sigma^0 \) with fluid part \( Y_F \).

✗ Fast variable \( y = \frac{x}{\epsilon} \).

✗ Two-scale asymptotic expansions:

\[
\begin{align*}
\mathbf{u}^\varepsilon(x) &= \mathbf{u}^0(x, x/\varepsilon) + \varepsilon \mathbf{u}^1(x, x/\varepsilon) + \ldots, \\
P^\varepsilon(x) &= p^0(x) + \varepsilon p^1(x, x/\varepsilon) + \ldots, \\
\Phi^\varepsilon_j(x) &= \Phi^0_j(x) + \varepsilon \Phi^1_j(x, x/\varepsilon) + \ldots.
\end{align*}
\]
Theorem.

The solution satisfies

\[ u^\varepsilon(x) \approx u^0(x, \frac{x}{\varepsilon}), \quad P^\varepsilon(x) \approx p^0(x) + \varepsilon p^1(x, \frac{x}{\varepsilon}), \quad \Phi^\varepsilon_j(x) \approx \Phi^0_j(x) + \varepsilon \Phi^1_j(x, \frac{x}{\varepsilon}), \]

where \((u^0, p^0, p^1, \{\Phi^0_j, \Phi^1_j\})\) is the solution of the two-scale homogenized problem (which admits a unique solution).

Remark.

The difficulty is to extract from the two-scale homogenized problem a macroscopic homogenized model and to study its Onsager properties.

Remark.

The (oscillating) concentrations are recovered from the ionic potentials by

\[ n^\varepsilon_i(x) \approx \frac{n^0_i(\infty) \gamma^0_i(\infty)}{\gamma^0_i(\frac{x}{\varepsilon})} \exp\{-z_i(\Psi^0(\frac{x}{\varepsilon}) + \Phi^0_i(x) + \Psi^{ext,*}(x))\}. \]
Two-scale homogenized problem

\[-\Delta_y u^0(x, y) + \nabla_y p^1(x, y) = -\nabla_x p^0(x) - f^*(x)\]

\[+ \sum_{j=1}^{N} z_j n_j^0(y) (\nabla_y \Phi^1_j(x, y) + \nabla_x \Phi^0_j(x) + E^*(x)) \text{ in } \Omega \times Y_F,\]

\[\text{div}_y u^0(x, y) = 0 \text{ in } \Omega \times Y_F, \quad \text{div}_x \left( \int_{Y_F} u^0 \, dy \right) = 0 \text{ in } \Omega,\]

\[-\text{div}_y n_i^0(y) \left( \sum_{j=1}^{N} K_{ij} z_j (\nabla_y \Phi^1_j(x, y) + \nabla_x \Phi^0_j(x) + E^*(x)) + Pe_i u^0(x, y) \right) = 0\]

\[-\text{div}_x \int_{Y_F} n_i^0(y) \left( \sum_{j=1}^{N} K_{ij} z_j (\nabla_y \Phi^1_j(x, y) + \nabla_x \Phi^0_j(x) + E^*(x)) + Pe_i u^0(x, y) \right) \, dy = 0\]

\[u^0(x, y) = 0 \text{ on } \Omega \times \partial Y_F, \quad \sum_{j=1}^{N} K_{ij} z_j (\nabla_y \Phi^1_j + \nabla_x \Phi^0_j + E^*) \cdot \nu = 0 \text{ on } \Omega \times \partial Y_F.\]

The macroscopic forcing terms are in red and blue.
Factorization of the two-scale functions

We want to separate the slow $x$ and fast $y$ variables. Our approach is different from that of Looker and Carnie.

We decompose

$$u^0(x, y) = \sum_{k=1}^{d} \left( -v^{0,k}(y) \left( \frac{\partial p^0}{\partial x_k} + f^*_k \right)(x) + \sum_{i=1}^{N} v^{i,k}(y) \left( E^*_k + \frac{\partial \Phi^0_i}{\partial x_k} \right)(x) \right)$$

$$p^1(x, y) = \sum_{k=1}^{d} \left( -\pi^{0,k}(y) \left( \frac{\partial p^0}{\partial x_k} + f^*_k \right)(x) + \sum_{i=1}^{N} \pi^{i,k}(y) \left( E^*_k + \frac{\partial \Phi^0_i}{\partial x_k} \right)(x) \right)$$

$$\Phi^1_j(x, y) = \sum_{k=1}^{d} \left( -\theta^{0,k}_j(y) \left( \frac{\partial p^0}{\partial x_k} + f^*_k \right)(x) + \sum_{i=1}^{N} \theta^{i,k}_j(y) \left( E^*_k + \frac{\partial \Phi^0_i}{\partial x_k} \right)(x) \right)$$

where $(v^{i,k}, \pi^{i,k}, \theta^{i,k}_j)$, for $0 \leq i \leq N$, are solutions of cell problems.
Definition of effective (or homogenized) quantities

We define the following effective hydrodynamic velocity:

\[ u(x) = \frac{1}{|Y_F|} \int_{Y_F} u^0(x, y) \, dy. \]

We also introduce the effective electrochemical potential of the \( j \)th species

\[ \mu_j(x) = -z_j \left( \Phi_j^0(x) + \Psi^{ext,*}(x) \right), \]

and the effective ionic flux of the \( j \)th species

\[ j_j(x) = \frac{1}{|Y_F|} \int_{Y_F} n_j^0(y) \left( \sum_{l=1}^N K_{jl} \frac{z_l}{\text{Pe}_j} \left( \nabla_y \Phi_l^1(x, y) + \nabla_x \Phi_l^0(x) + \mathbf{E}^*(x) \right) + u^0 \right) \, dy \]

We are now able to write the homogenized equations for the above effective fields.
Theorem (homogenized equations)

The macroscopic equations in $\Omega$ are

\[ \text{div}_x \mathbf{u} = 0 \quad \text{and} \quad \text{div}_x \mathbf{j}_i = 0, \quad \text{for } i = 1, \ldots, N, \quad \text{with} \]

\[
\begin{pmatrix}
\mathbf{u} \\
\{\mathbf{j}_i\}
\end{pmatrix}
= -\mathcal{M}
\begin{pmatrix}
\nabla p^0 + \mathbf{f}^* \\
\{\nabla \mu_i\}
\end{pmatrix}
\quad \text{and} \quad
\mathcal{M} =
\begin{pmatrix}
K & \frac{J_1}{z_1} & \cdots & \frac{J_N}{z_N} \\
L_1 & \frac{D_{11}}{z_1} & \cdots & \frac{D_{1N}}{z_N} \\
\vdots & \vdots & \ddots & \vdots \\
L_N & \frac{D_{N1}}{z_1} & \cdots & \frac{D_{NN}}{z_N}
\end{pmatrix}
\]

Furthermore the tensor $\mathcal{M}$ is symmetric positive definite (Onsager properties).
The matrices $\mathbb{J}_i$, $\mathbb{K}$, $\mathbb{D}_{ji}$ and $\mathbb{L}_j$ are defined by their entries

$$\{\mathbb{J}_i\}_{lk} = \frac{1}{|Y_F|} \int_{Y_F} v^{i,k}(y) \cdot e^l \, dy,$$

$$\{\mathbb{K}\}_{lk} = \frac{1}{|Y_F|} \int_{Y_F} v^{0,k}(y) \cdot e^l \, dy,$$

$$\{\mathbb{D}_{ji}\}_{lk} = \frac{1}{|Y_F|} \int_{Y_F} n_j^0(y) \left( v^{i,k}(y) + \sum_{m=1}^{N} K_{jm} \frac{z_m}{Pe_j} \left( \delta_{im} e^k + \nabla_y \theta^{i,k}_m(y) \right) \right) \cdot e^l \, dy,$$

$$\{\mathbb{L}_j\}_{lk} = \frac{1}{|Y_F|} \int_{Y_F} n_j^0(y) \left( v^{0,k}(y) + \sum_{m=1}^{N} K_{jm} \frac{z_m}{Pe_j} \nabla_y \theta^{0,k}_m(y) \right) \cdot e^l \, dy.$$
First cell problem: imposed pressure gradient

\[
\begin{align*}
-\Delta_y v^{0,k}(y) + \nabla_y \pi^{0,k}(y) &= e^k + \sum_{j=1}^{N} z_j n_j^0(y) \nabla_y \theta_j^{0,k}(y) \quad \text{in } Y_F \\
\text{div}_y v^{0,k}(y) &= 0 \quad \text{in } Y_F, \quad v^{0,k}(y) = 0 \quad \text{on } \partial Y_F, \\
-\text{div}_y n_i^0(y) \left( \sum_{j=1}^{N} K_{ij}(y) z_j \nabla_y \theta_j^{0,k}(y) + \text{Pe}_i v^{0,k}(y) \right) &= 0 \quad \text{in } Y_F \\
\sum_{j=1}^{N} K_{ij}(y) z_j \nabla_y \theta_j^{0,k}(y) \cdot \nu &= 0 \quad \text{on } \partial Y_F.
\end{align*}
\]
Second cell problem: **imposed electrostatic field**

\[
\begin{aligned}
-\Delta_y v^{l,k}(y) + \nabla_y \pi^{l,k}(y) &= \sum_{j=1}^{N} z_j n_j^0(y) (\delta_{lj} e^k + \nabla_y \theta_j^{l,k}(y)) \quad \text{in } Y_F, \\
\text{div}_y v^{i,k}(y) &= 0 \quad \text{in } Y_F, \quad v^{i,k}(y) = 0 \quad \text{on } \partial Y_F, \\
-\text{div}_y n_i^0(y) \left( \sum_{j=1}^{N} K_{ij}(y) z_j (\delta_{lj} e^k + \nabla_y \theta_j^{l,k}(y)) + \text{Pe}_i v^{l,k}(y) \right) &= 0 \quad \text{in } Y_F, \\
\sum_{j=1}^{N} K_{ij}(y) z_j (\delta_{lj} e^k + \nabla_y \theta_j^{l,k}(y)) \cdot \nu &= 0 \quad \text{on } \partial Y_F.
\end{aligned}
\]
All computations are done with FreeFem++.

Aqueous solution of NaCl at 298° K.

Cation Na$^+$ with diffusivity $D_1^0 = 13.33 \times 10^{-10} m^2/s$.

Anion Cl$^-$ with diffusivity $D_2^0 = 20.32 \times 10^{-10} m^2/s$.

The concentrations of the species in the bulk are considered equal:
$n_1^0(\infty) = n_2^0(\infty) = 0.1\text{mole/l}$.

The dynamic viscosity $\eta$ is equal to $0.89 \times 10^{-3} kg/(m \text{ sec})$.

The pore size is $l = 5. e - 8 m = 50\text{nm}$.

The ion radius is $\sigma = 2\text{nm}$.

The surface charge density is (minus) $\Sigma^* = 0.129 C/m^2$. 

Ideal case: cation concentration (left), anion concentration (right)
Averaged ion concentration as a function of $n_1^0(\infty) = n_2^0(\infty)$
Rescaled anion concentration $\frac{N_2mean}{n_2^0(\infty)}$ as a function of $n_1^0(\infty) = n_2^0(\infty)$
Permeability tensor (rescaled): variation of $n_1^0(\infty) = n_2^0(\infty)$
Diffusion tensor for the cation: variation of $n_1^0(\infty) = n_2^0(\infty)$
Coupling tensors $\mathbb{L}_i$ : variation of $n_1^0(\infty) = n_2^0(\infty)$
Ion transport in porous media

Permeability tensor: variation of the pore size (nm)

![Graph showing permeability tensor variation](image)
Averaged cell concentration: variation of the pore size (nm). Donnan effect.
Variation of porosity: 0.19, 0.51 and 0.75
Variation of porosity: permeability
Diffusion versus porosity: cation (left), anion (right)