

Numerical investigation of electrokinetic effects on pore scale transport and dispersion through porous media

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Introduction

Dispersion coefficient is an important factor in the solute transport phenomena. However, solute dispersion induced by electrokinetic driven flow was not study at the pore scale. In separation science and chromatography, dispersion determines the removal and separation efficiency. It has low energy cost with small hydrodynamic dispersion.

To predict the removal efficiency of various porous media of electrolyte properties should be considered, which affect flow and transport at pore scale

In our study, we use numerical method to investigate electrokinetic flow and transport properties starting from the pore scale. A pore network modeling was introduced to study electrokinetic effects and provide three dimensional velocity and concentration field. And pore network represents a porous media and includes the microstructure information, such as pore size distribution, coordination number.

Research questions

1. How electrokinetic driven flow (EOF) differs from pressure driven flow (PDF)?
2. What are the most important porous media properties (such as aspect ratio) and electrokinetic ratio($k*d$) control flow and transport in porous media?

Methods

Governing equation is

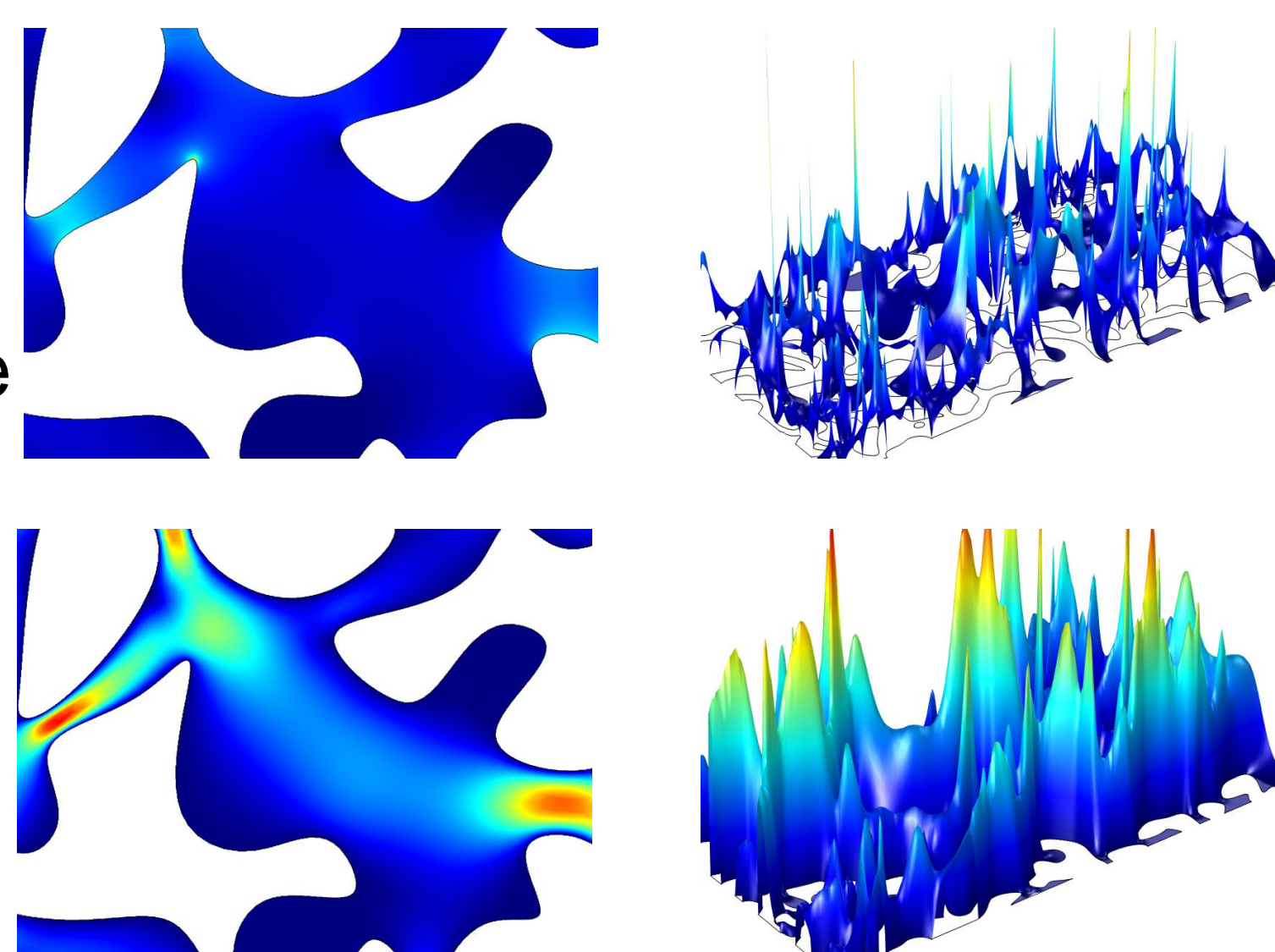
$$Q = L_{11}\Delta P + L_{12}\Delta V$$

Where Q is volumetric flow, ΔP is pressure difference, ΔV is potential difference, the coupling coefficient are

$$L_{11} = \frac{\pi d^4}{8\mu L}$$

$$L_{12} = \frac{\pi d^2 * \epsilon_0 \epsilon_r \zeta}{\mu L} G_1$$

$$G_1 = 1 - \frac{2I_1(\kappa d)}{\kappa d I_0(\kappa d)}$$



Where $k*d$ is larger than 100, G_1 can equal to 1, is thin double layer limit.

Velocity used as an input for advection diffusion equation in each pore. Optimized the breakthrough curve at outlet with analytical solution of solute transport equation, we obtain the dispersion coefficient.

	Pore network modeling	FEM Method	Hlushkou, D et al 2007
Structure	Heterogeneous	Heterogeneous	Random
Porosity	.37	.42	.38
Electrokinetic ratio ($k*d$)	>100	>100	>>100
Coordination number	3.25	3	
Tortuosity	.59	.59	.68
Longitudinal dispersion	Optimized from analytical solution	$\theta \frac{\partial c}{\partial t} + \theta v \frac{\partial c}{\partial x} = \theta D_L \frac{\partial^2 c}{\partial x^2}$	$D_L = \frac{1}{2} \frac{d\sigma^2}{dt}$

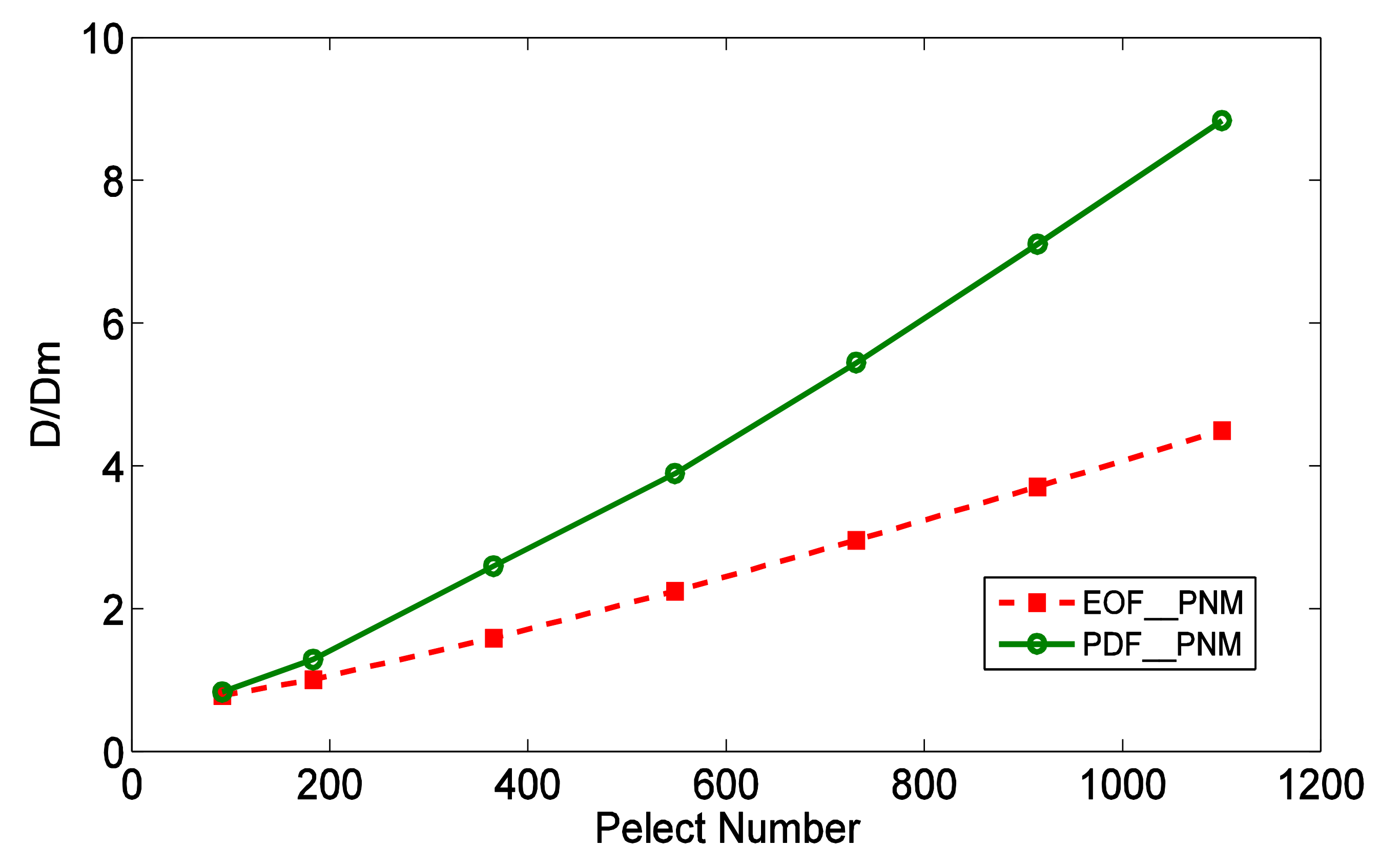
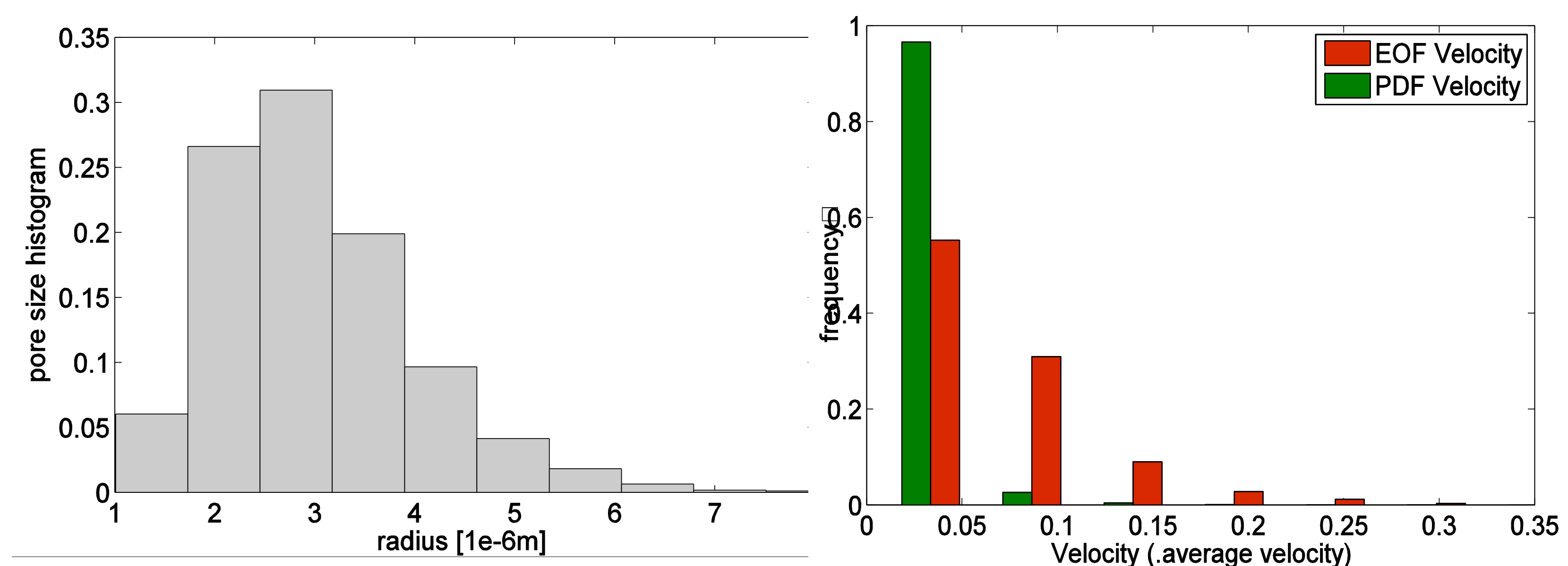
Results and discussion

The velocity distribution is different applying different driving force.

Most of PDF velocity is slow flow close to the wall, likely to have a long tail with large gradient.

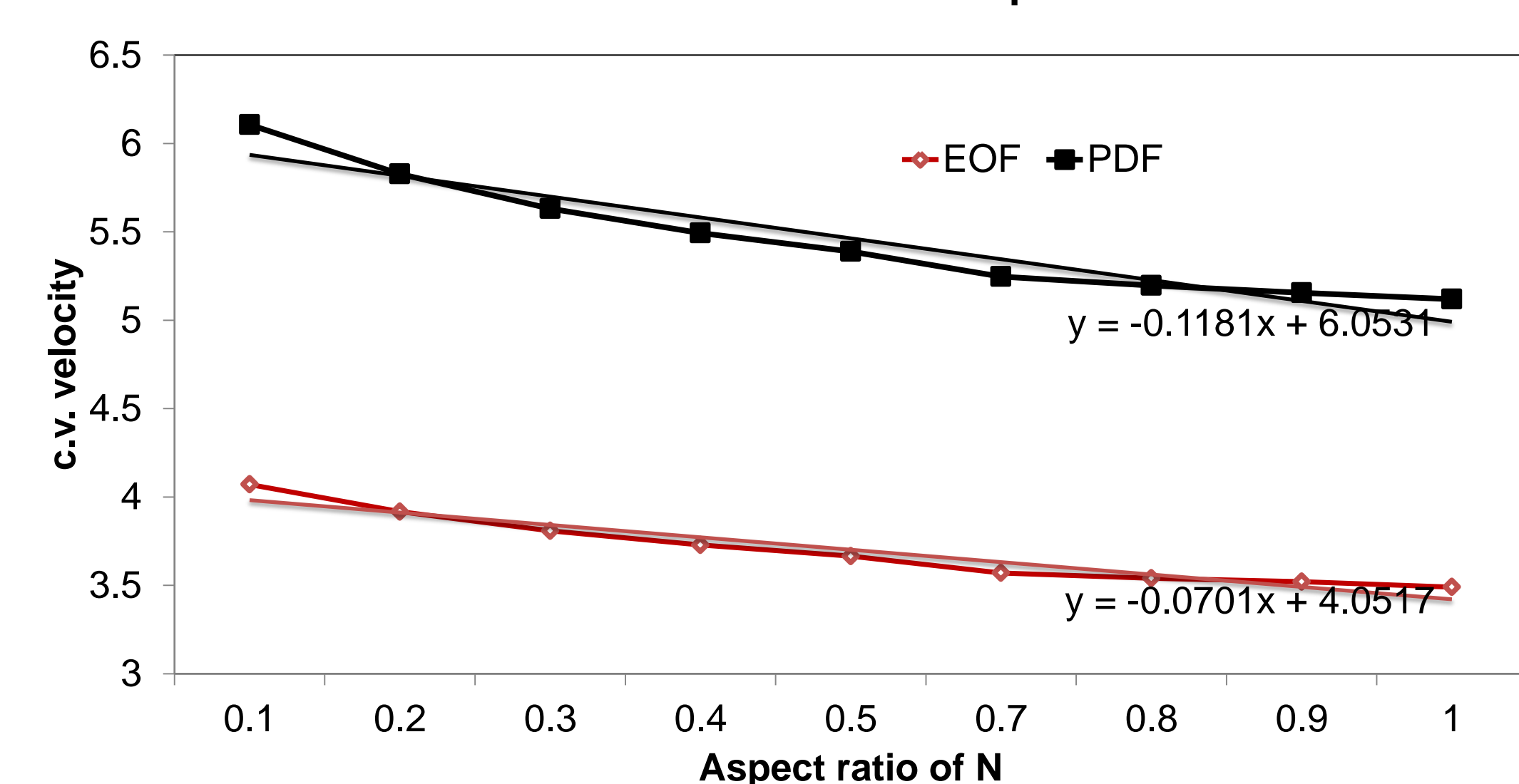
EOF velocity is more uniform distributed and close to mean value, in a relative narrow range.

The distinction between PDF and EOF is caused by pore scale velocity profile.



Conclusion

1. Dispersion coefficient induced by PDF differs from EOF.
2. Hydrodynamic dispersion is normally larger than electrokinetic dispersion. Mainly due to different velocity distribution profile, electrokinetic flow is more uniform distributed.
3. From pore networks modeling, the main factor for the dispersion coefficient change under same electrochemical background is coefficient variation of velocity.
4. The aspect ratio plays roles in the dispersion coefficient.
5. Electrokinetic radius has effects on the dispersion coefficient.



Dutta, D. (2008), Electrokinetic transport of charged samples through rectangular channels with small zeta potentials, *Anal Chem*, 80(12), 4723-4730.
Hlushkou, D., S. Khirevich, V. Apanasovich, A. Seidel-Morgenstern, and U. Tallarek (2007), Pore-scale dispersion in electrokinetic flow through a random sphere packing, *Anal Chem*, 79(1), 113-121.