EFFECTS OF SURFACE CHARGE DENSITY AND DISTRIBUTION ON THE NANOCHANNEL ELECTRO-OsmOTIC FLOW

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Other project

Development of MEAM potential for Al-Si-Mg-Cu-Fe alloys
B. Jelinek, S. Groh, A. Moitra, M. Horstemeyer, J. Houze, S-G. Kim, G. Wagner, M. Baskes
http://arxiv.org/abs/1107.0544

Scripts to reproduce some of the potential tests
http://code.google.com/p/ase-atomistic-potential-tests
using Atomistic Simulation Environment (ASE)
https://wiki.fysik.dtu.dk/ase
motivation for using ASE - talk at the NIST 2011 workshop
http://www.ctcms.nist.gov/potentials/activities.html

CAVS cyberinfrastructure site https://ccg.hpc.msstate.edu
Fixed Si channel walls, innermost layer charged negatively
Dimensions of a solute region 4.66x4.22x3.49 nm, PBC x,y.
108 Na\textsuperscript{+}, 38 Cl\textsuperscript{-}, 2144 SPC/E H\textsubscript{2}O molecules (not shown)

Velocity profiles

![Velocity profiles graph](image)
Velocity predicted from charge density

Stokes equation:

\[
\frac{d}{dz} \left[ \eta(z) \frac{du_x(z)}{dz} \right] = -F_d(z)
\]

Blue:
inverse power viscosity

\[
\eta(z) = \left[ 1 - \left( \frac{z}{h} \right)^2 \right]^{-p} \eta_{\text{exp}}
\]

Red:
constant viscosity

Black circles:
Molecular Dynamics
Velocity predicted from charge density

\[ F_d(z) = e \left[ c_{Na^+}(z) - c_{Cl^-}(z) \right] E_{ext} \]
Velocity predicted from charge density

Stokes equation:

\[
\frac{d}{dz} \left[ \eta(z) \frac{du_x(z)}{dz} \right] = -F_d(z)
\]

\[
F_d(z) = e \left[ c_{Na^+}(z) - c_{Cl^-}(z) \right] E_{ext}
\]
Velocity predicted from charge density

Stokes equation:

\[
\frac{d}{dz} \left[ \eta(z) \frac{du_x(z)}{dz} \right] = -F_d(z)
\]

Dark blue line: velocity prediction from MD charge density

Velocity predicted from charge density

Stokes equation:

$$\frac{d}{dz} \left[ \eta(z) \frac{du_x(z)}{dz} \right] = -F_d(z)$$

Dark blue line: velocity prediction from MD charge density, assumes constant viscosity

Viscosity estimation

Stokes equation:

$$\frac{d}{dz} \left[ \eta(z) \frac{du_x(z)}{dz} \right] = -F_d(z)$$
Viscosity estimation

Stokes equation:

\[ \frac{d}{dz} \left[ \eta(z) \frac{du_x(z)}{dz} \right] = -F_d(z) \]

Integrated:

\[ \eta(z) |_{z=z_0} = \frac{-\int_0^{z_0} F_d(z) \, dz}{\left. \frac{du_x(z)}{dz} \right|_{z=z_0}} \]
Viscosity estimation

Stokes equation:

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\frac{d}{dz} \left[ \eta(z) \frac{du_x(z)}{dz} \right] = -F_d(z)
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Integrated:

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\eta(z) \big|_{z=z_0} = \frac{-\int_0^{z_0} F_d(z) \, dz}{\frac{du_x(z)}{dz} \bigg|_{z=z_0}}
\]

Velocity approximation:

\[
u_{x\text{fit}}(z) = \sum_{n=0}^{7} a_n \cos \left( n\pi \frac{z}{h} \right)
\]

Viscosity estimation

Stokes equation:

\[ \frac{d}{dz} \left[ \eta(z) \frac{du_x(z)}{dz} \right] = -F_d(z) \]

Integrated:

\[ \eta(z)\big|_{z=z_0} = - \int_0^{z_0} F_d(z) \, dz \]

Velocity approximation:

\[ u_{x,\text{fit}}(z) = \sum_{n=0}^{7} a_n \cos \left( n\pi \frac{z}{h} \right) \]


\[ u_{\text{fit}}(y) = u_m \exp \left[ \frac{(y - y_m)^4}{y_1^4} \right] + \sum_{n=0}^{11} a_n \cos \frac{\pi y n}{L} \]
Viscosity estimation

Stokes equation:

$$\frac{d}{dz} \left[ \eta(z) \frac{du_x(z)}{dz} \right] = -F_d(z)$$
Viscosity estimation

Stokes equation:

$$\frac{d}{dz} \left[ \eta(z) \frac{du_x(z)}{dz} \right] = -F_d(z)$$

Blue: inverse power viscosity

$$\eta(z) = \left[ 1 - \left( \frac{z}{h} \right)^{2} \right]^{-P} \eta_{exp}$$
Velocity predicted from charge density

Stokes equation:

$$\frac{d}{dz} \left[ \eta(z) \frac{d u_x(z)}{d z} \right] = -F_d(z)$$

Blue:
inverse power viscosity

$$\eta(z) = \left[ 1 - \left( \frac{z}{h} \right)^2 \right]^{-p} \eta_{exp}$$
Velocity predicted from charge density

Stokes equation:

\[
\frac{d}{dz} \left[ \eta(z) \frac{du_x(z)}{dz} \right] = -F_d(z)
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Blue:
inverse power viscosity

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\eta(z) = \left[ 1 - \left( \frac{z}{h} \right)^2 \right]^{-p} \eta_{\text{exp}}
\]

Red:
constant viscosity
Zeta potentials vs. surf. charge density for uniform partial surface charge

Zeta potential is proportional to the water velocity in the channel center. Assumptions:

\[ \zeta = \frac{u_x (z_{\text{center}}) \eta}{\varepsilon_0 \varepsilon_r E_x} \]

MD Zeta potential:

Zeta potential is proportional to the water velocity in the channel center.

Assumes \( u_x \) is linear in \( E_x \).
Zeta potentials vs. surf. charge density for discrete partial surface charge

Zeta potential is proportional to the water velocity in the channel center. Assumes $u_x$ is linear in $E_x$.

$\zeta = \frac{u_x(z_{center})\eta}{\varepsilon_0\varepsilon_r E_x}$
Conclusions

Studied factors significantly affecting nanochannel electro-osmotic flow by MD simulations

Obtained velocity profiles, ionic concentrations, and viscosity profiles

Demonstrated an improved prediction of velocity profile from charge density with non-constant viscosity

Revealed the dependence of the flow on surface charge density, distribution, and ionic concentrations