Modeling Membrane Filtration for Water Recovery

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Potable Water Production

- Potable water quality/availability is a serious issue
  - 1 billion without reliable access to clean drinking water
  - up to 5 million die yearly of water borne diseases [1]
- Long duration space flight will require recycling of water to decrease liftoff weight
- Membrane filtration (RO) shows promise
  - semi-permeable membrane
  - removes foulants, including bacteria, viruses and salts

[1] ***Water, sanitation and hygiene links to health*. WHO, 2004. available from: http://www.who.int/water_sanitation_health/publications/facts2004/en/index.html.**

Limitations of Membrane Filtration

- Organic and Colloidal Fouling
  - fouling results in decreased permeate flux
  - combined fouling results from different foulants interacting to foul at a greater than additive rate [2]

- Maintenance
  - crossflow temporarily aids in membrane cleaning
  - fouling leads to costly maintenance requiring system shut down

- Power consumption
  - higher pressure required to maintain permeate flow rate

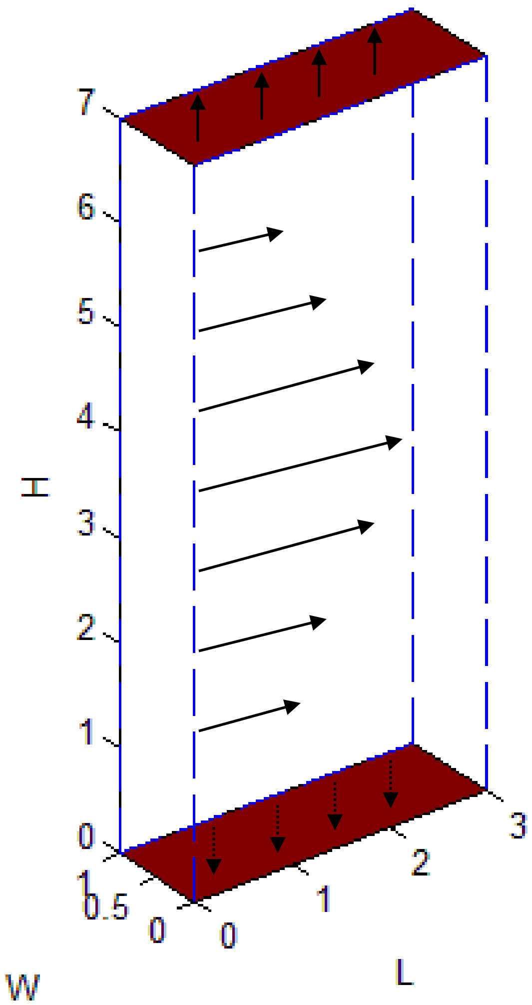
[2] Harris, A., *A Mechanistic Study on the Coupled Organic and Colloidal Fouling of Nanofiltration Membranes*, MS thesis in *Civil and Environmental Engineering*. 2008, Rice University: Houston, TX.

Solution Domain

- Cell dimensions scale with volume fraction and particle radius

- Continuum flow field:
  - one dimensional crossflow
  - quasi-steady

- Particle boundary conditions:
  - axial and no-flow directions (L and W) have periodic boundary conditions
  - reflective boundary condition at membrane



Force Bias Monte Carlo

- Probability and move acceptance

$$P_x = v_x(\sigma) / v_x\big|_{\max}$$

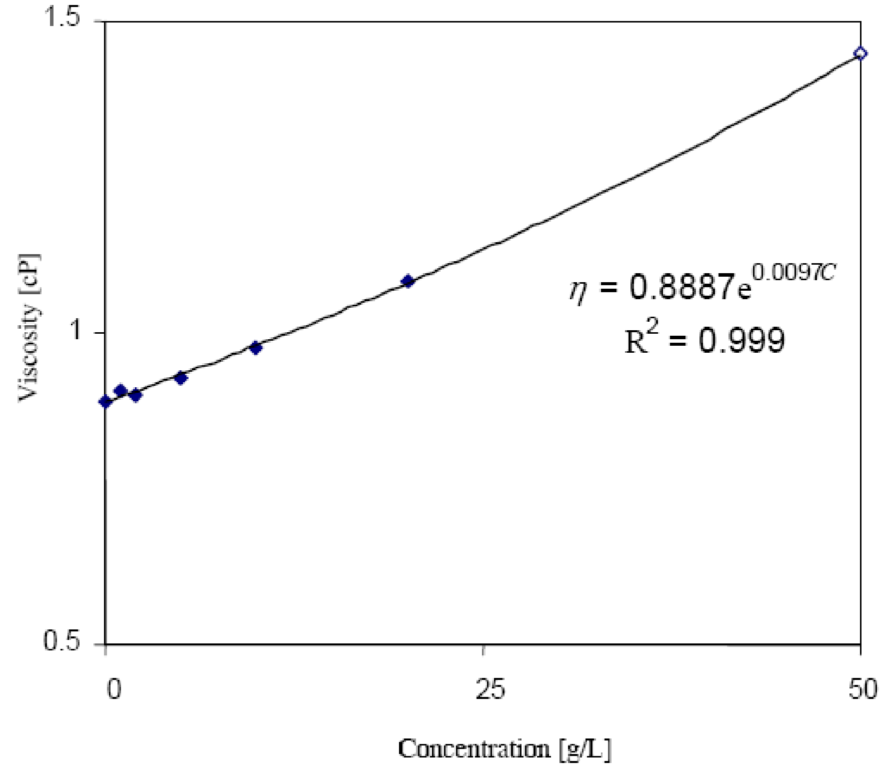
$$P_z = \min\left[1, \exp\ -\beta\Delta E - \beta\lambda \mathbf{F}_h \cdot \Delta\mathbf{r}\ \right]$$

$$\mathbf{F}_h = \frac{k_b T v_z\ \ \sigma\ \ K^{-1}\ \ \phi}{D_B + D_{SI}}\hat{\mathbf{z}}$$

- Probability of movement to lower energy state is 1
  - otherwise the exponential is used

Continuum Flow Representation

- Viscosity $\eta(C) = \eta_0 \exp(\alpha C)$
  - generalized Newtonian
  - experimentally determined coefficients [3]
  - higher volume fractions shown to follow exponential trend

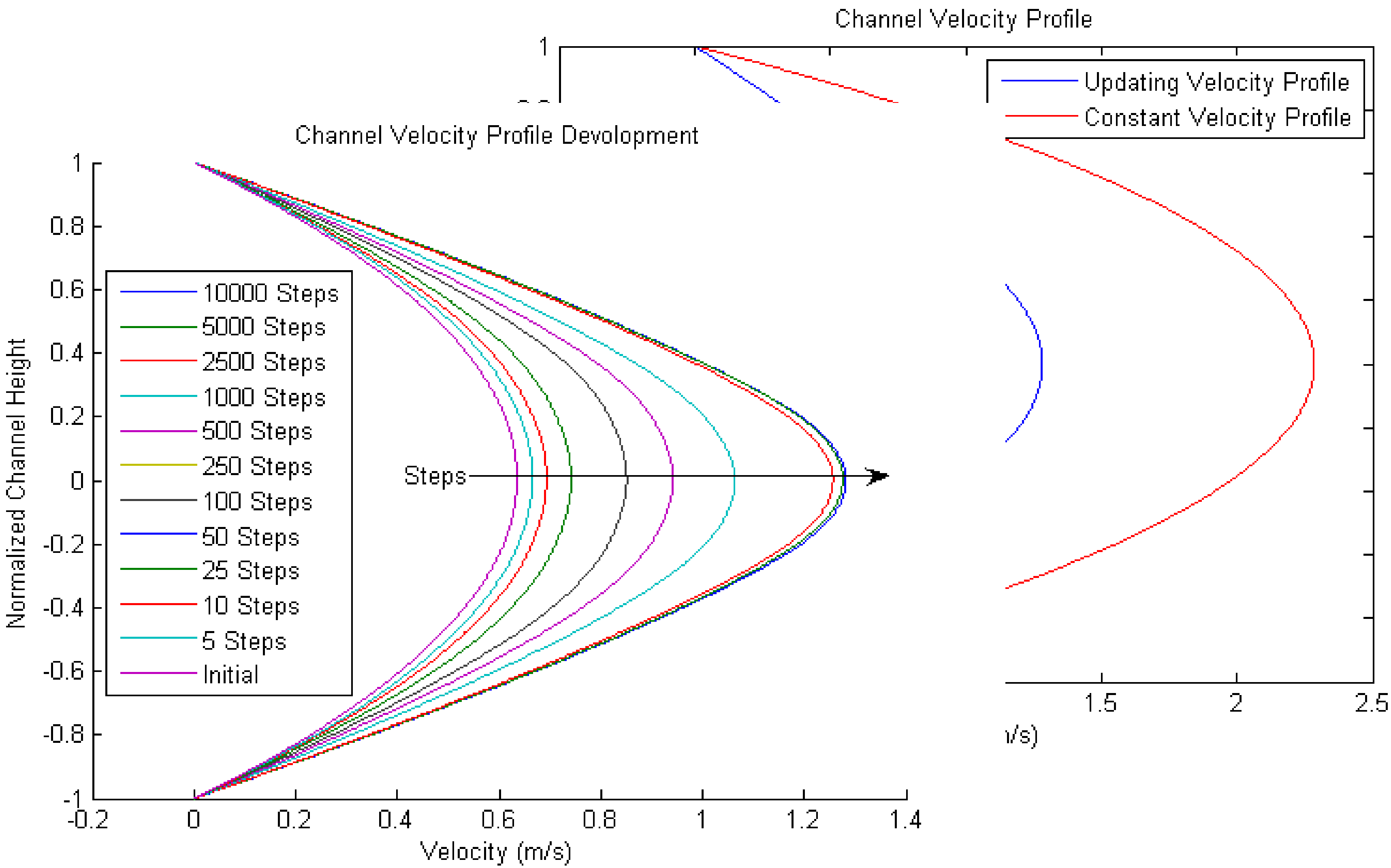


- Boundary conditions at membrane
  - no slip
  - v_w □ 0

- Spectral collocation solution
  - Chebyshev polynomials
  - Chebyshev-Gauss-Lobatto grid

[3] Hale, J.S., A. Harris, Q. Li, and B.C. Houchens. *The fluid mechanics of membrane filtration*. in *2007 ASME International Mechanical Engineering Congress and Exposition*. 2007. Seattle, WA.

Dynamically Updating Velocity



Particle-Particle Van der Waals

- Van der Waals potential
  - general form [4]

$$V_{VDW-SS} = -\frac{A_{H-SS}}{3}\left[\frac{1}{s^2-4}+\frac{1}{s^2}+\frac{1}{2}\ln\left(1-\frac{4}{s^2}\right)\right]$$

  - long-range interaction [4]

$$V_{VDW-SS}\quad s\quad = -A_{H-SS}\frac{16}{9}\frac{1}{s^6}$$

[4] Parsegan, V.A., *Van der Waals Forces: A Handbook for Biologists, Chemists, Engineers, and Physicists*. 2006, New York, NY: Cambridge University Press.

Particle-Particle Electrostatic Double Layer

- Electrostatic double layer potential
  - close-range [5]

$$V_{EDL-SS} = \frac{32\pi R\varepsilon_0\varepsilon_r k_b{}^2 T^2}{z^2 e^2}\gamma^2 \exp\ -\kappa l$$

$$\gamma = \tanh\left(\frac{ze\zeta}{k_b T}\right)$$

$$\kappa = \sqrt{\frac{2\times 10^3 N_A e^2 z^2 C_{EL}}{\varepsilon_0\varepsilon_r k_b T}}$$

  - long-range [5]

$$V_{EDL-SS} = \frac{64\pi R^2\varepsilon_0\varepsilon_r k_b{}^2 T^2}{2R+l\ \ z^2 e^2}\gamma^2 \exp\ -\kappa l$$

[5] Elimelech, M., J. Gregory, X. Jia, and R.A. Williams, *Particle Deposition & Aggregation: Measurement, Modeling and Simulation*. Colloid and Surface Engineering: Applications in the process industries; Controlled Particle, Droplet and Bubble Formation, ed. R.A. Williams. 1995, Woburn, MA: Butterworth-Heinemann.

Particle-Particle Electrostatic Double Layer

- Full range equation
  - Assume identical particles

$$V_{EDL-SS} = \frac{2\pi\varepsilon_0\varepsilon_r\zeta^2 R\ \ s-1}{s}\ln\left[1+\frac{\sqrt{e^{\kappa R\ \ 2-s}}}{s-1}\right]$$

$$\kappa = \sqrt{\frac{2\times 10^3 N_A e^2 z^2 C_{EL}}{\varepsilon_0\varepsilon_r k_b T}}$$

Particle-Surface Interactions

- Van der Waals potential

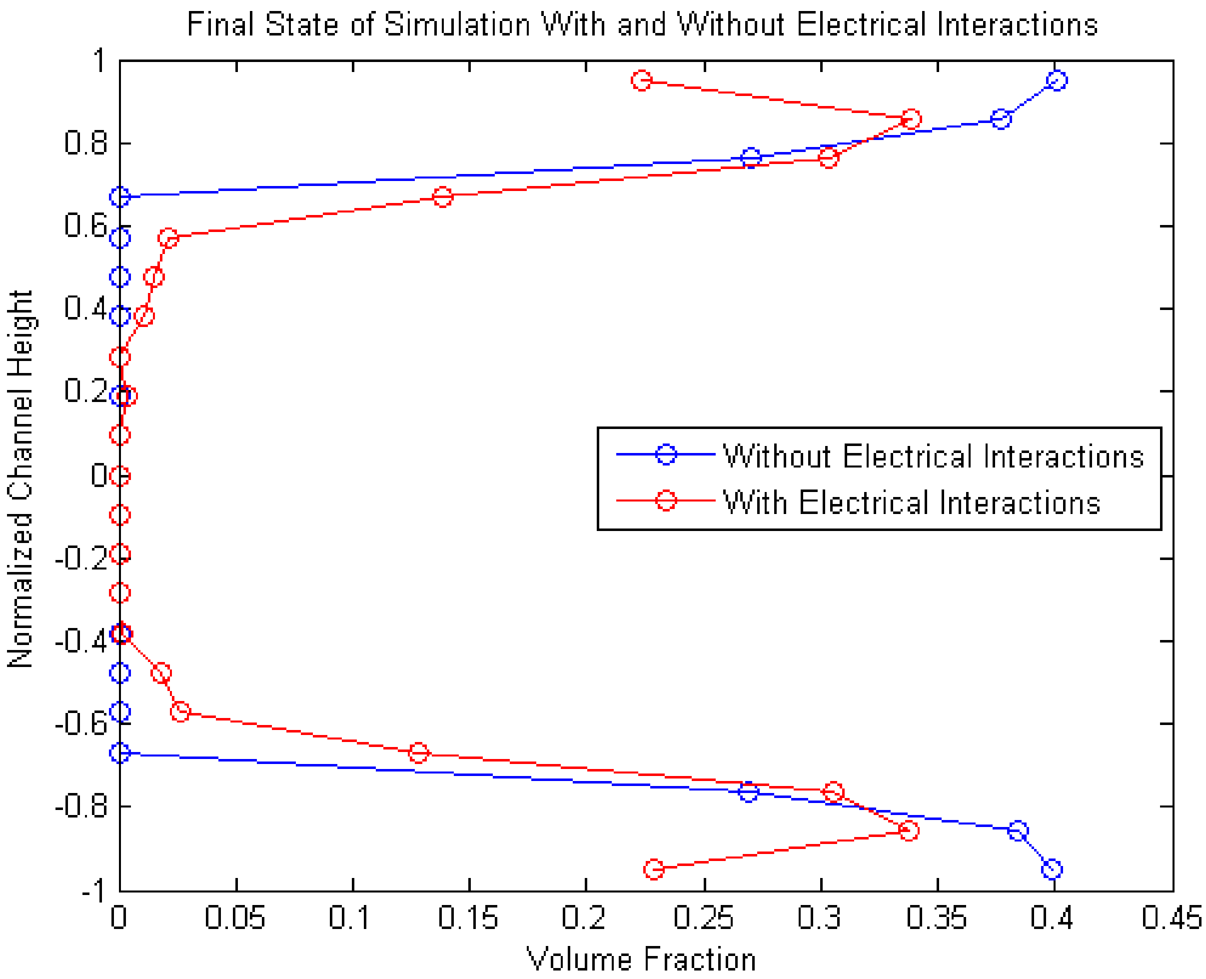
$$V_{VDW-SP} = -\frac{A_{H-SP}}{6}\left[\frac{1}{h}+\frac{1}{2+h}+\ln\left(\frac{h}{2+h}\right)\right]$$

- Electrostatic double layer

$$V_{EDL-SP} = \frac{64\pi R\varepsilon_0\varepsilon_r k_b{}^2 T^2}{z_{p1} z_{p2} e^2}\gamma_1\gamma_2 \exp\ -\kappa l$$

  – special case of sphere-sphere interaction

Concentration Profile with and without Electric Interactions

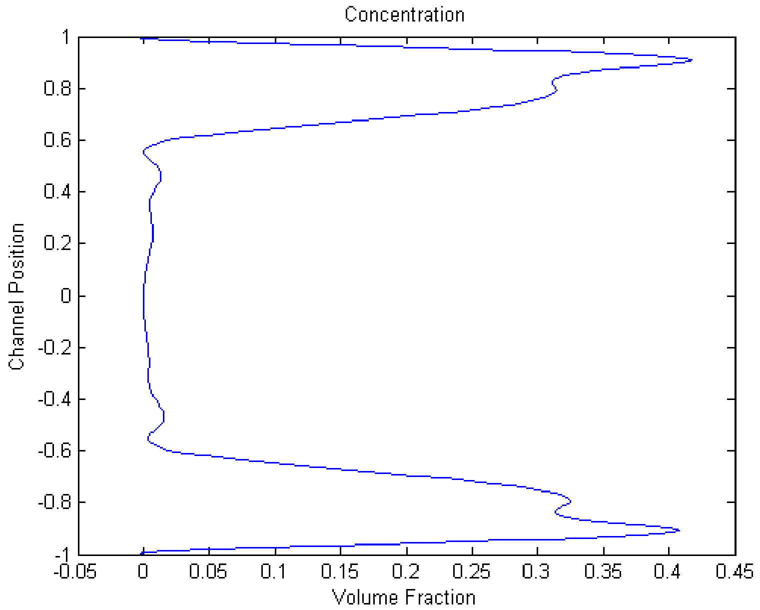


Surface Roughness

- Surface roughness of the membrane can substantially affect the motion of particles in the flow
- Fix particles to wall to approximate roughness
  - Allows a large variety of roughness possibilities
  - Key question: random distribution versus uniform distribution

Numerical Refinement

- Wall phenomena
  - Artifact of concentration calculation
  - Change concentration calculation (volume)
- Limited effect on the flow field
- Actually improved speed



N-Body/Parallel Optimization

- Previous work had moved particle by particle, evaluating a movement probability independent of other particle motion
- New movement process attempts new position before calculating move acceptance probability
- N-body algorithms exist
  - Lump particles in far field for faster evaluation
  - Fast Multipole Method (FMM) best candidate [6]
- Requires a new data handling structure
- Designed for "large" systems

[6] Greengard, L., *The Rapid Evaluation of Potential Fields in Particle Systems*. ACM Distinguished Dissertations. 1988, Cambridge, MA: Massachusetts Institute of Technology.

Parallel Optimization

- Change many small passes to a few large passes
- Each time a potential evaluation is carried out we need a sync, broadcast, and gather
- New data handling allows for N-body algorithms
- Exploit symmetry not previously available

$$H = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ E_{1,2} & 0 & 0 & 0 & 0 & 0 \\ E_{1,3} & E_{2,3} & 0 & 0 & 0 & 0 \\ E_{1,\ldots} & E_{2,\ldots} & E_{3,\ldots} & 0 & 0 & 0 \\ E_{1,N-1} & E_{2,N-1} & E_{3,N-1} & E_{\ldots,N-1} & 0 & 0 \\ E_{1,N} & E_{2,N} & E_{3,N} & E_{\ldots,N} & E_{N-1,N} & 0 \end{bmatrix}$$

$$F = H + H^T = \begin{bmatrix} 0 & E_{1,2} & E_{1,3} & E_{1,\ldots}{}^T & E_{1,N-1} & E_{1,N} \\ E_{1,2} & 0 & E_{2,3} & E_{2,\ldots}{}^T & E_{2,N-1} & E_{2,N} \\ E_{1,3} & E_{2,3} & 0 & E_{3,\ldots}{}^T & E_{3,N-1} & E_{3,N} \\ E_{1,\ldots} & E_{2,\ldots} & E_{3,\ldots} & 0 & E_{\ldots,N-1}{}^T & E_{\ldots,N}{}^T \\ E_{1,N-1} & E_{2,N-1} & E_{3,N-1} & E_{\ldots,N-1} & 0 & E_{N-1,N} \\ E_{1,N} & E_{2,N} & E_{3,N} & E_{\ldots,N} & E_{N-1,N} & 0 \end{bmatrix}$$

Future Work

- Determine appropriate number of particles fixed to wall to approximate real world surface roughness

- Increase simulation scale (more particles, longer channel)

- Application of FMM to large systems

References

[1] *Water, sanitation and hygiene links to health*. 2004 [cited 2008; Available from: http://www.who.int/water_sanitation_health/publications/facts2004/en/index.html.

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