Large Scale Monte Carlo Simulation of Cross-flow Membrane Filtration for Removal of Particulate Materials

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Motivation: A shortage of water due to an ever increasing world population and intensified demands for agricultural and industrial uses has resulted in wastewater reuse becoming a primary source of water. Consequently, quality as well as quality of treated water is one of the most serious public concerns. Membrane filtration has emerged as a cost competitive alternate to producing clean water in comparison to conventional methods of water and wastewater treatment. In order to optimize the operation as well as minimize investment and maintenance costs, a pilot plant is commonly used in designing and optimizing membrane systems although it does not always represent performance of full-scale systems. As such, lab-scale experiments and computer simulations are commonly used to provide basic scientific understanding of filtration phenomena. Compared to pilot plant operations and lab experiments, computer simulations are faster and more cost-effective. The objective of our project is to develop a large-scale cross-flow membrane filtration model to investigate the morphology of particulate materials in the membrane filtration systems.

Methods: In the membrane channel, from the inlet to the outlet, there is a fully developed parabolic laminar flow profile, which is accurately approximated as a simple shear flow near the membrane surface. A particle moves in the transverse direction due to fast crossflow on the order of 0.1 meter/sec. When the permeate flux flows through the porous membrane, particles are push down from bulk phase to the membrane surface. Consequently, particle concentration near the membrane surface increases, forming a certain concentration gradient. Therefore, particles retained near the membrane surface diffuse back to bulk phase. These particles interact each other undergoing electromagnetic interactions if charged. Uncharged particles collide with each other, holding a certain thermal energy, and contributing to self or collective diffusion.

The Monte Carlo method is used to simulate particle movement. At the beginning, the particle of interest *j* is located at position *m*. For the Metropolis Method, particle *j* is proposed to randomly moved to a new location *n* using algorithm: $r_j^n = r_j^m + (2a_0 - 1)\delta r_{\max}$, where a_0 is a uniform random number between 0 and 1, $\delta r_{\max}$ is the maximum allowable displacement. The proposed displacement is evaluated for acceptance or rejection according to the change in potential energy. If the change is less than zero, the proposed move is downhill and accepted. Otherwise, the movement is uphill and is accepted according to transition probability.

The Monte Carlo algorithm is modified to Biased Monte Carlo Simulation [1] when crossflow is applied to an open membrane filtration system. Basically, particle movements are biased in the direction of the flow field since the hydrodynamic influence on the particle motion procreates a biased probability distribution in the direction of the ambient field, so a hydrodynamic force-biased Monte Carlo simulation is developed to investigate particle removal in the membrane channel.

Two types of biased probability distribution are considered in our model—tangential bias and normal bias. In a tangential bias distribution, near the epicenter of the membrane channel, crossflow is much faster compared to permeate flux so particle diffusion against the crossflow is negligible. Therefore, particle movements are allowed only in the direction of the crossflow and the transport is convection-dominated. However, near the membrane surface, the no-slip boundary condition is used since the flow velocity is close to zero, and particles can easily perform their random Brownian motion. Spatial probability distribution of a particle is therefore 50 - 50 percent in the crossflow direction, and transport is diffusion-dominated. Between the epicenter and membrane surface, diffusion and convection are equally important. In a normal biased distribution, particle movement and configuration are in a dynamic equilibrium state. When a particle moves from one position to a new position, the displacement is dot-producted with the total force, providing a transition probability. If the probability is greater than a randomly generated number, then the trial movement is accepted.

All particles experience three forces: drag force, gravity, and diffusive force. Drag force is based on Stokes law and Happel's correction factor is used to modify the quantity of the drag force based on local volume fraction of particles near the target particle. Gravitational force is based on particle size and the density difference between the particle and water. The diffusive force, which is phenomenological, is due to the concentration gradient.

Use of HPC resources: Calculating the particle movements for a large scale Monte Carlo simulation of membrane filtration requires high-performance computing (HPC) resources to calculate individual displacement of particles. A master-slave algorithm was tested in the programming, meaning that one of node is responsible for task decomposition, while the other nodes are responsible for the calculations. After each step of the calculations, the slaves send the message to master and the master re-composes the calculation task. Our model was developed and implemented on a PC-based Linux system. We also use the Hurricane system at Maui High Performance Computing Center (MHPCC) for testing and simulations.

Results and Future Work: We developed a the model to investigate particulate material removal using membrane filtration. One of our results is shown in Figure 1. The simulation results were compared with experimental observations of critical flux from a a a published review paper [3]. Critical flux is the permeate flux below which no fouling occurs. In Our simulated critical flux is about 10 $\mu m/\sec$ for a hard sphere of 0.1 μm . The experimental data showed that the critical flux ranged from 8 to 12 $\mu m/\sec$, which is in relatively good agreement with our simulation. So Crossflow membrane filtration for particulate removal was investigated using Monte Carlo simulations. And the influence of the flow field on many particle motions is captured by the force-biased probability distribution.

Currently, only systems with constant particle numbers are simulated, and the interaction between particles is not included, especially since the model is a serial code. For the future work, a grand canonical Monte Carlo algorithm of interacting particles for fluctuating particle numbers will be implemented. Finally, we will parallellize the serial code.using HPC resources for future work. If possible, we will submit our job on Jaws system at MHPCC to obtain a full-scale [2] and faster simulation.

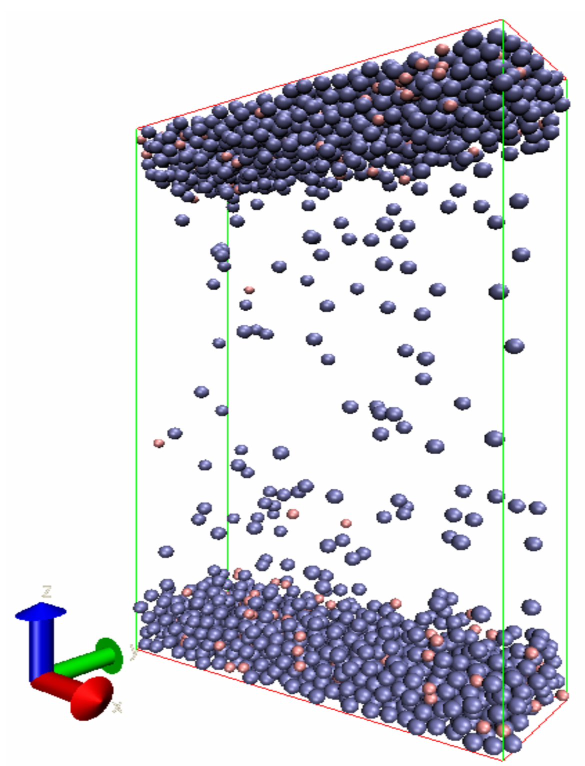

Figure 1 Simulation result of particle deposition

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References:

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