

Simulation of a Magnetophoretic Device for the Separation of Colloidal Particles in Magnetic Fluids

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Abstract: Magnetophoresis of non-magnetic particles is the induced motion of non-magnetic particles suspended in magnetic media on the application of a magnetic field gradient. It involves many driving forces arising from different transport phenomena. Magnetophoresis can be used in special separation devices to separate colloidal particles based on their sizes.

Multiphysics computational programs, such as COMSOL, are ideal for the modeling and simulation of those devices. In this work, we used the calculated magnetic field for a quadruple configuration of permanent magnets to solve the recently-developed magnetophoretic model for the transfer of the non-magnetic colloidal particles due to diffusion, convection, and magnetophoretic forces. The model also takes into account the electrostatic repulsion between the particles. The device chosen for the simulation was similar to a separation device used in an experiment to separate fluorescent polystyrene beads in the size range of 500 to 2000 nm.

The two-dimensional results show excellent correlation with the published experimental results. The successful use of COMSOL now opens the door for simulating new devices to arrive at the best configuration of the magnets and flow pathway before building those devices for experimental trials.

Keywords: Magnetophoresis, Colloidal Separations, Magnetic Fluids

1. Introduction

Magnetophoresis of non-magnetic particles is the induced motion of non-magnetic particles suspended in magnetic media on the application of a magnetic force gradient. Upon the application of the magnetic field, the non-magnetic particles are driven against the magnetic field gradient and are replaced by the surrounding magnetic fluid, which has a higher magnetic susceptibility. This magnetophoretic force is proportional to the volume of the

displaced particles. In a way, magnetophoresis is a phenomenon analogous to buoyancy. Thus, the difference in the magnitude of the magnetophoretic forces provides a means to establish the separation of colloidal non-magnetic particles based on the differences in their volumes just as the difference in density provides a means to classify particles according to their densities by flotation. This technique is promising especially for use in analysis. (Watarai et al. 2004)

Multiphysics computational programs are ideal for the modeling and simulation of magnetophoresis, since various physical phenomena influence the separation process. In addition to the magnetophoresis forces that impact the movement of the particles, particles are affected by diffusion and convection as they move with the flow of the magnetic fluid. Inter-particle interactions also contribute to their movement. COMSOL in particular is a good tool to simulate separation devices since it allows for solving non-standard partial differential equations. Thus the user can create his or her partial-differential-equations system and not necessarily choose one or more of the pre-packaged physical models.

In this work, we used COMSOL to solve the convection, diffusion and magnetophoretic partial differential equations for a magnetophoretic separation device. The device geometry was based on published experimental work in which polystyrene particles were separated in a quadruple configuration of permanent magnets [Sharpe 2006]. In addition to the convection, diffusion and magnetophoretic forces, the model used took into account the electrostatic forces between the particles as well.

2. The Magnetophoresis Separation Device

The classification of non-magnetic colloidal particles based on their size can be attained by suspending the colloidal particles in a magnetic fluid and flowing the mixture in a magnetic field

gradient. The device used is schematically depicted in Figure 1. The device consists of four quadruple permanent magnets configuration. The two magnets facing each other are placed to have the north pole directed to the centerline, while the two other magnets the south pole. The 2-cm diameter cylinder that is placed in the center of the device has a 0.5-cm diameter outlet tube placed at its center in the top opening of the cylinder. The mixture that contains a magnetic fluid and the non-magnetic colloidal particles flows from the bottom of the device upwards towards the outlet at the top. The stream that contains the large concentrated colloidal particles flows out from the center tube, while the stream dilute in the large colloidal particle flows out from the annulus.

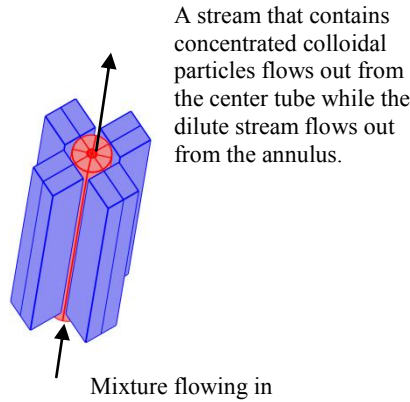


Figure 1. A schematic representation of the magnetophoretic device. The mixture is pumped through the red cylinder from the bottom. The outlet is at the top of the red cylinder and consists of a center tube for the concentrated stream and annulus for the dilute stream. The quadruple permanent magnet configuration is shown in blue.

This magnetic separation device is similar to the one used by Sharpe (2004) to experimentally concentrate fluorescent latex beads. We simulate the same device to be able to compare the COMSOL model with the experimental results and then we use the model to predict further possible separations with the same device.

Our goal was to construct a three-dimensional model for this separation device to enable us to capture subtle phenomena like the entrance effect shown experimentally by Sharpe. This work, however, presents only the two-dimensional results. The three-dimensional work will follow in a separate publication.

2. The Magnetophoresis Model

The magnetophoresis model takes into account the diffusion, convection, magnetophoresis and interparticle forces that influence the transfer of the non-magnetic colloidal particles. A full description of the model is found elsewhere (Fateen 2002, Gonzalez et al. 2004 and Gonzalez 2009). A brief description is presented here.

The dimensional form of the diffusive flux equation is

$$\underline{\mathbf{J}}_p = \frac{-W_f CD_{pf}}{\rho RT} [RT + \Psi^2 C_p] \underline{\nabla} C_p - \frac{W_f CD_{pf} \bar{v}_p}{RT} \left[C_p g \left(1 - \frac{\rho_p}{\rho}\right) + \frac{C_p}{\rho} \mu_o M \underline{\nabla} H \right]$$

where D_{pf} is the diffusivity of the non magnetic particles in the magnetic fluid, C is the total concentration of the fluid, W_f is the molecular weight of the magnetic fluid, \bar{v}_p is the partial molar volume of the particles, C_p is the concentration of the particles, R is the gas constant, T is the temperature, μ_o is the permeability of the free space, M is magnetization of the magnetic fluid, ρ_p is the density of the particles, ρ is the density of the magnetic fluid solvent, and H is the magnetic field. The term Ψ^2 represents the electrostatic force constant. The first term represents both the diffusional flux for a non-ideal fluid with the electrostatic interactions contributing to the excess chemical potential while the second term represents the effects of gravity and magnetic field on the flux.

The steady state governing equation for the concentration of the non-magnetic particles is

$$\underline{\mathbf{v}} \cdot \underline{\nabla} C_p + \underline{\nabla} \cdot \underline{\mathbf{J}}_p = 0$$

Where $\underline{\mathbf{v}}$ is mass average velocity of the magnetic fluid relative to the coordinate system

of the interest, and $\underline{\mathbf{J}}_p$ is the molar flux of the particles relative to the mass average velocity $\underline{\mathbf{v}}$. The non-dimensional form of the equation that was used in our simulation is as follows

$$(\tilde{v}_z(\tilde{r}) - \tilde{g}) \frac{\partial \tilde{C}_p}{\partial \tilde{z}} = \frac{1}{\tilde{r}} \frac{\partial}{\partial \tilde{r}} \tilde{r} \left[\tilde{D} + \tilde{\Psi}^2 \tilde{C}_p \right] \frac{\partial \tilde{C}_p}{\partial \tilde{r}} + \frac{1}{\tilde{r}} \frac{\partial}{\partial \tilde{r}} \tilde{r} \tilde{\beta} \tilde{M} \frac{d\tilde{H}}{d\tilde{r}} \tilde{C}_p$$

where $\tilde{C}_p = \frac{C_p}{C_{p0}}$, $\tilde{r} = \frac{r}{r_o}$, $\tilde{z} = \frac{z}{L}$, $\tilde{v}_z = \frac{v}{v_{\max}}$,

$$\tilde{M} = \frac{M}{M_s}, \text{ and } \tilde{H} = \frac{H}{H_0}$$

C_{p0} is the initial concentration of the non magnetic particles, r_o is the full radius of the tube, L is the full length of the tube, v_{\max} is the maximum linear velocity of the particles in the tube, M_s is the saturation magnetization and H_0 is the maximum magnetic field applied to the tube. The three non-dimensional constants in the equation are as defined by Sharpe 2004. The above equation shows that convection impacts the axial transport, while diffusion and magnetophoresis impacts the radial transport. Axial dispersion was neglected in comparison with convection.

Since Reynolds number is small, the velocity profile of our model was modeled by $v_z = v_{\max}(1 - r^2)$, which contains the assumption of constant axial velocity.

The Magnetization was obtained from

$$M = \left(\frac{M_s}{H_t + H} \right) H$$

where H_t is the magnetic field at which the magnetization of the magnetic fluid is equal to half the saturation magnetization.

The Magnetic field of our model was taken from the experimental measurement of Sharpe (2004)

$$H = (0.2212r^2 + 0.3662r + .0436) / \mu_o$$

3. Use of COMSOL Multiphysics

The convection and diffusion application mode in the mass balance of the chemical engineering module was used for solving this model. The extra term of the magnetic forces was added to this application mode through the 'Equation Systems' option.

The original equation of the convection and diffusion application mode is:

$$\frac{\partial c_i}{\partial t} + \nabla(-D_i \cdot \nabla c_i + c_i \cdot \mathbf{u}) = R_i$$

For steady state with rearrangement we get

$$\nabla(-D_i \cdot \nabla c_i) = R_i - \mathbf{u} \cdot \nabla c_i$$

In the conservative flux source term, the diffusivity was modified to add the depletion forces parameters and the magnetic forces term was added in the conservative flux source term.

The non dimensional gravity group \tilde{g} was added to the source term of the equation system.

The velocity profile was inserted as the axial Velocity (\mathbf{v}) in the subdomain. The magnetic field profile and magnetization were added in the global expressions.

The boundary conditions used were:

- At the inlet boundary $z=0$, $\tilde{C}_p = 1$
- At the outlet boundary $z=L$, Convective flux boundary condition was selected.
- Symmetry boundary condition was used at the axis and insulation at the wall

The convergence of the model was frequently obtained by adjusting the tuning parameter for artificial isotropic diffusion.

4. Results

Figure 2 shows a typical result of the non-dimensional concentration profile inside the magnetophoretic device, while Figure 3 shows

how the concentration profile develops along the radial direction as the particles move upwards in the separation device.

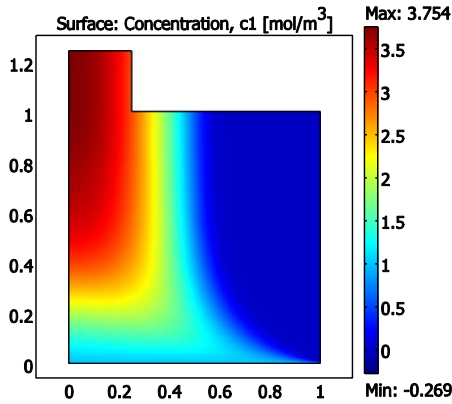


Figure 2. The non-dimensional concentration profile inside the magnetophoretic device for a typical set of parameters. Negative values are an artifact of the numerical solution.

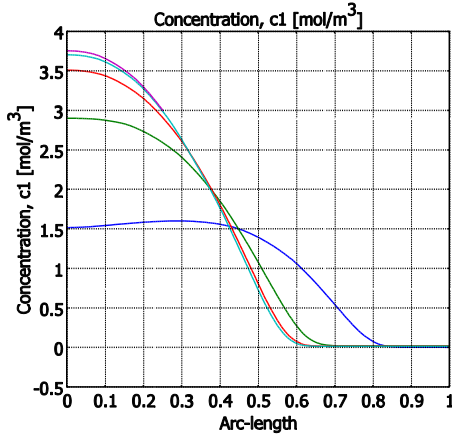


Figure 3. The concentration radial profile as the particle move upwards towards the exit of device. The inlet boundary condition for the concentration is 1.

To compare with the experimental data, we used boundary integration to calculate the normal flux from the inner quarter of the radius at the top of the device. This normal flux is then divided by the normal flux for the rest of the boundary to obtain the separation percentage as computed by Sharpe 2004. Figure 4 compares between the experimental data and the model predictions. The electrostatic parameter Ψ^2 was adjusted to 0.05 to provide a good fit for the data.

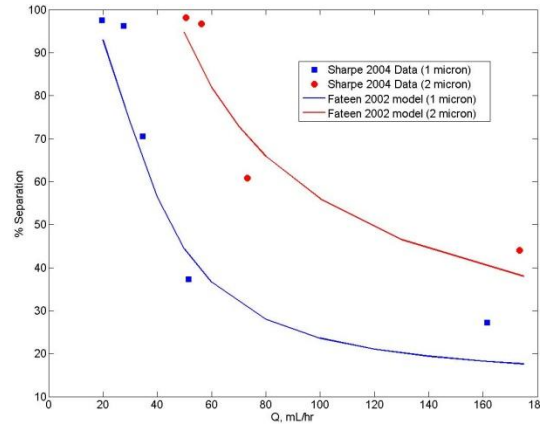


Figure 4. Comparison between the model predictions (solid lines) with Sharpe (2004) experimental data.

The model also enabled us to simulate the separation between different sized particles flowing in the same mixture. For a certain separation device, the model can be used to optimize the separation between 0.5 and 1 micron by finding the flow rate required to obtain the best separation. Figure 5 shows the effect of flow rate on the separation percentage of the 0.5 and 1 micron particles, while Figure 6 shows the relative separation factor of the two particles as a function of the flow rate. The relative separation factor is defined as the separation efficiency of the large particle divided by that of the small particle.

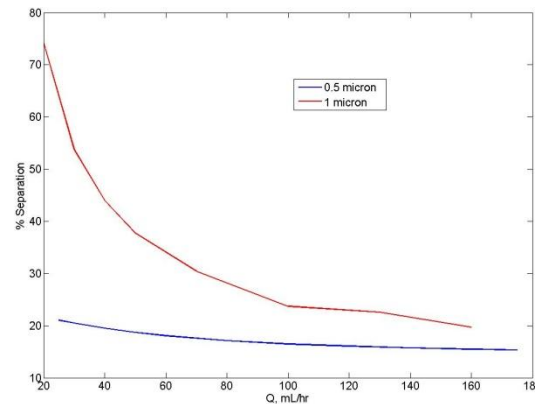


Figure 5. Using the model to predict the device's separation performance for a mixture of particles with sizes 0.5 and 1 microns.

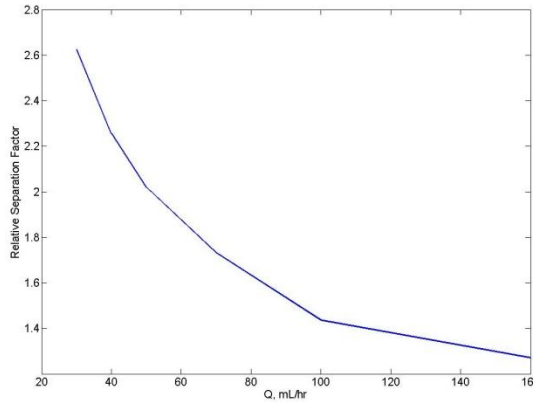


Figure 6. Relative separation factor for the 1-micron particle compared to the 0.5-micron particle versus the flow rate.

From Figure 6, a flow rate of 35 mL/hr would result in a separation factor of 2.5. In practice, better separation can be attained by repeating the process for the concentrated mixture as needed to reach the required separation, i.e. perform multistage separation.

To continue building the model, it is important to couple it with other COMSOL modules such as the AC/DC magnetostatic and the Incompressible Navier-Stokes modules. We started by incorporating Navier-Stokes module in a slightly modified geometry of the separation device to investigate the outlet effect by coupling the velocity calculated by NS module with the magnetophoretic model. Even though the results for the coupled case did not change significantly from the uncoupled case, it was important that we were able to combine the two modules to use them together when designing more efficient separation devices. Figure 7 shows the velocity profile and Figure 8 shows the concentration profile for the coupled model.

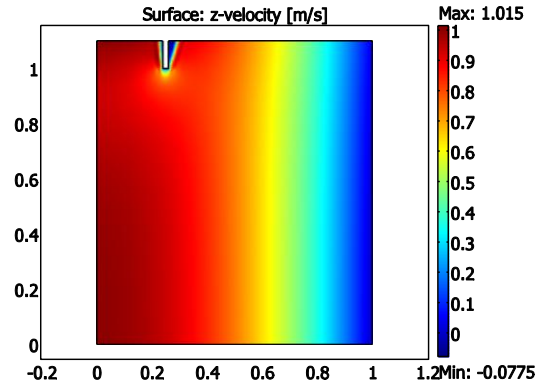


Figure 7. Using the model to predict the device's separation performance for a mixture of particles with sizes 0.5 and 1 microns.

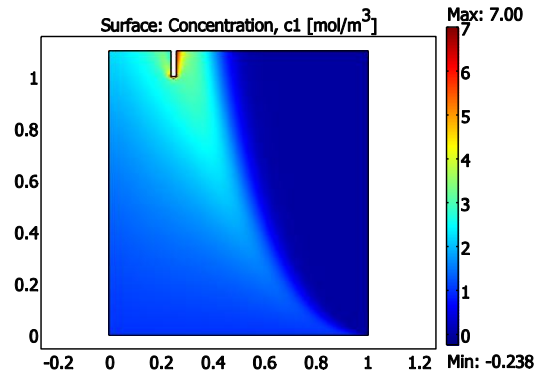


Figure 8. Using the model to predict the device's separation performance for a mixture of particles with sizes 0.5 and 1 microns.

7. Conclusions

In this work COMSOL was used to solve the magnetophoretic transport model for a separation device that separates micron and submicron colloidal particles. The results of the simulation were reasonably compared with experimental data. The model was used to probe the possibility of separating two different sized particles by the same separation device. Navier-Stokes model was also coupled with the magnetophoretic model to produce similar results. The next step in our work will be to include the magnetostatic model and to repeat the simulation in three dimensions. If the 3-D model proves successful, different designs of more efficient separation devices will be

envisaged and simulated with COMSOL using the models developed and tested in this work.

8. References

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