Two Dimensional Orbital Mixing for a Fluid

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Introduction

This report was written to complete research done at the University of Washington's Chemical Engineering Department on orbital mixing of a 96-well microplate. The interest in this research came from Rosetta Software. Our objective is to compare our model produced on COMSOL software to a paper written in biotechnology progress by Svenja Weiss, et. al.[1] It will be useful to understand and model this mixing as a way to run pharmaceutical and other chemical plants as efficiently as possible.

It is common for a pharmaceutical or chemical to run thousands of tests in order to discover new drugs or chemicals. These companies desire identical and reproducible results with very small variation between the same tests. While identical results are desirable, an efficient process can also help a company run at its maximum capacity. This research intends to model orbital mixing and then find the most effective way to run the mixing process.

Materials and Methods

As seen in Figure 1. the 96-well microplate is a small device which holds 96 individual wells with a volume of 0.2 mL. The shaking diameter is 12 mm and shaking occurs at 500, 700 and 900 revolutions per minute. The radius of an individual well has been estimated by dimensional analysis to measure 3.66 mm. The density of the fluid and the dynamic viscosity were estimate to have the properties of water 1 g/cm^3 and 0.001 Pa s respectively. We were then able to calculate the rotational velocities for 500, 700 and 900 rpm to be 52.3, 73.3 and 94.2 radians per second.

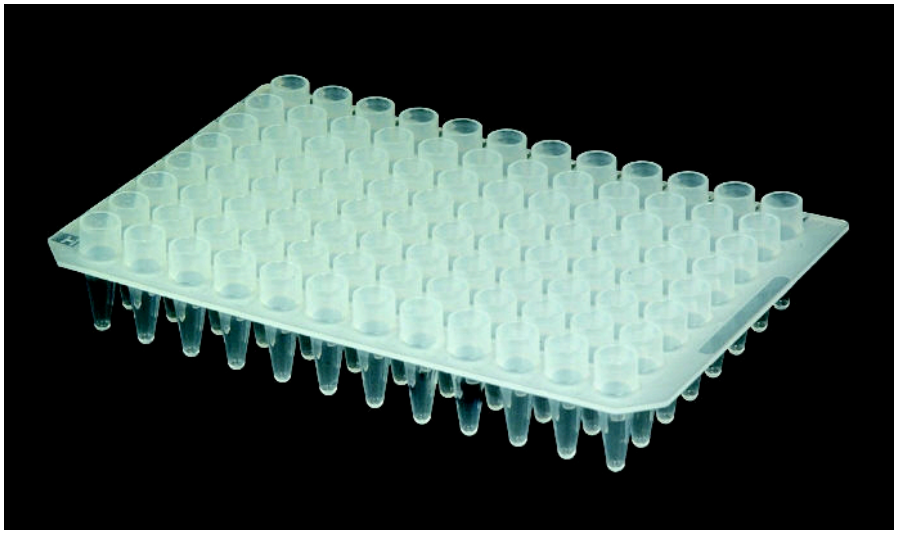

Figure 1. Photograph of a 96-Well Microplate

There are two approaches which can be taken to model orbital mixing on COMSOL multiphysics software. Our research first intended on using the equation of motion. The equation used to describe the forces in this model is:

$$\frac{Du}{Dt} = \left[\frac{\partial u}{\partial t} + u \cdot \nabla u\right] = -2\Omega \times u - \Omega \times (\Omega \times x) - \frac{1}{\rho}\nabla p + \frac{\eta}{\rho}\nabla^2 u$$

Where the Centrifugal Force is: $-2\Omega \times u$ and the Coriolis Force is: $-\Omega \times (\Omega \times x)$. These two forces calculated the velocity forces or orbital mixing. Our attempts to model this in COMSOL became difficult conceptualize the coordinate system COMSOL used.

We used a programmed model called ALE moving mesh in COMSOL to model velocity forces. The momentum transport was modeled using the Navier-Stokes equation (NS) for incompressible fluids, given in Equation 1, and the convective and diffusive transport was modeled using steady-state convection and diffusion equations, given in Equation 2. The momentum transport was solved first and the results obtained were used in solving the convective and diffusive transport. All settings and boundary conditions are displayed in Table 1.

$$\rho \frac{Dv}{Dt} = -p + \mu\nabla^2 \mathrm{v} + \rho \mathrm{g} \qquad \text{Equation 1}$$

$$(\nabla \cdot \mathrm{v}) = 0$$

ρ = constant density of fluid

v = velocity vector

p = pressure

μ= constant dynamic viscosity

g = gravitational force vector

$$D\nabla^2 c = \mathrm{v} \cdot \nabla c \qquad \text{Equation 2}$$

D = constant diffusion coefficient

c = concentration

v = velocity vector

Table 1. Parameters set in COMSOL multiphysics

Constants:	**Navier-Stokes: subdomain settings**
Omega=52.3	Density: 1000 kg/m^3
rad_rotation=1.2	Dynamic viscosity: .001 Pa s
vel=omega*rad_rotation	Volume force: 0
	$v(t_o)$ = vel*0.75
Global Expressions:	
radius=sqrt(X^2+Y^2)	**Boundary Conditions: inflow/outflow velocity**
	u_o=-omega*sqrt(X^2+Y^2)*sin(thetazero+omega*t)
Subdomain Expressions:	v_o=omega*sqrt(X^2+Y^2)*cos(thetazero+omega*t)
thetazero=asin(Y/sqrt(X^2+Y^2))	
	Concentration/Diffusion:
Solver Parameters	δ_{ts}=1
Analysis: transient, time dependen	D isotropic= 1e-5
Times= 0:0.001:0.12	u=u
Relative = 0.01	v=v
Absolute=0.001	intial concentration: 1 mol/g for inner circle
	0 mol/g for outer circle

Results

The modeling was in two dimensions with one large circle and one smaller circle, which was inside the large circle. The initial concentration was 1 mol/cm^3 in the small circle with a concentration of zero outside the inner circle. The time to solve for was 0.12 seconds, which is one revolution at 500 rpms. The mesh obtained under these conditions had 3656 elements and 39306 degrees of freedom. COMSOL solved this problem in one and a half hours.

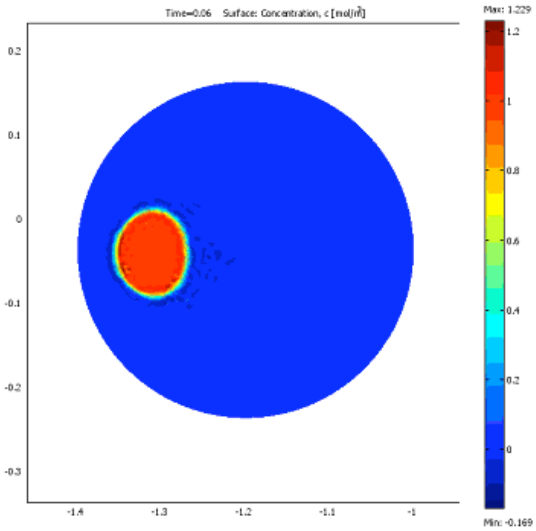

Figure 2. Photograph of model after 180 degrees rotation

As seen in Figure 2. the model is shown at 0.06 seconds or 180 degrees of rotation from its starting point. The concentrated circle is has flattened on the inner portion and moved towards the wall of the well. These results were confirmed by the second model shown in Figure 3. which shows the smaller circle has moved closer to the wall of the well and the inner part of the concentrated circle has flattened out.

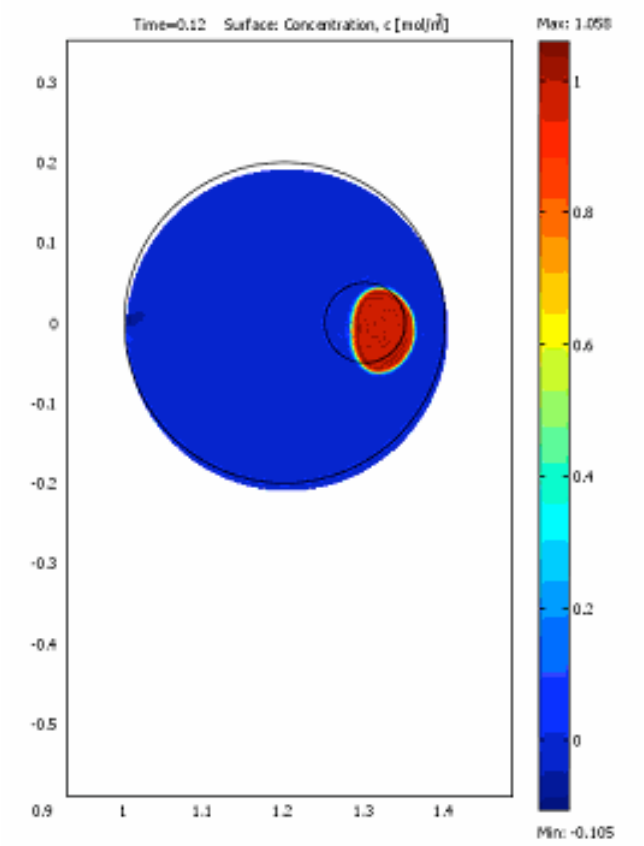

Figure 3. After 360 degrees shows that the concentrated circle has moved closer to the wall and the inner portion has flattened out from its original shape.

To verify that the model was accurate the following tests were done: Check velocity fields, took out the ALE equation for a moving mesh and asked if the solution made sense logically. The velocity streamline shown in Figure 4. shows the vectors of the well rotation after 360 degrees.

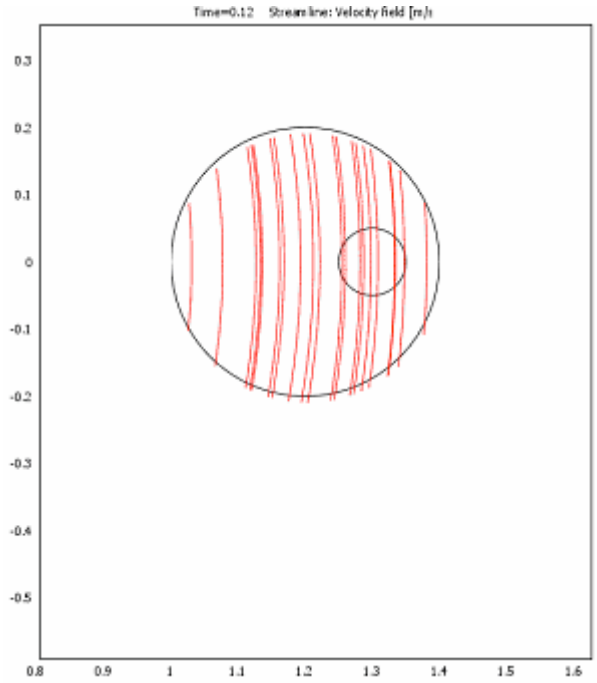

Figure 4. The velocity streamline after 360 degrees of rotation.

The velocity streamline in Figure 4. shows that the model is moving in a circular direction. Another test to verify the model is to make the concentration velocities to be a solid body rotation; these are the same as the boundary conditions for the NS and the ALE mesh movement. The NS equation was then deleted as seen in Figure 5. the model was then ran for 0.08 seconds. This test was looking for the concentration profile with diffusion only, which is believed to have very little effect on the in our model.

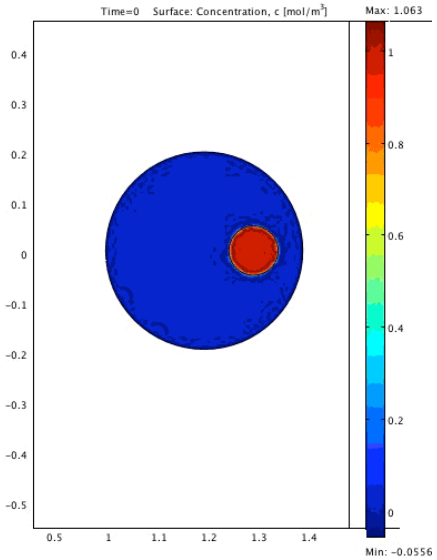

Figure 5. Picture of model without Navier-Stokes equation at time 0

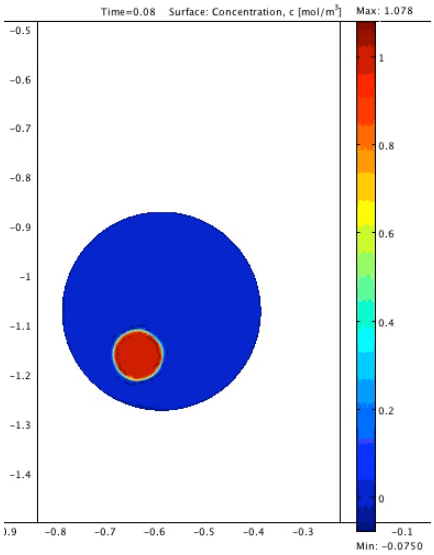

Figure 6. Picture of model taken without Navier-Stoke equation at time 0.08 seconds

As verified in Figure 6. the model without the NS equation gave a circle after 0.08 seconds, this verifies that diffusion has little effect on the concentration profile. The flattening shown in Figure 3. is from the NS velocity forces only.

As determined by the tests the model is functioning correctly. The objective of this research was to compare the mixing to the photographs in Wiess's paper in Biotechnology Progress. This requires a three dimensional model, which we were not able to obtain under time restrictions of one quarter of research.

Conclusions

The model obtained in this research has nearly achieved its objective. The next step is to add the design of the well in three dimensions. The difficulties which we came across during research were conceptualizing the coordinates in COMSOL; this was time consuming. Now that we have a grasp on how to solve this problem using the equation of motion we could attempt to solve the problem in a moving coordinate system. Because it would not be using the ALE of a moving mesh from COMSOL, it may compute a solution faster.

We now know that mixing by velocity forces of the Navier-Stokes equation had a much greater effect on mixing than diffusion forces. It has been shown that orbital mixing in a well pushes the concentrated portion towards the wall and the inner porting of the concentration circle flattens. We were not able to get our model into three dimensions so we could not compare the model to the paper or test different mixing methods. This problem is very hard for a computer to solve as seen by our results only taken at 0.12 seconds, but there was a lot of progress made and with a little more time we could complete all of the objectives, including best mixing methods and comparison of our model to Weiss's paper.

References

[1] Svenja Weiss, Gernot T. John, Ingo Klimant, and Elmar Heinzle Modeling of Mixing in 96-well Microplates Observed with Fluorescence Indicators. Biological Progress. 821-830 (2002)

[2] Batchelor, G.R., An Introduction to Fluid Dynamics, Cambridge p. 139-140 (1967)