Orbital Mixing In Comsol Using Coriolis and Centrifugal Forces

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Introduction

Every year pharmaceutical and chemical companies run millions of tests using 96-well microplates. This research looked at orbital mixing, in hopes of finding a better mixing technique which will maximize concentration homogeneity in minimal time. Having the most efficient technique is always desirable for these tests, this will save time and it keeps companies profitable. The interest in this research came from Rosetta Software company. Our objective is to compare our model produced from 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.

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.

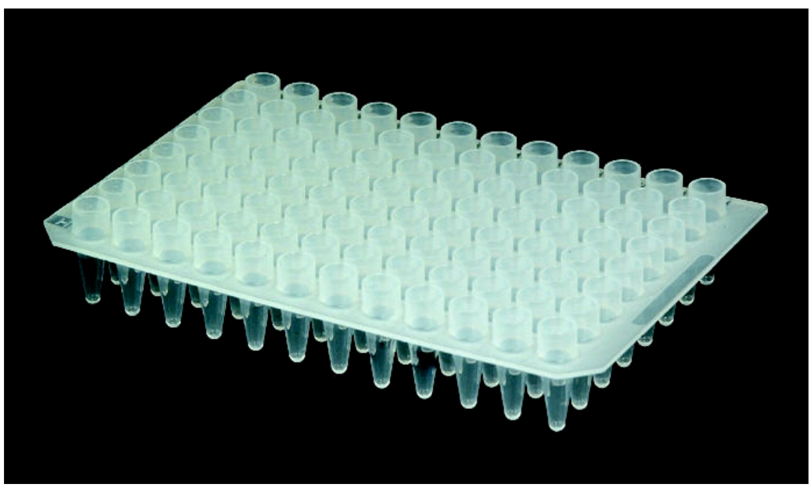

Figure 1. Photograph of a 96-Well Microplate

There are two approaches which were considered to model orbital mixing on COMSOL multiphysics software. Our research in the fall used ALE moving mesh in COMSOL to model velocity forces.[3] After determining that the ALE method was a strenuous calculating method for COMSOL, we determined using a fixed coordinates system with Equation 1 shown below to describe the velocity forces would hopefully make calculations easier:

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

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 for orbital mixing.

We used a programmed model called The Momentum Transport was modeled using the Navier-Stokes equation (NS) for incompressible fluids, given in Equation 2, and the convective and diffusive transport was modeled using steady-state convection and diffusion equations, given in Equation 3. 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.

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

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

ρ = constant density of fluid
v = velocity vector
p = pressure
μ = constant dynamic viscosity
g = gravitational force vector

$$D\nabla^2 c = \mathrm{v} \cdot \nabla c \qquad \text{Equation 3}$$

D = constant diffusion coefficient
c = concentration
v = velocity vector

Table 1. Parameters set in COMSOL multiphysics

Constants				**Navier-Stokes subdomain settings**				
Ω	52.3			Fx	(coriolis_x+centrifugal_x)			
shaking D	0			Fy	(coriolis_y+centrifugal_y)			
a	0.3			**Boundary Conditions inflow/outflow velocity**				
Subdomain Expressions				symmetry				
x_o	R*sin(omega*t)+x			u_o	-omega*a*y/SQRT(x^2+y^2)			
y_o	R*cos(omega*t)+y			v_o	omega*a*x/sqrt(x^2+y^2)			
coriolis_x	2*omega*v			**Concentration/Diffusion**				
coriolis_y	=-2*omega*u			δ_{ts}	1			
centrifugal_x	-(R*cos(omega*t)+x)*omega^2			D isotropic	1.00E-10			
centrifugal_y	(R*sin(omega*t)+y)*omega^2			u	u-omega*(R*sin(omega*t)+y)			
length	sqrt((R+x)^2+y^2)			v	v+omega*(R*cos(omega*t)+x)			
Solver Parameters								
Analysis	transient, time dependent							
Times	0:0.01:0.96							
Relative	0.01							
Absolute	0.001							
Boundary Expressions								
theta	atan(y/(R+x))							
x_o	length*sin(theta+omega*t)							
y_o	length*cos(theta+omega*t)							
length	sqrt((R+x)^2+y^2)							

Results

This section will show and discuss all experimental results from the research done. The main case looked at for this quarter was done for a time 0.96 seconds or 8 revolutions at 500 rpm.

Case 1

Elements: 1140
Degrees of freedom: 7596
Solving time: 1.5 hours

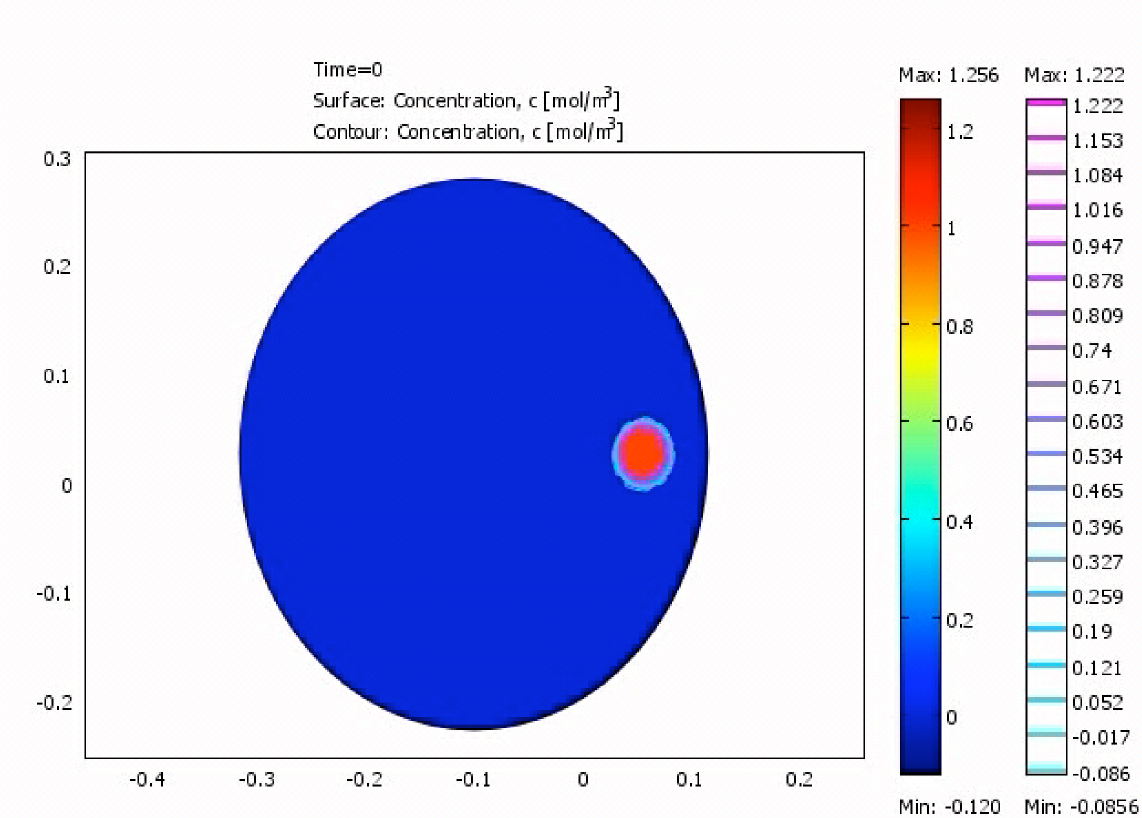

Figure 1. This shows the initial profile for case 1. The inner circle has a concentration set at 1 mol/m^3 while the outer circle is set with no concentration

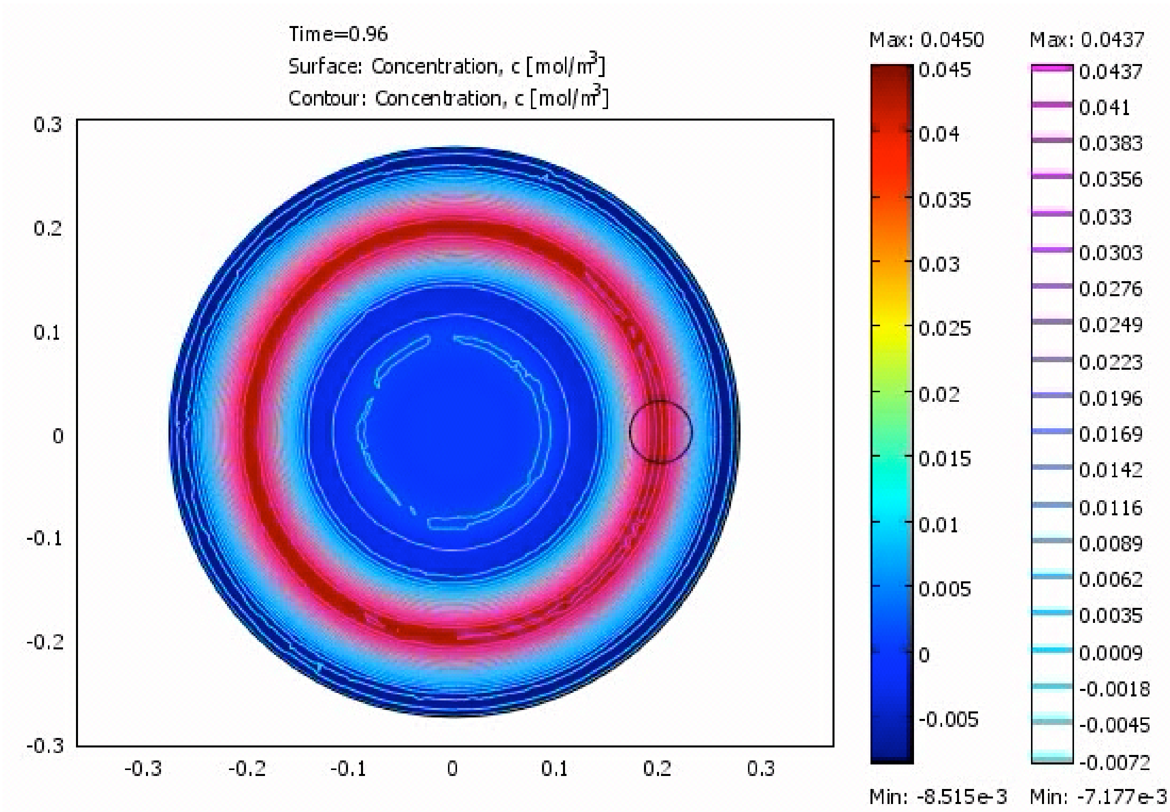

Figure 2. This shows the final profile for case 1. The concentration is highest at the distance from center of the original concentrated drop.

As seen in figures 1 and 2 there is a significant amount of mixing for this model. The concentration is highest at the radius from the initial concentration profile. It was determined that better mixing may occur if a concentration profile of equal area were to stretch the diameter of the circle results for this can be seen in Case 2 below.

Case 2
Elements: 4010
Degrees of freedom: 26685
Solving time: 3 hours

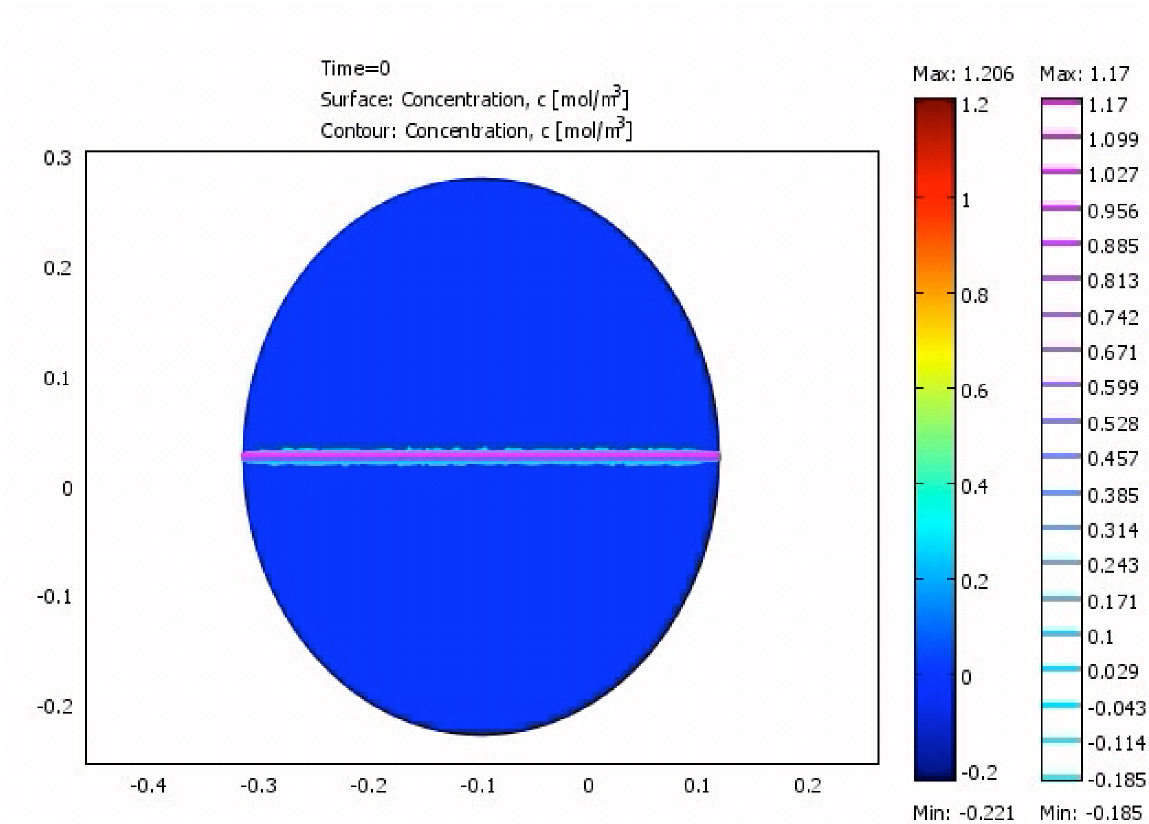

Figure 3. This shows the initial profile for case 2. The inner line has a concentration set at 1 mol/m^3 while the outer circle is set with no concentration.

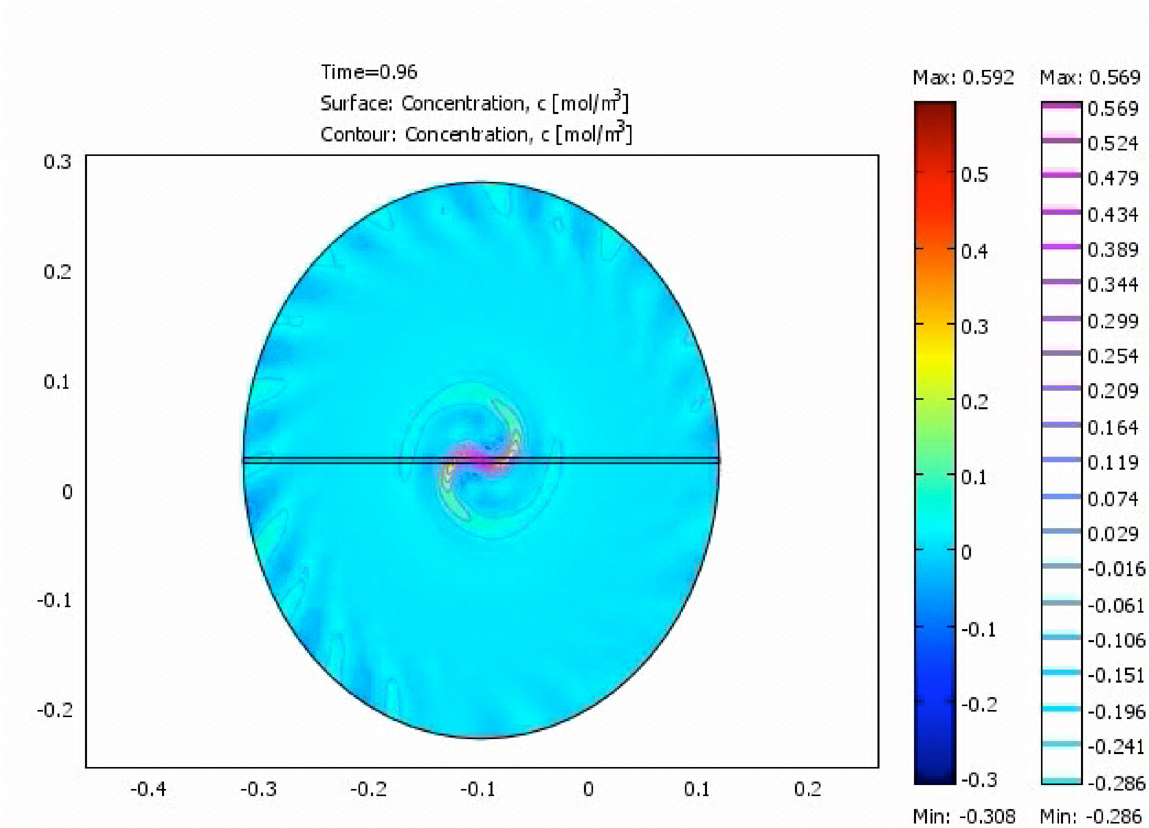

Figure 4. This shows the final profile for case 2. The concentration is highest at the center of the well due to the fact that there is no velocity at the center of the well.

As seen in figures 3 and 4, a greater homogenized mixing was obtained. The greatest amount of inhomogeneity was at the center of the well which is expected because there is no velocity at the center.

A couple simple checks for the solution can be done if the angular velocity is changed and if the mesh is refined. In case 3 shown below both checks were done to verify the results.

Case 3
Elements 4560
Degrees of freedom: 30008
Solvin time: 3.4 hours

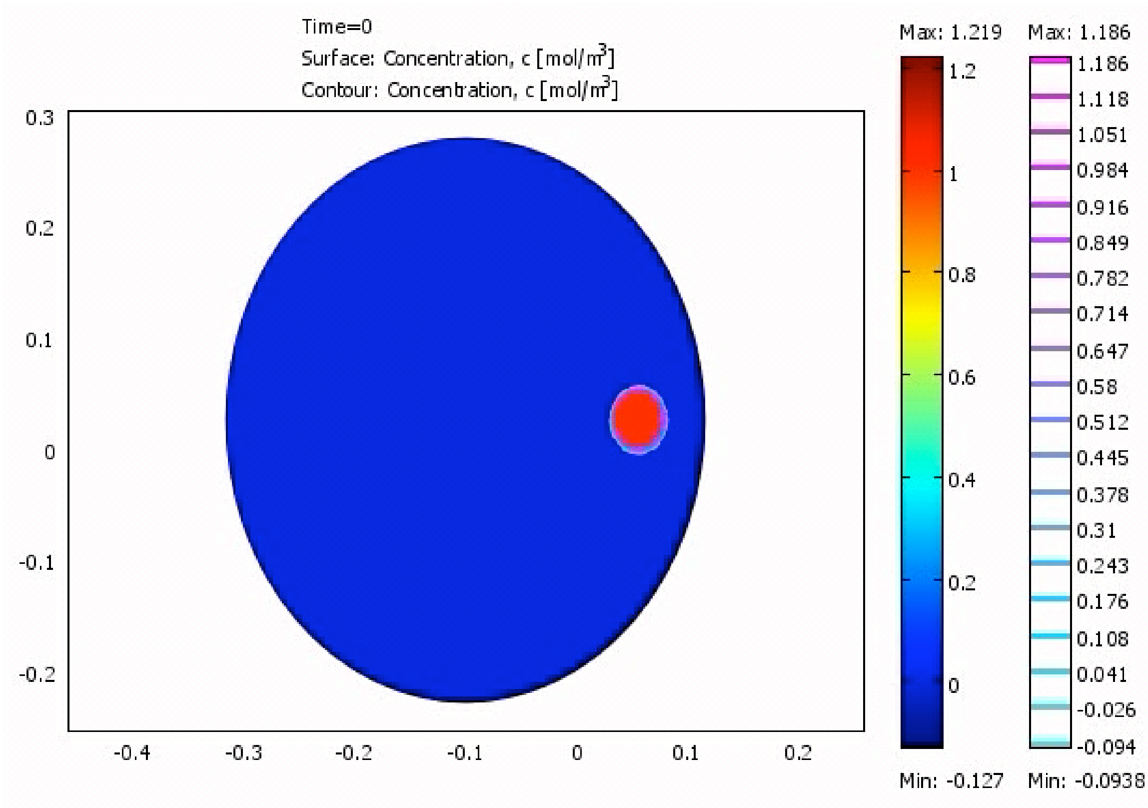

Figure 5. This shows the initial profile for case 3. The inner circle is has a concentration set at 1 mol/m^3 while the outer circle is set with no concentration.

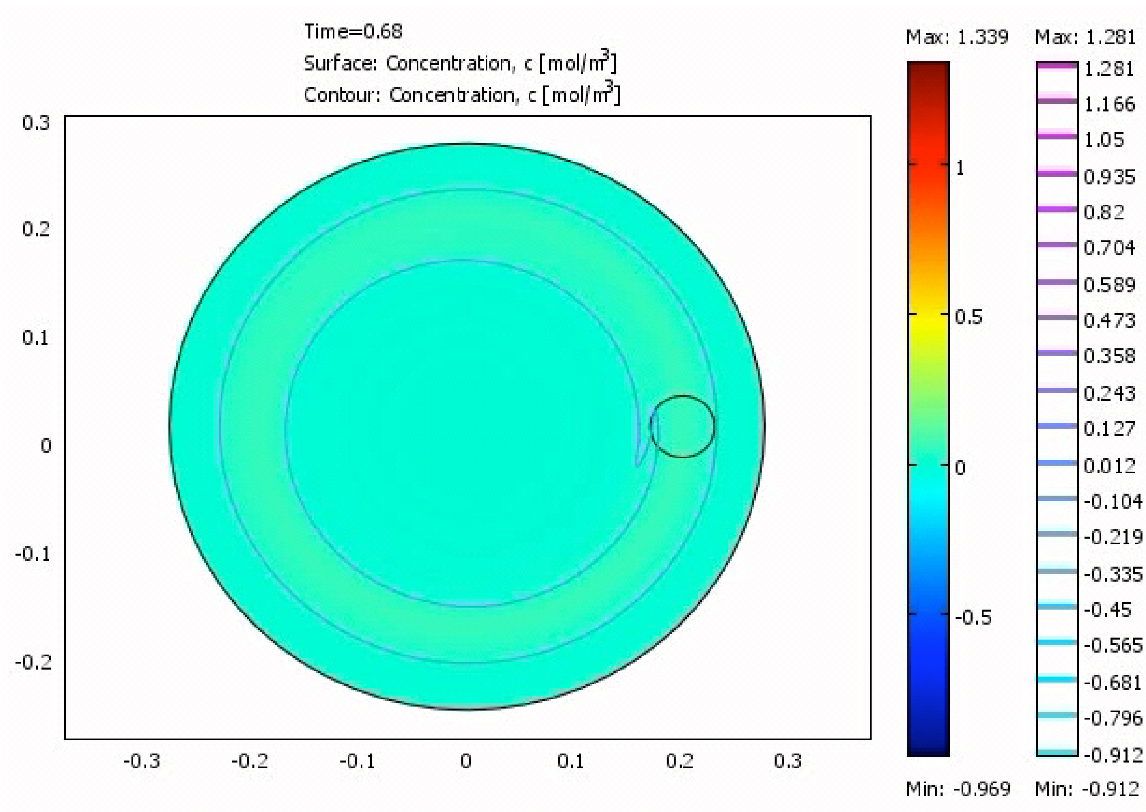

Figure 6. This shows the final profile for case 3. The concentration is highest at the distance from center of the original concentrated drop.

As seen in figures 5 and 6, results are similar to those shown in figures 1 and 2. The greater mesh refinement has given a better concentration distribution

Case 4

This attempt was to solve for the problem in three dimensions, but it was very difficult for Comsol to model. An attempt to model mixing after 10μs with a coarse mesh was obtained after 3 hours, however, mixing for 10μs is not long enough to see any mixing effects. An attempt to model mixing for more than 10μs was done, but the solution did not converge due to inverted matrices.

Earlier research from last fall gave the results shown in Figure 7 below:

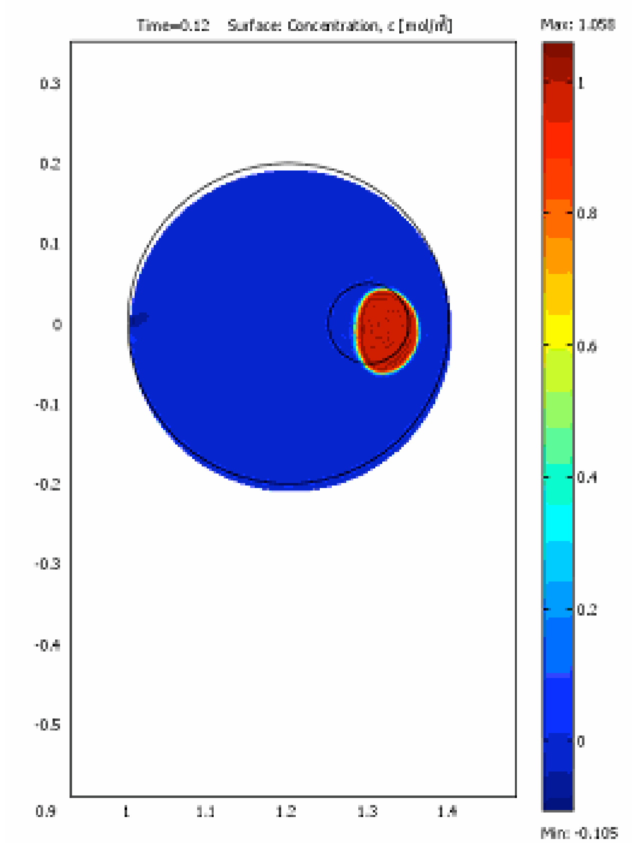

Figure 7. After 360 degrees, the profile shows that the concentrated circle has moved closer to the wall and the inner portion has flattened out from its original shape.

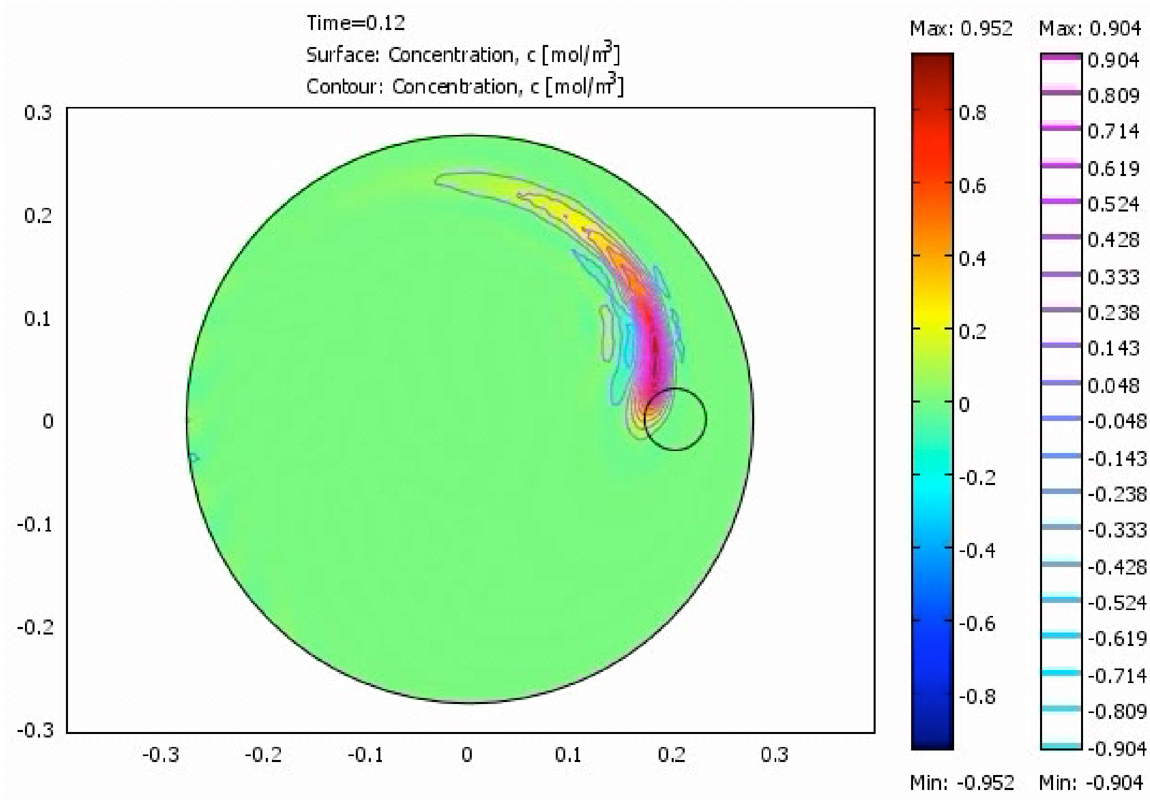

Figure 8. This shows the concentration profile after 0.12 seconds for 500 rpm simulation using the Coriolis and centrifugal forces.

It can be seen that little mixing occurred in this case using ALE in Figure 7. Although this mixing was only after one revolution the comparison to the results obtained using the Coriolis and centrifugal forces was different in Figure 8.

Conclusions

After completing the second quarter of research on this problem, the conclusions have not changed very much. Although using the Coriolis and centrifugal equations helped shorten the solving time for Comsol. This problem is still very difficult and time consuming. Trying this problem using a non-dimensional unit method could further simplify the problem and make a 3 dimensional case feasible. However, there were some notable differences between using ALE and the new equations. As seen in the results section research done in the fall did not have the same kind of mixing that we found in this quarter's research. It was shown that homogenized mixing is better obtained when a concentrated fluid is placed over the diameter of the well.

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)
3. Lillie, Shawn, Two Dimensional Orbital Mixing for a Fluid, Undergraduate Research (Finlayson) at the University of Washington (2006)

Appendices

Sample calculations:

$$500\frac{rev}{\min}\frac{2\pi\ rad}{1\,rev}\frac{1\min}{60\sec} = 52.3\frac{rad}{\sec}$$