Mixing in Flow Devices:

Spiral microchannels in two and three dimensions

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I. Introduction

The purpose of this research project is to study the mixing effect in microchannels as spirals and helices. Computer-generated geometries are constructed in Comsol Multiphysics in two dimensions and later three dimensions in the same ranges of Reynolds number and Peclet number.

The study is first carried out in two-dimension objects using dimensionless variables. The first geometry is a curved channel in a C-shape and the second one is a spiral channel that is actually a combination of several C-shaped channels of different curvatures. Later, study of three-dimension helix is done by a similar method. The problem is firstly solved in small range of Reynolds number for laminar flow; then at a fixed Reynolds number of 1 while varying the Peclet number from 100 to 1000. The characteristics of mixing in the channel are determined based on five quantities: mixing cup concentration and its variance, optical average concentration, optical variance and the pressure drop across channel. The definitions and methods to calculate these values are presented in the next section.

II. Theory and Methods

Theory

Flow in microfluidic devices is laminar in a low range of Reynolds number. The geometries are constructed to achieve fully developed flow for Reynolds number from 1 to 100. The Peclet number is the measurement of the relationship between diffusion and convection. This project is carried on in the range of Peclet number from 100 to 1000.

The geometries are solved based on the nondimensional Navier-Stokes equation

$$\operatorname{Re}\frac{\partial u'}{\partial t'} + \operatorname{Re}u' \cdot \nabla' u' = -\nabla' p' + {\nabla'}^2 u' \qquad (\text{Equation 1})$$

in which the dimensionless variables are defined as below

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$$u' = \frac{u}{u_s} \rightarrow u = u_s u'$$
 (Equation 2)

$$p' = \frac{p}{p} \rightarrow p = p_s p'$$
 (Equation 3)

$$x' = \frac{x}{x} \to x = x_s x'$$
 (Equation 4)

$$\nabla' = x_s \nabla \to \nabla = \frac{1}{r} \nabla'$$
 (Equation 5)

The standard units of the variables in this problem are given as below

- Velocity standard: $u_s = 0.005 \text{ m/s}$
- Distance standard: $x_s = 200$ m
- Fluid density: $\rho = 1000 \text{ kg/m}^3$

- Viscosity $\eta = 0.001$ Pa.s
- Diffusivity: $D = 10^{-9} \text{ m}^2/\text{s}$

From the above values, the Reynolds number for the dimensional problem is 1 and the Peclet number is 1000.

The geometries are constructed so that both dimensionless diameter of the channels and average inlet velocity are 1. The mixing cup concentration and its variance are used to evaluate how well the geometry works. In this report, this concentration and its variance will be determined by the product of concentration and velocity integrated on the surface of the concerned boundary. The following formulas are used in the calculation with velocity integration included

$$c_{mixing \, cup} = \frac{\int_{A} c(x, y, z) v(x, y) dx dy}{\int_{A} v(x, y) dx dy}$$
(Equation 8)
$$c_{var \, iance} = \frac{\int_{A} \left[c(x, y, z) - c_{mixing \, cup} \right]^2 v(x, y) dx dy}{\int_{A} v(x, y) dx dy}$$
(Equation 9)

With average velocity assumed to be 1 over any crossed-sectional area along the path, the velocity is not taken into account and the above formulas become

$$c_{mixing \, cup, optical} = \frac{\int_{A} c(x, y, z) dA}{\int_{A} dA}$$
(Equation 10)
$$c_{var \, iance, optical} = \frac{\int_{A} \left[c(x, y, z) - c_{mixing \, cup} \right]^{2} dA}{\int_{A} dA}$$
(Equation 11)

Equations 10 and 11 calculate the optical average concentration integrated over the crossed section of the channel and its optical variance.

After the models in interest are run in Comsol, the pressure drop between the inlet and outlet of the channel is recorded. This value is dimensionless according to the problem setup. In order to get the pressure drop in Pascals, the pressure standard is taken into account:

$$p = p_s p' = \frac{\mu u_s}{x_s} p'$$
 (Equation 12)

From the given standards, the pressure standard can be calculated as

$$p_s = \frac{\mu u_s}{x_s} = \frac{(0.001 Pa \cdot s)(0.005 \, m/s)}{200 \mu m} = 0.025 Pa$$
(Equation 13)

Methods

A. Two-Dimensional Models

Step 1: Constructing the geometry in COMSOL Multiphysics.

The geometry is constructed in COMSOL under the setting of Model Navigator: "Chemical Engineering Module/ Momentum Transport/ Laminar Flow/ Incompressible Navier-Stokes/ Steady State Analysis". The option of solving for convection and diffusion is added later. Its dimensions are resembled the literature drawings as much as possible (Figure 1).



Figure 1. Illustration of Dean flow effects in a curved microchannel. ("Fluid mixing in planar spiral microchannels", Arjun P. Sudarsan and Victor M. Ugaz, The Royal Society of Chemistry journal, 2006).

For the first geometry including only one arc between the inlets and outlet, the ratio between the radius of curvature and the diameter of the channel is approximately 3. The two inlets' diameter is a half of the mixing section's one. In dimensionless system, the diameter of the curved mixing section is 1 and the diameter of the inlets is _. The inner radius of the mixing section is 2.5 and the outer one is 3.5 (these radii imply that the radius of the centerline of the arc has a radius of 3, satisfying the approximation ratio stated earlier).



Figure 2. Reproduction of the channels illustrated in the literature (Figure 1 above). The radii of curvature are estimated from the picture given in the paper. The channel's radius is set to 1.

The second geometry is a two-arc spiral constructed in the same manner. Its diameter is 1. The larger arc's outer diameter is 20 and the smaller one's is 17. The object is constructed by making four separate C-shaped arcs and creating a composite object from them. The internal boundaries are kept for later evaluation of mixing effect along the equivalent path.



Figure 3. Spiral channel with four turns. Its radius is 1. It is constructed from four C-shaped channels with different radii of curvature. Mixing cup concentration, its variance, optical concentration and optical variance are evaluated at boundaries 12, 13, 14 and 15 shown above. The tabulated results can be found in Appendix A.

Step 2: Setting Physical and Boundary Conditions.

Before putting the physical properties and boundary conditions in, all of the subdomains in the geometry should be grouped together.

1. Step 2.1: Conditions for the Navier-Stokes Equation

<u>Subdomain Settings</u>: The density of fluid in this setting is directly related to the Reynolds number the problem is solved at. This is proved from the definition of Reynolds number in terms of dimensionless variables:

$$x_{s} = D = 1$$

$$u_{s} = \langle u \rangle = average \ velocity = 1$$

$$Set \ \mu = 1$$

$$Re = \frac{\rho u_{s} x_{s}}{\mu} = \frac{\rho \cdot 1 \cdot 1}{1}$$
(Equation 6)

In 2D problem, the geometries are solved at Re = 1; therefore, the density is set to be 1 when the dynamic viscosity is 1.

Boundary Settings:

- The two inlet boundaries are set as Boundary Type: "Inlet" Boundary Condition: "Velocity" Quantity: Initial value u_o = 0.02
- The outlet boundary is set as Boundary Type: "Outlet" Boundary Condition: "Pressure" Quantity: Initial value P_o = 0

In some cases, this setting does not convert. The Boundary Condition can be set as "Laminar inflow" in stead of "Inlet".

2. Step 2.2: Add one more model

From the menu Multiphysics/ Model Navigator, choose Mass Transport/ Convection and Diffusion/ Steady State Analysis to the convection and diffusion equations into the problem.

3. Step 2.3: Conditions for Convection and Diffusion Equations

Switch to the newly added model to enter its properties.

<u>Subdomain Settings</u>: The diffusivity is inversely proportional to the Peclet number. The Peclet number when written in terms of dimensionless variables proves this relationship:

$$Pe \equiv \frac{v_s x_s}{D} = \frac{1 \cdot 1}{D}$$
 (Equation 7)

The expected range for Pe number is from 100 to 1000 as mentioned above. This 2D problem is solved at Pe = 100. Therefore, the diffusion coefficient is set as 1/100.

The x-velocity is u and the y-velocity is v.

Boundary Settings:

- The two inlet boundaries are set as Boundary Condition: "Concentration" Quantity: Initial value C_o = 1 for one boundary and C_o = 0 for the other
- The outlet boundary is set as

Boundary Condition: "Convective flux"

Step 3: Solving for the five desired quantities

After defining the mesh, the Navier-Stokes equation is solved first. Then, its solution is used as the initial values to solve the convection and diffusion model.

B. Three-Dimensional Model

After the two-dimensional solutions are collected, the three-dimensional geometry is solved by a similar method. The geometry is constructed, then the Navier-Stokes equation is solved for momentum transport/velocity profile before the mass transfer model of "Convection and Diffusion" is solved for concentration profile. **Step 1:** *Constructing the geometry in COMSOL Multiphysics.*

Because of the difficulties in constructing a three-dimensional spiral channel from the one studied in the two-dimensional case, a spiral channel is used instead. Theoretically, this model still follows the same concept of constructing the geometry by combing several C-shaped channels in series. The cross-section of the pipe is round and set up at diameter of 1 for the purpose of solving the problem in dimensionless variables.

_Open Comsol Script and issue the command "C>>h=helix3(0.5,10,10,2*10,12)" which gives the following output:

h =

3D solid object subdomains: 1 faces: 98 edges: 196 vertices: 100

Then, in Comsol Multiphysics workspace, the helix is imported by "File/Import/Geometry Objects..." The helix appears with its center at the origin of the coordinates.



Figure 4. Three-dimensional geometry studied in this project.

III. Results

Three geometries are studied: two of them are in two-dimensions (C-shaped and spiral channels) and the last one is in three-dimensions (helix). For each geometry, mixing effect is evaluated by five quantities defined from equation 8 to equation 12. The tabulated results are presented by the tables in Appendix A. Firstly, at one fixed Pe value (Pe=100), laminar flow corresponding to the range of Re from 1 to 30 is examined. The calculated values show that low Re numbers do not have significant effect on mixing. Therefore, the study is carried on at one fixed Re number (Re=1) and in the range of Pe number from 100 to 1000.



Variance for mixing in spiral channel

Figure 5. Representation of variances in the two-dimensional and three-dimensional geometries studied in this project. These values show the same trend and can collapse into one curve and have the same characteristics. This implies that it is possible to use two-dimensional simulation for modeling mixing channel.

Examples of concentration profiles for both the 2D and 3D cases are presented in the following section of this report.



Figure 6. Concentration profile of the spiral mixing channel. This illustration is taken from the simulation in which Re is kept at 1 and Pe is set to be 500. Two different feed streams at different concentrations are fed to the channel. Mixing parameters are evaluated by Comsol at each turn of the channel, corresponding to four equivalent length z's.



Min: -0.0549

Figure 7. Concentration profiles in the helix solutions at Re=1 and Pe=500. The study of 3D channel is only carried out at one fixed Re and varying Pe from 100 to 1000.

Comparison of results from refining the meshes

The data for each trial (in tables A1 - A3) are collected at the largest possible mesh of each setting up condition. Figures 8 and 9 below show two concentration profile of the same helix in figure 7 above, but one is at the highest possible mesh when the other is at the first mesh. Larger mesh provides more accurate solutions.

During the process of this project, computer memory is the main limitation to solve these problems at higher mesh. In most of the time, the computer cannot solve a meshed that is refined more than three times. Therefore, the optical values in the spiral channel are larger than the expected ones. Resolving the geometry at higher meshes will get the solution closer to expectation.



Figure 8. Concentration profiles in the helix solutions (Re=1, Pe=500) at largest mesh.



Figure 9. Concentration profiles in the helix solutions (Re=1, Pe=500) at lowest mesh.

				optical c _{mixing}	optical
Re	Pe	Mesh elements	DOF	cup	variance
30	100	136	331	0.3597	0.01053
30	100	544	1205	0.3386	0.00931
30	100	2176	4585	0.3326	0.00894
30	100	8704	17873	0.3307	0.00885
30	100	34816	70561	0.3302	0.00882

Table 1. Effect of different mesh sizes the calculated quantities.

Table 1 shows how concentration and its variance decrease when the number of mesh elements is getting larger. Dividing the mesh smaller provides a more accurate calculation. As stated earlier, the results of the optical values in the 2D spiral channel exceed expectations (concentration of 0.5 and variance of 0.25) because the mesh is not divided small enough. The larger of number of elements, the smaller those values get. However, due to computer memory limitation, this study considers the presented result acceptable since they're still showing the same behaviors and trends such as the best mixing occurs at lower Peclet numbers.

IV. Literature Comparison

In order to construct the geometry for studying the mixing effect in spiral channels, the paper "Fluid mixing in planar microchannels" written by Arjun P. Sudarsan and Victor M. Ugaz was used as a reference. This paper was published in the journal *The Royal Society of Chemistry* in 2006. The authors, Surdarsan and Ugaz, studied fluid mixing at varied flow rates in the range of Reynolds number from 0.02 to 18.6. Their results were presented in terms of mixing intensity versus the channel length. The mixing intensity was defined as

mixing intensity=
$$\frac{\text{width of mixed interface}}{\text{width of channel}}$$

In our project, the range of Reynolds number, from 0 to 30, is larger than the range studied in the paper but the geometry has less number of arcs in one spiral than in the experiment described in the paper. This project only studied a spiral channel with two arcs at Re = 1, 5, 10, 20 and 30. The number of arcs expanded the length of the channel so that mixing could occur better. The paper stated that diffusion was primary at lower Re numbers and the secondary Dean Effects contributed in the levels of mixing at higher ones. In our model in Comsol Multiphysics, convection and diffusion were taken into account for mixing. At low Re numbers such as around 1, the mixing cup concentration and variance were larger than the higher Re. They dropped when Re number was changed from 1 to 5. In the range from Re = 5 to Re = 30, these two values kept decreasing slightly but magnitude of their differences were still lower than when Re number changed from 1 to 5.

The paper concluded that multiple sections of spirals with fewer arcs have better mixing at higher Reynolds numbers. The result in our project supported this statement.

Our study were also carried out at a constant Re = 1 and varied Peclet number. The diffusivity of the fluid in the literature experiment was not available for comparison.

V. Suggestions for Improved Mixing

The result shows that increasing the equivalent length also raises mixing effect. Therefore, lining up several channels in series or adding more turns into the existing spiral/helix will increase the outlet concentration. The experiment in the literature also demonstrates a similar concept.

VI. Conclusions

The variances in both 2D and 3D cases can collapse into one curve as presented in Figure 1 in logarithmic scale. For laminar flow (1 < Re < 30), there is no major impact in mixing when Re is adjusted. In the studied range if Pe (100 to 1000), all of the models suggests that mixing occurs the best at the lower limit. Because the conclusions from the 3D solution mirrors the ones from 2D case, it is possible to model microfluidic channels in two dimensions and still be able to characterize the mixing effect.

The shape of the curve of logarithm of variance versus the quantity z'/Pe is the same as the one of T-sensor. However, the scale is quite different because of the setup of the problem and the specification of the geometries.

IV. Appendices

A. Mixing characteristics from Comsol simulations presented by five quantities: pressure drop, mixing cup concentration and its variance, optical concentration and optical variance.

Run	Re	Pe	_P' (D'less)	_P (Pa)	C _{mixing cup}	variance	optical c _{mixing cup}	optical variance
1	1	100	138.3	0.3458	0.5227	0.0099	0.4767	0.0116
2	5	100	139.8	0.3494	0.4990	0.0151	0.4927	0.0201
3	10	100	140.0	0.3501	0.4825	0.0099	0.4804	0.0133
4	20	100	143.5	0.3588	0.4179	0.0090	0.4142	0.0121
5	30	100	146.6	0.3664	0.3648	0.0078	0.3597	0.0105
6	1	100	138.3	0.3458	0.4787	0.0087	0.4767	0.0116
7	1	200	138.3	0.3458	0.4788	0.0395	0.4738	0.0525
8	1	300	138.3	0.3458	0.4779	0.0656	0.4771	0.0876
9	1	500	138.3	0.3458	0.4762	0.0983	0.4724	0.1265
10	1	750	138.3	0.3458	0.4823	0.1238	0.4785	0.1538
11	1	1000	138.3	0.3458	0.4717	0.1329	0.4682	0.1598

Table A1. Results for the C-shaped 2D geometry.

				Boundary 14						
Run	Re	Pe	z'/Pe	_P' (D'less)	_P (Pa)	C mixing cup	variance	optical concentration	optical variance	
1	1	100	0.0766	1455	3.637	0.5029	1.823E-03	0.7540	9.856E-02	
2	5	100	0.0766	1470	3.675	0.3997	1.639E-03	0.6001	6.342E-02	
3	10	100	0.0766	1489	3.723	0.4929	4.075E-04	0.7391	9.206E-02	
4	20	100	0.0766	1526	3.816	0.4858	4.119E-04	0.7283	8.944E-02	
5	30	100	0.0766	1565	3.911	0.4774	1.860E-03	0.7156	8.923E-02	
6	1	100	0.0766	1455	3.637	0.5029	1.823E-03	0.7540	9.856E-02	
7	1	200	0.0383	1455	3.637	0.5045	1.914E-02	0.7562	1.350E-01	
8	1	300	0.0255	1455	3.637	0.5122	2.177E-02	0.7662	1.522E-01	
9	1	500	0.0153	1455	3.637	0.5055	7.929E-02	0.7586	2.590E-01	
10	1	750	0.0102	1455	3.637	0.5090	1.094E-01	0.7601	3.079E-01	
11	1	1000	0.0077	1455	3.637	0.5093	1.280E-01	0.7604	3.376E-01	

 Table A2. Results for the 2D spiral channel.

				Boundary 13							
Run	Re	Pe	z'/Pe	_P' (D'less)	_P (Pa)	C mixing cup	variance	optical concentration	optical variance		
1	1	100	0.1414	1870	4.675		3.566E-04	0.7531	9.526E-02		
2	5	100	0.1414	1888	4.720	0.3798	2.405E-04	0.5710	5.484E-02		
3	10	100	0.1414	1905	4.763	0.4907	5.000E-05	0.7360	9.040E-02		
4	20	100	0.1414	1943	4.857	0.4824	5.057E-05	0.7235	8.737E-02		
5	30	100	0.1414	1981	4.954	0.4689	3.515E-04	0.7040	8.334E-02		
6	1	100	0.1414	1870	4.675	0.5021	3.566E-04	0.7531	9.526E-02		
7	1	200	0.0707	1870	4.675	0.5020	8.339E-03	0.7524	1.116E-01		
8	1	300	0.0471	1870	4.675	0.5097	1.071E-02	0.7613	1.234E-01		
9	1	500	0.0283	1870	4.675	0.5009	5.604E-02	0.7483	2.090E-01		
10	1	750	0.0188	1870	4.675	0.4994	8.739E-02	0.7488	2.665E-01		
11	1	1000	0.0141	1870	4.675	0.4990	1.076E-01	0.7482	3.025E-01		

				Boundary 12							
Run	Re	Pe	z'/Pe	_P' (D'less)	_P (Pa)	C _{mixing cup}	variance	optical concentration	optical variance		
1	1	100	0.2062	2285	5.713	0.5021	3.566E-04	0.7531	9.526E-02		
2	5	100	0.2062	2305	5.763	0.3864	2.405E-04	0.5710	5.484E-02		
3	10	100	0.2062	2321	5.802	0.4913	5.000E-05	0.7360	9.040E-02		
4	20	100	0.2062	2359	5.897	0.4835	5.057E-05	0.7235	8.737E-02		
5	30	100	0.2062	2398	5.994	0.4724	3.515E-04	0.7040	8.334E-02		
6	1	100	0.2062	2285	5.713	0.5021	3.566E-04	0.7531	9.526E-02		
7	1	200	0.1031	2285	5.713	0.5020	8.339E-03	0.7524	1.116E-01		
8	1	300	0.0687	2285	5.713	0.5097	1.071E-02	0.7613	1.234E-01		
9	1	500	0.0412	2285	5.713	0.5009	5.604E-02	0.7483	2.090E-01		
10	1	750	0.0275	2285	5.713	0.4994	8.739E-02	0.7488	2.665E-01		
11	1	1000	0.0206	2285	5.713	0.4990	1.076E-01	0.7482	3.025E-01		

				Boundary 15						
Run	Re	Pe	z'/Pe	_P' (D'less)	_P (Pa)	C _{mixing cup}	variance	optical concentration	optical variance	
1	1	100	0.2827	3504	8.759	0.5021	7.217E-07	0.7531	9.453E-02	
2	5	100	0.2827	3525	8.812	0.3880	3.801E-07	0.5819	5.644E-02	
3	10	100	0.2827	3540	8.849	0.4914	1.965E-08	0.7371	9.055E-02	
4	20	100	0.2827	3578	8.945	0.4835	7.937E-06	0.7253	8.768E-02	
5	30	100	0.2827	3617	9.042	0.4729	6.950E-07	0.7093	8.385E-02	
6	1	100	0.2827	3504	8.759	0.5021	7.217E-07	0.7531	9.453E-02	
7	1	200	0.1414	3504	8.759	0.5019	3.832E-04	0.7528	9.524E-02	
8	1	300	0.0942	3504	8.759	0.5070	9.394E-04	0.7608	9.881E-02	
9	1	500	0.0565	3504	8.759	0.5011	1.717E-02	0.7510	1.286E-01	
10	1	750	0.0377	3504	8.759	0.5025	4.293E-02	0.7530	1.796E-01	
11	1	1000	0.0283	3504	8.759	0.5028	6.457E-02	0.7532	7.532E-01	

Table A3. Results for the 3D 5-turn helix.

				C _{mixing}		optical	optical
Re	Ре	z'/Pe	_P (Pa)	cup	variance	concentration	variance
1	100	0.2827	8.737	0.4752	1.498E-08	0.7128	8.468E-02
1	200	0.1414	8.737	0.4470	4.878E-05	0.6705	7.505E-02
1	300	0.0942	8.737	0.4369	7.101E-04	0.6552	7.333E-02
1	500	0.0565	8.737	0.4360	6.066E-03	0.6531	8.625E-02
1	750	0.0377	8.737	0.4414	1.799E-02	0.6596	1.175E-01
1	1000	0.0283	8.737	0.4466	3.132E-02	0.6660	1.522E-01

B. Sample Calculations

The standard units of the variables in this problem are given

- Velocity standard: $u_s = 0.005 \text{ m/s}$
- Distance standard: $x_s = 200 \text{ m}$
- Fluid density: $= 100 \text{ kg/m}^3$
- Viscosity: = 0.001 Pa.s
- Diffusivity: $D = 10^{-9} \text{ m}^2/\text{s}$

From the above values, the Reynolds number for the dimensional problem is 1 and the Peclet number is 1000.

For one trial:

In "Postprocessing" menu, use the option "Boundary Integration".

Choose the boundary needed to be evaluated.

Find the pressure drop from the inlet to the recent boundary (pressure is represented as "p"): The number Comsol gives out is the dimensionless pressure drop p' = 1455 (Table A2, run 1).

Convert that value to dimensional quantity by

$$p_{s} = \frac{\mu u_{s}}{x_{s}} = \frac{(0.001 Pa \cdot s)(0.005 m/s)}{200 \mu m} = 0.025 Pa$$
$$p = p_{s}p' = \frac{\mu u_{s}}{x_{s}}p' = (0.025 Pa)(1455) = 3.637 Pa$$

Mixing cup concentration: Firstly, evaluate the quantity "v" over the whole boundary. This value is the denominator of equation 8. Then, use equation 8 as the function "c*v/(value of 'v') to get the concentration.

Variance: Substitute the just found mixing cup concentration into equation 9 and follow the same method.