

Micro-Mixing by Rectangular Expansion Channel

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June 10, 2008

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Introduction

The purpose of the research is to obtain best mixing properties on rectangular expansion geometry channel. The geometry will be study in 2-dimension, and then it will be extrude for 3-dimensions. By varying the Reynolds and Peclet number, the mixing cup concentration and the variance will be calculated. Also, the variance was calculated by varying the path length of the flow.

Background

For the research, non-dimensional method of the incompressible Navier-Stokes equation is used to calculate the pressure drop. Also, Convection and Diffusion equation of the Comsol is used for calculating the concentration. Following set of non-dimensional equations is used to calculate the non-dimensional properties.

$$u' = \frac{u}{u_s} \rightarrow u = u_s u' \quad \text{Eq. 1}$$

$$p' = \frac{p}{p_s} \rightarrow p = p_s p' \quad \text{Eq. 2}$$

$$x' = \frac{x}{x_s} \rightarrow x = x_s x' \quad \text{Eq. 3}$$

$$\nabla' = x_s \nabla \rightarrow \nabla = \frac{1}{x_s} \nabla' \quad \text{Eq. 4}$$

For the purpose of represent the mixing properties, the values of the mixing cup and variance are calculated by using equation 5 and 6.

$$c_{\text{mixing cup}} = \frac{\int_A c(x, y, z) v(x, y) dx dy}{\int_A v(x, y) dx dy} \quad \text{Eq. 5}$$

$$c_{\text{variance}} = \frac{\int_A [c(x, y, z) - c_{\text{mixing cup}}]^2 v(x, y) dx dy}{\int_A v(x, y) dx dy} \quad \text{Eq. 6}$$

Optical terms of each equation 5 and 6 are same equation without the velocity terms.

Method (Comsol)

Step 1:

1. Space dimension: 2D
2. Application Modes
 - A. Chemical Engineering Module
 - Momentum balance
 - Incompressible Navier-Stokes
 - Steady-state analysis

Step 2:

1. Draw

- A. Draw Object
- B. Create Composite object

In step 2, Fig. 1 was drawn.

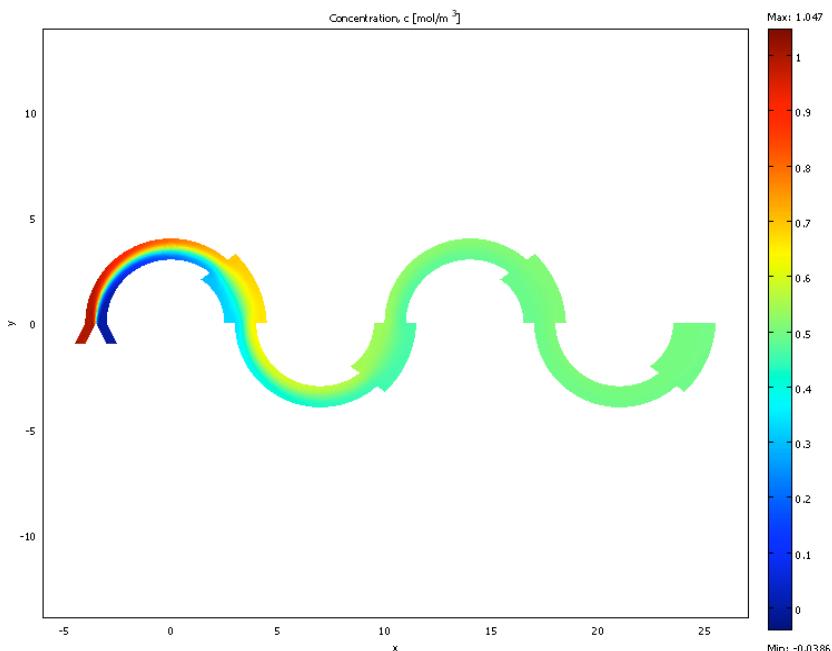


Figure 1: Solved 2D-geometry of mixing fluid

The dimensions of the figure are shown on Fig. 2.

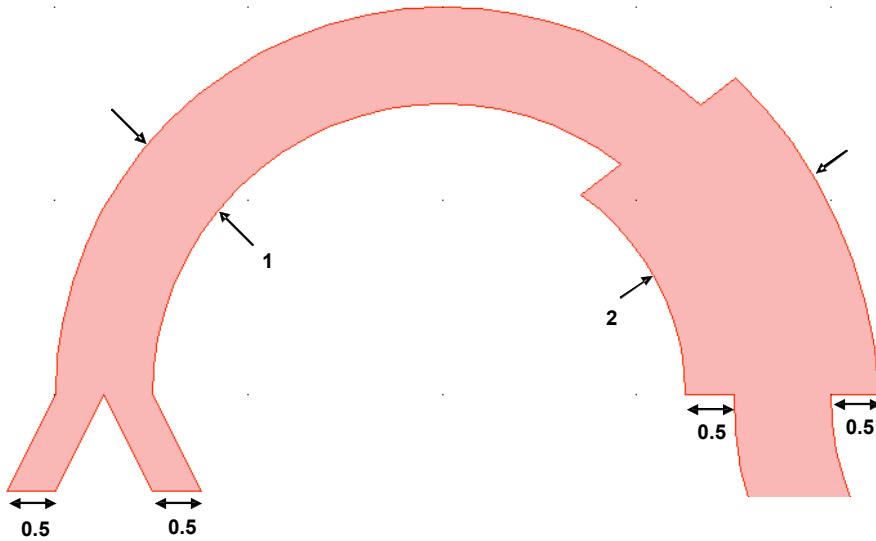


Figure 2: Dimension of the figure used

Step 3:

1. Multiphysics

A. Model Navigator

i. Space dimension: 2D

ii. Application Modes

Chemical Engineering Module

Mass Transport

Convection and Diffusion (steady state)

B. Add the application mode on same Geom (Geom1 (2D) in my case)

Then the mesh was initialized and refined. The mesh consists of 1720 elements.

Step 4:

1. Mesh

A. Initialize mesh

B. Refine mesh (# of degrees of freedom = 12208, # of elements = 1720)

After the mesh was refined, the subdomain and boundary setting were set up. First, settings of the incompressible Navier Stokes were set up.

Step 5:

1. Choose the “Incompressible Navier-Stokes” in the model tree

2. Physics

A. Subdomain settings

$\rho = 1, 10, 50, \text{ or } 100$ (Reynold's number was varied)

$$\begin{aligned}\bar{=} & 1 \\ \bar{F}_x &= 0 \\ \bar{F}_y &= 0\end{aligned}$$

B. Boundary settings

Boundary 1

Boundary type: inlet
Boundary condition: Laminar inflow
 $u_0 = 1$

Boundary 5

Boundary type: inlet
Boundary condition: Laminar inflow
 $u_0 = 1$

Boundary 23

Boundary type: outlet
Boundary condition: Pressure
 $P_0 = 0$

Other boundaries were set to

Boundary type: wall
Boundary condition: no slip

After the settings of the Navier-Stokes were done, Convection and Diffusion was set up.

Step 6:

1. Choose the “Convection and Diffusion” in the model tree
2. Physics

A. Subdomain settings

D (isotropic) = $1/Pe$, ($Pe = 100, 200, 300, 500, 700$, or 1000 were varied)
Under the D (anisotropic),

$$\begin{aligned}R &= 0 \\ u &= u \\ v &= v\end{aligned}$$

B. Boundary settings

Boundary 1

Boundary condition: Concentration
 $c_0 = 1$

Boundary 5

Boundary condition: Concentration
 $c_0 = 0$

Boundary 23

Boundary condition: Convective flux

Other boundaries were set to

Boundary condition: Insulation/Symmetry

Step 7:

1. Solve

A. Solve problem

The method for 3D is same as 2D's, except the geometry. For 3D, the 2D geometry is extruded to 3D with height of one.

Results

The value of $c_{mixing\ cup}$ and $c_{variance}$ with and without velocity term are obtained by boundary integration at the outlet boundaries. The concentration of mixing cup and variance of difference Reynold's number and Peclet number are shown on Appendix I for 2D and 3D. Also, the diagrams with the path length and variances are shown on Appendix I.

The pressure drop is shown on following table 1.

Table 1: Pressure drop at different path length or the location of the expansions

Expansion Location	$\Delta P [=] \text{ Pa}$			
	1	2	3	4
Re = 1	4.539	7.206	9.871	12.482
Re = 10	4.650	7.333	10.014	12.530
Re = 50	4.846	7.734	10.605	13.168
Re = 100	5.209	8.290	11.361	14.411

Note: The location of the expansion is a convention to show the pressure drop. It is determined by the numbering the expansions from left to right.

Discussion

Most calculations of the mixing cup and the variance are focused on the 2D. However, the 3D geometry is used to compare the result between the 2D and 3D and check any difference between them. For the 3D, one figure of the variance is drawn and compared to the 2D. Fig. 3 shows the comparison between the 2D and 3D at the Reynold's number one.

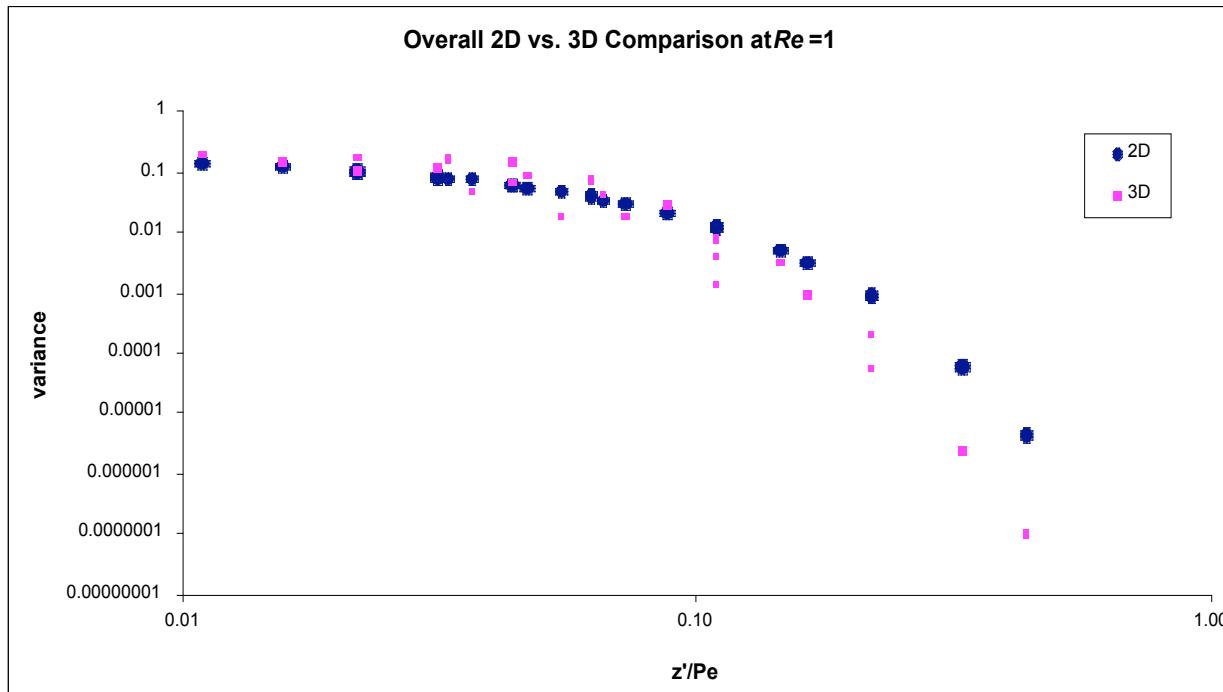


Figure 3: Comparison of variance between the 2D and 3D at $Re=1$

At the low ratio between the path length and the Peclet number, the difference of the variance between the 2D and 3D is very small where the difference is increasing as the ratio increase. The source of the difference will be the inaccurate calculation due to the coarse mesh. Another source is the vertical vortices, dean vortices. The dean vortices are considered because of the geometry difference between the 2D and 3D. 2D and 3D geometry has horizontal vortices, expansion vortices. However, 2D does not have dean vortices while 3D has it. Since the vortices make better mixing in the channels, vortices need to be studied more. However, most source of error considered is the inaccurate calculation due to the mesh refinement. The reason is that the vortices in this study does not considered as big factor for mixing due to the small heights compared to the length and expansions.

For more detail discussion, four cases of 2D are studied which is shown in Appendix I. As the results shows, the better mixing is obtained at higher Re and low Pe . The reason is that the expansion vortices are getting bigger with higher velocity at the expansions. If the vortices are bigger, then the mixing at the inlet of the expansion will occur more than slow velocity with

smaller vortices. As the results shows, the following figures obtained from the Comsol also show the same trend, even for 3D case.

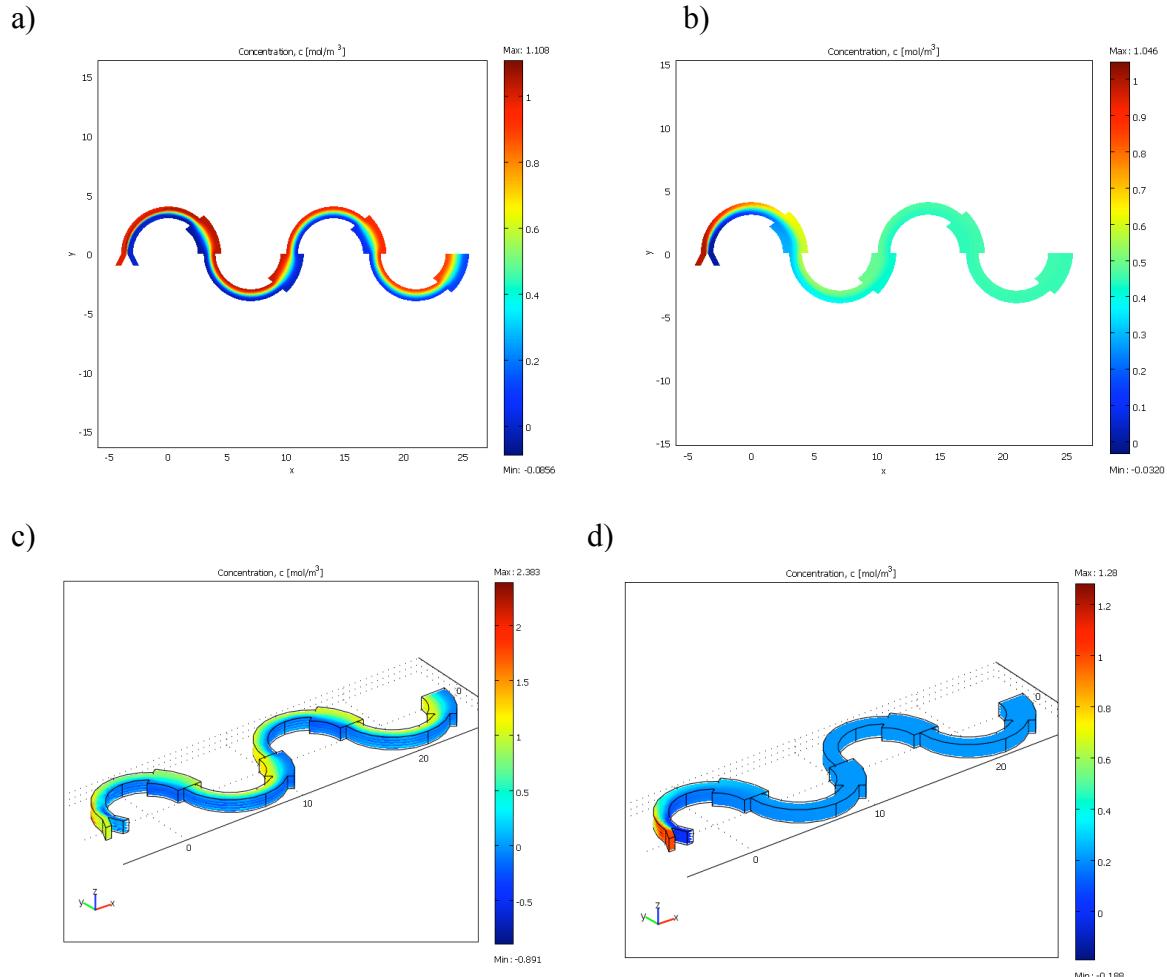


Figure 4: Comparison of concentration mixing at different Re and Pe for 2D and 3D: a) Re = 1, Pe = 1000 b) Re = 100, Pe = 100 c) Re = 1, Pe = 1000 d) Re = 100, Pe = 100
Note: the concentration bar on the side of each graph is different.

The diagrams obtained between the path length and the variances are check by compare to the T-sensor variance diagram from the book. Obtained diagrams have similar trend as the book's diagram.

Conclusion

By performing this research, the better mixing was obtained at higher Reynold's number and higher ratio between the path length and the Peclet number. Expansion channels are useful mixing channel for the higher velocity fluids.

Recommendation

Few recommendations for further research on this geometry are made on the following list.

- Vary the width of the expansions
- Do more fine mesh calculation on for 3D and compare with 2D
- Vary the height for 3D to see the dean vortices' effect

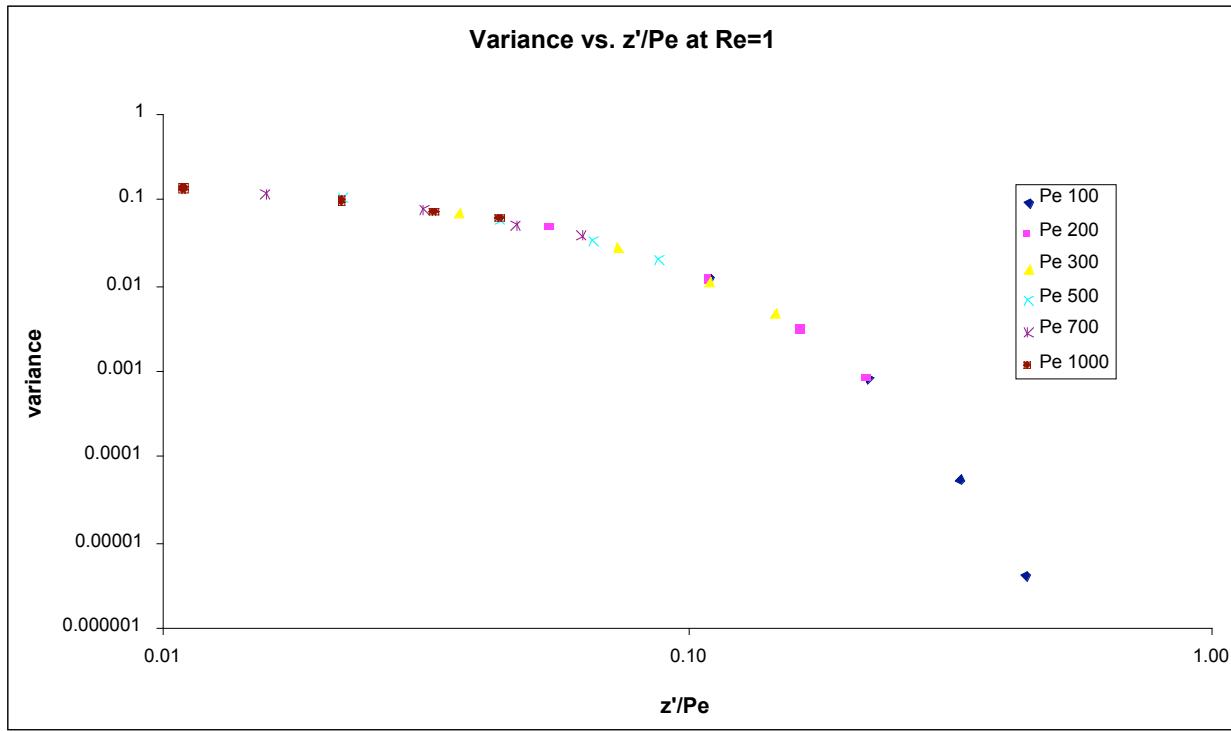
Appendix I

2D: Re = 1

of elements 1720
DEGREES OF FREEDOM 12208

Object	z'	z'/Pe	Expression					
			c*v	c	$(c - c_{mix})^2 * v$	$(c - c_{mix})^2$	v	1
1	11.00	0.11	0.443359	0.460945	0.012238	0.017334	0.957318	1
2	21.99	0.22	0.442748	0.460228	0.000819	0.001151	0.963469	1
3	32.99	0.33	0.440586	0.460163	0.000054	0.000077	0.957158	1
4	43.98	0.44	0.438750	0.917331	0.000004	0.000012	0.953668	1.993763
Pe			<hr/>					
1	11.00	0.05	0.439836	0.457270	0.044897	0.063729	0.957318	1
2	21.99	0.11	0.436707	0.455634	0.011420	0.016148	0.963469	1
3	32.99	0.16	0.436125	0.454819	0.002884	0.004115	0.957158	1
4	43.98	0.22	0.432886	0.905557	0.000802	0.002300	0.953668	1.993763
Pe			<hr/>					
1	11.00	0.04	0.438225	0.457124	0.069238	0.098469	0.957318	1
2	21.99	0.07	0.434338	0.454615	0.027485	0.039173	0.963469	1
3	32.99	0.11	0.434664	0.452810	0.010889	0.015644	0.957158	1
4	43.98	0.15	0.430017	0.900081	0.004716	0.013641	0.953668	1.993763
Pe			<hr/>					
1	11.00	0.02	0.437389	0.459380	0.097771	0.138372	0.957318	1
2	21.99	0.04	0.433194	0.456137	0.055196	0.079588	0.963469	1
3	32.99	0.07	0.434407	0.452529	0.031423	0.045628	0.957158	1
4	43.98	0.09	0.428031	0.897039	0.019493	0.057014	0.953668	1.993763
Pe			<hr/>					
1	11.00	0.02	0.437677	0.461977	0.113285	0.158763	0.957318	1
2	21.99	0.03	0.433474	0.458892	0.074129	0.107578	0.963469	1
3	32.99	0.05	0.435063	0.453942	0.049321	0.072136	0.957158	1
4	43.98	0.06	0.427904	0.898373	0.035770	0.105394	0.953668	1.993763
Pe			<hr/>					
1	11.00	0.01	0.438604	0.465262	0.126477	0.174506	0.957318	1
2	21.99	0.02	0.434417	0.462969	0.092183	0.134327	0.963469	1
3	32.99	0.03	0.436190	0.456663	0.068905	0.101509	0.957158	1
4	43.98	0.04	0.428646	0.902962	0.056281	0.167119	0.953668	1.993763

C _{mixing cup}		C _{variance}	
w/v	w/o v	w/v	w/o v
0.4631	0.4609	0.012784	0.017334
0.4595	0.4602	0.000850	0.001151
0.4603	0.4602	0.000056	0.000077
0.4601	0.4601	0.000004	0.000006
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0.4594	0.4573	0.046899	0.063729
0.4533	0.4556	0.011853	0.016148
0.4556	0.4548	0.003013	0.004115
0.4539	0.4542	0.000841	0.001154
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0.4578	0.4571	0.072325	0.098469
0.4508	0.4546	0.028527	0.039173
0.4541	0.4528	0.011376	0.015644
0.4509	0.4514	0.004945	0.006842
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0.4569	0.4594	0.102130	0.138372
0.4496	0.4561	0.057289	0.079588
0.4539	0.4525	0.032829	0.045628
0.4488	0.4499	0.020440	0.028596
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0.4572	0.4620	0.118336	0.158763
0.4499	0.4589	0.076940	0.107578
0.4545	0.4539	0.051529	0.072136
0.4487	0.4506	0.037508	0.052862
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0.4582	0.4653	0.132116	0.174506
0.4509	0.4630	0.095678	0.134327
0.4557	0.4567	0.071989	0.101509
0.4495	0.4529	0.059015	0.083821

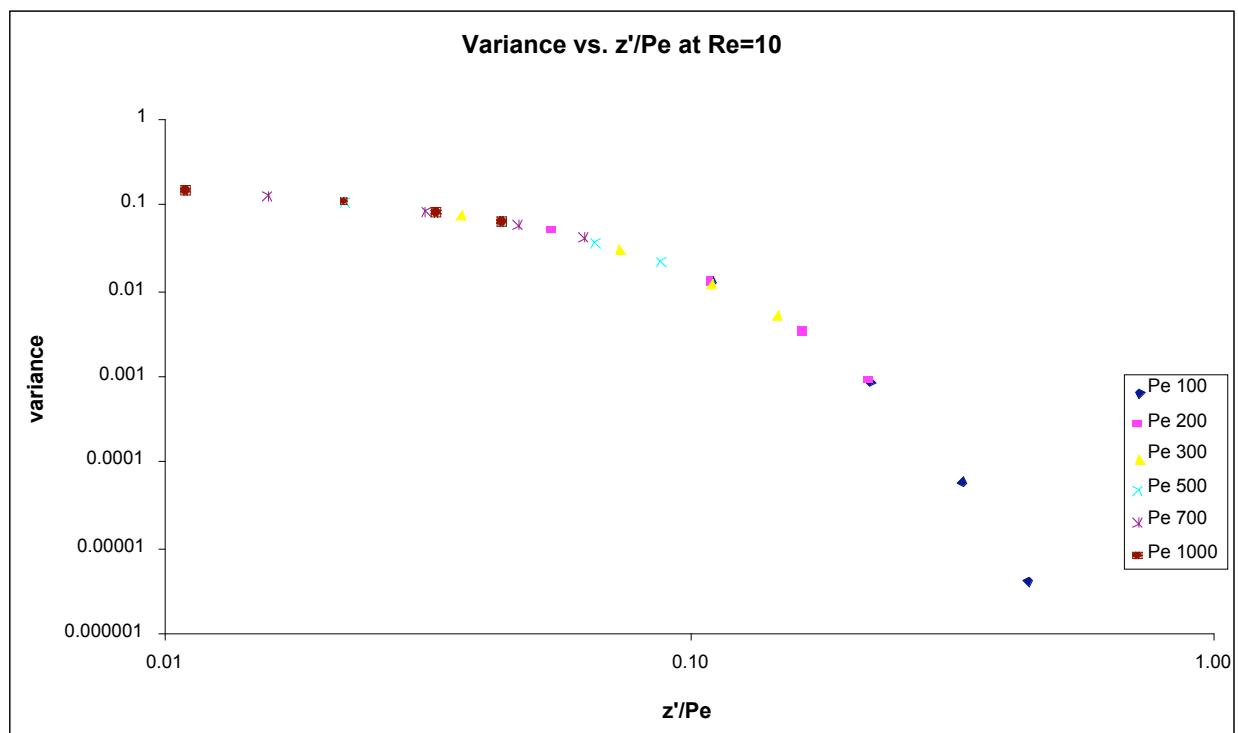


2D: $Re = 10$

of elements 1720
DEGREES OF FREEDOM 12208

Object	z'	z'/Pe	Expression					
			c*v	c	$(c - c_{mix})^2 * v$	$(c - c_{mix})^2$	v	1
1	11.00	0.11	0.48426	0.491404	0.013055	0.017111	0.975974	1
2	21.99	0.22	0.486613	0.498635	0.000886	0.001157	0.978366	1
3	32.99	0.33	0.485066	0.496707	0.000060	0.000078	0.975930	1
4	43.98	0.44	0.497817	0.991417	0.000004	0.000012	1.001389	1.993763
Pe			200					
1	11.00	0.05	0.48296	0.486566	0.048751	0.064004	0.975974	1
2	21.99	0.11	0.48713	0.502204	0.012614	0.016513	0.978366	1
3	32.99	0.16	0.484278	0.494089	0.003240	0.004258	0.975930	1
4	43.98	0.22	0.497959	0.994817	0.000901	0.002426	1.001389	1.993763
Pe			300					
1	11.00	0.04	0.482236	0.484542	0.075493	0.099157	0.975974	1
2	21.99	0.07	0.48757	0.504755	0.030559	0.040190	0.978366	1
3	32.99	0.11	0.483555	0.491542	0.012291	0.016225	0.975930	1
4	43.98	0.15	0.498517	1.000398	0.005322	0.014414	1.001389	1.993763
Pe			500					
1	11.00	0.02	0.481421	0.482839	0.106929	0.139506	0.975974	1
2	21.99	0.04	0.488022	0.507747	0.061816	0.081858	0.978366	1
3	32.99	0.07	0.482559	0.488065	0.035622	0.047377	0.975930	1
4	43.98	0.09	0.499617	1.010274	0.022042	0.060252	1.001389	1.993763
Pe			700					
1	11.00	0.02	0.481004	0.482025	0.124180	0.160317	0.975974	1
2	21.99	0.03	0.488265	0.509489	0.083429	0.110855	0.978366	1
3	32.99	0.05	0.482015	0.486058	0.056098	0.075019	0.975930	1
4	43.98	0.06	0.500462	1.017463	0.040501	0.111501	1.001389	1.993763
Pe			1000					
1	11.00	0.01	0.48071	0.481278	0.139136	0.176880	0.975974	1
2	21.99	0.02	0.488523	0.511112	0.104334	0.138789	0.978366	1
3	32.99	0.03	0.48161	0.484376	0.078735	0.105883	0.975930	1
4	43.98	0.04	0.501367	1.024888	0.063877	0.177301	1.001389	1.993763

$C_{mixing\ cup}$	$C_{variance}$	
	w/v	w/o v
0.4962	0.4914	0.013376
0.4974	0.4986	0.000906
0.4970	0.4967	0.000061
0.4971	0.4973	0.000004
0.4948	0.4866	0.049951
0.4979	0.5022	0.012893
0.4962	0.4941	0.003320
0.4973	0.4990	0.000899
0.4941	0.4845	0.077351
0.4984	0.5048	0.031235
0.4955	0.4915	0.012594
0.4978	0.5018	0.005315
0.4933	0.4828	0.109561
0.4988	0.5077	0.063183
0.4945	0.4881	0.036501
0.4989	0.5067	0.022011
0.4928	0.4820	0.127237
0.4991	0.5095	0.085274
0.4939	0.4861	0.057482
0.4998	0.5103	0.040445
0.4925	0.4813	0.142561
0.4993	0.5111	0.106641
0.4935	0.4844	0.080677
0.5007	0.5140	0.063788

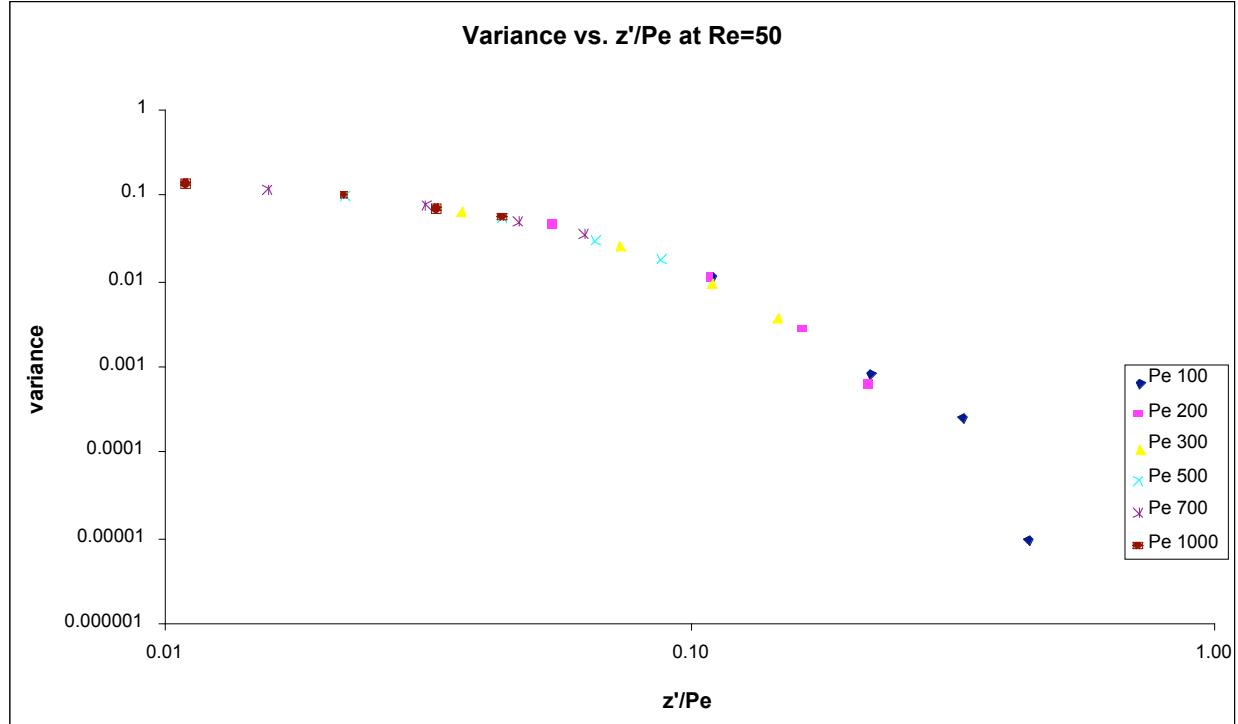


2D: $Re = 50$

of elements 1720
DEGREES OF FREEDOM 12208

Object			Expression						
	z'	z'/Pe	c*v	c	$(c - c_{mix})^2 * v$	$(c - c_{mix})^2$	v	1	
1	11.00	0.11	0.432923	0.448206	0.010788	0.014159	0.944067	1	
2	21.99	0.22	0.446717	0.473617	0.000824	0.001118	0.948257	1	
3	32.99	0.33	0.441886	0.467407	0.000255	0.000262	0.944174	1	
4	43.98	0.44	0.466633	0.935984	0.000010	0.000031	0.995502	1.993763	
	Pe 200								
1	11.00	0.05	0.421352	0.427662	0.041401	0.055010	0.944067	1	
2	21.99	0.11	0.45464	0.488871	0.010050	0.013642	0.948257	1	
3	32.99	0.16	0.437388	0.458723	0.002517	0.003191	0.944174	1	
4	43.98	0.22	0.468808	0.960675	0.000623	0.002088	0.995502	1.993763	
	Pe 300								
1	11.00	0.04	0.416719	0.4199	0.064736	0.086733	0.944067	1	
2	21.99	0.07	0.46278	0.502762	0.024811	0.033252	0.948257	1	
3	32.99	0.11	0.433751	0.450627	0.009264	0.012501	0.944174	1	
4	43.98	0.15	0.474389	1.004505	0.003974	0.012552	0.995502	1.993763	
	Pe 500								
1	11.00	0.02	0.412958	0.414878	0.093187	0.123692	0.944067	1	
2	21.99	0.04	0.473131	0.520759	0.052312	0.070631	0.948257	1	
3	32.99	0.07	0.42809	0.438715	0.028283	0.038384	0.944174	1	
4	43.98	0.09	0.484167	1.084615	0.017821	0.056609	0.995502	1.993763	
	Pe 700								
1	11.00	0.02	0.41151	0.413697	0.109424	0.143695	0.944067	1	
2	21.99	0.03	0.478819	0.531333	0.072318	0.098104	0.948257	1	
3	32.99	0.05	0.424086	0.431109	0.045628	0.062197	0.944174	1	
4	43.98	0.06	0.49083	1.143338	0.034038	0.109351	0.995502	1.993763	
	Pe 1000								
1	11.00	0.01	0.410652	0.413516	0.124062	0.160634	0.944067	1	
2	21.99	0.02	0.483465	0.540631	0.092499	0.125854	0.948257	1	
3	32.99	0.03	0.41992	0.423984	0.065266	0.089365	0.944174	1	
4	43.98	0.04	0.497155	1.203916	0.055451	0.181055	0.995502	1.993763	

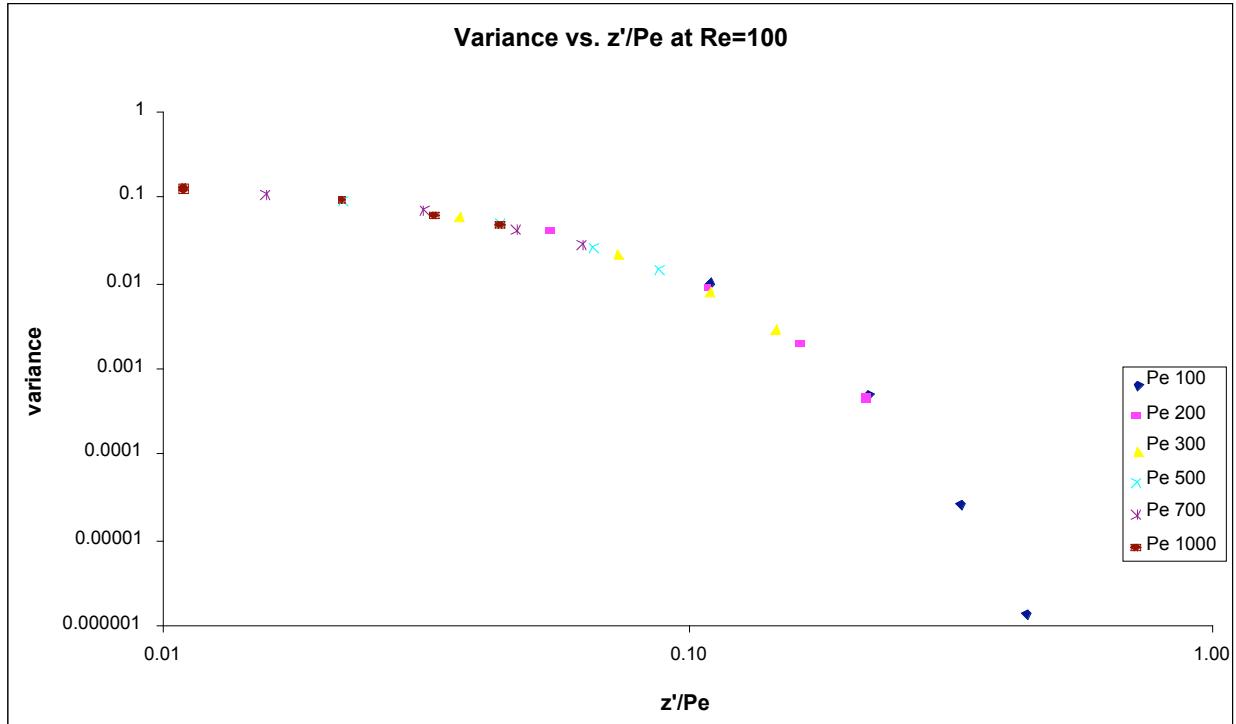
$C_{mixing\ cup}$	$C_{variance}$	
	w/v	w/o v
0.4586	0.4482	0.011427
0.4711	0.4736	0.000869
0.4680	0.4674	0.000270
0.4687	0.4695	0.000010
$C_{mixing\ cup}$	w/v	w/o v
0.4463	0.4277	0.043854
0.4794	0.4889	0.010598
0.4632	0.4587	0.002666
0.4709	0.4818	0.000626
$C_{variance}$	w/v	w/o v
0.4414	0.4199	0.068571
0.4880	0.5028	0.026165
0.4594	0.4506	0.009812
0.4765	0.5038	0.003992
$C_{mixing\ cup}$	w/v	w/o v
0.4374	0.4149	0.098708
0.4989	0.5208	0.055166
0.4534	0.4387	0.029955
0.4864	0.5440	0.017902
$C_{variance}$	w/v	w/o v
0.4359	0.4137	0.115907
0.5049	0.5313	0.076264
0.4492	0.4311	0.048326
0.4930	0.5735	0.034192
$C_{mixing\ cup}$	w/v	w/o v
0.4350	0.4135	0.131412
0.5098	0.5406	0.097546
0.4447	0.4240	0.069125
0.4994	0.6038	0.055702
$C_{variance}$	w/v	w/o v
0.4350	0.4135	0.160634
0.5098	0.5406	0.125854
0.4447	0.4240	0.089365
0.4994	0.6038	0.090811



2D: $Re = 100$

# of elements	1720
DEGREES OF FREEDOM	12208

C _{mixing cup}		C _{variance}	
w/ v	w/o v	w/v	w/o v
0.4352	0.4192	0.010127	0.013310
0.4565	0.4601	0.000529	0.000694
0.4516	0.4508	0.000028	0.000036
0.4527	0.4537	0.000001	0.000003
<hr/>			
0.4147	0.3853	0.040097	0.052276
0.4706	0.4848	0.008838	0.011546
0.4445	0.4379	0.001930	0.002526
0.4563	0.4716	0.000437	0.000796
<hr/>			
0.4062	0.3722	0.063037	0.081628
0.4848	0.5073	0.022816	0.029886
0.4382	0.4251	0.008046	0.010540
0.4648	0.5071	0.002986	0.005861
<hr/>			
0.3991	0.3636	0.090606	0.115568
0.5032	0.5372	0.049611	0.065558
0.4278	0.4053	0.025409	0.033424
0.4799	0.5655	0.014165	0.025471
<hr/>			
0.3964	0.3617	0.106378	0.133775
0.5136	0.5552	0.070056	0.093199
0.4203	0.3922	0.041678	0.055016
0.4902	0.6113	0.027863	0.050730
<hr/>			
0.3947	0.3619	0.120715	0.149235
0.5224	0.5714	0.091564	0.122481
0.4123	0.3796	0.060421	0.080029
0.5000	0.6642	0.046618	0.090127



3D: $Re = 1$

of elements 1720
DEGREES OF FREEDOM 12208

Object	z'	z'/Pe	Expression						1
			c*v	c	$(c - c_{mix})^2 * v$	$(c - c_{mix})^2$	v	1	
1	11.00	0.11	0.344773	0.387300	0.00119300	0.00168200	0.891531	1	
2	21.99	0.22	0.348202	0.387385	0.00004840	0.00006759	0.899174	1	
3	32.99	0.33	0.346677	0.387294	0.00000202	0.00000284	0.895151	1	
4	43.98	0.44	0.369854	0.772149	0.00000009	0.00000023	0.954966	1.993763	
		Pe 200							
1	11.00	0.05	0.349555	0.395211	0.015594	0.021859	0.891531	1	
2	21.99	0.11	0.356174	0.396958	0.003456	0.004804	0.899174	1	
3	32.99	0.16	0.353352	0.395046	0.000780	0.001091	0.895151	1	
4	43.98	0.22	0.377137	0.786026	0.000193	0.000478	0.954966	1.993763	
		Pe 300							
1	11.00	0.04	0.356573	0.406211	0.040657	0.056708	0.891531	1	
2	21.99	0.07	0.366983	0.409782	0.016046	0.022332	0.899174	1	
3	32.99	0.11	0.361087	0.404377	0.006388	0.008940	0.895151	1	
4	43.98	0.15	0.385453	0.799369	0.002797	0.006924	0.954966	1.993763	
		Pe 500							
1	11.00	0.02	0.377010	0.434410	0.090571	0.125572	0.891531	1	
2	21.99	0.04	0.395187	0.443383	0.057263	0.080402	0.899174	1	
3	32.99	0.07	0.382089	0.429306	0.036230	0.051112	0.895151	1	
4	43.98	0.09	0.407990	0.835282	0.025185	0.062716	0.954966	1.993763	
		Pe 700							
1	11.00	0.02	0.395352	0.457574	0.127187	0.176111	0.891531	1	
2	21.99	0.03	0.420930	0.474521	0.098700	0.139862	0.899174	1	
3	32.99	0.05	0.402104	0.452307	0.076574	0.109172	0.895151	1	
4	43.98	0.06	0.430286	0.871730	0.065135	0.162996	0.954966	1.993763	
		Pe 1000							
1	11.00	0.01	0.418635	0.483844	0.172044	0.237948	0.891531	1	
2	21.99	0.02	0.452954	0.512771	0.153664	0.219315	0.899174	1	
3	32.99	0.03	0.427939	0.479098	0.138608	0.200657	0.895151	1	
4	43.98	0.04	0.460499	0.921438	0.136046	0.341607	0.954966	1.993763	

w/v	C _{mixing cup}		C _{variance}	
	w/o v	w/v	w/v	w/o v
0.3867	0.3873	0.001338	0.001682	
0.3872	0.3874	0.000054	0.000068	
0.38728	0.3873	0.000002	0.000003	
0.38730	0.3873	0.0000001	0.0000001	
0.3921	0.3952	0.017491	0.021859	
0.3961	0.3970	0.003844	0.004804	
0.3947	0.3950	0.000871	0.001091	
0.3949	0.3942	0.000202	0.000240	
0.4000	0.4062	0.045604	0.056708	
0.4081	0.4098	0.017845	0.022332	
0.4034	0.4044	0.007136	0.008940	
0.4036	0.4009	0.002929	0.003473	
0.4229	0.4344	0.101590	0.125572	
0.4395	0.4434	0.063684	0.080402	
0.4268	0.4293	0.040474	0.051112	
0.4272	0.4189	0.026373	0.031456	
0.4435	0.4576	0.142661	0.176111	
0.4681	0.4745	0.109767	0.139862	
0.4492	0.4523	0.085543	0.109172	
0.4506	0.4372	0.068207	0.081753	
0.4696	0.4838	0.192976	0.237948	
0.5037	0.5128	0.170895	0.219315	
0.4781	0.4791	0.154843	0.200657	
0.4822	0.4622	0.142462	0.171338	

