Semester Long Internship Report

On

Steady State CFD Method For Residence Time Distribution In Different Tubular Geometries To Evaluate The Mixing

Submitted by

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Acknowledgment

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Introduction

It is very important to have a consistent and rational method to quantify radial mixing to evaluate and compare different tubular flow geometries for their capabilities for mixing under different operating conditions. Mixing is achieved by two physical processes- diffusion and convection. Diffusion plays an important role in mixing at molecular level and short distances. For micromixers where the radial distances are very small, diffusion leads to increased radial mixing for diffusing chemical species (with diffusion coefficient of the order of O(-10) m2/s and radial Peclet number <100) even under the laminar flow condition in straight tube where there is no radial flow. But for non-diffusing chemical species (with diffusion coefficient of O(-15) or less, Radial Pe >>100), convection is the only way for improved radial mixing. Convection in radial direction can be caused by either turbulent flow or by using different methods in laminar flow. In laminar flow, energy consumption is low compared to turbulent flow. So, using laminar flow needs different methods to cause and increase radial mixing. This includes active methods (which use external energy and moving equipment) and passive methods (no external energy or moving equipment). In passive methods, one of the ways to increase radial mixing is to cause radial flows using curvature. Currently our project includes straight tube (STR – Straight Tube Reactor), helical coil (CTR – coiled Tube Reactor) and helical coil with regular bends (CFI – Coiled Flow Inverter). Straight tube does not have any radial flow under laminar flow. So, mixing of non-diffusing chemical species requires radial flow as done in CTR. This is expected to further increase by introducing regular bends in the same coil (CFI).

Now we can easily measure no mixing and complete mixing simply by looking at it. But anything is difficult to measure qualitatively. So, to make this process quantitative, we resort to two methods – RTD calculations and unmixed feed case. In RTD Calculations, normally a step input of uniform concentration of non-diffusing massless tracer is simulated at inlet with fully developed flow at inlet and time of first arrival and variation of tracer concentration at outlet with time is recorded. So, the whole simulation is unsteady state and once steady state of tracer concentration at outlet is reached, simulation is stopped.

This has several disadvantages – it requires many simulations in terms of each time step. They may be very large numbers if the time step size needs to be very small. So, if single simulation file is very large due to complicated and/ or large geometry, then the overall computational resources in terms of computational power, storage and time requirements would be very large. So a new method of measuring RTD is proposed where instead of flat concentration profile, a parabolic concentration profile of massless non-diffusing tracer is injected at inlet in step input manner.

The dimensionless time of first appearance for laminar is = 0.5 and for plug flow is = 1.0. For plug flow, which is indicative of uniform radial mixing, we want this value for any mixer to be as near as 1.0. Instead of transient, a single steady state simulation is required and volume average concentration at outlet needs to be calculated.

Governing Equations and Solver

1) simpleFoam

- Category: Incompressible
- SteadyState
- Laminar/Turbulent

Equations:

The solver employs the SIMPLE algorithm to solve the continuity equation:

$$\nabla \cdot \mathbf{u} = 0$$

And momentum equation:

$$\nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - \nabla \cdot \mathbf{R} = -\nabla p + \mathbf{S}_u$$

Where,

$\mathbf{u}$ = Velocity

p = Kinematic pressure

$\mathbf{R}$ = Stress tensor

$\mathbf{S}_u$ = Momentum source

Input requirements:
Mandatory fields:

- P: kinematic pressure [m2/s2]
- U: velocity [m/s]

2) scalarTransportFoam

- Category: Basic
- SteadyState/Transient
- Incompressible

Equations:

Evolves a transport equation for the scalar

$$\frac{\partial}{\partial t}(T) + \nabla \cdot (\mathbf{u}T) - \nabla \cdot (D_T \nabla T) = S_T$$

Input requirements:
Mandatory fields:

- U: velocity[m/s]
- T: scalar[-]

TransportProperties:

- DT: Diffusion coefficient[m2/s]

Simulation Procedure

Consider a pipe of diameter 1 mm with a length of 1.252 m. There are 3 geometries made using this pipe which are STR, CTR and CFI respectively. We have to perform both steady and unsteady state flow simulations by using these geometries. Below a table is given where the Renolds number is given with respect to geometry.

Table 1 [Types of geometries and flow details]

Geometry	Flow	Re no.
STR	Laminar	0.06
		10
		1000
	Turbulent	10000
	Plug	10000
CTR	Laminar	0.06
		10
		1000
CFI	Laminar	0.06
		10
		1000

The simulation procedure involved the following key steps:

(i) Geometry and Mesh Setup: The geometries of STR, CTR, and CFI were defined, and appropriate meshes were created to represent the flow fields accurately.

(ii) Boundary Conditions: Inlet and outlet boundary conditions were specified for each geometry, with the Reynolds number being a critical parameter.

(iii) Flow Regime Selection: Flow regimes were determined based on the provided Reynolds numbers, distinguishing between laminar and turbulent flow conditions.

(iv) Steady-State and Unsteady-State Simulations: Both steady-state and unsteady-state simulations were conducted for each geometry to examine flow characteristics, mixing, and radial flow.

(v) Data Collection and Analysis: Key parameters were monitored and recorded during simulations. Unsteady-state data were analysed to understand transient behaviour and the evolution of flow over time.

(vi) Comparison and Evaluation: The results obtained from different geometries were compared to assess the effectiveness of each geometry in achieving radial mixing.

Geometry and Mesh

Tabel 2 [Details of Geometries]

Reactor Type	Length(m)	Curvature Ratio	No. of Turns	Pitch (m)	Number of bends
STR	1.252	-	-	-	0
CTR	1.262	5	40	0.003	0
CFI	1.285	5	40	0.003	9

Curvature ratio is the ratio between radius of coil and inner radius of tube.

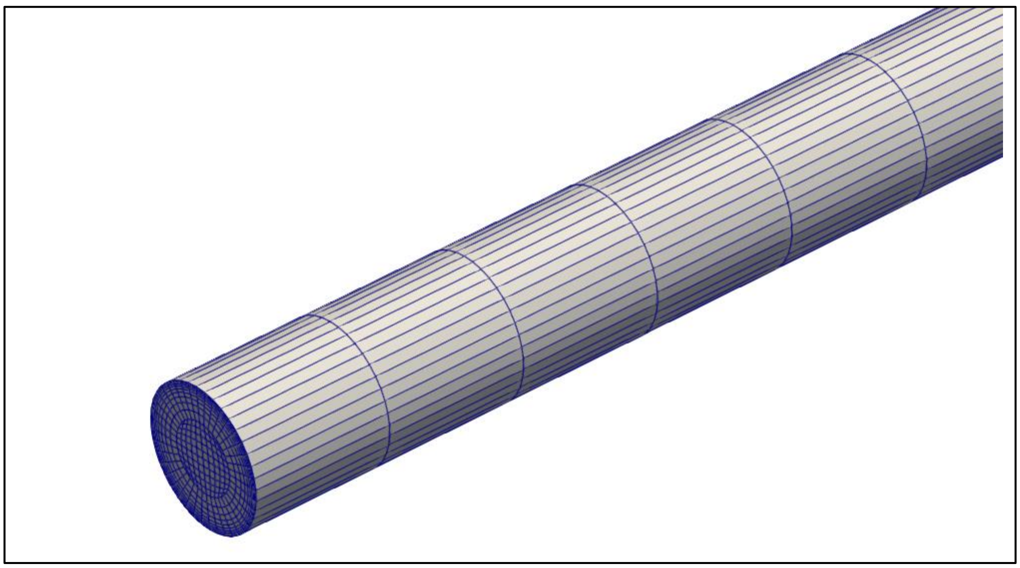


Figure 1 [STR]

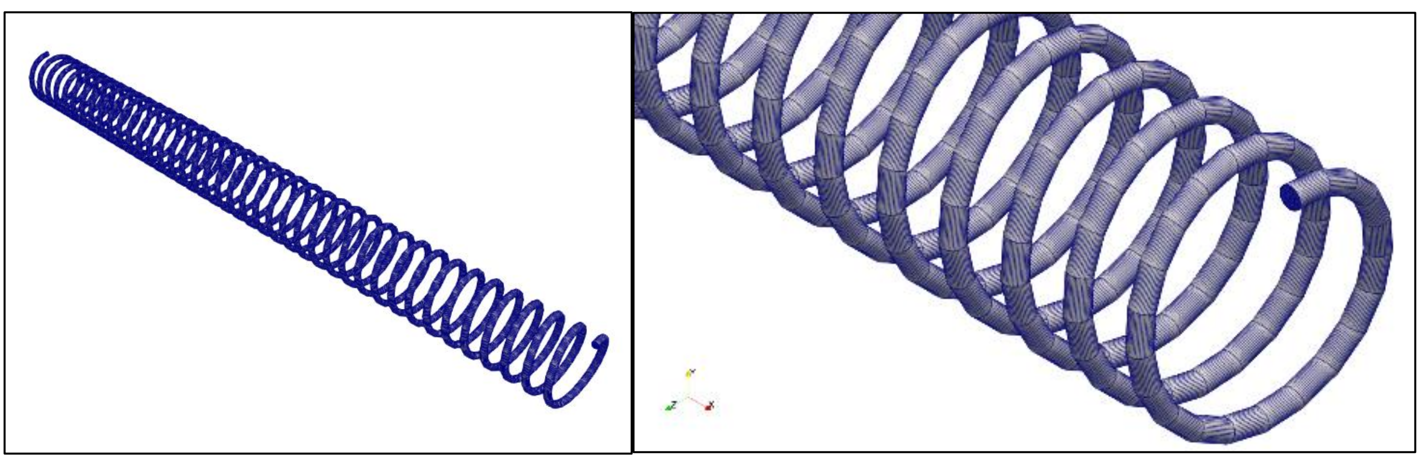


Figure 2 [CTR]

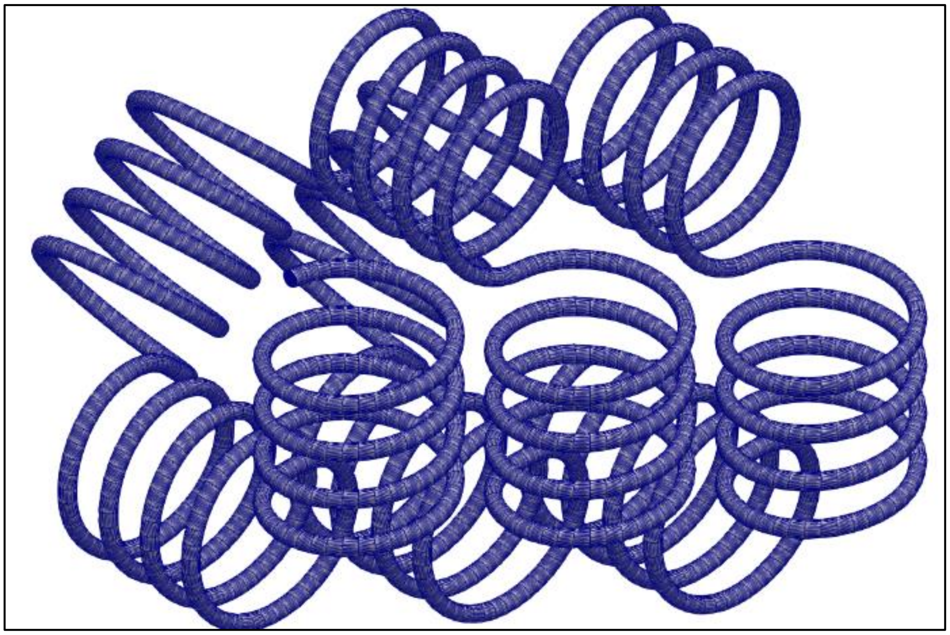


Figure 3 [CFI]

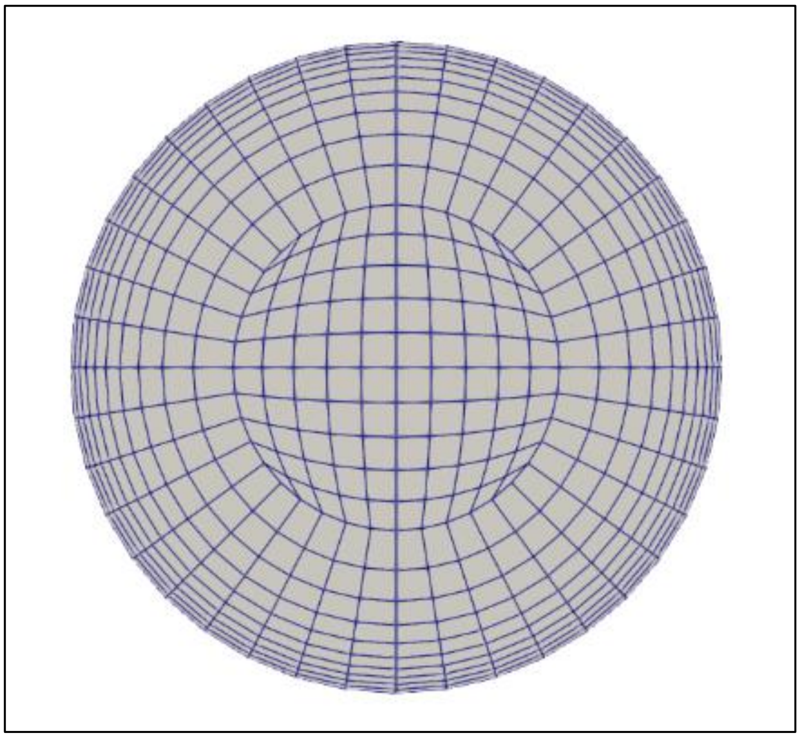


Figure 4 [O-grid Meshing]

Formulation

To calculate Cavg/Cmax in a pipe we can integrate as follows,

(i) For Laminar flow conditions -

$$\boldsymbol{C_{avg} = \frac{\int_0^R 2\pi r \cdot U_{(r)} \cdot C_{(r)}\, dr}{\frac{\pi R^2}{2} U_{max}}}$$

$$\boldsymbol{C_{avg} = \frac{\int_0^R 2\pi r \cdot \left[U_{max}\left(1 - \left(\frac{r}{R}\right)^2\right)\right] \cdot \left[C_{max}\left(1 - \left(\frac{r}{R}\right)^2\right)\right] dr}{\frac{\pi R^2}{2} U_{max}}}$$

$$\boldsymbol{C_{avg} = \frac{2}{3} C_{max}}$$

(ii) For Plug flow condition -

$$\boldsymbol{C_{avg} = \frac{\int_0^R 2\pi r \cdot U_{(r)} \cdot C_{(r)}\, dr}{\pi R^2 U_{avg}}}$$

$$\boldsymbol{C_{avg} = \frac{\int_0^R 2\pi r \cdot U \cdot \left[C_{max}\left(1 - \left(\frac{r}{R}\right)^2\right)\right] dr}{\frac{\pi R^2}{2} U}}$$

$$\boldsymbol{C_{avg} = \frac{1}{2} C_{max}}$$

For laminar flow, theoretical value of C_avg/C_max = 0.667, and for plug flow with flat velocity profile, it is = 0.5. So, for plug flow, this ratio should be as near to 0.5 as possible for any mixer. So this way we can easily evaluate and compare the state of radial mixing in the above mentioned three geometries for non-diffusing massless tracer.

In steady state flow simulations, to keep the variation of concentration profile intact we used parabolic velocity profile as inlet boundary conditions. For parabolic velocity profile code can be written as follows.

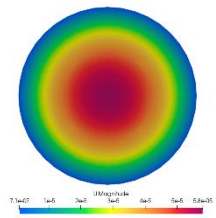
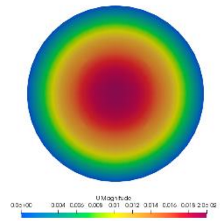
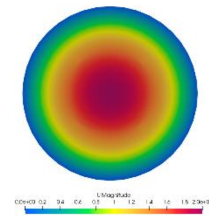
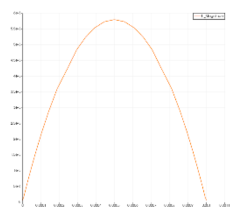
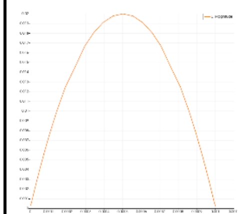
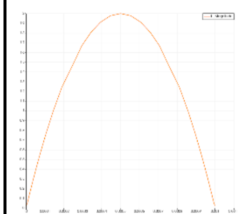
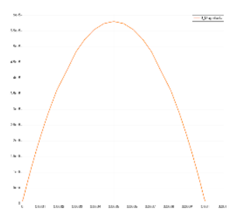
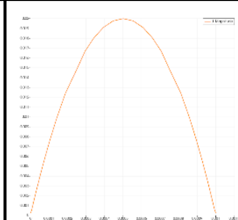
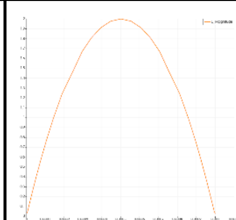
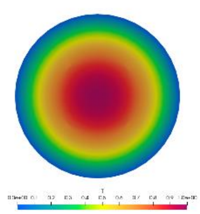
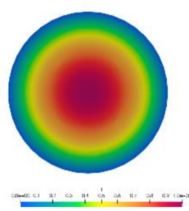
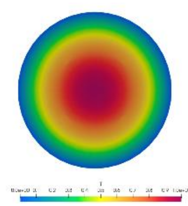
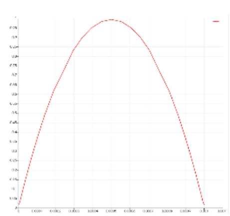
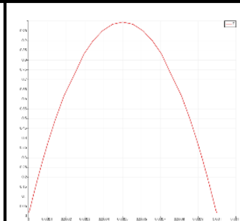
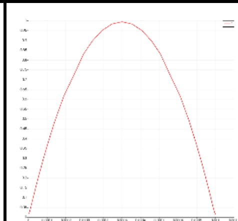
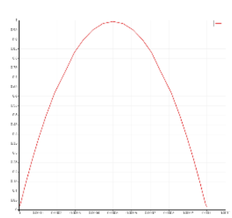
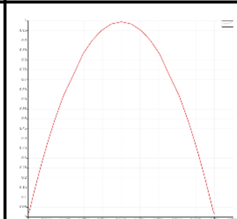
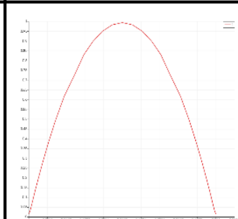
```
inlet
{
        type    codedFixedValue;
        value   $internalField;
        name    parabolicVelocity;
        code
        #{
                const vectorField& Cf = patch().Cf();
                vectorField& field = *this;
                const scalar c = 0;
                const scalar r = 0.0005;
                const scalar Umax = 0.000058;
                forAll(Cf, faceI)
                {
                        const scalar x = Cf[faceI][0];
                        const scalar y = Cf[faceI][1];
                        field[faceI] = vector(0, 0, Umax*(1-((pow((y-c)/r,2))+(pow((x-c)/r,2)))));
                }
        #};
}
```

Figure 5 [Code for parabolic velocity profile]

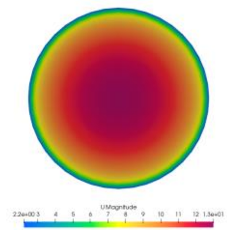
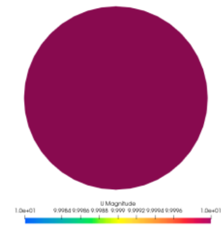
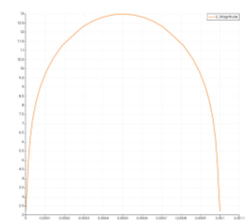
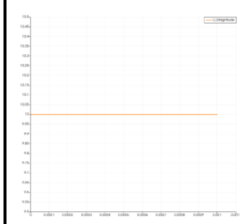
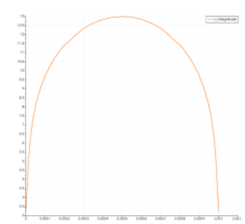
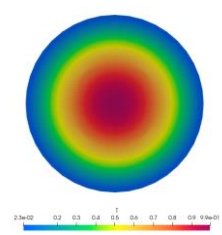
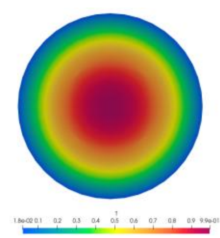
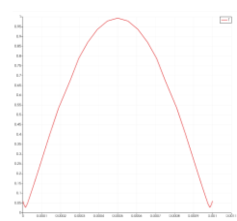
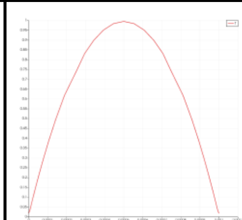
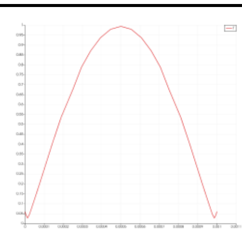
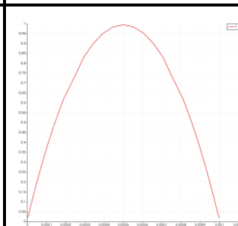
Results

Steady-State Simulations:

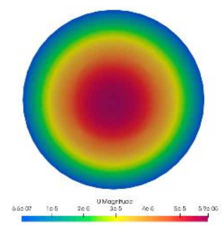
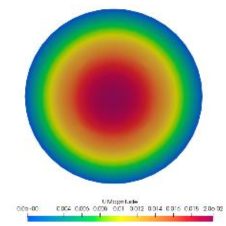
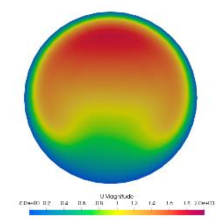
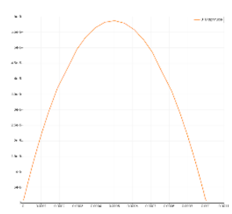
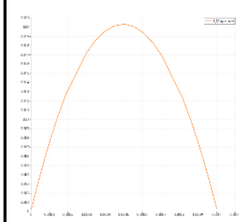
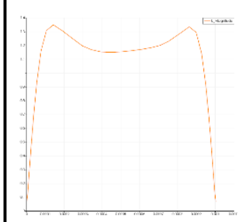
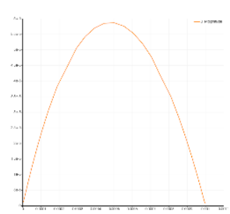
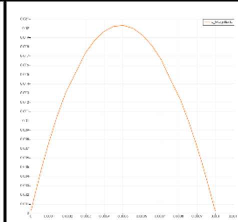
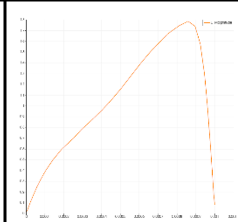
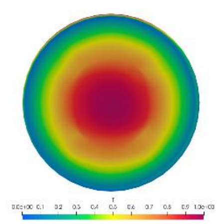
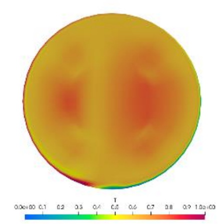
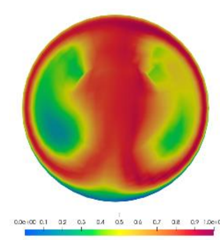
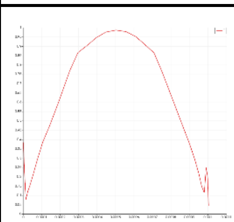
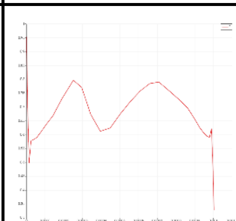
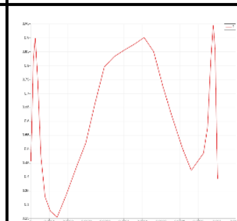
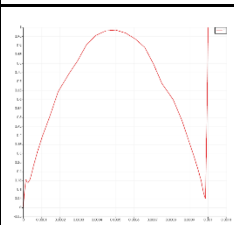
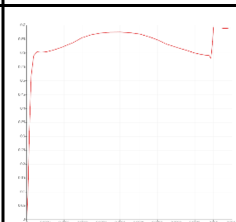
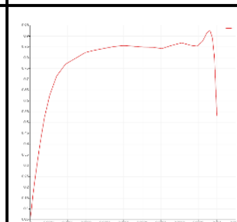
Tabel 3 [Results of STR geometry with laminar flows]

STR	orientation	Re 0.06	Re 10	Re 1000
U	XY plane			
	X-axis			
	Y-axis			
C	XY plane			
	X-axis			
	Y-axis			

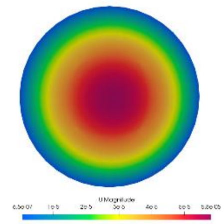
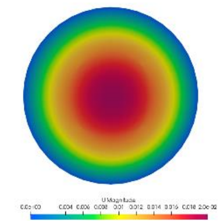
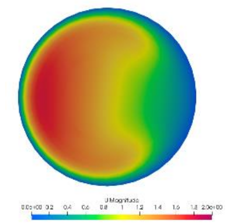
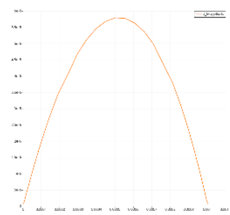
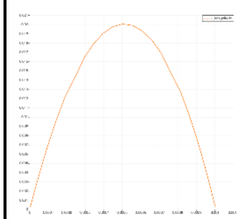
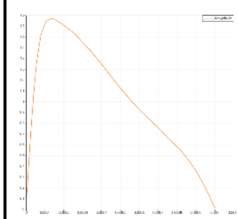
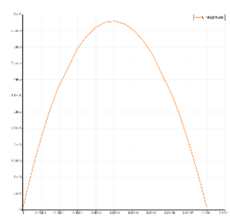
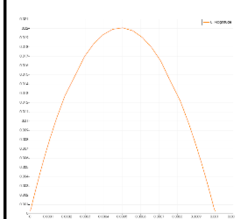
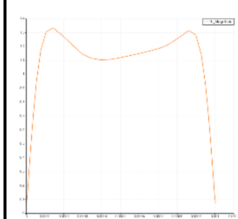
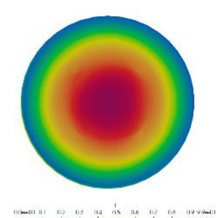
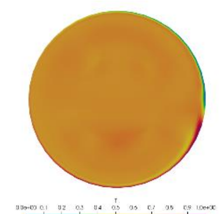
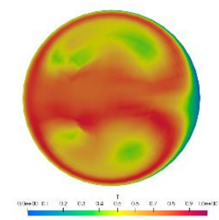
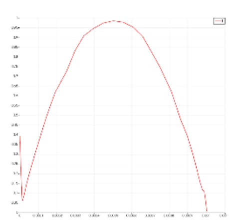
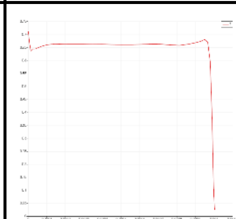
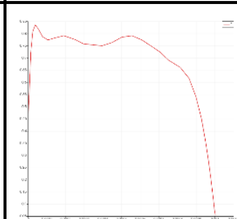
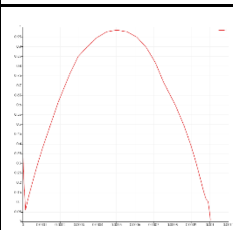
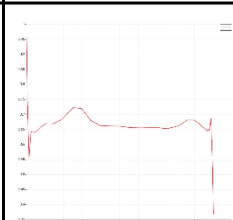
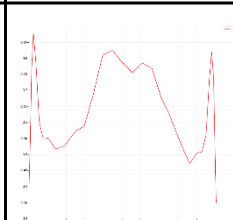
Tabel 4 [Results of STR geometry with turbulent and plug flow]

STR	orientation	Re 10000(Turbulent)	Re 10000(Plug)
U	XY plane		
	X-axis		
	Y-axis		
C	XY plane		
	X-axis		
	Y-axis		

Tabel 5 [Results of CFR geometry]

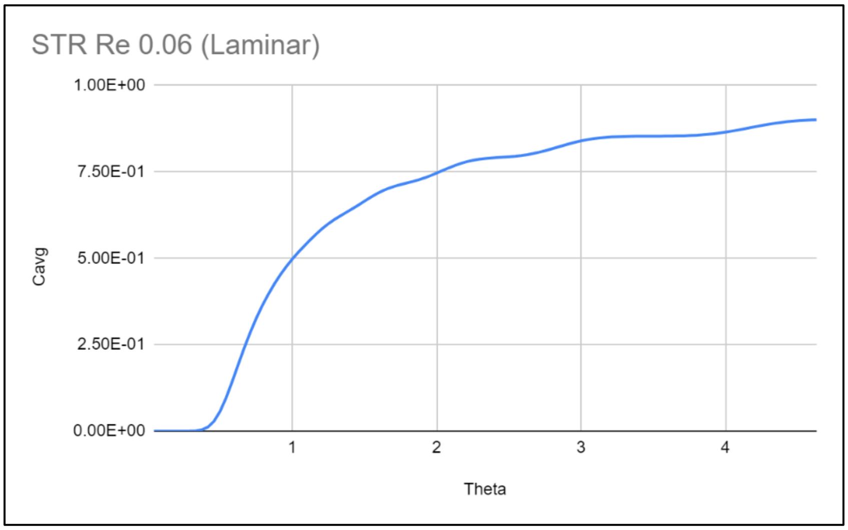
CFR	orientation	Re 0.06	Re 10	Re 1000
U	XY plane			
	X-axis			
	Y-axis			
C	XY plane			
	X-axis			
	Y-axis			

Tabel 6 [Results of CFI geometry]

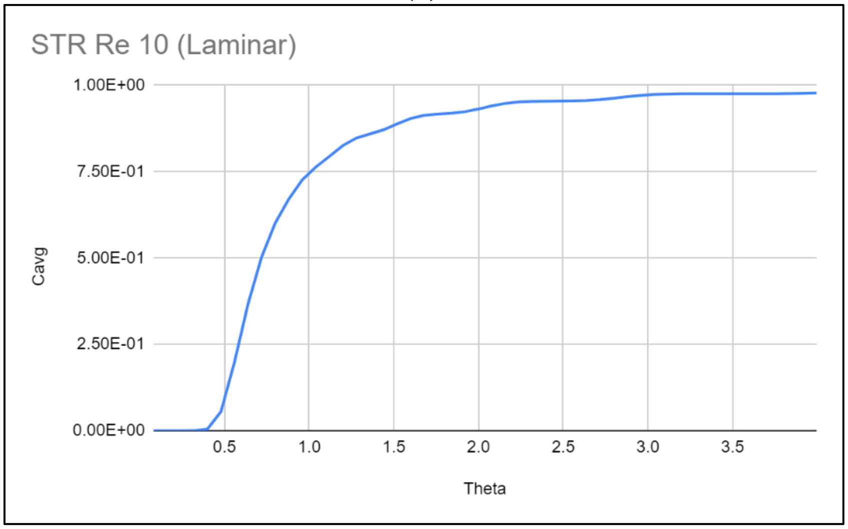
CFIR	orientation	Re 0.06	Re 10	Re 1000
U	XY plane			
	X-axis			
	Y-axis			
C				
	X-axis			
	Y-axis			

Unsteady-State Simulations:

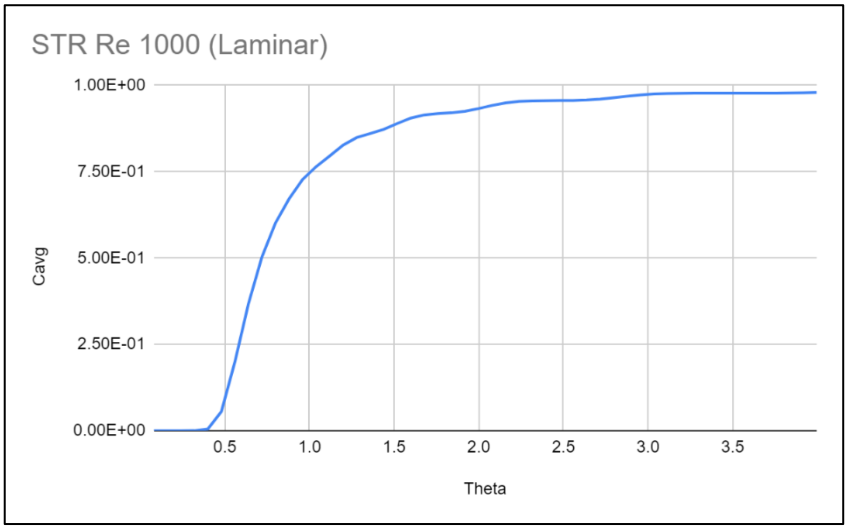
(i) STR:



(a)

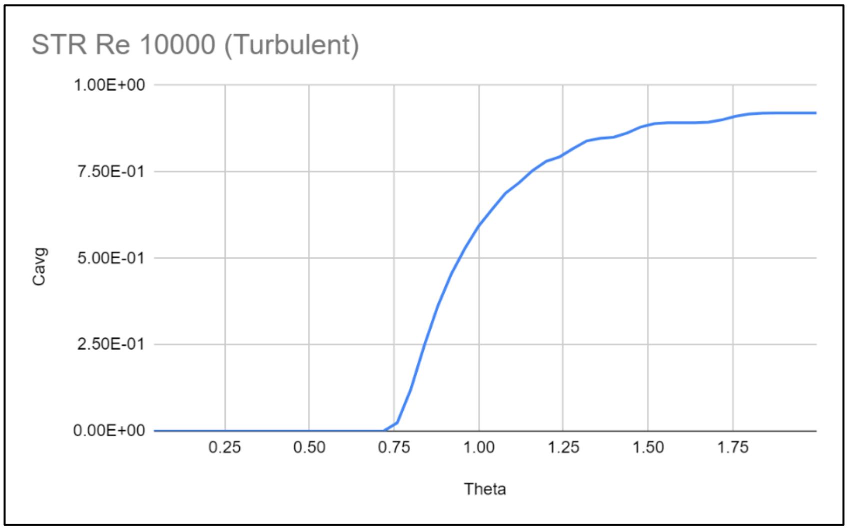


(b)

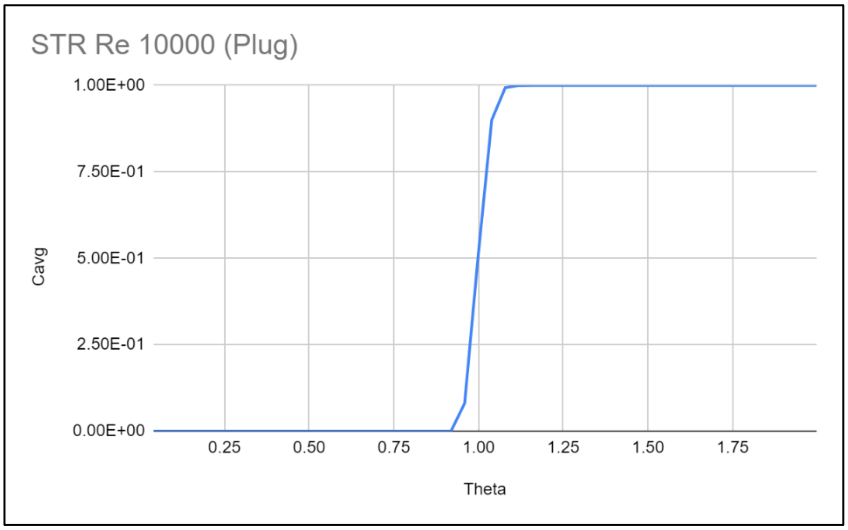


(c)

Figure 6 [Cavg Vs. Theta for STR with laminar flows]



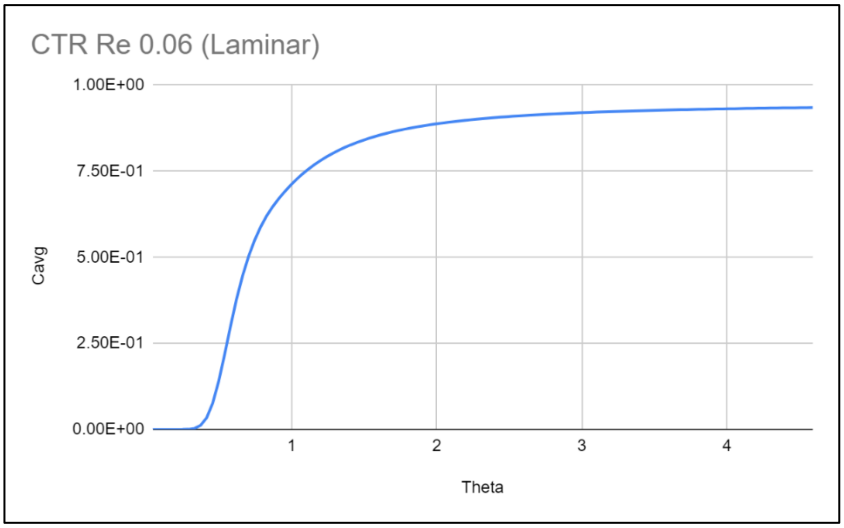
(a)



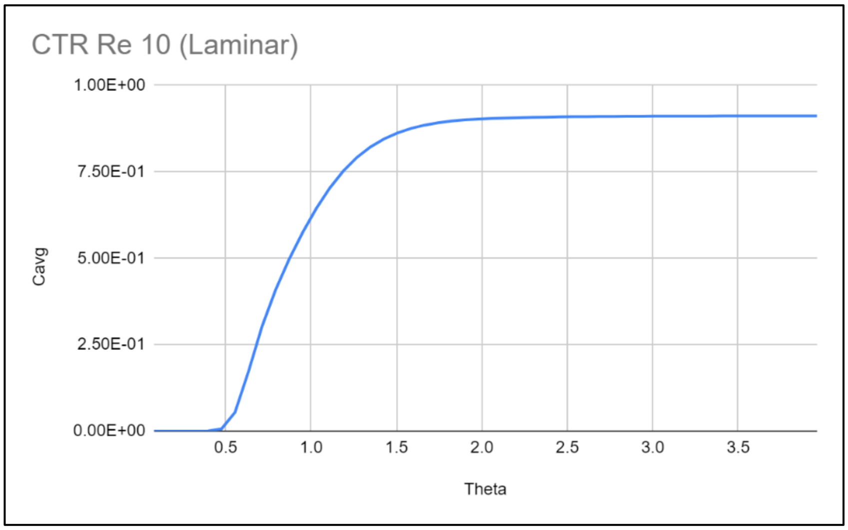
(b)

Figure 7 [Cavg Vs. Theta for STR with turbulent and plug flow]

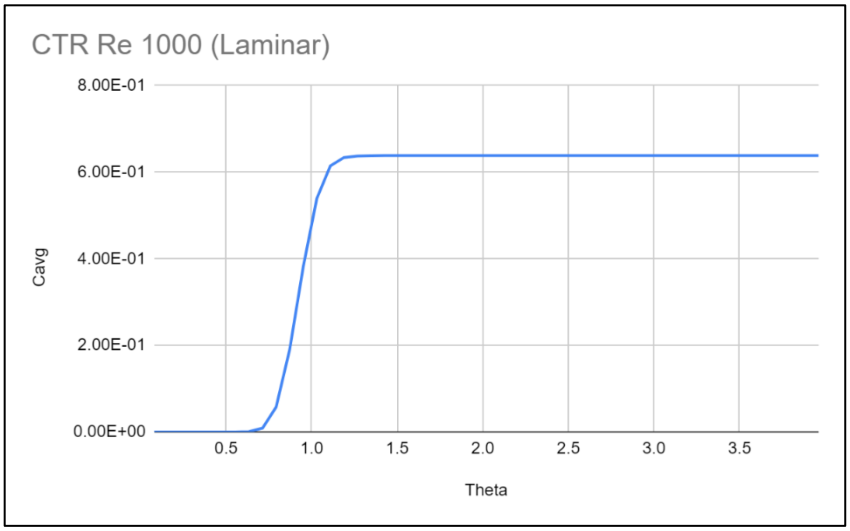
(ii) CTR:



(a)



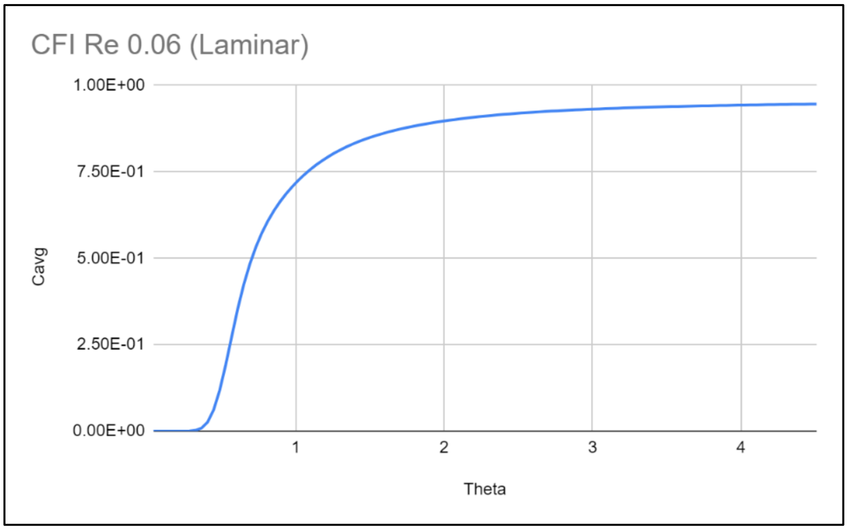
(b)



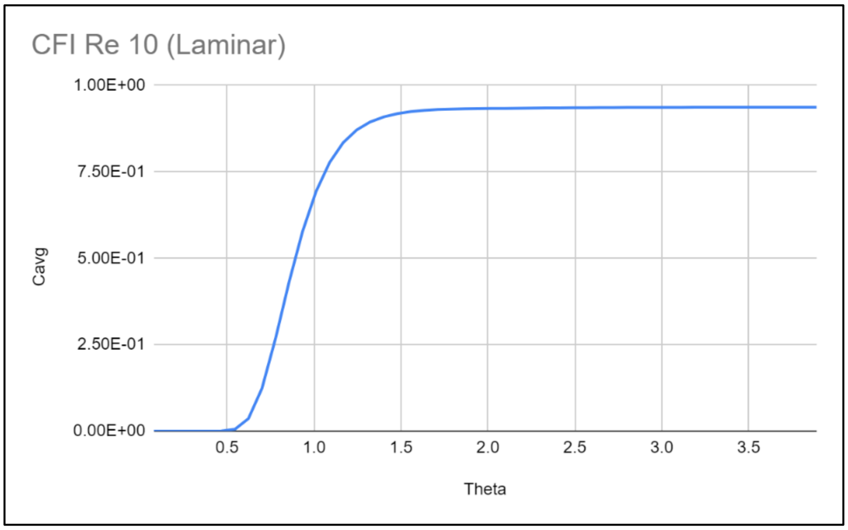
(c)

Figure 8 [Cavg Vs. Theta for CTR with laminar flows]

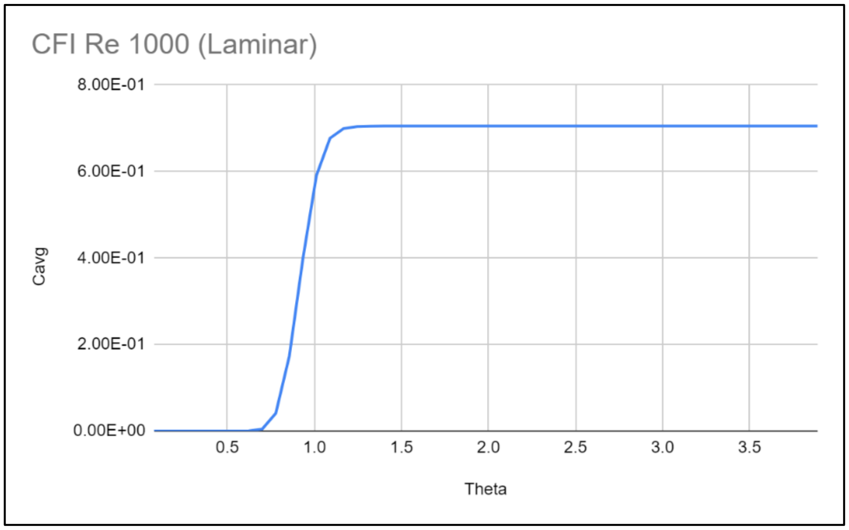
(iii) CFI:



(a)



(b)



(c)

Figure 9 [Cavg Vs. Theta for CFI with laminar flows]

Tabel 7 [C/Cmax and theta for all cases]

Geometry	Flow	Re no.	c/cmax	theta
STR	Laminar	0.06	0.6702	0.5006
		10	0.6702	0.5595
		1000	0.6701	0.5594
	Turbulent	10000	0.5071	0.8
	Plug	10000	0.5066	1
CTR	Laminar	0.06	0.6658	0.5377
		10	0.6651	0.5547
		1000	0.6391	0.5547
CFI	Laminar	0.06	0.6745	0.5281
		10	0.6648	0.5447
		1000	0.6579	0.5447

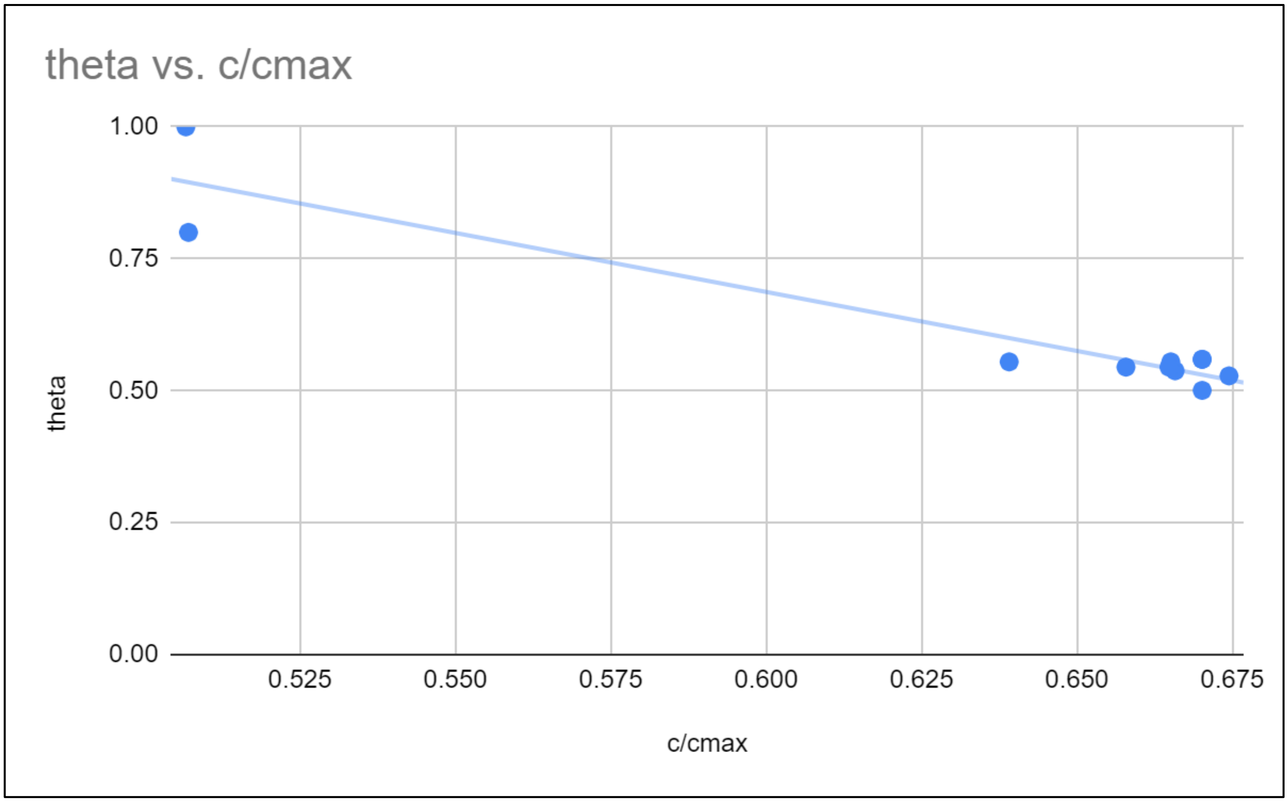


Figure 10 [Theta Vs. C/Cmax plot with all cases]

Correlation study focused on the relationship between R2 and theta, with the following key findings:

- A strong correlation (R2 = 0.893) was established between R2 and theta.
- The correlation between theta and C/Cmax was determined as follows:
  - $\theta = 2.5 - 3 * (C/Cmax)$ at C/Cmax = 0.5, and $\theta = 1$
  - $\theta = 2/3$ at C/Cmax = 0.5
- Suggestions for Improvement:
  - Reducing the time steps in transient simulations to gather finer-grained data.
  - Obtaining more data points near critical values of θ, such as θ = 1 (C/Cmax = 0.5) and θ = 2/3, to refine the correlation model.

Conclusion

In conclusion, this report has outlined a comprehensive simulation procedure involving different pipe geometries and the development of a correlation model between R2 and theta. The correlation study indicates a strong relationship, while further improvements are suggested for increased accuracy. The results of this study are valuable for understanding fluid flow, mixing, and radial flow characteristics in various pipe geometries.

To further advance this research, the following recommendations are made:

- Implement the suggested improvements in data collection to refine the correlation model.
- Explore additional flow conditions and geometries to expand the applicability of the correlation.
- Continue investigating the impact of geometry on flow characteristics and mixing.

Summary

This report comprehensively covers a study on fluid flow and mixing in different pipe geometries. It includes a simulation procedure and a correlation study to understand the behavior of flow in Straight Tube Reactor (STR), Coiled Tube Reactor (CTR), and Coiled Flow Inverter (CFI) under various flow conditions.

According to the results we received CTR geometry performed very good mixing considering the laminar flow with Re 1000. Although both the CTR and CFI geometry are equally good for mixing under laminar flows. If we consider the STR geometry in laminar flows there were no significant improvements because of its construction.

References

Garg, D. K., Serra, C. A., Hoarau, Y., Parida, D., Bouquey, M., & Muller, R. (2020, June 2). Numerical Investigations of Different Tubular Microreactor Geometries for the Synthesis of Polymers under Unmixed Feed Condition. *Macromolecular Theory and Simulations*, *29*(4). https://doi.org/10.1002/mats.202000008

Garg, D. K., Serra, C. A., Hoarau, Y., Parida, D., Bouquey, M., & Muller, R. (2020, August 9). Numerical Investigations of Perfectly Mixed Condition at the Inlet of Free Radical Polymerization Tubular Microreactors of Different Geometries. *Macromolecular Theory and Simulations*, *29*(6). https://doi.org/10.1002/mats.202000030