

# **To observe the effect of hydrodynamic flow and mixing during heating and cooling on heat transfer coefficient in a Straight Tube, Coiled Flow and Coiled Flow Inverter micromixer using OpenFOAM**

**Harish Jayaraj P**

Bachelor's Student, Rajalakshmi Engineering College

## **Abstract**

The objective of this project is to calculate and compare the Heat Transfer Coefficient (HTC) for various tubular flow microreactor geometries, i.e. straight tube reactor (STR), coiled tube reactor (CTR), coiled flow inverter reactor (CFIR). The study is done at different Reynolds numbers of 0.1, 10, 1000 for both heating and cooling conditions with a temperature difference of 5 and 20 K between the wall and the fluid at the inlet. *buoyantSimpleFoam* is used for the laminar simulation. Geometry is created using SolidWorks and the mesh is generated using the ANSYS Meshing module. After the simulation, it is observed that for a given geometry, HTC values remain the same for both heating and cooling for both temperature differences. The HTC values are found to be a function of Re and increase with Re, the HTC values are found to be in the following order:  $CTR > CFIR > STR$ .

## **References**

1. Garg, Dhiraj K., et al. "Numerical investigations of perfectly mixed conditions at the inlet of free radical polymerization tubular microreactors of different geometries." *Macromolecular Theory and Simulations* 29.6 (2020): 2000030.

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## **Abstract**

The objective of this project is to calculate and compare the Heat Transfer Coefficient (HTC) for various tubular flow microreactor geometries, i.e. straight tube reactor (STR), coiled tube reactor (CTR), coiled flow inverter reactor (CFIR). The study is done at different Reynolds numbers of 0.1, 10, 1000 for both heating and cooling conditions with a temperature difference of 5 and 20 K between the wall and the fluid at the inlet. *buoyantSimpleFoam* is used for the laminar simulation. Geometry is created using SolidWorks and the mesh is generated using the ANSYS Meshing module. After the simulation, it is observed that for a given geometry, HTC values remain the same for both heating and cooling for both temperature differences. The HTC values are found to be a function of Re and increase with Re, the HTC values are found to be in the following order: CTR > CFIR > STR.

## 1. Introduction

The case study aims to simulate a hydrodynamic flow of water at various Reynolds numbers ( $Re$  0.1, 10 and 1000) through 3 different geometries namely Straight Tube Reactor (STR), Coiled Tube Reactor (CTR) and Coiled Flow Inverter Reactor (CFIR) with a temperature difference of 5 and 20 K between walls and the fluid for both heating and cooling. The purpose of the simulation is to calculate the Heat Transfer Coefficient (HTC) for all the geometries at various Reynolds Numbers and temperature differences. SolidWorks was used to prepare the geometry and ANSYS was used for meshing which was later imported into *polyMesh* directory in an OpenFOAM readable format using *fluent3DMeshToFoam* command. *buoyantSimpleFoam* was used for simulations and it was post-processed using *paraView* to obtain contour plots and graphs.

## 2. Problem Statement

To observe the effect of hydrodynamic flow and mixing during heating and cooling on heat transfer coefficient in a Straight Tube, Coiled Flow and Coiled Flow Inverter micromixer using OpenFOAM. The purpose of this study is to conduct steady-state numerical simulations of hydrodynamic flow and heat transfer within three different reactor geometries: Straight Tube Reactor (STR), Coiled Tube Reactor (CTR), and Coiled Flow Inverter Reactor (CFIR). The study aims to investigate the effects of varying Reynolds numbers and temperature differences on the Heat Transfer Coefficient (HTC) for each geometry. This could help in selecting the right geometry and right Reynolds number for maximum Heat Transfer Coefficient. The geometric details are given in Table 1.

Reactor type	Length [m]	Curvature ratio <sup>a)</sup>	No. of turns	Pitch [m]	Number of bends
STR	1.252	–	–	–	0
CTR	1.262	5	40	0.003	0
CFIR	1.285	5	40	0.003	9

*Table 1: Geometric Parameters of the Geometries*

### 3. Governing Equations

buoyantSimpleFoam is a steady-state solver and thus uses the SIMPLE algorithm as the name suggests. SIMPLE (Semi Implicit Method for Pressure Linked Equations) is a method used for solving steady state simulations. The Equations are given as follows:

Momentum Equation:

$$\frac{\partial}{\partial t}(u) + \nabla \cdot (u \times u) = -\nabla p \quad (1)$$

Continuity Equation:

$$\nabla \cdot u = 0 \quad (2)$$

Discretization of the continuity equation gives the constraint:

$$\nabla \cdot \phi = 0 \quad (3)$$

The velocity correction equation is given by:

$$u = \frac{H}{A} - \frac{1}{A} \nabla p \quad (4)$$

The pressure equation is given by:

$$\nabla \cdot \left[ \left( \frac{1}{A} \right)_f \nabla p \right] = \nabla \cdot \left( \frac{H}{A} \right)_f \quad (5)$$

Due to hydrostatic effects, a modified  $p$  is used in the momentum equation for calculation.

The modified  $p$  accounts for the hydrostatic pressure effects, hence it can be represented as:

$$p' = p - \rho(g \cdot h) \quad (6)$$

In this simulation *rhoconst* method is used for density variations where the density is kept constant. Hence the momentum equation is modified as:

$$\frac{\partial}{\partial t}(\rho u) + \nabla \cdot (\rho u \times u) - \nabla \cdot (\mu_{eff} \nabla u) = -\nabla p' \quad (7)$$

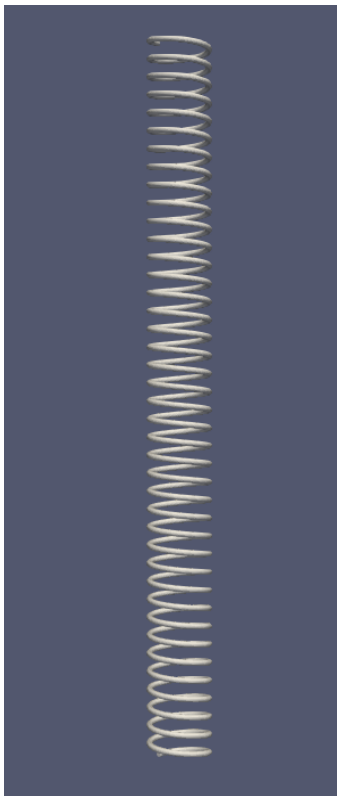
The RAS Laminar model was used in this simulation. This is mathematically given as:

$$\frac{\partial}{\partial t}(\rho) + \nabla \cdot (\rho \bar{u}) = 0 \quad (8)$$

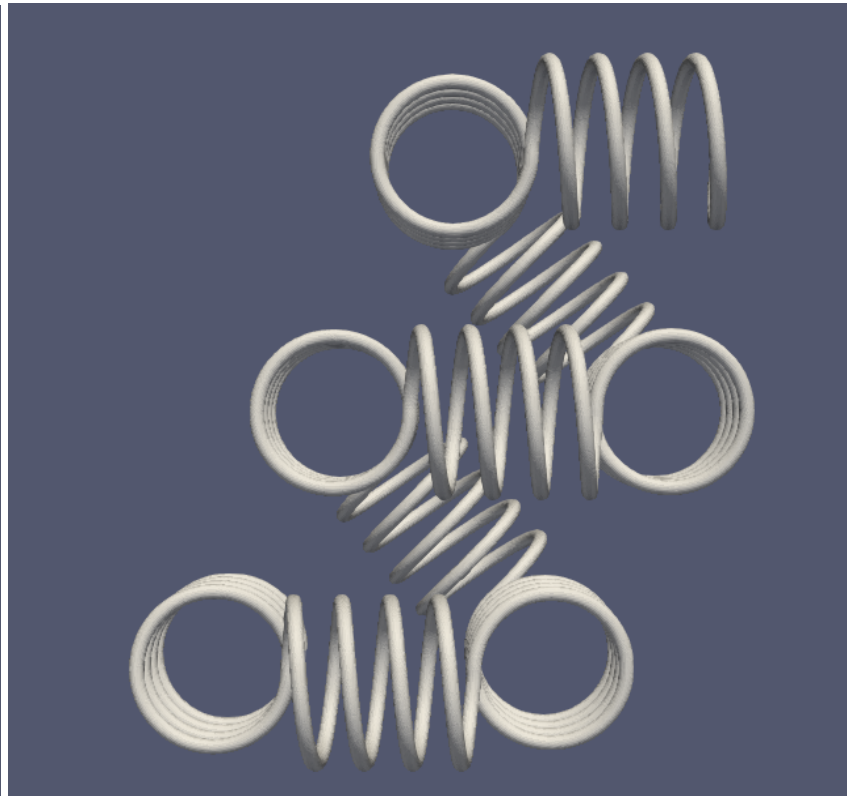
## 4. Simulation Procedure

### 4.1 Geometry and Mesh

The geometry was prepared using SolidWorks. For STR and CTR (Fig1), an O-grid was generated since an unstructured mesh was not accurate in the solution. Hence a multibody geometry was prepared with a square of 0.3mm and a diameter of 1mm. For CFIR (Fig.2), an unstructured mesh was generated since the geometry was complicated for structured mesh and also since the no. of cells were too high for a quality mesh than for the unstructured mesh. All the geometries have only 3 patches: Inlet, outlet and walls (all surfaces other than the inlet and outlet face).



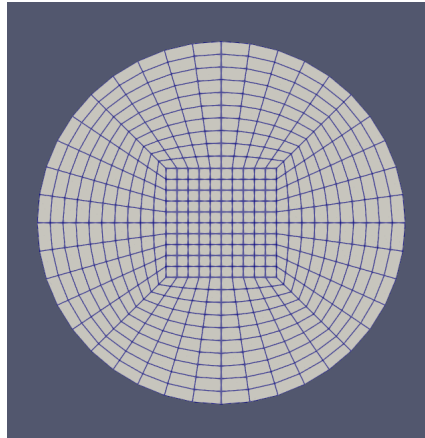
CTR  
(fig 1.)



CFIR  
(fig 2.)

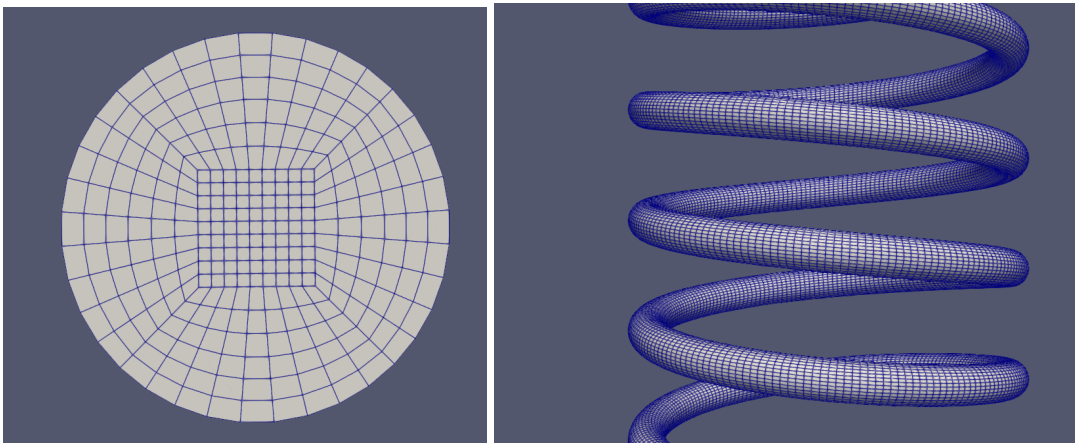
The cross section mesh can be seen in the below figure

Straight Tube Reactor (Structured Mesh):



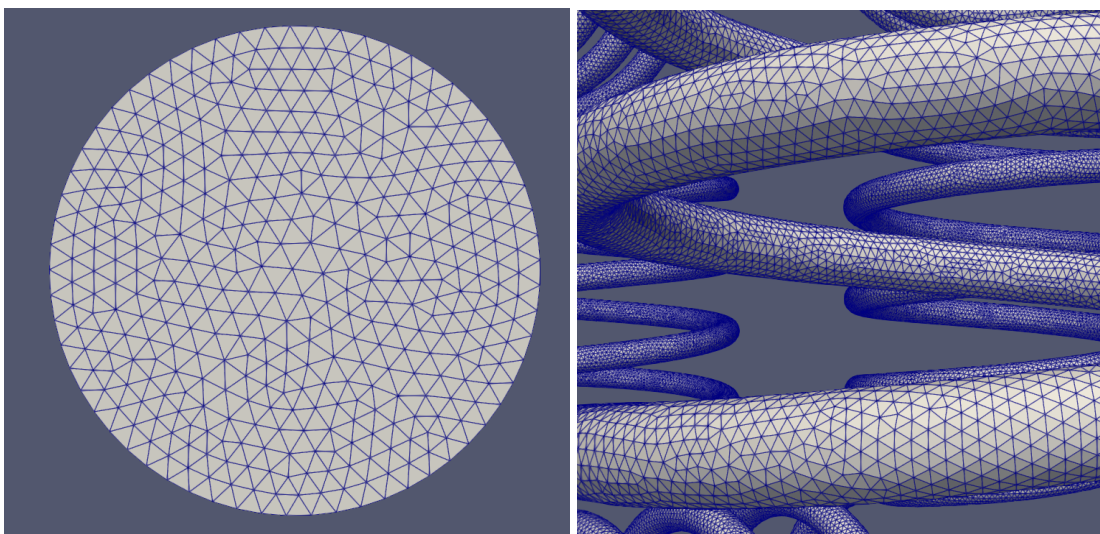
(fig 3.) STR Structured Mesh

Coiled Tube Reactor (Structured Mesh):



(fig 4.) CTR Structured Mesh

Coiled Flow Inverter Reactor (Unstructured Mesh):



(fig 5.) CFIR Structured Mesh

## 4.2 Initial and Boundary Conditions

The initial and boundary conditions can be categorised for each geometry in Table 2 and 3. Here for each of the given velocities, each corresponding temperature conditions were taken and the combinations were simulated respectively. The inlet, wall and outlet pressure was always set as 0 Pa for all the cases.

Geometry	Velocity [m/s]	Temperature Conditions	
		Wall [K]	Inlet [K]
Straight Tube Reactor	1. Re 0.1 = 1e-4	1. 335	1. 340
	2. Re 10 = 1e-2	2. 320	2. 340
	3. Re 1000 = 1	3. 345	3. 340
		4. 360	4. 340
Coiled Tube Reactor	1. Re 0.1 = 1e-4	1. 335	1. 340
	2. Re 10 = 1e-2	2. 320	2. 340
	3. Re 1000 = 1	3. 345	3. 340
		4. 360	4. 340
Coiled Flow Inverter Reactor	1. Re 0.1 = 1e-4	1. 335	1. 340
	2. Re 10 = 1e-2	2. 320	2. 340
	3. Re 1000 = 1	3. 345	3. 340
		4. 360	4. 340

Table 2: Boundary Conditions for case files in 0 folder

Standard Boundary Conditions for all Cases:

Parameter	Location	Type	Condition
Temperature	outlet		zeroGradient
Velocity (internalField => uniform (0 0 0))	wall outlet		noSlip zeroGradient
pressure (internalField => uniform 0)	inlet outlet wall	calculated calculated calculated	\$internalField \$internalField \$internalField
p_rgh (internalField => uniform 0)	inlet outlet wall	fixedFluxPressure prghPressure fixedFluxPressure	uniform 0 p => uniform 0 value => uniform 0 uniform 0

Table 3: Boundary Conditional parameters for case files in 0 folder

### 4.3 Solver

The solver used was *buoyantSimpleFoam*. The directory of the solver tutorial is:

“\$FOAM\_TUTORIALS\heatTransfer\buoyantSimpleFoam\hotRadiationRoom”

*buoyantSimpleFoam* is a heatTransfer solver which accounts for velocity (U), pressure (p) and temperature (T). It also has an option to include the body force effects of gravity in the simulation. It is a steady state solver which uses the SIMPLE (Semi Implicit Method for Pressure Linked Equations) algorithm. Remaining parameters used in each of the case files are discussed below in Table 4. This setup file is kept common for all 3 geometries and only the BCs were changed.

**thermoPhysicalProperties:** (*constant/thermoPhysicalProperties*):

type	heRhoThermo
mixture	pureMixture
equationOfState	rhoConst
energy	sensibleEnthalpy
molWeight	18 [kg/mol]
rho	997.74 [kg m <sup>-3</sup> ]
Cp	4185.5 [J kg <sup>-1</sup> K <sup>-1</sup> ]
Hf	-285.83 [kJ/mol]
mu	0.001 [kg m <sup>-1</sup> s <sup>-1</sup> ]
Pr	6.9

Table 4: Values for parameters in *thermoPhysicalProperties* file in *constant* folder

**turbulenceProperties** (*constant/turbulenceProperties*)

simulationType      =>      laminar

**g** (*constant/g*)

value                      =>      (0 0 0)

**decomposeParDict** (*system/decomposeParDict*)

The PC used for running the case file had 8 cores. Hence the geometry was decomposed into 8 *simple* segments to implement the MPI. (numberOfSubdomains => 8)

STR:

```
n      (8 1 1);
```

CTR:

```
n      (1 8 1);
```

CFIR:

```
n      (2 2 2);
```

The *fvSolution* and *fvSchemes* were kept as default and the residual control was set to  $10e-4$  for all parameters.

## 5. Results and Discussions

In Fig. 6, the temperature profile of fluid from inlet onwards along the flow direction is shown for STR, with  $Re=0.1$   $\Delta T = 5K$ , and cooling case. As can be seen, the fluid temperature is decreasing linearly and attaining wall temperature in a short distance. So, only a small amount of surface area is effectively required to achieve desired heat transfer. Thus, instead of using complete surface area for HTC calculation, the area value should be one where actual heat transfer is occurring. Besides, since the fluid temperature profile is straight while the wall temperature is constant, hence the average temperature difference for HTC calculation can be the arithmetic average of inlet and outlet temperature difference.

Temperature plot along the axis:

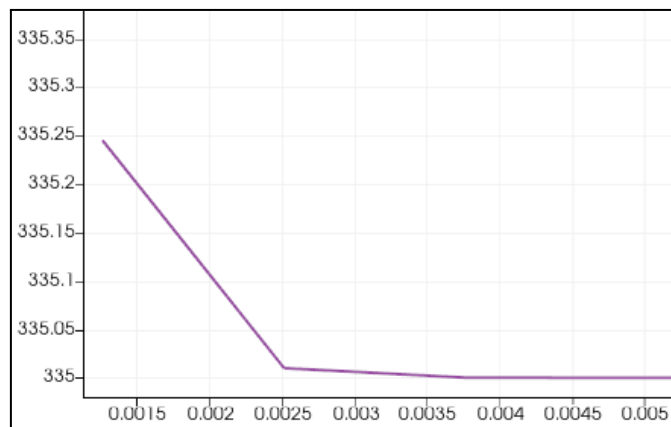


fig. 6. Temperature along axis (STR) for  $Re = 0.1$ ,  $\Delta T = 5K$ , Cooling

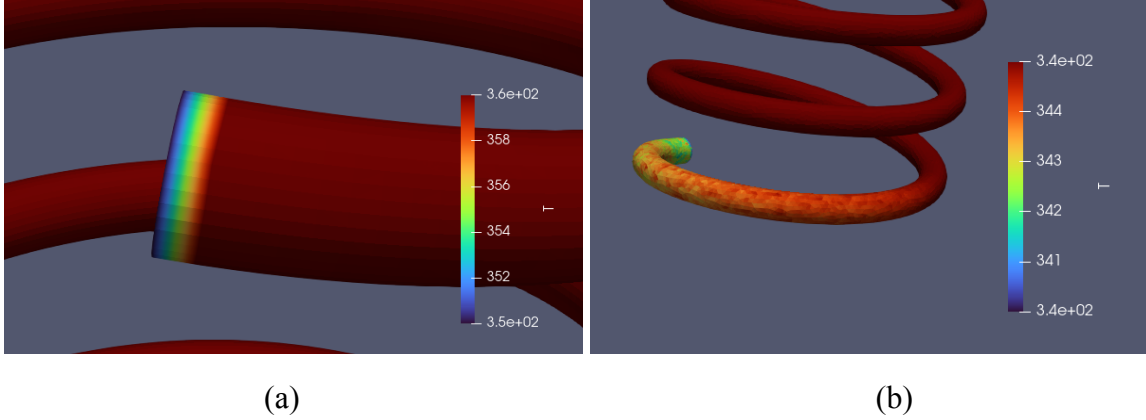


fig. 7. (a) CTR (b) CFIR  $Re = 0.1$ ,  $\Delta T = 5K$ , Heating

A similar behaviour with the change in temperature was also observed in CTR and CFIR. Fig. 7. & 8. shows the temperature contour plot of the fluid (internal mesh) at the outermost fluid layer. From the plots, the distance from inlet at which the fluid temperature reaches the wall temperature can be calculated. The distance from the inlet at which the fluid temperature reached wall temperature varied with the value of  $\Delta T$  and the Reynolds number at the inlet for CFIR, but remained the same for STR and CTR irrespective of change in Reynolds number and  $\Delta T$ . This distance at which the temperature of fluid reaches the wall temperature was calculated for each geometry for each Reynolds number and  $\Delta T$  for both heating and cooling, so that the surface area of the reactor which actually contributes to the heat transfer can be isolated from the rest of length of the reactor which doesn't contribute to the heat transfer and the HTC value was calculated only for that surface area.

This method of calculation was done for each case for all the geometries and the obtained values are tabulated in table 5. Analytical method of calculation was carried out for each case and the details of the calculation are discussed below.

The formula used to calculate the Average HTC is given as,

$$m \times C_p \times \Delta T = HTC_{avg} \times A \times \Delta T_{avg} \quad (9)$$

in which,

$$m = \rho \times V \times A_{cs} \quad (10)$$

$$A = \pi \times d \times L \quad (11)$$

$$\Delta T_{avg} = \Delta T/2 \quad (12)$$

$$A_{cs} = \frac{\pi}{4} d^2 \quad (13)$$

Where,

$m$  = Mass flow rate at the inlet (kg/s)

$A$  = Cross section area (m<sup>2</sup>)

$C_p$  = Specific heat (J/K/kg)

$\Delta T$  = Difference of temperature between inlet fluid and outlet fluid (K)

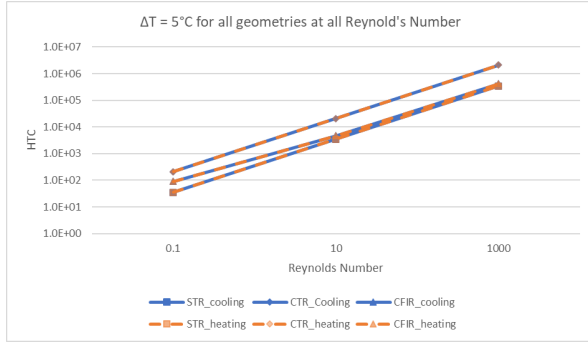
$d$  = Diameter of the tube (m)

$L$  = Length of the reactor taken for calculation (m)

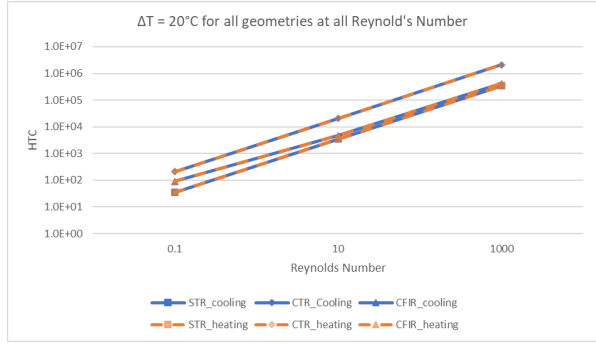
$V$  = Average Velocity at the inlet (m/s)

Geometry	Re	deltaT (K)	Length (m)	Surface area (m <sup>2</sup> )	m (kg/s)	Cp (J/K/kg)	LMTD (K)	HTC (W/m <sup>2</sup> /K)
STR	0.1	5	0.006	1.88E-05	7.83E-08	4185.5	2.5	3.48E+01
	0.1	20	0.006	1.88E-05	7.83E-08	4185.5	10	3.48E+01
	10	5	0.006	1.88E-05	7.83E-06	4185.5	2.5	3.48E+03
	10	20	0.006	1.88E-05	7.83E-06	4185.5	10	3.48E+03
	1000	5	0.006	1.88E-05	7.83E-04	4185.5	2.5	3.48E+05
	1000	20	0.006	1.88E-05	7.83E-04	4185.5	10	3.48E+05
CTR	0.1	5	0.001	3.14E-06	7.83E-08	4185.5	2.5	2.09E+02
	0.1	20	0.001	3.14E-06	7.83E-08	4185.5	10	2.09E+02
	10	5	0.001	3.14E-06	7.83E-06	4185.5	2.5	2.09E+04
	10	20	0.001	3.14E-06	7.83E-06	4185.5	10	2.09E+04
	1000	5	0.001	3.14E-06	7.83E-04	4185.5	2.5	2.09E+06
	1000	20	0.001	3.14E-06	7.83E-04	4185.5	10	2.09E+06
CFIR	0.1	5	0.0023	7.22E-06	7.83E-08	4185.5	2.5	9.08E+01
	0.1	20	0.0023	7.22E-06	7.83E-08	4185.5	10	9.08E+01
	10	5	0.0045	1.41E-05	7.83E-06	4185.5	2.5	4.64E+03
	10	20	0.0045	1.41E-05	7.83E-06	4185.5	10	4.64E+03
	1000	5	0.005	1.57E-05	7.83E-04	4185.5	2.5	4.18E+05
	1000	20	0.005	1.57E-05	7.83E-04	4185.5	10	4.18E+05

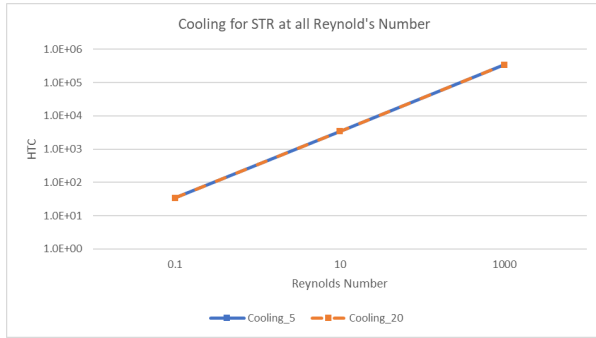
Table 5.  $HTC_{avg}$  Calculation



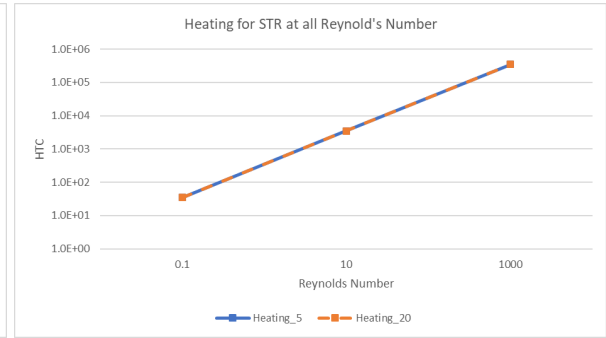
(a)



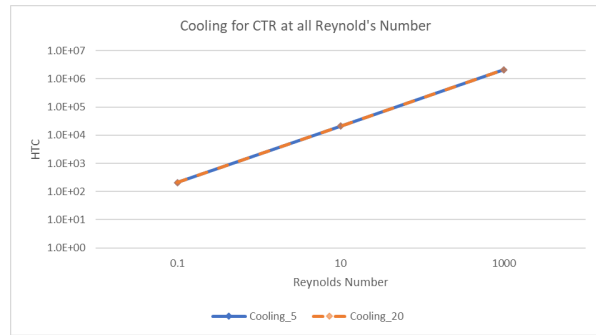
(b)



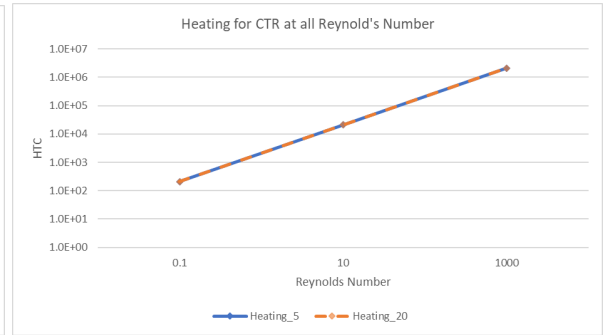
(c)



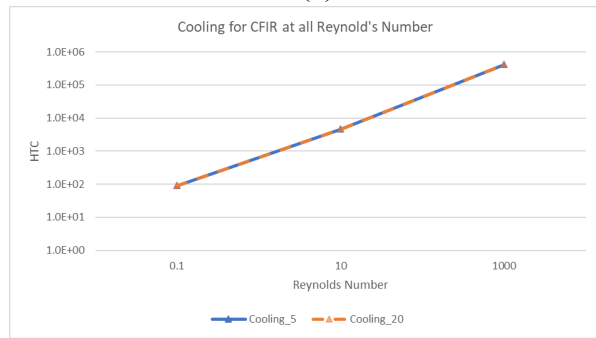
(d)



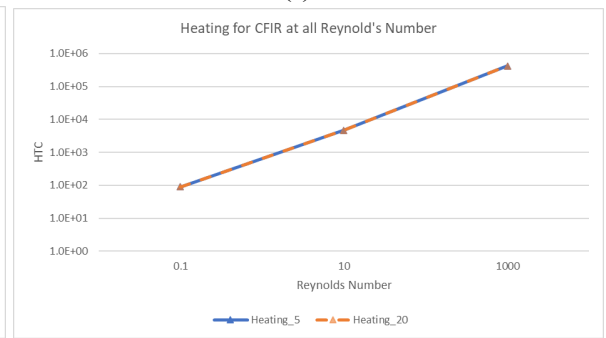
(e)



(f)



(g)

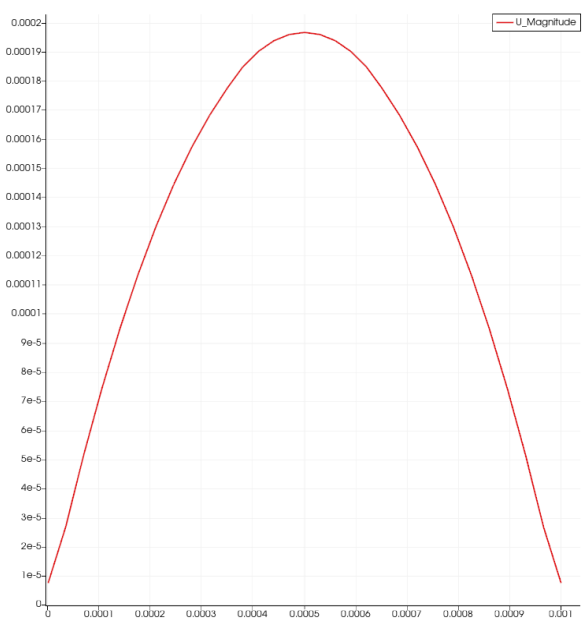


(h)

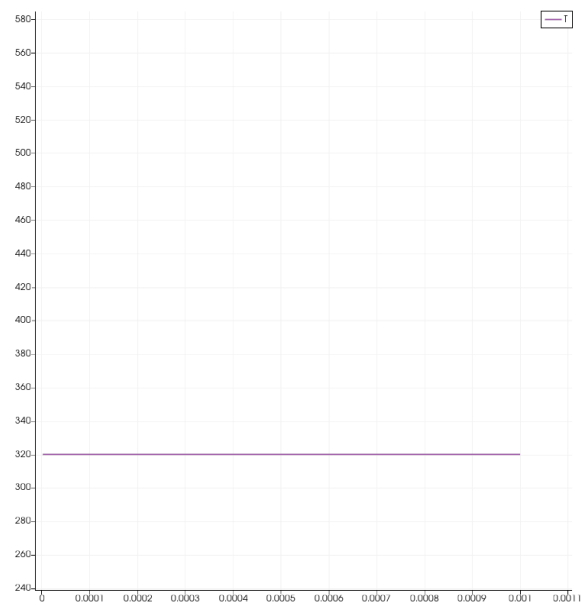
Fig. 8.  $HTC_{avg}$  Vs. Reynolds Number plots for all Geometries at various  $\Delta T$

Based on the obtained plots in *Fig. 8*, It can be seen that the  $HTC_{avg}$  value is the order of  $CTR > CFIR > STR$  for all Reynolds numbers irrespective of heating or cooling and the  $\Delta T$  (*Fig. 8., a,b*). The individual graphs (*Fig. 8., c-h*) shows that the  $HTC_{avg}$  increases with increase in Reynolds number irrespective of  $\Delta T$ . The high values of HTC is realistic as the constant wall temperature belongs to the phase change case- Steam Condensation for heating and Boiling for cooling case. During phase change cases, HTCs are usually very high of the order ( $10^4$  W/m<sup>2</sup>/K). Small radial dimensions might have enhanced it further.

Both the below plots were plotted at the outlet face along the diameter of STR geometry. The velocity plot (*fig 9*) at the outlet is parabolic. This graph is plotted for the STR case with  $Re=0.1$  with inlet temperature being 340 [K] and wall temperature being 320 [K] ( $\Delta T=20$ ). As it could be observed in *Fig 10*. The temperature has reached a steady state equal to the wall temperature of 320 [K] at the outlet. Hence a straight line with uniform temperature is obtained. Similar behavior was observed for all the cases simulated for all geometries.



*Fig 9. Velocity profile*



*Fig 10. Temperature profile*

## References

1. Garg, Dhiraj K., et al. "Numerical investigations of perfectly mixed conditions at the inlet of free radical polymerization tubular microreactors of different geometries." *Macromolecular Theory and Simulations* 29.6 (2020): 2000030.
2. Kumar, Vimal, et al. "Pressure drop and heat transfer study in tube-in-tube helical heat exchanger." *Chemical Engineering Science* 61.13 (2006): 4403-4416.
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