

Eulerian-Lagrangian Modelling of Particle Fouling in Microchannel

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Abstract

Toward process intensification, using continuous flow microreactors offers an interesting approach. However, fouling in microreactors during continuous production is a problem, especially in food industries. Understanding the fouling process at the microscale is a highlighted subject of ongoing research of microscale reactive flows. The present study aims to develop a numerical model for the prediction of the fouling process in micro-structured metallic devices. The study also includes the use of various particle geometric configurations, surface properties of the micro-structured devices, flow field and temperature field of the flow. The study uses a customised form of pimpleFoam solver to incorporate Lagrangian Particle Tracking. A simple geometry involving an L shaped channel is taken for the present study, and proposed results include a variation of pressure drop and particles deposition rate. Thus, from this study, we hope to understand the fouling process in microchannels so that efficient design configurations of these structures that can have useful applications in the food industry.

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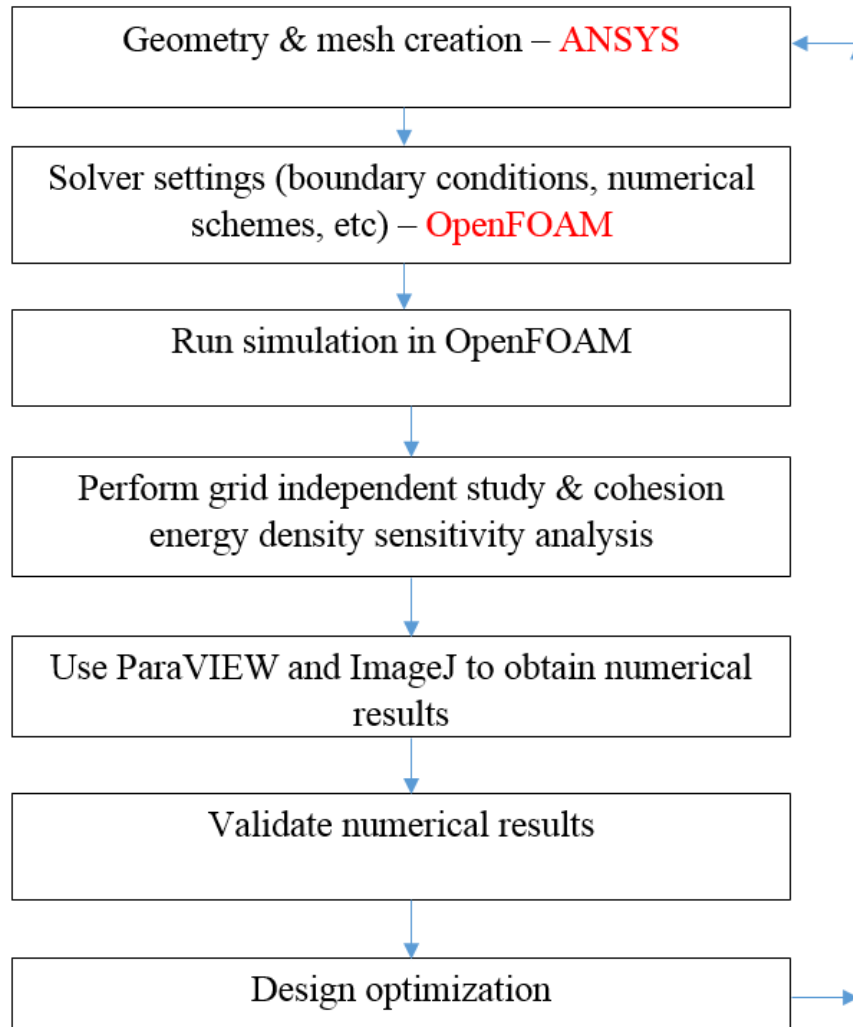
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1. Introduction

This work deals with predicting the fouling trend in microstructure devices using numerical CFD simulation based in OpenFOAM. The goal of this work is to combine particle drag and impact mechanics and fluid dynamics to model complex fouling mechanisms in idealized micro-structured metallic devices while achieving numerical accuracy and consistency. To achieve this aim, a coupling Lagrangian-Particle-Tracking (LPT) is proposed based on a newly developed solver from the OpenFOAM software package. The flow field of the continuous phase is described based on fluid boundary conditions. Particle trajectories in the dispersed phase are calculated within a Lagrangian reference frame, for which the Discrete Phase Model with the two-way coupling approach is used. The influence of particle deposition and accumulation on pressure drop is to be assessed. The model validity is to be verified with the results of fouling experiments which have been conducted by the project partner.

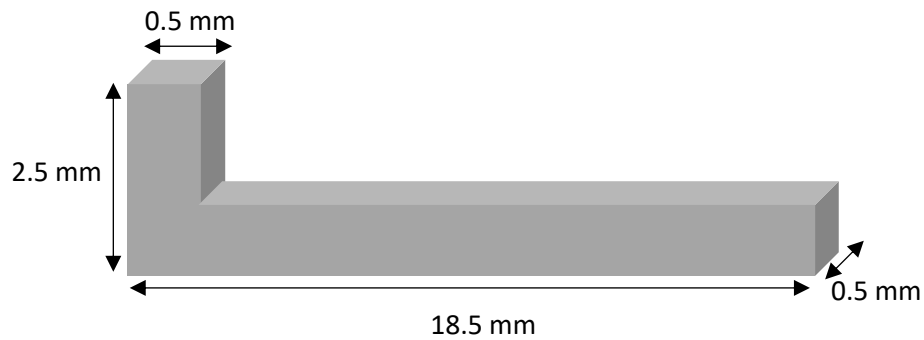
2. Numerical/Experimental/Design Analysis Details

The numerical procedure is shown in the following block diagram, and each step will be explained in the coming sections of the present report.



2.1 Geometry and Mesh creation

The geometry of the computational domain is an L shaped channel containing an inlet, walls and an outlet as shown below.

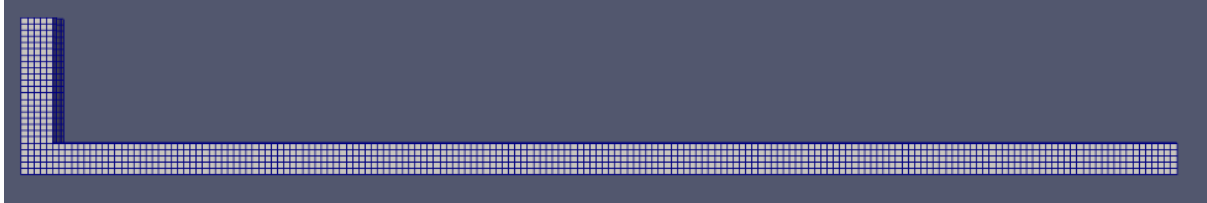


- The geometry and mesh creation was done using the blockMeshDict dictionary in OpenFOAM.
- Inlet-Outlet and Walls were defined as patches and walls, respectively.

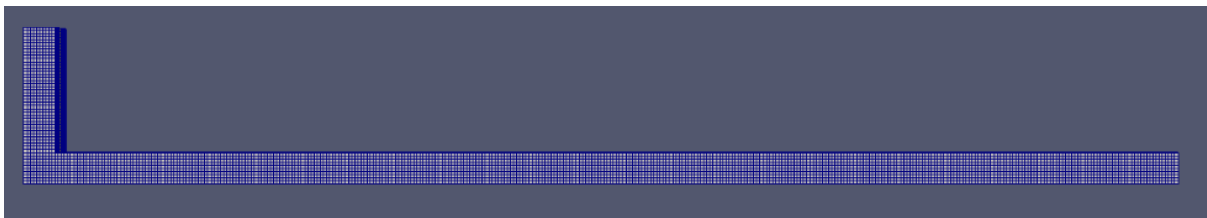
2.2 Grid Sensitivity Analysis

Cases:

1. Case I: 0.1 mm uniform mesh size



2. Case II: 0.05 mm uniform mesh size



3. Case III: 0.025 mm uniform mesh size



All three cases were run for the following conditions:

- mass flow rate = 5 g/min
- $Re = 509.863$ (laminar)
- $u = 0.336$ m/s
- Duration = 0.1 s

Clock Time for the three cases was as follows:

Case I: 21 s

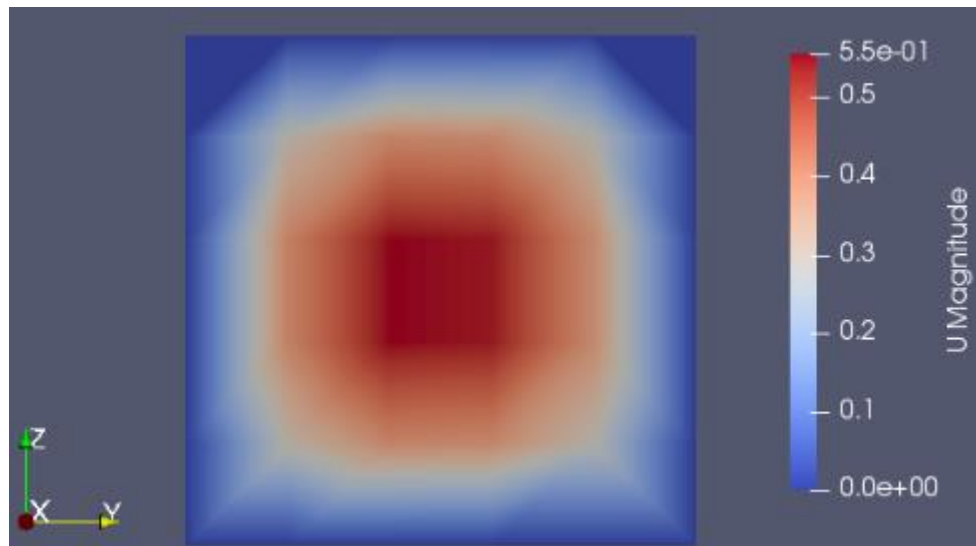
Case II: 362 s

Case III: 3724 s

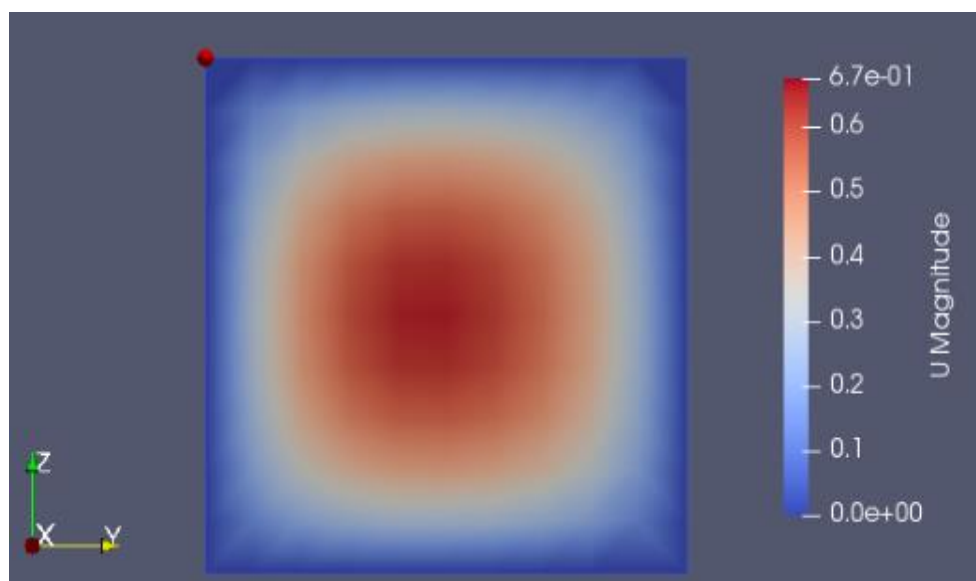
Qualitative Analysis

For performing the mesh sensitivity analysis, a slice plane was taken at $x = 0.01$ m with normal pointing in the positive X-axis direction.

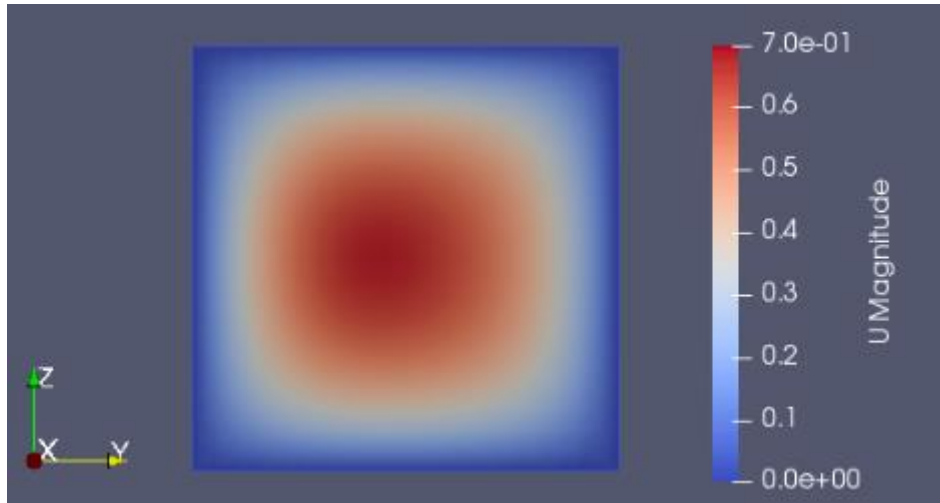
U_x contour of each of the three cases can be seen as follows:



Case I



Case II

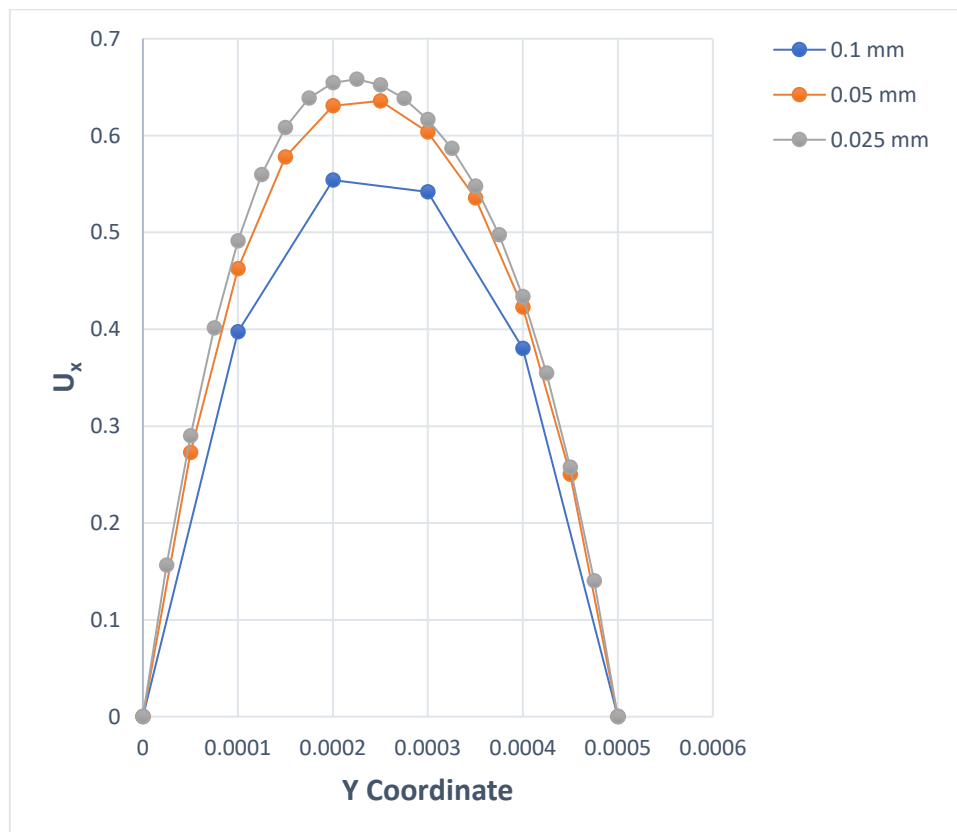


Case III

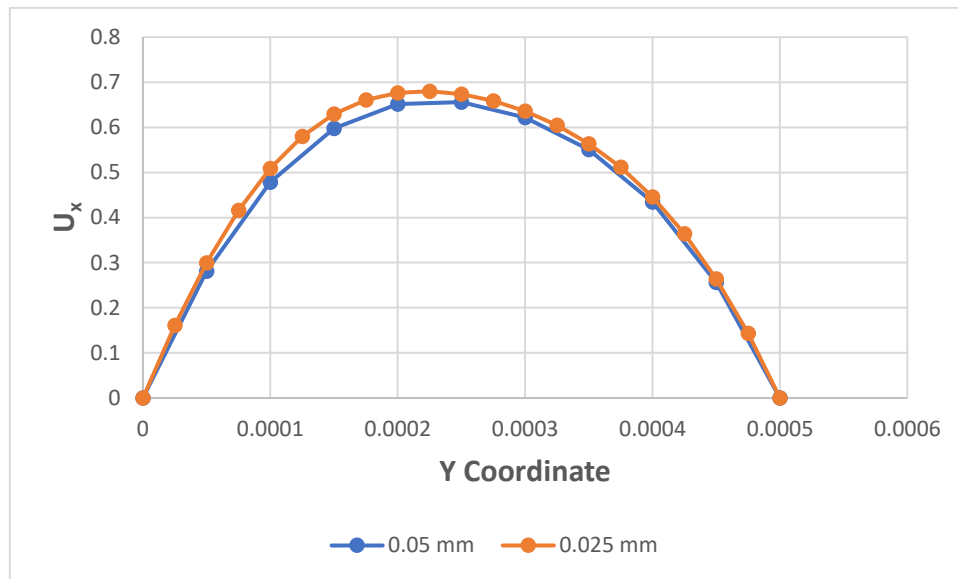
From the three cases, we can see that the result that most smoothly captures the velocity profile is Case III.

Quantitative Analysis

- The values of velocity at each data point on the aforementioned plane was exported from ParaView as a CSV file.
- Keeping the Z and X coordinates constant at -0.0003 m and 0.01 m a graph was plotted showing the variation of U_x vs Y coordinate:



- Keeping the Z and X coordinates constant at -0.00025 m and 0.01 m a graph was plotted showing the variation of U_x vs Y coordinate:



Pressure Drop (N/m^2)

4.1 Case I: 591.525

4.2 Case II: 703.345

4.3 Case III: 763.953

From the above data, we can see that pressure drop significantly changes Case I and Case II but does not change as much between Case II and Case III.

From the graphs above and the pressure drop data, it can be inferred that the uniform grid size of 0.025 m most accurately captures the velocity contour expected. However, from the clock time, it can be seen that Case III takes almost ten times more time as that of Case II without much change in computed velocity values. So, going with the case II grid size would be an optimum decision considering computational costs required.

2.3 Solver Settings

2.3.1 Solver Development

The current study used OpenFOAM (Open-source Field Operation And Manipulation), a C++ toolbox for the development of customized numerical solvers, and pre-/post-processing utilities for the solution of continuum mechanics problems, most prominently including computational fluid dynamics (CFD).

The solver used in the present study is pimpleLPTFoam, a customised form of pimpleFoam (large time-step transient solver for incompressible, flow using the PIMPLE (merged PISO-SIMPLE) algorithm) developed by Robert Kasper [5.2]. The developed solver incorporates Lagrangian Particle Tracking (LPT). In experimental fluid mechanics, Lagrangian Particle Tracking refers to the process of determining long 3-Dimensional trajectories of small neutrally buoyant particles (flow tracers) that are freely suspended within a turbulent flow field. These are usually obtained by 3-D Particle Tracking Velocimetry. A collection of such particle trajectories can be used for analysing the Lagrangian dynamics of the fluid motion, for performing Lagrangian statistics of various flow quantities etc.

In computational fluid dynamics, the Lagrangian Particle Tracking (or in short LPT method) is a numerical technique for simulated tracking of particle paths Lagrangian within a Eulerian phase. It is also commonly referred to as Discrete Particle Simulation (DPS). Some simulation cases for which this method is applicable are sprays, small bubbles, dust particles, and is especially optimal for dilute multiphase flows with large Stokes number.

Phase-Coupling Mechanisms:

The phase coupling mechanisms strongly influences the behaviour of the continuous and dispersed phases

- One-way coupling: Fluid flow affects particles trajectories
- Two-way coupling: Fluid flow affects particles trajectories which in turn affects the fluid flow
- Four-way coupling: Mutual interaction between fluid and particles and also particle-particle collision considered.

Description of Fluid Flow:

- **Lagrangian Description-** In the Lagrangian description of fluid flow, individual fluid particles are "marked," and their positions, velocities, etc. are described as a function of time. As the particles move in the flow field, their positions and velocities change with time. The physical laws, such as Newton's laws and conservation of mass and energy, apply directly to each particle. If there were only a few particles to consider, the Lagrangian description would be desirable. However, fluid flow is a continuum phenomenon, at least down to the molecular level. It is not possible to track each "particle" in a complex flow field. Thus, the Lagrangian description is rarely used in fluid mechanics.
- **Eulerian Description-** In the Eulerian description of fluid flow, individual fluid particles are not identified. Instead, a control volume is defined, as shown in the diagram. Pressure, velocity, acceleration, and all other flow properties are described as fields within the control volume. In other words, each property is expressed as a function of space and time, as shown for the velocity field in the diagram. In the Eulerian description of fluid flow, one is not concerned about the location or velocity of any particular particle, but rather about the velocity, acceleration, etc. of whatever particle happens to be at a particular location of interest at a particular time. Since fluid flow is a continuum phenomenon, at least down to the molecular level, the Eulerian description is usually preferred in fluid mechanics. Note, however, that the physical laws such as Newton's laws and the laws of conservation of mass and energy applied directly to particles in a Lagrangian description. Hence, some translation or reformulation of these laws is required for use with a Eulerian description.

The present study incorporated four-way coupling with Eulerian-Lagrangian method for Lagrangian Particle Tracking to customise pimpleFoam solver to pimpleLPTFoam solver.

2.3.2 Initial Conditions ^[5.3]

- Pressure (p file): The internalField is given a uniform 0 value throughout cell volumes of the mesh. The inlet patch is provided zeroGradient; the outlet is given fixedValue of 0 and walls are also provided with zeroGradient boundary conditions. zeroGradient is a homogeneous Neumann boundary condition which means that the quantity has a zero gradient in a direction perpendicular to the boundary.
- Velocity (U file): The standard boundary conditions for incompressible flow in a channel are taken here with 0.336 m/s, 0.672 m/s and 3.36 m/s average speed of the flow-through inlet. noSlip and zeroGradient boundary conditions are taken at the walls and outlet respectively.

Particle fluid details

<i>Solid-fluid Details</i>	Protein particles	water
Density (kg/m ³)	1000	992.25
Diameter (μm) *	1	-
Young's Modulus (MPa)	500	-
Poisson Ratio	0.20	-
Kinematic Viscosity (m ² /s)	-	6.59e-7
Cohesion Energy	20000	-
Density		
Coefficient of Restitution [CoR]	0.4	-
Coefficient of Friction [CoF]	0.5	-

parcelsPerSecond =1e6

$$\dot{m}_{H_2O} = 5 \frac{g}{min}, 10 \frac{g}{min}, 50 \frac{g}{min}$$

For Reynolds number in laminar region turbulence model in OpenFOAM constant folder is set to Laminar model and for turbulent, k-omega SST model is used.

If Reynolds number is above 1150 then we need to consider turbulent flow ^[5.1]. For turbulent flow the following parameters have to be defined in the initial conditions folder, namely:

- Turbulence Kinetic Energy (k) = $\frac{3}{2} (I|U|)^2$

Where,

$$I = \text{Turbulence Intensity} = 0.16 \cdot \text{Re}^{-0.125}$$

- Turbulence Dissipation Rate (ϵ) = $(C_\mu^{0.75} k^{1.5})/L$

Where,

$$C_\mu = \text{A model constant equal to 0.09}$$

$$L = \text{A reference length scale} = 0.07 \cdot 0.05 \text{ mm}$$

- Turbulence Specific Dissipation Rate (ω) = $k^{0.5}/(C_\mu^{0.25} \cdot L)$

Average Velocity (U)

The average velocity can be calculated based on the given mass flow rate and area of cross-section of the flow domain data.

$$U = \frac{\dot{m}_{H2O}}{A \cdot \rho}$$

Where,

$$A = \text{Area of cross section of flow} = 0.25 \cdot 10^{-6} \text{ m}^2$$

$$\rho = \text{Density of fluid} = 992.5 \text{ Kg/m}^3$$

Therefore, for the three given mass flow rates we get the average velocities as

$$U_1 = 0.336 \text{ m/s}$$

$$U_2 = 0.672 \text{ m/s}$$

$$U_3 = 3.36 \text{ m/s}$$

Reynolds Number

$$Re_1 = \frac{Uh}{\mu} = 509.836 \text{ (Laminar [6.7])}$$

$$Re_2 = \frac{Uh}{\mu} = 1019.672 \text{ (Laminar [6.7])}$$

$$Re_3 = \frac{Uh}{\mu} = 5098.36 \text{ (Turbulent [6.7])}$$

Where,

$$h = \frac{4.A}{P} \text{ (P is perimeter of cross section) = 0.5 mm}$$

$$\mu = \text{Kinematic viscosity (given)}$$

Turbulence Modelling [5.8]

For average velocity 3.36 m/s the Reynolds number is found to correspond to turbulent conditions and so k-omega SST turbulence model is chosen for turbulence modelling.

• k	=	$\frac{3}{2} (I U)^2$	= 0.05122 m ² s ⁻²
• l	=	$0.16 * Re^{-0.125}$	= 0.055
• ω	=	$k^{0.5} / (C\mu^{0.25} * L)$	= 1062.5107

For turbulence modelling, there are several models that can be used; some of them are k-epsilon, k-omega and k-omega SST. These can be used considering several factors such as Reynolds number, wall boundary consideration etc. [5.4,5.5]

The k-omega SST model can be used for low Reynolds flow applications without additional damping functions, SST stands for Shear Stress Transport. The SST formulation also switches to a k-epsilon behaviour in the free-stream, which avoids that the k-omega problem, which is very sensitive to the inlet free-stream turbulence properties. The k-omega SST model also accounts for its smooth behaviour in adverse pressure gradients and separating flow. It produces some

large turbulence levels in regions with large normal strain, like stagnation regions and regions with strong acceleration. This effect is much less pronounced than with a normal k-epsilon model though. The SST model has the ability to account for the transport of the principal shear stress in adverse pressure gradient boundary-layers. Thus, we chose the k-omega SST model for our study.

2.3.3 Constant Folder

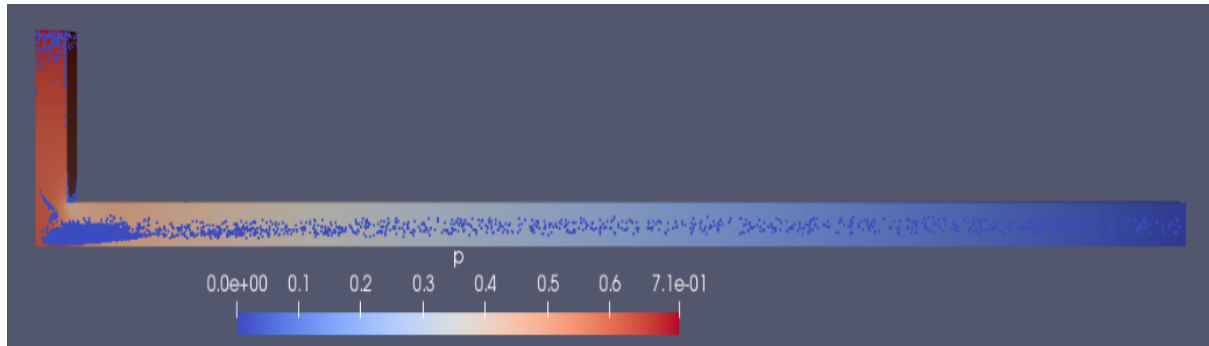
- g file: This contains the value and direction of acceleration due to gravity that needs to be considered for the simulation. In this simulation, we have considered g to be 9.8 m/s^2 in the negative y-axis direction.
- kinematicCloudProperties file: This file contains properties of particles to be injected in the fluid domain. ^[5.6]
- RASProperties file: This file contains the RAS model to be used. ^[5.7]
- transportProperties file: This file contains the transport model, viscosity and density of the fluid to be used. Newtonian model is used here as the viscosity of fluid remains constant.
- turbulenceProperties file: It contains the simulationType (Laminar, RAS, etc.).
- polyMesh folder: This is generated on performing blockMesh operation and geometry creation. It contains the information regarding boundary, faces, neighbours, owner and points.

2.3.4 System folder

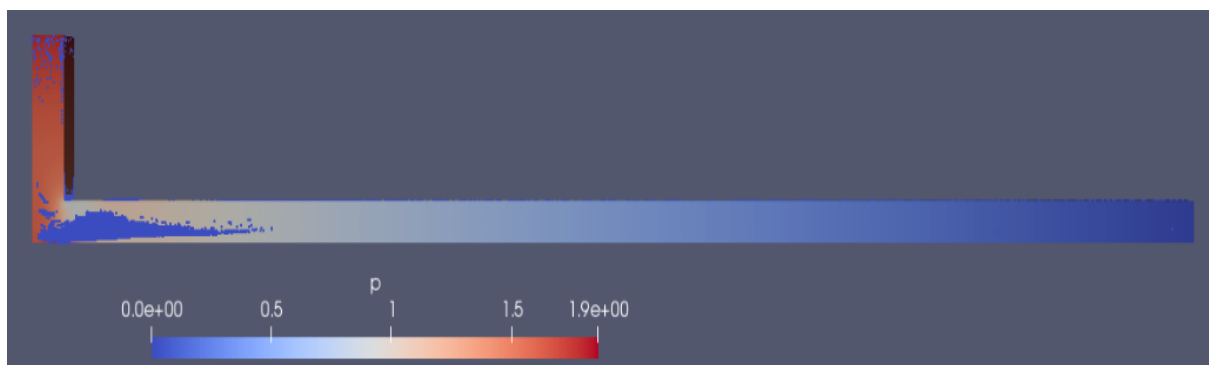
- blockMeshDict file: This contains the geometry creation code.
- controlDict file: This contains information such as solver to be used, startTime, endTime, deltaT, writeControl, writeInterval etc. We have considered an adjustable time step based on the maximum Courant number as 0.5.
- fvSchemes file: This contains various schemes to be used for solving the partial differential equations involved in the simulation. Standard schemes have been used in the present case based on a number of references taken.
- fvSolution file: This contains the equation solvers, tolerances and algorithms.

3. Results and Discussion

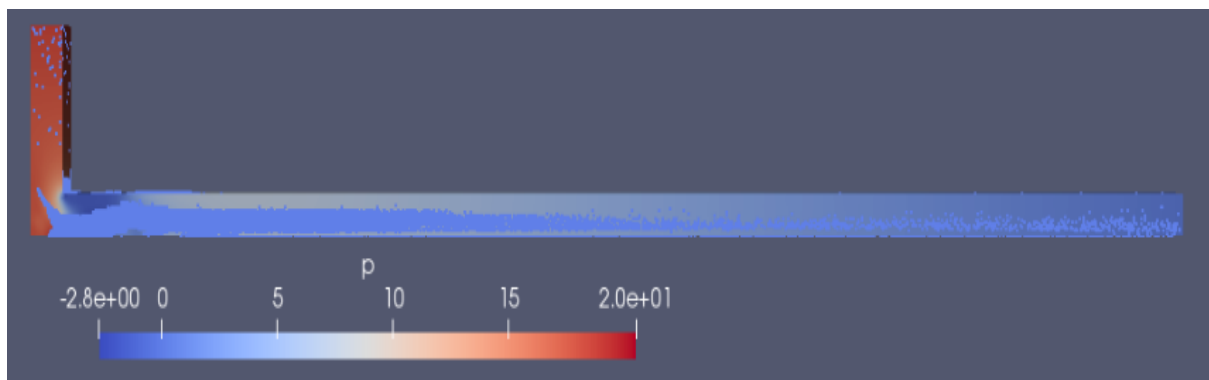
3.1 Pressure Drop



Case I



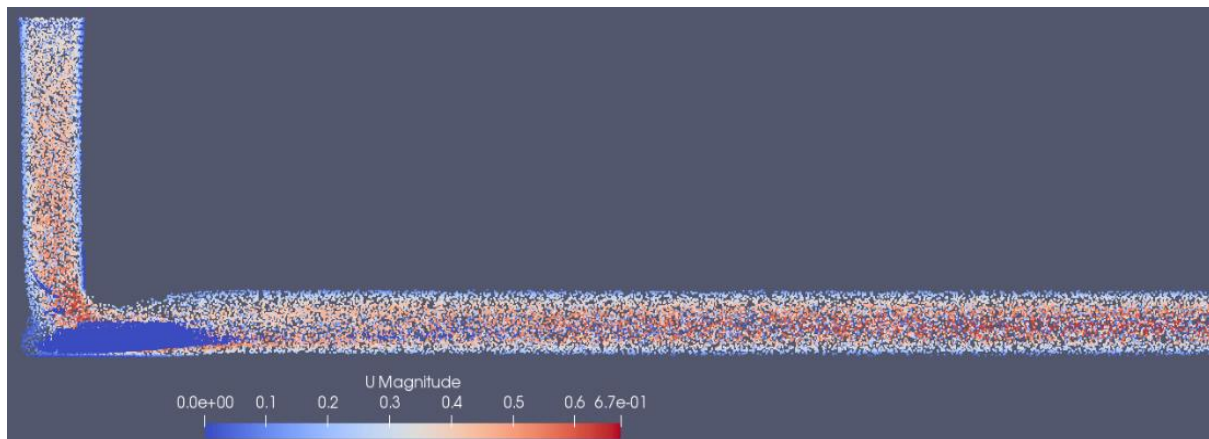
Case II



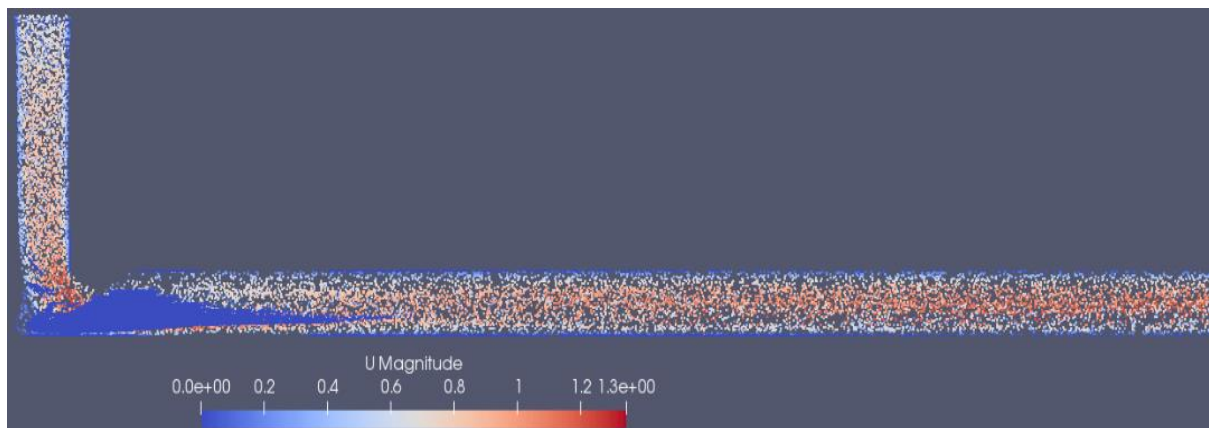
Case III

The increase in pressure drop in each of the above cases can be attributed to increasing mass flow rates, which in turn cause higher flow velocity, which is a function of pressure drop between two points in the flow domain (inlet and outlet in the present case).

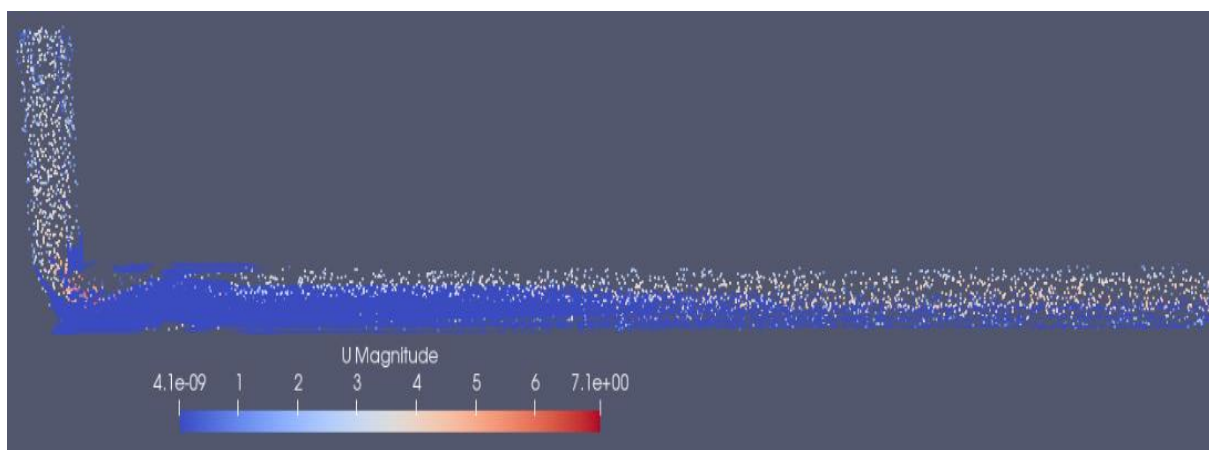
3.2 Particles Velocity Magnitude



Case I



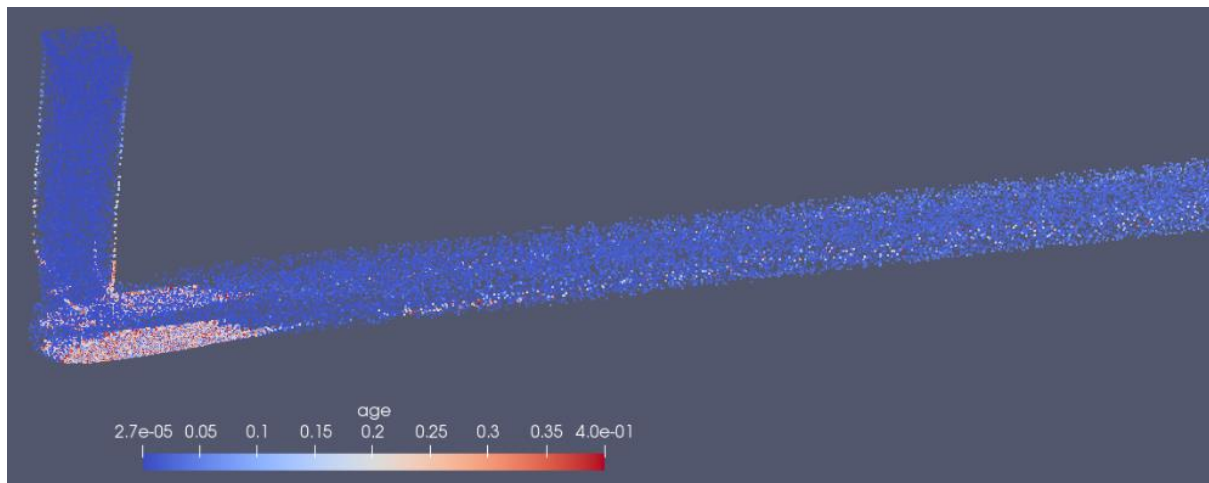
Case II



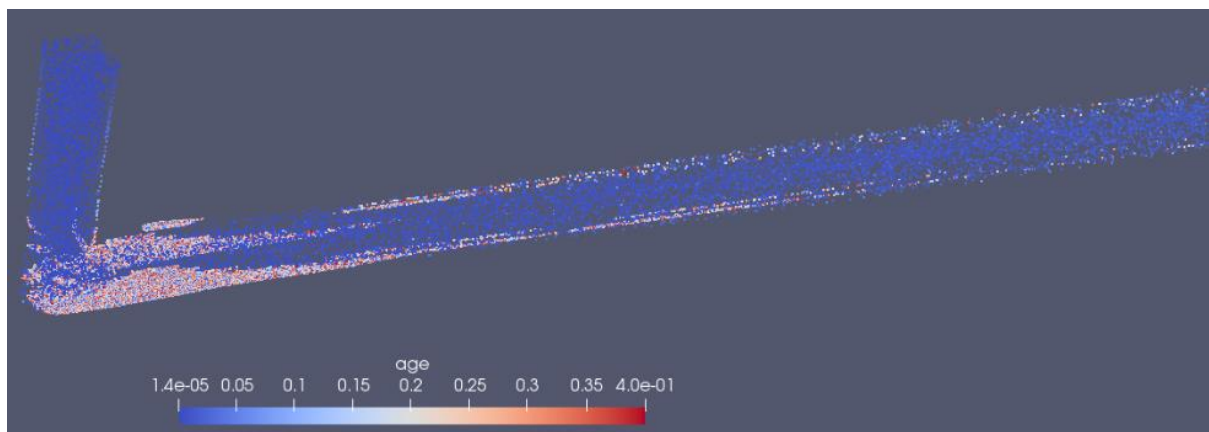
Case III

As expected from the three cases, the particles velocity magnitude is dependent on flow velocity magnitudes (which were calculated earlier). The dark blue points indicate particles that have attained zero velocity, which denote the fouling process.

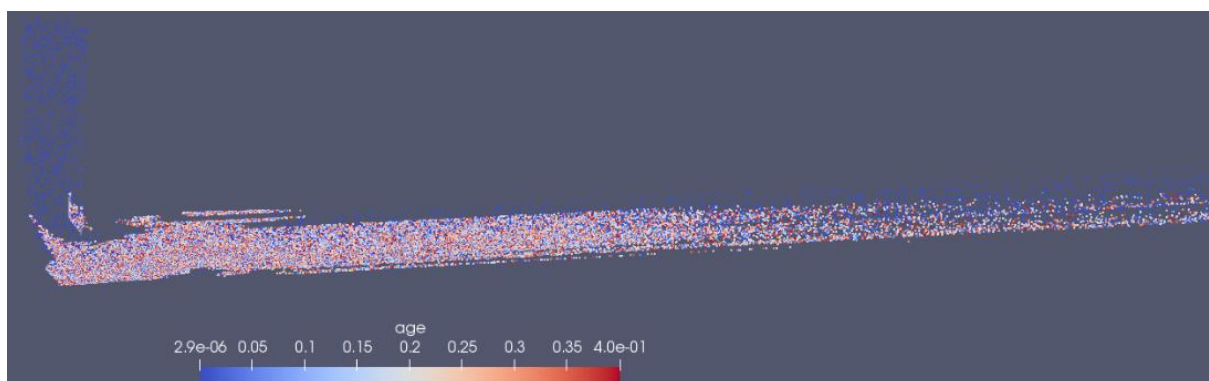
3.3 Particles age (s)



Case I



Case II

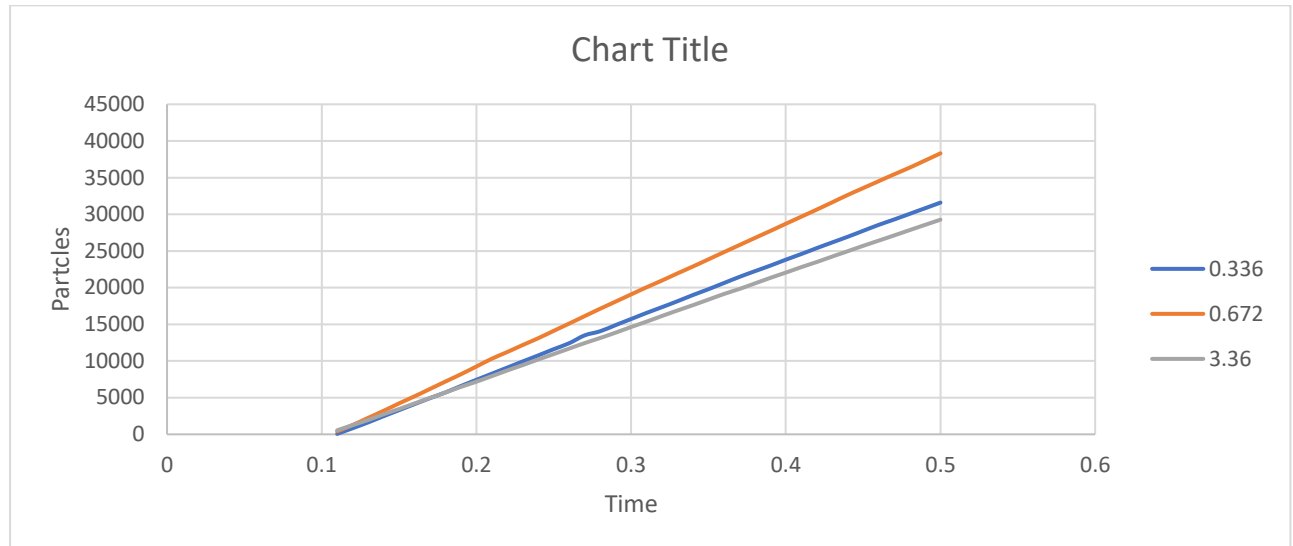


Case III

The above three visualisations capture the particles age in seconds, i.e. the amount of time a particle has been present inside the flow domain. We can observe particles of higher age have accumulated at the bottom wall of the microchannel, attributing the fouling process.

3.4 Particle Deposition Rate

The particle deposition rate on the bottom wall was the main objective of this study.



From the above graph, we can infer that the particle deposition rate increases with an increase in the average fluid velocity in the laminar region and decreases with an increase in average fluid velocity in the turbulent region. This can be attributed to the chaotic nature of the flow in the turbulent region, which may inhibit particles from being deposited.

Higher Deposition Rates can be achieved if we decrease the coefficient of restitution and increasing the coefficient of friction between the walls and particles. Also, by increasing particles cohesion energy density, particles will be more likely to cling on to each other and thus increase the particles deposition rate.

4. Conclusion and Future Work

The present study encompasses Lagrangian Particle Tracking in the pimpleFoam solver and thus has been used to study particle fouling process in a simple L shaped geometry. This type of study finds applications predominantly in food industries where fouling is a significant problem. Incorporating energy equation in the developed solver to account for heat transfer between particles, fluid and the domain boundaries can be worked upon in the future. This incorporation may lead to a more robust study whereby particle fouling, as well as heat transfer, can be studied.

5. References

- 5.1 <https://www.pulsus.com/scholarly-articles/fluids-flow-stability-in-ducts-of-arbitrary-crosssection.pdf>
- 5.2 https://www.foamacademy.com/wp-content/uploads/2016/11/GOFUN2017_ParticleSimulations_slides.pdf
- 5.3 <https://www.cfdsupport.com/Turbomachinery-CFD-manual/node149.html>
- 5.4 <https://engineering.stackexchange.com/questions/4111/reynolds-number-for-a-rectangular-duct>
- 5.5 <https://www.cfd-online.com/Forums/main/75554-use-k-epsilon-k-omega-models.html>
- 5.6 <https://www.cfd-online.com/Forums/openfoam-pre-processing/174534-kinematiccloudproperties-details.html>
- 5.7 <https://www.openfoam.com/documentation/guides/latest/doc/guide-turbulence-ras-k-epsilon.html>
- 5.8 <https://www.openfoam.com/documentation/user-guide/turbulence.php>