Application of OpenFoam to study flow through cylindrical pipe with baffle and relating it to Oscillatory Baffled Reactors(OBR)

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Mini-Report

CONTENTS

Introduction:

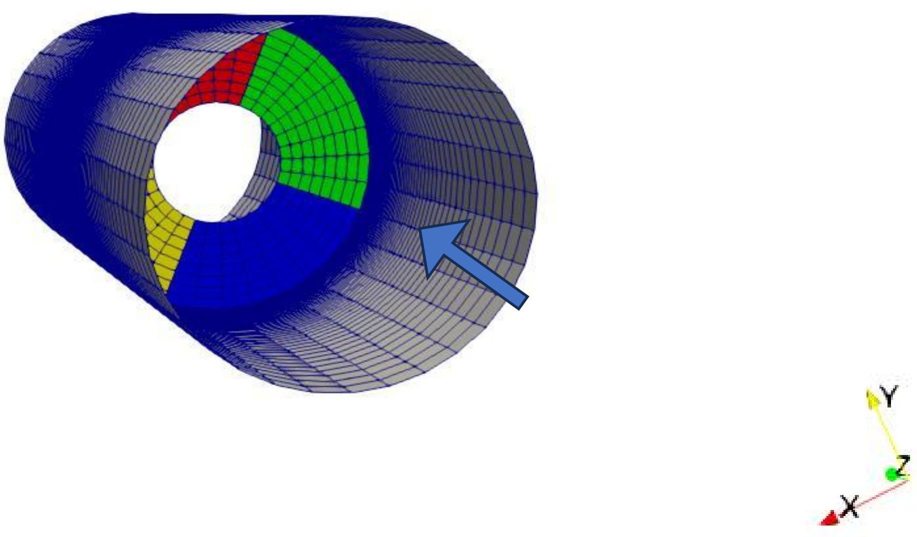
An oscillatory baffled reactor (OBR) is a type of continuous-flow reactor that employs oscillatory flow to enhance mixing and mass transfer within the reactor. Unlike conventional reactors, which rely on turbulent flow for mixing, OBRs utilize controlled oscillations to induce chaotic flow patterns, leading to improved mixing efficiency and reaction kinetics. This innovative design consists of a series of baffles or obstacles within the reactor that oscillate back and forth, causing fluid motion characterized by rapid changes in velocity and direction. The oscillatory motion promotes the formation of microscale vortices and enhances fluid dispersion, resulting in reduced mass transfer limitations and improved reaction selectivity. OBRs find applications in various chemical processes, including homogeneous and heterogeneous catalysis, chemical synthesis, and bioconversion reactions, offering advantages such as higher reaction rates, reduced energy consumption, and enhanced product quality. This introduction sets the stage for exploring the principles, applications, and advancements of oscillatory baffled reactors in modern chemical engineering and process intensification.

Application of OPENFOAM:

In the computational fluid dynamics (CFD) simulations conducted using OpenFOAM, the geometry of a pipe with a baffle has been constructed utilizing the blockMesh utility. This process involves discretizing the computational domain into a mesh composed of blocks, which allows for the representation of complex geometries with structured hexahedral cells. The inclusion of a baffle within the pipe geometry serves to induce flow disturbances and enhance mixing characteristics, mirroring the physical configuration of an oscillatory baffled reactor (OBR). Subsequently, appropriate boundary conditions have been assigned to the inlet, outlet, walls, and baffle surfaces to accurately simulate the flow behavior and interactions within the system. These boundary conditions govern parameters such as velocity, pressure, and turbulence properties at the boundaries of the computational domain. To solve the governing equations describing fluid flow, two distinct solvers, namely pimpleFoam and SimpleFoam, have been employed. The pimpleFoam solver is suitable for transient, turbulent flows with time-varying pressure-velocity coupling, making it well-suited for capturing the dynamic behavior within the pipe-baffle system. On the other hand, SimpleFoam is a steady-state solver commonly used for laminar or turbulent flows where steady-state solutions are sought. By utilizing these solvers in conjunction with appropriate meshing techniques and boundary conditions, comprehensive insights into the flow characteristics and mixing performance within the pipe-baffle configuration can be obtained, aiding in the design and optimization of oscillatory baffled reactors and similar fluid processing systems.

Geometry:

In the computational modeling undertaken for this study, the geometry of a cylindrical reactor with two distinct inner diameters of 0.1546 cm and 0.375 cm, both with a common length of 2 cm, has been constructed using OpenFOAM's blockMesh utility. The specifications for this geometry are defined in the blockMeshDict file, where parameters such as vertex coordinates, block sizes, and boundary patches are outlined. Additionally, a baffle has been integrated into the cylinder's midpoint to induce flow disruption and enhance mixing. This baffle, characterized by a centrally located hole with a diameter matching the smaller inner diameter of 0.1546 cm, is also defined within the blockMeshDict file as a solid obstacle with an aperture. By configuring the computational domain in accordance with these specifications, we aim to investigate the impact of the baffle on flow patterns, residence time distribution, and mixing efficiency within the cylindrical reactor configuration. Such insights are crucial for optimizing the design and performance of oscillatory baffled reactors and analogous fluid processing systems.



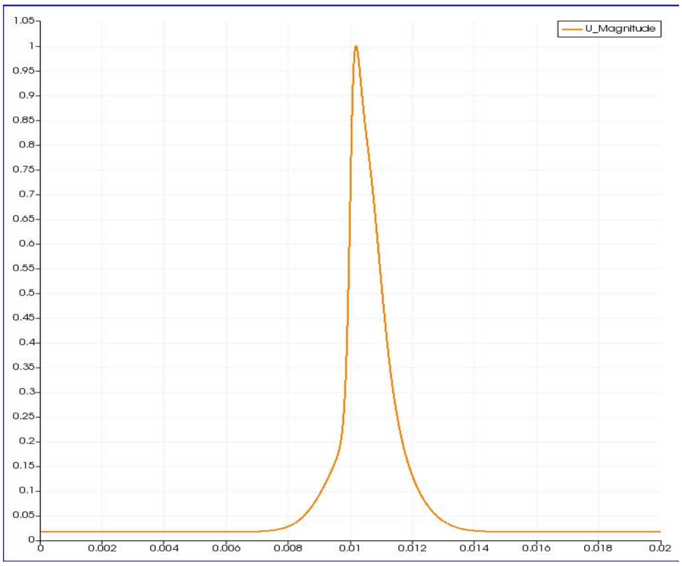
3. Boundary conditions:

In the computational setup, boundary conditions are crucial for accurately representing the flow dynamics within the domain. At the inlet and outlet boundaries, cyclic boundary conditions are applied to emulate the continuous and seamless flow through the computational domain. These cyclic boundary conditions ensure that the flow field is consistent and periodic, allowing for a realistic representation of the fluid behavior within the system. Specifically, at the inlet boundary, prescribed velocity and pressure conditions are imposed to initiate the flow, while at the outlet boundary, the same conditions are enforced to maintain continuity as fluid exits the domain. Along the walls, a no-slip boundary condition is applied for velocity, preventing fluid from slipping past the solid boundaries. For pressure, a zero-gradient boundary condition is utilized, assuming no variation perpendicular to the boundary surface. Together, these boundary conditions, including the cyclic boundary condition, govern the flow behaviour and interactions within the computational domain, contributing to accurate and reliable simulation results.

4. Methodology and Solver:

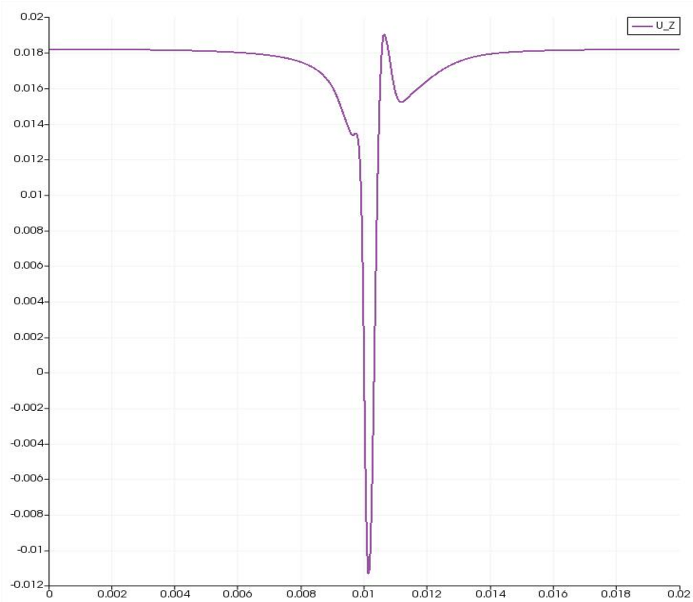
In the computational analysis conducted using OpenFOAM, the pimpleFoam solver has been employed to derive results for the specified problem. This solver is particularly well-suited for handling transient, turbulent flows, making it an appropriate choice for capturing the dynamic behavior within the system. However, for this specific scenario, the solver has been configured to simulate laminar flow conditions, reflecting the relatively low flow velocities and smooth flow patterns anticipated within the cylindrical reactor geometry. To enhance the accuracy of the simulation and account for additional effects, such as flow enhancement, an fvOptions file has been introduced into the constant folder. Within this file, a momentum source term has been incorporated to represent an average inlet velocity of 2 cm/s, effectively augmenting the flow velocity at the inlet boundary. By integrating this momentum source, the simulation aims to account for any deviations from idealized laminar flow conditions, thereby providing a more comprehensive understanding of the flow behavior and mixing characteristics within the system.

5. Results



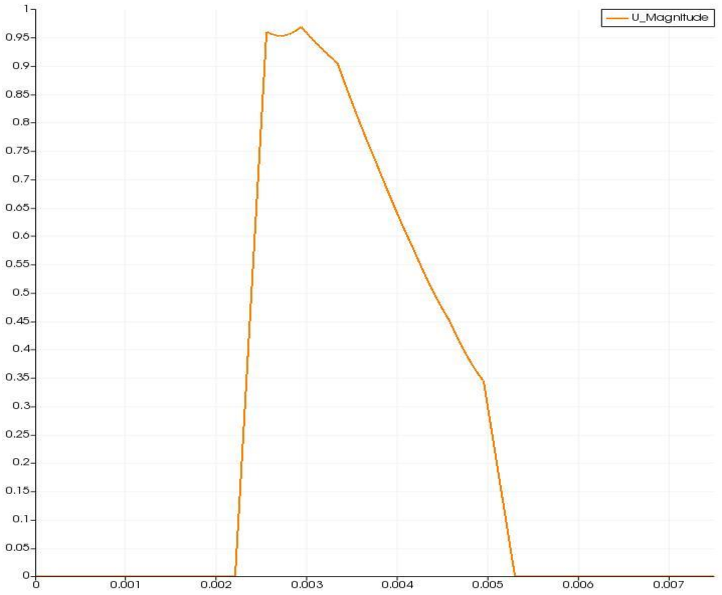
U-mag Vs Z

We can see that the magnitude of velocity is increasing around z=1cm.As there is a baffle at that location and less area for fluid flow. Hence equation of continuity verifies for increased flow rate.



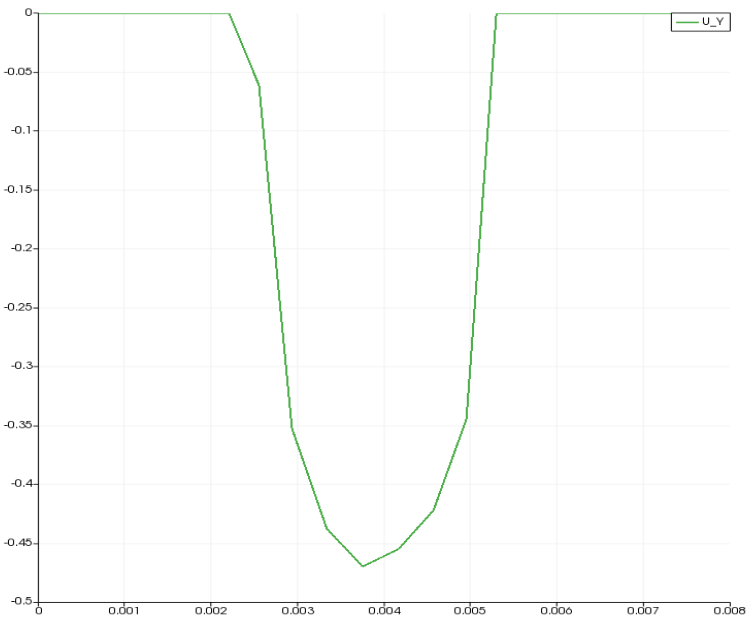
U_Z Vs Z

We can see that velocity in z-dirn decreases in z-dirn and also become negative near the baffle.It means that after redirecting from baffle, some fluid particles flow in negative dirn, and there is some sort of flow separation.



U-mag Vs Y

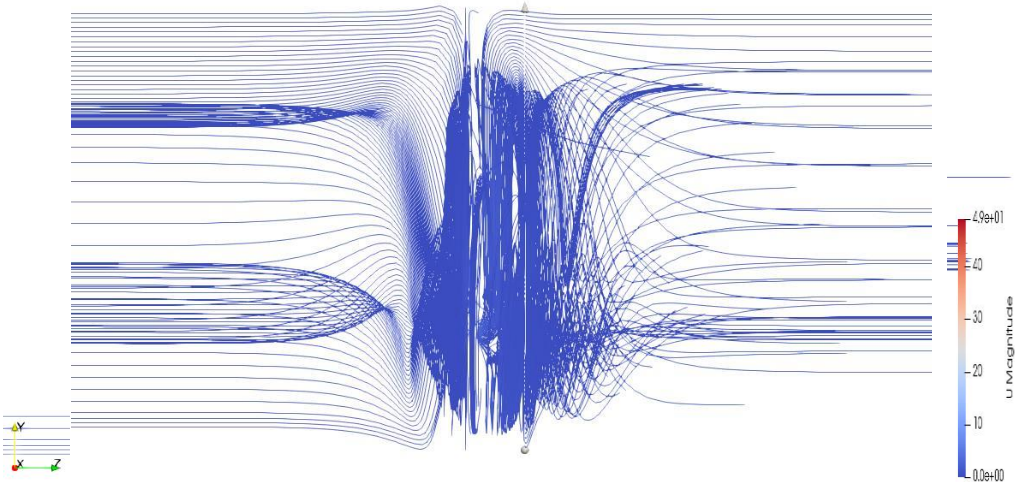
The magnitude of velocity in y dirn is zero at baffle walls. The velocity is present near the hole of the baffle



U_Y Vs Y

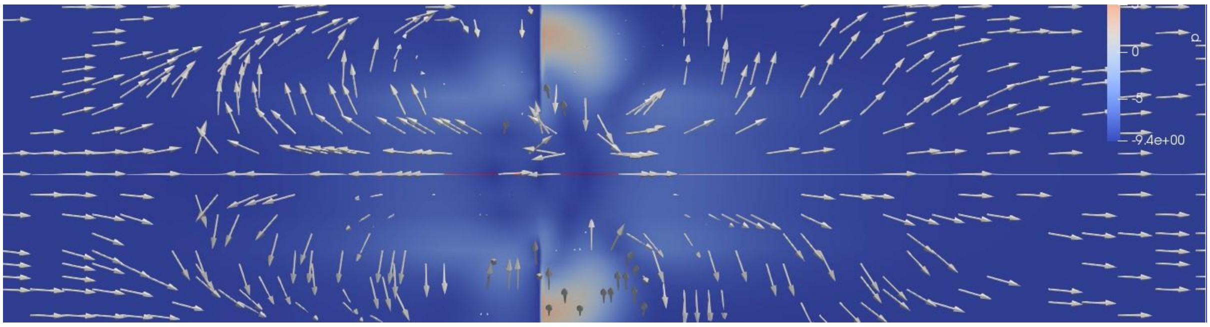
At the location of baffle, the fluid particle flow in negative y-dirn .It means there can be a recirculatory motion (a formation of vortex there)

Streamlines:



Comments: We can see the vortex formation near the walls. There is mixing of fluid particles near the baffle. There is some sort of separation also where fluid particles are moving opposite to the flow.

Glyph vector view:



Comments: We can easily see the vortex formation and mixing between different layers of fluid. Very less fluid particles are passing to other side through the baffle hole.

6. Conclusion and Future work:

In conclusion, our study highlights the significant role of vortex formation near the baffle surface in promoting mixing within the cylindrical reactor system. The presence of the baffle induces complex flow patterns characterized by the generation of vortices, which effectively enhance fluid mixing by facilitating the intermingling of different fluid streams. Notably, we observed fluid particles moving in opposite directions around the baffle, contributing to the creation of eddies and promoting the dispersion of species within the reactor. This phenomenon underscores the importance of baffle design and placement in optimizing mixing efficiency and reaction kinetics in similar fluid processing systems.

Moving forward, several avenues for future research present themselves. Firstly, a detailed investigation into the influence of baffle geometry, such as size, shape, and placement, on vortex formation and mixing efficiency could provide valuable insights for reactor design optimization. Additionally, exploring the impact of varying flow rates and fluid properties on vortex dynamics and mixing performance would contribute to a comprehensive understanding of the system behavior under different operating conditions. Furthermore, coupling computational simulations with experimental validation could validate the observed phenomena and provide practical guidelines for enhancing reactor performance in industrial applications. Overall, future research endeavors should focus on refining our understanding of fluid dynamics near baffles and leveraging this knowledge to develop more efficient and reliable mixing strategies for diverse chemical processes.

7. References:

https://pubs.acs.org/doi/10.1021/acs.iecr.2c02830