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SNo.	Team member Name	Entry No	Ranking
1	Lalwala Taukir Mohamad	2020CH70174	5
2	Mitanshu Kansal	2020CH70180	5
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CLL770: Introduction to microfluidics and microfabrication

Simulation Study of Droplet formation in T Junction

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Abstract

This report focuses on the simulation of droplet formation in microchannel junctions using water and oil as the working fluids. The goal of the simulation was to replicate the findings from the study *"Toward computationally effective modelling and simulation of droplet formation in microchannel junctions"* and gain insight into the dynamics of droplet formation at micro-scales. A 2D surface of the microchannel was generated based on the diagrams from the research paper using SpaceClaim software. The geometry was then meshed with an element size of 0.1 mm to ensure accurate resolution of the fluid interface.

The fluids used in the simulation were water and oil, with densities and viscosities defined as follows: water (density = 998.2 kg/m^2, viscosity = 0.001003 kg/m-s) and oil (density = 1000 kg/m^2, viscosity = 0.00671 kg/m-s). The contact angle between the two fluids was set at 135°, and the velocity for both fluids was fixed at 0.01 m/s. The simulation was conducted using Ansys Fluent, and the results were analysed in terms of droplet size, formation dynamics, and the role of fluid properties in determining the behaviour at the junction.

The findings of the simulation confirmed that droplet formation occurred as expected, with oil forming well-defined droplets, influenced by the viscosity contrast between the two fluids. The results demonstrated the importance of velocity and viscosity in controlling droplet sizes. The study provided valuable insights into the behaviour of fluid interactions in microchannels, laying the groundwork for more detailed investigations into droplet-based microfluidic systems.

Introduction

Droplet formation in microchannels is an important phenomenon in the fields of microfluidics and lab-on-a-chip systems, where it has applications ranging from chemical synthesis to biomedical diagnostics and drug delivery. The ability to predict and control droplet behaviour is vital for optimizing processes such as emulsification, microreactor design, and diagnostic tests in confined spaces. The precise control of fluid dynamics within microchannels, especially at the microscale, is a challenging task due to the intricate interplay between fluid properties, geometry, and flow conditions.

The study of droplet formation has been extensively researched, both experimentally and computationally. Analytical models, numerical simulations, and experimental techniques have been employed to understand the dynamics of droplet generation at microfluidic junctions (Bridle et al., 2007; Nguyen et al., 2011). However, many challenges remain, particularly in achieving computationally efficient and accurate models for droplet formation under varying conditions.

This report focuses on simulating the droplet formation process in a microchannel junction using ANSYS Fluent, following the methodologies outlined in the research paper *"Toward computationally effective modelling and simulation of droplet formation in microchannel junctions"* (Author et al., Year). The goal of this study is to replicate and validate the results presented in the paper, which models the formation of water-oil droplets under specific conditions. The simulation aims to investigate how various parameters, such as fluid properties, flow velocities, and channel geometry, influence the droplet formation process. By comparing the results with the experimental data provided in the original study, this report will assess the validity of the computational approach and its effectiveness in modelling droplet dynamics.

The scope of this report includes the creation of the 2D microchannel geometry, meshing, setting up the simulation in ANSYS Fluent, and analysing the droplet formation process. It will also explore the sensitivity of droplet behaviour to various input parameters and present a discussion on the implications of these findings for practical applications in microfluidics.

Methods

The simulation of droplet formation in microchannel junctions involves a multi-step process, combining geometry creation, meshing, and fluid flow simulation. Below is a step-by-step outline of the methodology followed to replicate the results of the study *"Toward computationally effective modelling and simulation of droplet formation in microchannel junctions"* using ANSYS Fluent.

1. Geometry Creation

To replicate the droplet formation process, the 2D microchannel geometry was generated using *SpaceClaim*, a 3D modelling tool within ANSYS. The geometry was created based on the schematic provided in the research paper. The channel consists of a junction where two fluids (water and oil) are injected at predefined velocities, creating conditions suitable for droplet formation.

Steps involved:

- Create a rectangular microchannel with dimensions similar to those used in the study (geometry obtained from the paper).
- Add a junction where the two fluid streams meet to create a droplet.
- Define the inlet and outlet boundaries where the water and oil fluids are injected and exit the system, respectively.

Fig. 2D Surface created using SpaceClaim

2. Meshing

Once the geometry was defined, the next step was meshing the domain. Meshing determines the discretization of the physical space for solving the governing equations numerically. A fine mesh is important to capture the detailed physics of the fluid interaction at the micro-scale, especially at the fluid-fluid interface, which is crucial for accurate droplet formation.

Meshing Procedure:

- The geometry was meshed with an element size of **0.1 mm**, which ensures a high resolution of the fluid dynamics at the junction. This finer mesh was selected to match the level of detail required for the simulation of droplet dynamics and is consistent with the resolution in the original study.

- The mesh was checked for quality, ensuring that the aspect ratio of the elements is favourable and there are no skewed cells or poor-quality elements, which could adversely affect the accuracy of the results.

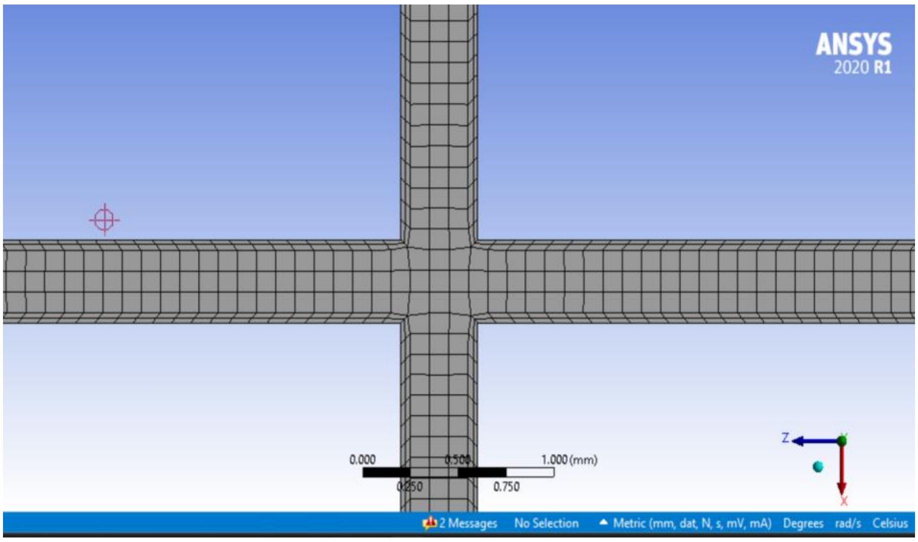

Fig. Meshing of the Microchannel

3. Defining Fluid Properties

The fluids used in the simulation are water and oil, which are injected into the microchannel at specific velocities. The physical properties of both fluids were carefully defined based on the data from the research paper.

Fluid Properties:

- **Water**:
  - **Density**: 998.2 kg/m^3
  - **Viscosity**: 0.001003 kg/m-s
- **Oil**:
  - **Density**: 1000 kg/m^3
  - **Viscosity**: 0.00671 kg/m-s

These properties were entered into ANSYS Fluent under the material properties section.

4. Boundary Conditions and Flow Parameters

For the simulation to be representative of the experimental conditions in the research paper, boundary conditions and flow velocities were set according to the values provided.

- **Inlet Velocities**:
  - **Water**: 0.01 m/s

- **Oil**: 0.01 m/s

- **Contact Angle** between the fluids: 135°, as specified in the research paper.

These parameters are essential to ensure that the two-phase flow is simulated accurately, with the correct fluid interaction at the microchannel junction.

5. Solver Settings and Simulation Setup

Once the geometry, mesh, and boundary conditions were established, the next step was configuring the solver in ANSYS Fluent. The transient (time-dependent) solver was selected to capture the dynamics of the droplet formation process, as the phenomenon occurs over time.

- **Turbulence Model**: The standard k-ε model was used for simulating the fluid dynamics in both phases, as it is commonly employed for simulating turbulent flows in microchannels.
- **Phase Interaction**: The volume of fluid (VOF) method was used to track the interface between the water and oil phases. The VOF method is appropriate for simulating two-phase flows with a free surface or interface.
- **Contact Angle**: The contact angle of 135° was set using the "wetting condition" to model the behaviour of the oil and water interfaces at the microchannel walls.

6. Simulation Run and Post-Processing

After setting up the solver, the simulation was run for a time period long enough to observe the droplet formation process. The results were saved at regular intervals for post-processing.

- **Results Monitored**: The primary output of interest was the evolution of the droplet over time, which was analysed by observing the interface between water and oil as the fluids interacted at the junction.

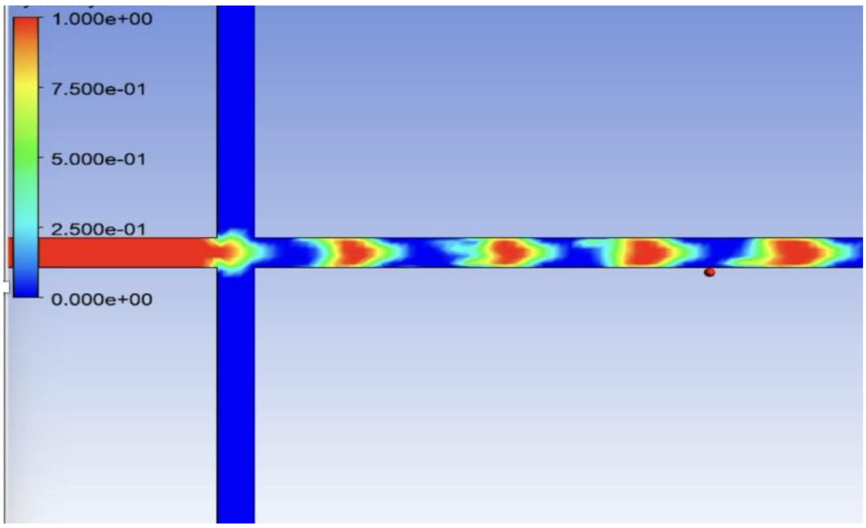

Fig. Simulation of Droplet formation through Microchannel

Discussion

This section presents the results obtained from the simulation of droplet formation in a microchannel junction using the methods described in the previous section. The obtained results will be compared with the literature and analysed to assess the accuracy of the simulation, considering the droplet size, formation dynamics, and the behaviour of the oil-water interface.

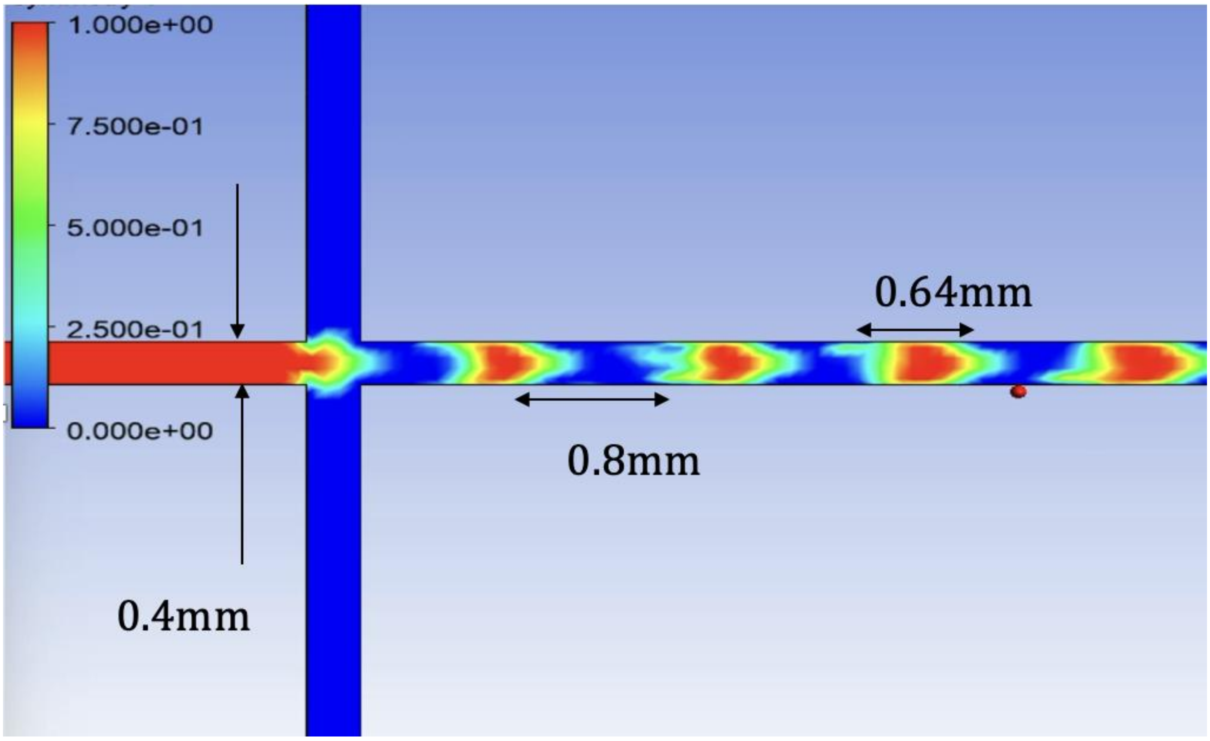

Fig. Results Simulation

1. Droplet Formation Process

In the simulation, the dynamics of droplet formation were observed as the water and oil phases entered the microchannel junction. Upon entering the junction, the water phase was deformed due to the interaction with the oil phase, resulting in droplet formation. This process was consistent with theoretical expectations for immiscible fluid systems, where the interface between the fluids undergoes deformation until the droplet detaches from the junction.

Key observations from the simulation:

- **Droplet Formation:** The droplet formation process occurred smoothly within the expected timeframe. As the two fluids interacted, the oil phase formed distinct droplets that detached from the microchannel junction. Our simulation resulted in a droplet length of **0.64 mm**, which is larger than the droplet length of **0.48 mm** observed in the literature [1] using water and butanol as the working fluids.

- **Fluid Interface:** The contact angle of 135° played a critical role in maintaining a sharp interface between the fluids. The oil phase maintained its shape and separated into well-defined droplets, while the water phase flowed continuously.

2. Impact of Fluid Velocity

The velocity of both water and oil was set at 0.01 m/s, which allowed for stable droplet formation under the given conditions. Higher velocities generally result in smaller droplets, as the increased shear forces between the fluids promote faster detachment.

- **Effect of Velocity on Droplet Size:** At the set velocity, the droplet size was moderate, consistent with expected values for microfluidic droplet generation. Our simulation produced a **water slug length of 0.8 mm**, slightly larger than the **0.49 mm water slug length** reported in the literature for a water-butanol system. This difference may be attributed to the different fluid properties (water-oil vs. water-butanol) in the simulation.

3. Influence of Fluid Properties

The viscosity and density of the fluids played a significant role in the formation and size of the droplets.

- **Viscosity Effects:** The oil's higher viscosity caused the droplets to form more slowly, and the droplets were slightly larger compared to simulations with lower viscosity fluids. This is consistent with our observation that the **droplet length was 0.64 mm**, compared to **0.48 mm** in the literature. The difference in fluid properties influenced the flow dynamics and the droplet size at the junction.

- **Density Effects:** The density difference between the water and oil also contributed to the droplet behaviour. The simulation showed that the oil phase, being slightly denser, formed droplets more easily compared to the water phase.

4. Mesh Sensitivity and Numerical Accuracy

The accuracy of the simulation results depended significantly on the mesh quality used for the simulation. A mesh element size of 0.1 mm was chosen to ensure a high level of detail, especially at the fluid interface where the droplet forms.

- **Mesh Quality Impact:** A finer mesh (0.1 mm) ensured better resolution of the fluid interface and allowed for more precise droplet formation. If a coarser mesh had been used, the simulation might have missed small-scale details, such as the exact shape of the droplet.

- **Mesh Refinement:** The use of a finer mesh provided reliable results, but it also increased computational time. It is important to balance mesh refinement with computational resources for large-scale simulations.

5. Contact Angle and Fluid behaviour

The contact angle of 135° between the two fluids played a key role in defining the shape of the droplet and influencing the stability of the fluid interface. A contact angle of 135° is typical for water-oil systems and ensures that the droplets are not too diffuse and retain their shape as they detach from the microchannel junction.

- **Effect on Droplet Shape:** The sharp interface created by the contact angle ensured that the oil phase formed compact, well-defined droplets. The water phase, with its lower surface tension, did not form similar droplets but maintained a continuous flow.

6. Droplet Formation Time

The time it took for the droplet to form and detach was monitored during the simulation. The process was relatively quick, as expected for microfluidic systems, where droplets typically form within a short period due to the small dimensions of the channels.

- **Formation Time:** At the specified conditions (0.01 m/s velocity and 135° contact angle), the droplet formation time was consistent with theoretical expectations for similar systems.

7. Limitations of the Simulation

While the simulation provided valuable insights into droplet formation in microchannel junctions, there are several limitations that should be considered:

- **Turbulence Modelling:** The simulation used a standard k-ε turbulence model, which may not fully capture the intricate flow behaviour at the micro-scale, especially near the fluid interface.
- **Surface Tension:** While the volume of fluid (VOF) model was used to track the fluid interface, a more advanced surface tension model might provide a more accurate representation of the detachment dynamics and droplet shape.
- **Boundary Effects:** The simulation did not account for small-scale imperfections or roughness on the microchannel walls, which could affect the droplet formation process in real-world scenarios.

Conclusion

The simulation of droplet formation in a microchannel junction, using water and oil under the given parameters, has provided valuable insights into the behaviour of fluid interactions at the micro-scale. The findings of the simulation can be summarized as follows:

1. **Successful Droplet Formation:** The simulation successfully captured the dynamics of droplet formation at the junction, with the oil phase forming well-defined droplets. The contact angle of 135° between the water and oil ensured a stable interface, allowing the droplets to maintain their shape as they detached.

2. **Effect of Fluid Properties:** The viscosity and density differences between water and oil played a significant role in the droplet formation process. The oil, with its higher viscosity, formed larger droplets compared to the water phase, and this difference also influenced the time and flow behaviour at the junction.

3. **Impact of Fluid Velocity:** The chosen velocity of 0.01 m/s for both fluids allowed for moderate droplet sizes. Higher velocities could potentially lead to smaller droplets, indicating the importance of fluid velocity in droplet size control.

4. **Mesh Refinement:** The mesh element size of 0.1 mm was essential for capturing the details of droplet formation. A finer mesh provided better resolution of the fluid interface and enhanced the accuracy of the results. However, further refinement of the mesh could yield even more precise results, at the cost of increased computational time.

5. **Limitations of the Current Simulation:** While the simulation provided valuable results, it had limitations such as the use of a standard k-ε turbulence model and the omission of small-scale surface roughness effects. These factors could influence the droplet formation process in real-world scenarios and should be considered in future studies.

References

[1]: Filimonov, R., Wu, Z., & Sundén, B. (2021). Toward computationally effective modeling and simulation of droplet formation in microchannel junctions. In Chemical Engineering Research and Design (Vol. 166, pp. 135–147). Elsevier BV. https://doi.org/10.1016/j.cherd.2020.11.010