Deformation of Non-Newtonian droplet in constricted microchannel

A Report Submitted in

Partial Fulfilment of the Requirements for the

7th Semester Final Year B.Tech. Project

Submitted by

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2024

DECLARATION

Thesis Title: **Deformation of Non-Newtonian droplet in constricted microchannel**

Degree for which the Thesis is submitted: **Bachelor of Technology**

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CERTIFICATE

It is certified that the work contained in this thesis entitled ‘ Deformation of Non-Newtonian droplet in constricted microchannel’ submitted by VAIBHAV GARG(2116133) and SIDDHANT TRIPATHI (2116147) for the award of B.Tech. End Semester Project Evaluation is absolutely based on their own work carried out under our supervision and that this work has not been submitted elsewhere for any degree.

Signature of Supervisor:

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ABSTRACT

Microfluidic systems have significantly advanced the understanding of fluid dynamics, particularly in the context of non-Newtonian fluids. Recent research highlights the critical influence of fluid properties such as viscosity, elasticity, and channel geometry on droplet behavior. Key factors such as shear forces, surface tension, and geometric configurations govern droplet formation, distribution, and mixing efficiency, enabling the design of optimized microfluidic devices for biomedical, emulsification, and industrial applications. Despite these advancements, several gaps remain. Existing studies inadequately address the effects of viscosity ratios, shear rates, and temperature on droplet deformation, as well as the comparative behavior of Newtonian and non-Newtonian droplets in Newtonian media. Furthermore, the impact of shrinkage and the interaction between various droplet types on deformation are not understood properly.

This study aims to bridge these gaps by systematically investigating the influence of critical physical parameters on droplet deformation. The objectives include analyzing the deformation of both Newtonian and non-Newtonian droplets in Newtonian media, exploring the effects of constrictions on droplet behavior, and drawing comparisons to enhance the fundamental understanding of microfluidic systems. The findings are expected to provide valuable insights for the design and optimization of microfluidic applications across diverse fields.

ACKNOWLEDGEMENT

We thank our supervisor Dr. Binita Nath, Assistant Professor, Department of Mechanical Engineering, Silchar National Institute of Technology for her constant support, approval and encouragement throughout our research. Her expertise and unwavering guidance were crucial in the decision making process of the project. Suggestions are useful to improve this research. We are grateful to all the faculty members of the Department of Mechanical Engineering, Silchar National Institute of Technology for their administrative support and academic guidance in all stages of this study. They are hardworking, talented and relentlessly determined. Without their dedication and cooperation, the completion of this research would not have been possible. time for our research work.

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1

Introduction

The study of droplet dynamics in microfluidic systems has garnered significant interest in recent years due to its pivotal role in a wide range of applications, including biomedical diagnostics, drug delivery, chemical synthesis, and food processing. Microfluidics, which involves the precise manipulation of fluids at the microscale, enables researchers and engineers to harness unique flow behaviors that arise from confined geometries. One particularly important aspect of this field is understanding how droplets of non-Newtonian fluids behave when passing through microchannel contractions, as the deformation and stability of these droplets are critical for their intended applications.

1.1 The vital parameters influencing the droplet deformation

In straight microchannel contraction, droplet deformation is influenced by few primary forces: viscous forces, surface tension, capillary forces and pressure forces. The fluid's resistance to flow, which is influenced by its viscosity, gives rise to viscous forces. Viscosity in non-Newtonian fluids can vary based on the shear rate, which can impact how droplets contract as they pass through the microchannel. The force operating at the interface between the droplet and the surrounding fluid is known as surface tension. It leads to cohesive forces among molecules of liquid, which minimize surface area. Apart from that Surface tension at the interface between a liquid droplet and the surrounding fluid, as well as interactions between the fluid molecules, are the causes of capillary forces. These forces are responsible for the droplet's shape and stability, particularly in confined geometries such as microchannels.

The pressure differences between the surrounding fluid and the droplet lead to pressure forces. A microchannel contraction leads to a drop in pressure considering the flow is constrained. The interplay of these forces collectively governs the behaviour of droplet deformation in microchannel systems.

1.2 Microchannel Geometry and Design

The geometry and design of microchannels are critical for controlling fluid flow and droplet formation. Configurations like T-junctions and flow-focusing channels allow for precise manipulation of droplet size and frequency. Key factors, such as channel dimensions and surface features, influence flow rates and droplet behaviour—narrow channels enhance capillary forces for smaller droplets, while wider channels can produce larger ones. The aspect ratio also plays a vital role in balancing inertial, viscous, and capillary forces. Optimizing these designs is essential for applications like targeted drug delivery, enhancing the performance of microfluidic devices.

1.3 Applications

The study of droplet deformation in microfluidic channels with constrictions has wide-ranging applications across fields such as engineering, healthcare, and environmental science:

Oil Recovery: Droplet deformation in porous media is crucial for enhanced oil recovery. Understanding how non-Newtonian fluids deform helps optimize oil extraction from reservoirs with complex pore geometries.

Innovation Potential: Innovations in droplet dynamics can lead to more efficient recovery techniques by reducing residual oil trapped in pores, minimizing environmental impact and maximizing resource extraction.

Microfluidic Sensors: Non-Newtonian fluid droplets are used in designing advanced biosensors for detecting pathogens and biomarkers. Deformation and manipulation of droplets can enhance the sensitivity and speed of these sensors in healthcare diagnostics.

Innovation Potential: Improved control over droplet shape and stability in microfluidic devices can lead to breakthroughs in early disease detection and point-of-care diagnostics, especially in developing wearable health monitors.

Cosmetic Industry: Emulsions and creams, often involving non-Newtonian droplets, rely on droplet behavior for product texture and efficacy. Optimizing droplet formation leads to better product consistency and delivery of active ingredients.

Innovation Potential: Understanding droplet deformation can revolutionize the creation of advanced emulsions in skincare, enabling more effective delivery of nutrients and activities in personal care products.

Wastewater Treatment: In environmental applications, controlling the deformation of non-Newtonian droplets during mixing and chemical reactions can enhance the treatment of industrial wastewater.

Innovation Potential: Developing systems that leverage droplet deformation can improve the efficiency of chemical treatment processes, reducing environmental pollution and optimizing resource recovery from waste streams.

1.4. Newtonian Fluid

A Newtonian fluid is a fluid whose flow behavior can be described by the relationship between stress and friction. Simply put, the viscosity (resistance to flow) of a Newtonian fluid remains constant regardless of the amount of shear applied. This means that no matter how much the fluid is stirred or slowed down, its viscosity does not change.

1.4.1 Characteristics of Newtonian Fluids:

1. **Constant Viscosity**: The fluid's viscosity remains unchanged regardless of the applied stress or shear rate.
2. **Linear Relationship**: There is a linear relationship between the shear stress and the shear rate.
3. **Time-Independent Behavior**: Newtonian fluids do not exhibit time-dependent behaviors such as thixotropy or rheopexy (which are seen in non-Newtonian fluids).

1.4.2 Governing Equation (Newton's Law of Viscosity):

The behavior of Newtonian fluids is described by **Newton's Law of Viscosity**, which states:

$$\tau = \mu \frac{du}{dy} \tag{1}$$

Where:

- τ is the **shear stress** (force per unit area, typically in Pascals).
- μ is the **dynamic viscosity** of the fluid (in Pa·s or N·s/m²).
- $\frac{du}{dy}$ is the **shear rate** or the velocity gradient (in s^{-1}).

1.4.3 Navier-Stokes Equation for Newtonian Fluid Flow:

The **Navier-Stokes equations** describe the motion of Newtonian fluids and are based on the principles of mass, momentum, and energy conservation. In the most general form, the Navier-Stokes equation for incompressible flow is:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f} \tag{2}$$

Where:

- ρ is the **density** of the fluid.
- $\mathbf{u}$ is the **velocity field** (vector quantity).
- ∇p is the **pressure gradient**.
- μ is the **dynamic viscosity**.
- $\nabla^2\mathbf{u}$ represents the **diffusion of momentum** due to viscosity (Laplacian of the velocity field).
- $\mathbf{f}$ represents any external forces (such as gravity).

This equation describes the balance of forces acting on a fluid element, accounting for inertia, pressure, viscous forces, and external forces.

1.5 Non-Newtonian Fluid

A non-Newtonian fluid is characterized by a viscosity that varies with shear rate

or stress, unlike Newtonian fluids with constant viscosity. These fluids can be shear-thinning (decreasing viscosity with increased shear) or shear-thickening (increasing viscosity with shear). In microchannel applications, this variability affects flow dynamics and droplet behaviour by influencing fluid-wall interactions. Shear-thinning fluids enhance droplet detachment under high shear, while shear-thickening fluids may hinder it. This variability also improves mixing efficiency, optimizing reaction kinetics in processes like emulsification. Overall, the relationship between non-Newtonian viscosity and capillary forces presents both challenges and opportunities in microfluidic design.

1.5.1 Characteristics of Non-Newtonian Fluids:

1. **Variable Viscosity:** The viscosity of non-Newtonian fluids is not constant; it changes with the rate of shear.
2. **Nonlinear Behavior:** The relationship between shear stress and shear rate is often nonlinear.

3. **Time-Dependent or Shear-Dependent Behavior:** Some non-Newtonian fluids exhibit time-dependent behaviors like thixotropy (shear-thinning over time) or rheopexy (shear-thickening over time).

1.5.2 Governing Equations for Non-Newtonian Fluids:

Since non-Newtonian fluids don't follow Newton's Law of Viscosity, their flow behavior is described using different models depending on the type of non-Newtonian fluid. Some of them are as follows-

1. Power-Law Model (for Shear-Thinning and Shear-Thickening Fluids):

This model is commonly used for fluids that exhibit either shear-thinning or shear-thickening behavior.

$$\tau = K\left(\frac{du}{dy}\right)^n \tag{3}$$

Where:

- τ is the **shear stress**.
- K is the **consistency index** (fluid-specific constant).
- $\frac{du}{dy}$ is the **shear rate**.
- n is the **flow behavior index** (where n<1 indicates shear-thinning, and n>1 indicates shear-thickening).

2. Bingham Plastic Model:

For fluids that behave like a solid until a yield stress is reached:

$$\tau = \tau_0 + \mu_p \frac{du}{dy} \quad \text{for} \quad \tau > \tau_0 \tag{4}$$

Where:

- τ_0 is the **yield stress**.
- μ_p is the **plastic viscosity**.

3. Herschel-Bulkley Model:

A more generalized model that combines features of the Power-Law and Bingham Plastic models:

$$\tau = \tau_0 + K\left(\frac{du}{dy}\right)^n \tag{5}$$

This model accounts for both yield stress and shear-thinning/thickening behavior.

1.5.3 Types of Non-Newtonian Fluids:

Non-Newtonian fluids can be categorized based on how their viscosity changes with the applied shear rate or stress:

1. Shear-Thinning Fluids (Pseudoplastic):

In these fluids, viscosity decreases with increasing shear rate. This means the fluid becomes "thinner" or easier to flow as more force is applied.

2. Shear-Thickening Fluids (Dilatant):

In these fluids, viscosity increases with increasing shear rate. They become more "thick" or resistant to flow as shear stress is applied.

3. Bingham Plastics:

These fluids behave like a solid until a certain amount of shear stress is applied. Once this yield stress is exceeded, they start flowing like a viscous fluid.

4. Thixotropic Fluids:

In these fluids, viscosity decreases over time under constant shear. If the applied stress is removed, they slowly regain their original viscosity.

5. Rheopectic Fluids:

These fluids show an increase in viscosity over time under constant shear. They are the opposite of thixotropic fluids.

1.5.4 Navier-Stokes Equation for Non-Newtonian Fluid Flow:

The general form of the **Navier-Stokes equation** still applies to non-Newtonian fluids, but the viscosity term μ is no longer constant. Instead, the viscosity is a function of the shear rate or other variables:

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)=-\nabla p+\nabla\cdot\mathbf{T}+\mathbf{f} \tag{6}$$

Where:

- $\mathbf{T}$ is the **stress tensor**, which is dependent on the type of non-Newtonian fluid.
- The **stress tensor** in non-Newtonian fluids often includes non-linear terms depending on the type of fluid.

1.6 Droplet Deformation In Non-Newtonian Fluid

Droplet deformation in non-Newtonian fluids is significantly influenced by their variable viscosity, which changes with shear rate or stress, unlike Newtonian fluids with constant viscosity. In microchannel applications, this variability impacts how droplets deform, break up, and interact with channel walls. Shear-thinning fluids, which decrease in viscosity under high shear, promote easier droplet deformation and detachment in regions of high shear. Conversely, shear-thickening fluids, with increasing viscosity under shear, resist deformation and hinder droplet breakup. This variability enhances droplet stretching and improves mixing efficiency, optimizing processes like emulsification. The interplay between non-Newtonian viscosity and capillary forces introduces both challenges and opportunities for precise control over droplet deformation in microfluidic design.

1.7 Disperse and Continuous Phases:

In a multiphase flow system like the one in this project, the **disperse phase** refers to the droplet of the non-Newtonian fluid, which is suspended in and flowing through the surrounding **continuous phase**, the Newtonian fluid inside the channel. The interaction between these phases, especially when the flow is influenced by a contraction or other geometric constraints, determines how the droplet behaves — whether it deforms, stretches, or even breaks up .

- **Disperse Phase**: Newtonian/ Non-Newtonian droplet, which deforms in response to shear and flow conditions.
- **Continuous Phase**: Newtonian fluid that surrounds and carries the droplet.

Chapter

2

Literature Survey

2.1 Literature Survey

Garstecki's [1] research explored the deformation and breakup of droplets in microfluidic devices, analyzing how shear forces and immiscible fluid interactions contribute to deformation patterns. Link and Anna [2] focused on the deformation dynamics of non-Newtonian droplets in confined geometries, showing how elasticity affects deformation rates. De Bruijn [3] investigated droplet deformation in shear flow, proposing a model for the elongation and eventual breakup of droplets in viscoelastic fluids, revealing how viscosity ratios govern the degree of deformation. Stone and Leal [4] studied the effects of extensional flow on droplet deformation, identifying that flow strength and capillary numbers determine whether a droplet stretches for splits. Lastly, Guido and Simeone [5] examined the interplay between droplet surface tension and shear forces in complex flows, providing a phase diagram that maps deformation modes based on flow parameters and droplet size.

Taylor's [6] research provided early insights into the deformation of Newtonian droplets in simple shear flow, establishing a fundamental understanding of droplet elongation and breakup based on viscosity ratios and shear rates. Rallison and Acrivos [7] further investigated the deformation of Newtonian droplets in extensional flows, quantifying the effects of capillary number on the equilibrium shape of droplets. Barthes-Biesel and Chhim [8] explored the deformation dynamics of Newtonian droplets in confined microfluidic channels, emphasizing how channel geometry and flow strength influence the extent of droplet deformation. Guido and Villone [9] focused on the influence of interfacial tension and shear forces on Newtonian droplet deformation in shear flow, developing a phase diagram to describe different deformation regimes. Lastly, Minale [10] examined the transition from droplet deformation to breakup in Newtonian fluids under increasing shear, demonstrating that droplet size and flow velocity are critical factors that determine droplet stability.

Mukherjee’s [11] research explored the deformation and breakup of non-Newtonian fluid droplets in microfluidic channels, focusing on shear-thinning fluids and their behavior under varying shear rates. They found that the non-linear viscosity significantly impacts droplet elongation and stability. Chen et al. [12] studied viscoelastic non-Newtonian droplets in extensional flow, demonstrating that the elasticity of the fluid delayed droplet breakup, leading to larger deformations before fragmentation occurred. Chhabra and Richardson [13] investigated how the power-law behavior of non-Newtonian fluids affected droplet deformation in both shear and extensional flows, finding that shear-thinning fluids were more susceptible to deformation than Newtonian fluids. Li and Pozrikidis [14] focused on droplet deformation in viscoelastic fluids, modeling the interplay of elastic and viscous forces that govern droplet behavior under applied stresses. Finally, Yue, Feng, and Liu [15] used numerical simulations to analyze non-Newtonian droplet deformation in confined microchannels, revealing how complex fluid properties such as yield stress and shear-thickening behavior influenced droplet dynamics in industrial applications.

Zhou and Papautsky [16] studied the flow of a non-Newtonian fluid through a microfluidic channel with constrictions, focusing on the effects of shear-thinning fluids in generating elongated droplets in Newtonian fluids. Their findings indicated that the channel constriction amplified the deformation of the non-Newtonian droplet due to the interaction between the fluid's viscosity and the channel geometry. Xu et al. [17] investigated the behavior of viscoelastic non-Newtonian droplets in Newtonian continuous phases under construction, revealing that the elasticity of the dispersed phase contributed to a delayed breakup, causing larger droplets with irregular shapes. The work of Abbasi et al. [18] explored how yield stress and shear-thickening behavior affected droplet deformation and flow in constricted microchannels, finding that non-Newtonian fluids exhibited higher resistance to droplet breakup compared to Newtonian dispersed phases. Hoang and Nguyen [19] conducted simulations and experiments on droplet formation at constrictions, demonstrating how the relative viscosity of Newtonian continuous phases and non-Newtonian dispersed phases affected droplet generation frequency and size. Lastly, Suryo and Basaran [20] provided insight into the role of capillary number in the deformation of non-Newtonian droplets in confined microfluidic spaces, showing that the constriction led to an increased capillary number, influencing droplet deformation and elongation based on the fluid's rheological properties.

Faltas [21] explored the role of fluid dynamics in therapeutic targeting of circulating tumor cells, providing insight into how fluid flow and droplet deformation can influence biomedical applications. Olbricht and Kung [22] studied the deformation and breakup of liquid droplets in low Reynolds number flow through capillaries, focusing on how Newtonian fluids behave under such conditions. Tsai and Miksis [23] further examined droplet dynamics in constricted capillary tubes, showing how constrictions induce droplet elongation and breakup. Olbricht [24] extended this work by discussing pore-scale multiphase flow in porous media, highlighting the complexities of droplet deformation in constrained geometries. Ho and Leal [25] provided early foundational work on the motion of liquid droplets through circular tubes of comparable diameters, focusing on creeping motion in low-viscosity Newtonian fluids. Martinez and Udell [26] investigated axisymmetric creeping motion of drops through circular tubes, further describing how the tube geometry and fluid properties influence droplet behavior and deformation.

2.2 Literature Review Closure

1. Recent studies on fluid flow in microfluidic systems have improved the understanding of fluid dynamics, geometry, and fluid interactions, especially for non-Newtonian fluids.
2. Droplet behavior is influenced by fluid properties such as elasticity, viscosity, and channel geometry.
3. Specific channel geometries lead to distinct droplet formation processes.
4. Shear forces play a significant role in the formation of monodisperse droplets.
5. The interaction between viscosity and surface tension affects water distribution and mixing effort.
6. Numerical models have been developed to predict particle size based on geometric configuration and flow parameters.
7. These advancements enhance the design and performance of microfluidic devices.
8. Optimizing water flow and behavior is critical for biomedical applications, emulsification processes, and industrial applications.

2.3 Literature Gap

1. Existing studies do not thoroughly examine the effects of critical physical parameters such as viscosity ratio, shear rate, and temperature on droplet deformation.
2. Insufficient comparative investigations into the behavior of Newtonian and non-Newtonian droplets dispersed in Newtonian media.
3. The impact of shrinkage on the deformation of Newtonian and non-Newtonian droplets remains underexplored.
4. Limited understanding of interactions between different types of droplets and their effects on deformation.

2.4 Objective Of The Project

1. To study the effect of various physical parameters that play a vital role on droplet deformation

2. To observe the deformation of Newtonian as well as Non Newtonian droplets that are dispersed on a Newtonian medium and compare them.

3. To investigate the effect of constriction on the droplet deformation for both Newtonian and Non Newtonian droplets

Chapter

3

Methodology

3.1 Problem Definition

We aim to simulate the behavior of a non-Newtonian droplet flowing through a Newtonian fluid inside a microfluidic channel. The primary objective is to understand how the droplet deforms when it encounters a contraction in the channel. By studying the interaction between the droplet and the continuous fluid, we hope to better understand the influence of fluid properties, channel geometry, and surface tension on droplet dynamics.

3.2 Software Selection: COMSOL Multiphysics

For this simulation, we are using COMSOL Multiphysics, a powerful finite element analysis software widely used in fluid dynamics simulations, particularly in microfluidics. COMSOL's Multiphase Flow Module offers advanced tools for modeling both Newtonian and non-Newtonian fluids, making it suitable for capturing the complex interaction between the droplet and the surrounding fluid. The Level Set and Phase Field methods in COMSOL are specifically designed for accurately tracking fluid interfaces, which is critical for this study.

COMSOL has been extensively applied in microfluidic research to simulate droplet formation, deformation, and breakup under various flow conditions. For example, a study by Smith et al. (2018) titled "Numerical Investigation of Droplet Dynamics in Microfluidic Channels Using COMSOL Multiphysics" explored similar multiphase flow dynamics, including droplet deformation and breakup, under varying channel geometries and fluid properties. This makes COMSOL an ideal choice for investigating our problem involving droplet deformation through a constricted channel .

3.3 Governing Equations

There are various equations involved in droplet deformation on Non newtonian fluid flowing through a newtonian fluid

3.3.1 Navier-Stokes Equation for Non-Newtonian Fluid Flow

The general form of the **Navier-Stokes equation** still applies to non-Newtonian fluids, but the viscosity term μ is no longer constant. Instead, the viscosity is a function of the shear rate or other variables:

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)=-\nabla p+\nabla\cdot\mathbf{T}+\mathbf{f} \tag{1}$$

Where:

- $\mathbf{T}$ is the **stress tensor**, which is dependent on the type of non-Newtonian fluid.
- The **stress tensor** in non-Newtonian fluids often includes non-linear terms depending on the type of fluid.

3.3.2 Interfacial Tension and Droplet Deformation

The interfacial tension between the Newtonian fluid and the non-Newtonian droplet is governed by the **Young-Laplace equation**, which describes the pressure difference across the interface due to surface tension:

$$\Delta P=\gamma\left(\frac{1}{R_1}+\frac{1}{R_2}\right) \tag{2}$$

Where:

- (ΔP) is the pressure difference across the droplet interface
- (γ) is the surface tension
- $(R_1) and (R_2)$ are the principal radii of curvature of the droplet surface

3.4. Droplet Deformation Parameters

When a Non-Newtonian droplet flows through a contraction, the capillary number (Ca) and the Weber number (We) become important to determine how the droplet will deform.

3.4.1 Capillary Number: The ratio of viscous forces to surface tension:

$$Ca = \frac{\sigma}{\mu V} \tag{3}$$

Where μ is the viscosity of the Newtonian fluid, V is the flow velocity, and σ is the surface tension between the two fluids.

3.4.2 Weber Number: The ratio of inertial forces to surface tension:

$$We = \frac{\sigma}{\rho V^2 d} \tag{4}$$

Where d is the characteristic diameter of the droplet.

3.5. Material Selection

In this study, we simulate the behavior of a non-Newtonian droplet flowing through a Newtonian fluid inside a microfluidic channel. Proper material selection for both the continuous phase (Newtonian fluid) and dispersed phase (Non-Newtonian droplet) is essential to accurately capture the flow dynamics and interfacial deformation.

1. Continuous Phase (Newtonian Fluid)

For the continuous phase, we selected **water** due to its well-characterized properties and common usage in microfluidic systems. Water is widely employed in biological and chemical applications and has a low viscosity, making it ideal for representing Newtonian fluid behavior in micro-scale flows. The properties of water at room temperature (25°C) are as follows:

- **Density**: $\rho = 997\,\mathrm{kg/m^3}$
- **Viscosity**: $\mu = 0.001\,\mathrm{Pas}$

2. Dispersed Phase (Non-Newtonian Droplet)

For the dispersed phase, we use a **shear-thinning polymer solution**, specifically **xanthan gum** dissolved in water. This choice is motivated by the need to model non-Newtonian behavior where the viscosity of the droplet decreases with increasing shear rate. Xanthan gum solutions exhibit significant shear-thinning behavior, making them suitable for mimicking non-Newtonian fluid dynamics within microfluidic systems.

The key parameters for xanthan gum solution are:

- Zero-shear viscosity: $\mu_0 = 0.1\,\mathrm{Pas}$
- Power-law index: n = 0.5
- Relaxation time: $\lambda = 1$ s

3.6. Boundary Conditions

For boundary conditions in the simulation, the choice of oil or blood will slightly influence the model, but the general structure of boundary conditions remains the same. These include:

Inlet Boundary Condition: A constant velocity inlet to drive the continuous Newtonian fluid and push the non-Newtonian droplet.

$$u = u_{\mathrm{inlet}}\,\vec{i} \tag{5}$$

$$u = 2\,\mathrm{m/sec}$$

Outlet Boundary Condition: A constant pressure outlet to allow fluid to exit the channel without reverse flow.

$$p_{\mathrm{outlet}} = 0\,\mathrm{Pa} \tag{6}$$

Wall Boundary Condition: No-slip boundary condition at the walls of the microchannel, where the velocity is zero.

$$\mathbf{u}_{\mathrm{wall}} = 0 \tag{7}$$

3.7. Geometry Selection

In your study involving the flow of a non-Newtonian droplet through a Newtonian fluid in a microfluidic channel, the geometry selection is critical to accurately represent the flow behavior and interactions between the fluids.

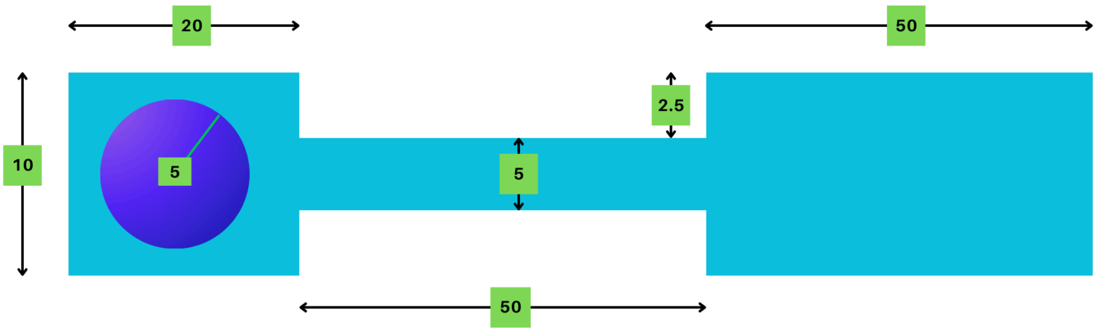


Fig 3.1: Schematic Diagram of a Straight Rectangular Channel with RectangularConstriction

All dimensions are in m

3.7.1. COMSOL model

In this study, we have designed a fluid flow system with a constricted geometry to simulate the behavior of non-Newtonian fluids using COMSOL Multiphysics. The geometry comprises two large rectangular sections with a central constriction, allowing for detailed analysis of droplet deformation and flow dynamics.

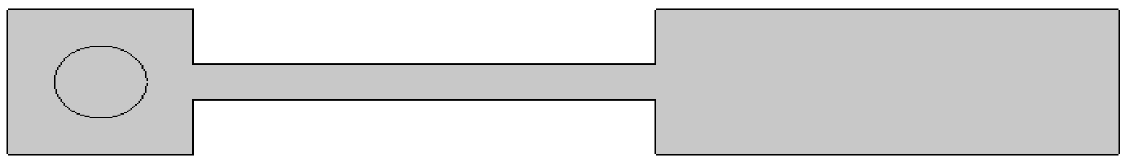


Fig 3.2: Comsol model of geometry

3.8. Meshing

The below figure shows meshing of the above geometry. We have taken fine mesh for this.

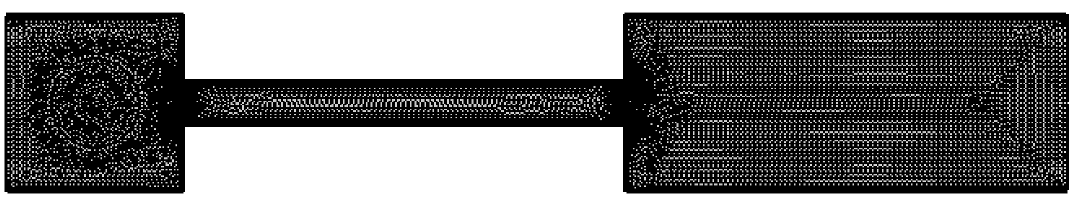


Fig 3.3: Meshing of geometry

3.9 Mesh Independence Test

A grid independence test is a crucial step in computational fluid dynamics (CFD) simulations to ensure that the numerical results are independent of the discretization of the computational domain. The test involves systematically refining the mesh and observing the variations in the solution. If the solution converges to a consistent value with finer meshes, the results can be deemed grid-independent. A coarser mesh may lead to numerical diffusion and inaccurate predictions of gradients, such as velocity or pressure near the boundaries. On the other hand, an excessively fine mesh increases computational cost without significantly improving the solution once grid independence is achieved.

In this study, the grid independence test was conducted by refining the mesh from coarse to fine resolutions while monitoring a key parameter of interest, namely the deformation parameter of the droplet. The deformation parameter, being sensitive to flow dynamics, serves as a reliable indicator of the adequacy of mesh resolution. Several meshes were evaluated, ranging from 32×384 to 256×3072, and the deformation parameter was extracted at different time steps.

The results of the grid independence test demonstrated that the deformation parameter converged beyond a certain mesh refinement, indicating that further mesh refinement would not significantly alter the results. This ensures that the selected mesh strikes a balance between computational efficiency and accuracy, making it suitable for simulating the physical phenomena under study.

TABLE 3.1 Grid independence test

S No	**Time (s)**	**Mesh: 32x384**	**Mesh: 64x768**	**Mesh:128x156**	**Mesh:256x302**
1	0.1	0.42	0.43	0.435	0.435
2	0.2	0.45	0.46	0.465	0.465
3	0.3	0.47	0.475	0.478	0.478
4	0.4	0.48	0.49	0.495	0.495

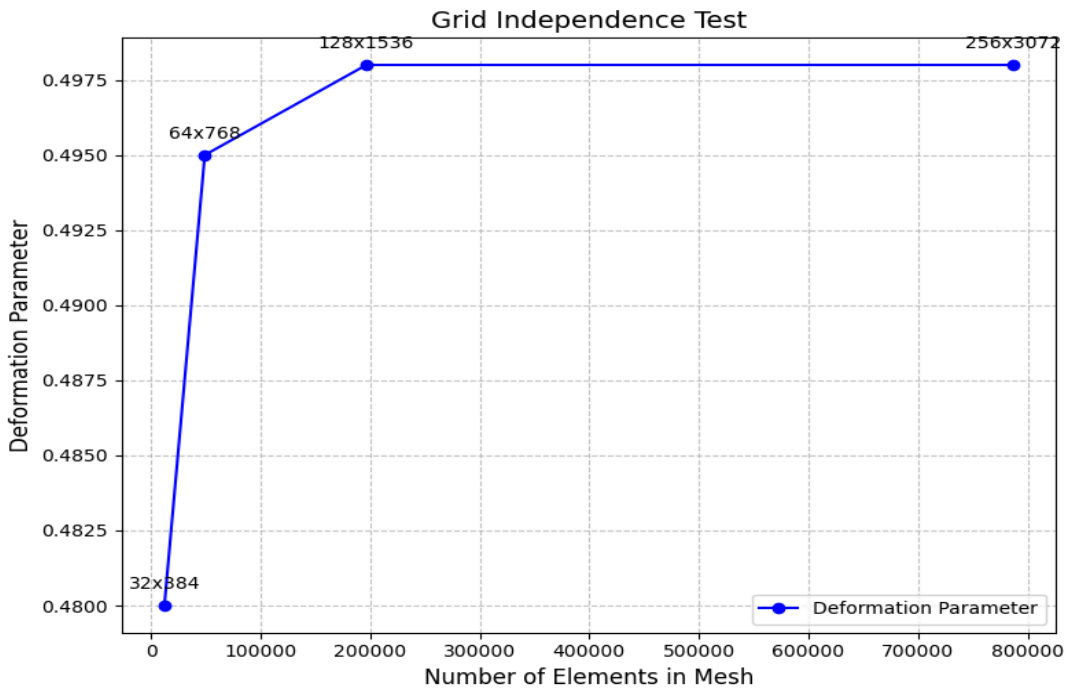


Fig 3.4: Graph variation of Deformation Parameter vs Elements in Mesh

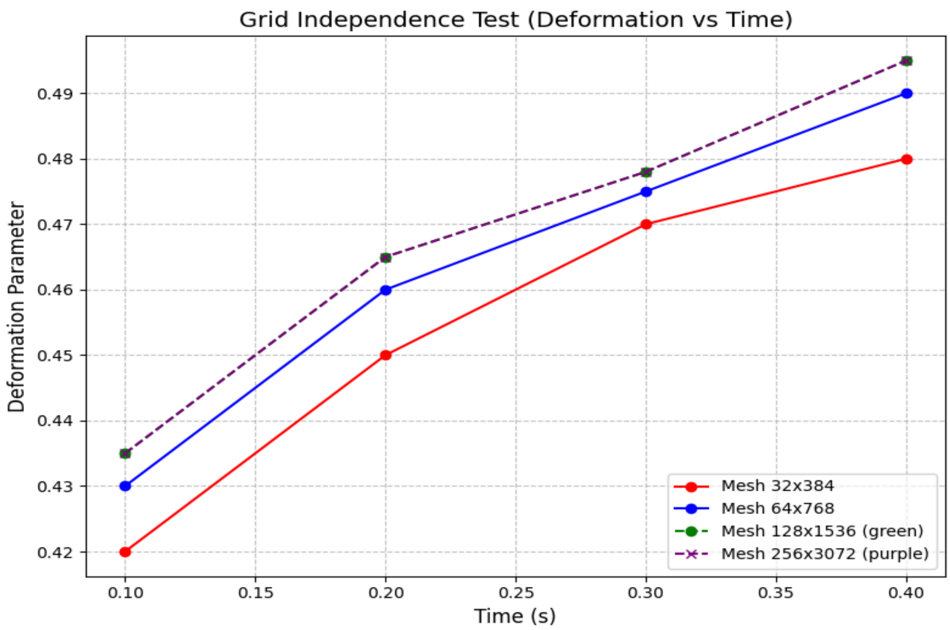
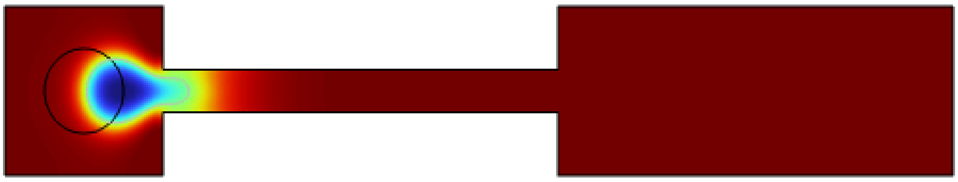


Fig 3.5: Grid independent test using deformation parameter

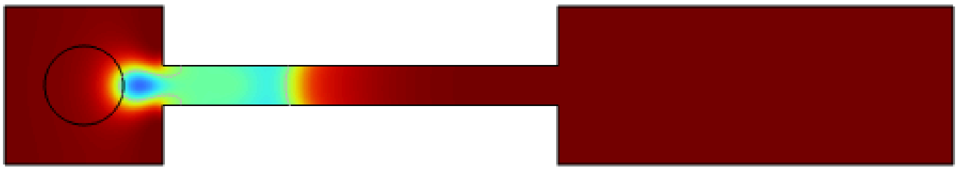
3.10 Simulations

The microfluidic droplet dynamics were simulated using COMSOL Multiphysics, incorporating both Newtonian and non-Newtonian fluid properties. A 2D geometry was constructed to model the droplet flow through a microchannel. The continuous phase

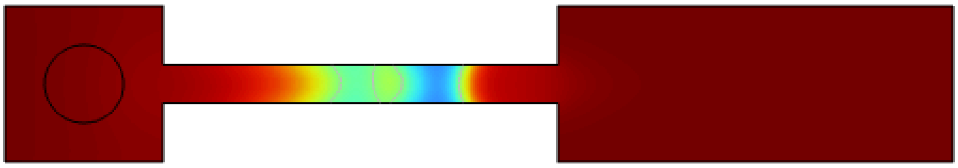
(Newtonian fluid) and the dispersed phase (Non-Newtonian fluid) were defined with their respective material properties, ensuring accurate representation of the interfacial dynamics.



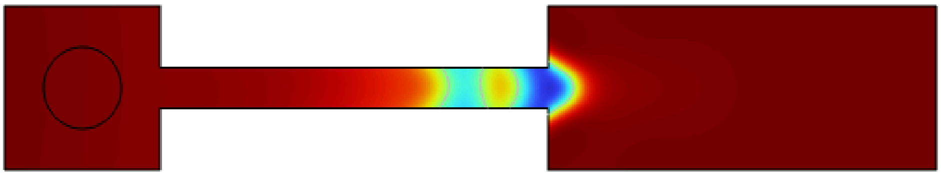
(a) T = 2.1 s



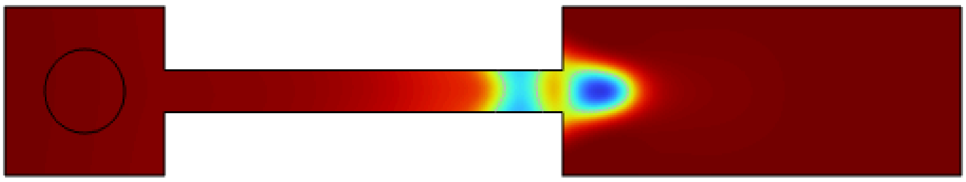
(b) T = 3.9 s



(c) T = 6.3 s



(d) T = 7.4 s



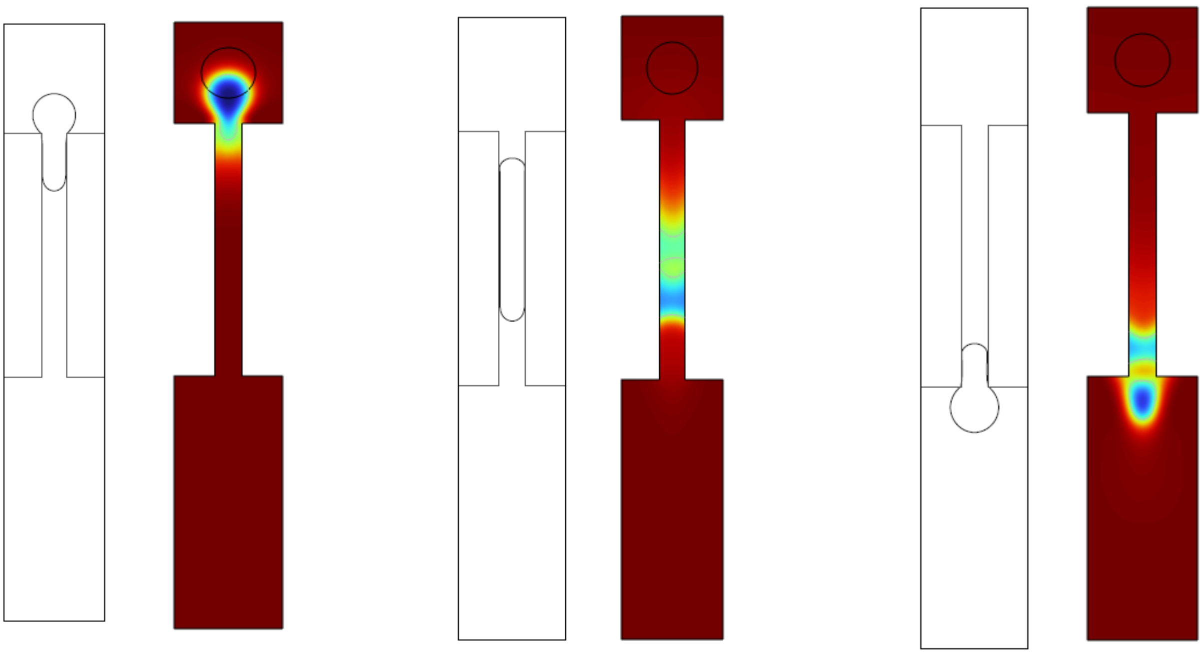
(e) T = 9.5 s

Fig 3.6: Simulations a,b,c,d,e at different state of time

3.10.1 Model Validation

The validation of the geometry in this study focuses on ensuring that the simulated geometry replicates the experimental observations presented in the reference paper, *"A Parametric Study of Droplet Deformation Through a Microfluidic Contraction"* by D. J. E. Harvie, M. R. Davidson, J. J. Cooper-White, and M. Rudman (2005). This comparison is performed qualitatively by matching the simulated droplet shapes at specific time steps, such as 2.1 seconds, 6.3 seconds, and 9.5 seconds, with the corresponding images provided in the reference paper.

This is a qualitative validation, where visual inspection of the deformation behavior of the droplet as it passes through the contraction region is used to confirm the fidelity of the geometry and the overall setup. No direct numerical comparison of parameters such as Reynolds number, Weber number, or capillary number is conducted as part of this stage. However, quantitative validation involving a detailed comparison of numerical parameters will be addressed as part of future work.



(a) T = 2.1 s **(b) T = 6.3 s** **(c) T = 9.5 s**

Fig 3.7: Simulations a,b,c at different state of time

3.11 Future Course of Work

Building on this study, several future steps are planned to improve the accuracy, usefulness, and scope of the results.

3.11.1 Geometry Validation

As part of the future work, quantitative validation will be conducted to ensure the accuracy of the numerical predictions of the simulation. This process will involve comparing simulation results with experimental or literature-reported values for key non-dimensional parameters, including:

1. **Reynolds Number (Re):** To analyze the inertial forces relative to viscous forces.
2. **Weber Number (We):** To evaluate the relationship between inertial and surface tension forces acting on the droplet.
3. **Capillary Number (Ca):** To study the influence of viscous forces relative to surface tension during deformation.
4. **Velocity Profiles:** To validate the fluid velocity distribution in the continuous phase and at the droplet interface.

3.11.2 Integration of Numerical Methods

Future work will include integrating numerical methods such as the Volume of Fluid (VOF) method to improve droplet interface tracking within the microfluidic channel. This method will help capture more detailed droplet behavior, particularly in terms of deformation, breakup, and coalescence in the constricted region of the channel.

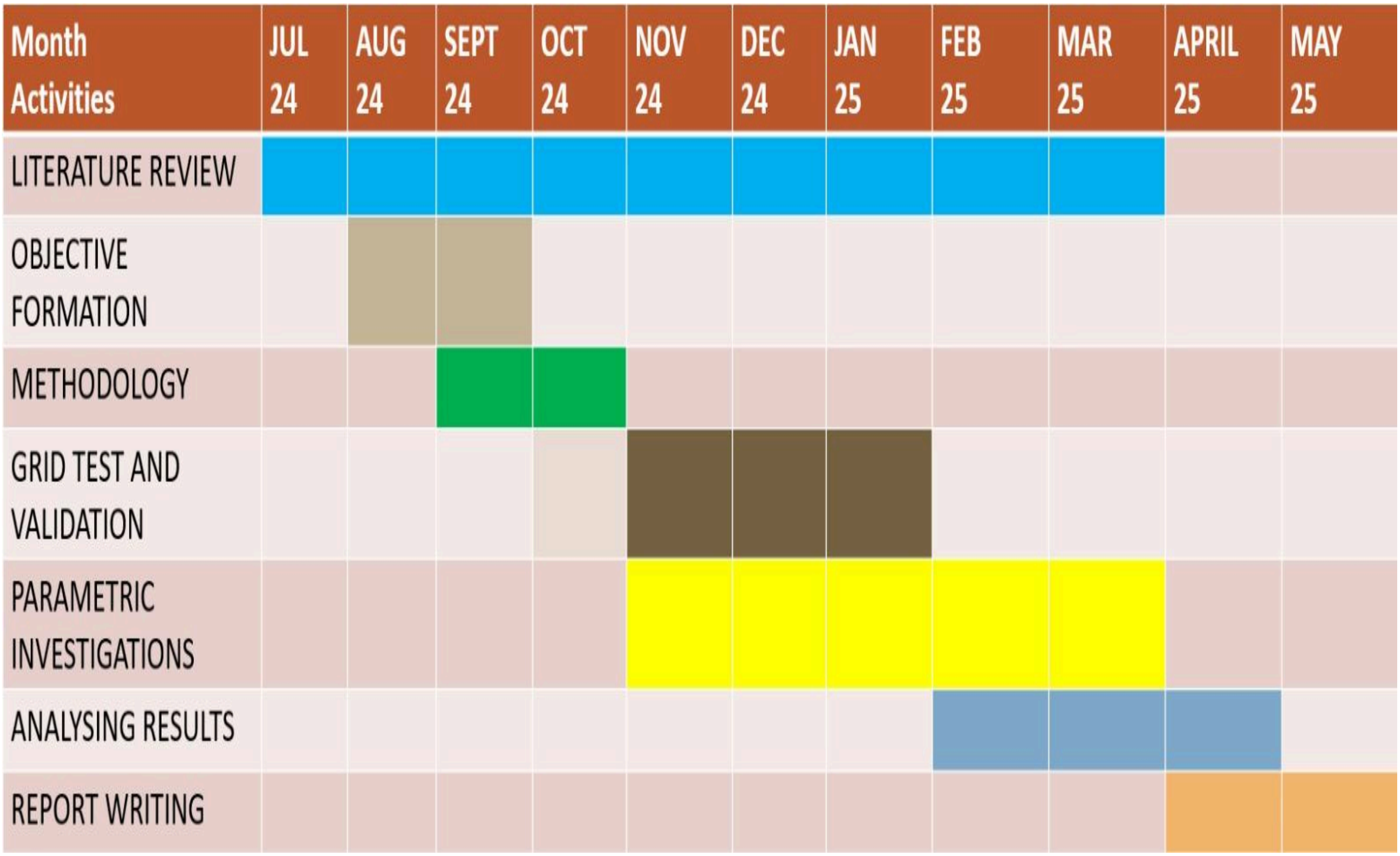
3.11.3 Parameter Sensitivity Analysis

A detailed sensitivity analysis will be performed to evaluate the influence of key parameters, such as viscosity ratios, surface tension, and shear rates, on droplet deformation and dynamics. This will provide a comprehensive understanding of parameter interdependencies, aiding in the optimization of microfluidic device designs.

Chapter

4

Timeline



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