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Numerical Simulation of a Bubble Rising in an Environment Consisting of Xanthan Gum

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Abstract

An improved numerical algorithm for front tracking method is developed to simulate a bubble rising in viscous liquid. In the new numerical algorithm, volume correction is introduced to conserve the bubble volume while tracking the bubble's rising and deforming. Volume flux conservation is adopted to solve the Navier–Stokes equation for fluid flow using finite volume method.

Non-Newtonian fluids are widely used in industry such as feed and energy industries. In this research we used Xanthan gum which is a microbiological polysaccharide. In order to obtain the properties of the Xanthan gum, such as viscosity, storage and loss modulus, shear rate, etc., it was necessary to do an amplitude sweep and steady flow test in a rheometer with a concentric cylinder as geometry.

Based on the data given and using a numerical regression, the coefficients required by Giesekus model are obtained. With these coefficients, it is possible to simulate the comportment of the fluid by the use of the developed algorithm. Once the data given by OpenFOAM is acquired, it is compared with the experimental data.

INTRODUCTION

Most of the times, there are air bubbles that are conformed due to industrial process as column reactors, fermentation, mineral processing and petrochemical processes. [1]

Despite of non-Newtonian fluids are frequently used in the industry, there is not much research about their behavior, and the existing studies are based mainly on experiments. Nevertheless, the experimentation is a process that cannot represent important details of the fluid, such as mass transfer and flow structure, details that can be obtained through the numerical simulation. Authors as Bhaga, Weber [2] and Funfschilling [3] analyzed the behavior of air bubbles and the deformation that they experiment. In the recent literature, Zhang [1] developed an algorithm to simulate a bubble rising in non-Newtonian fluid. Kishore [4] obtained through numerical simulation, the steady state drag coefficients and flow patterns of a Newtonian sphere fluid sedimenting in power-law liquids. But, all the mentioned studies used the power-law and Carreu models which are linear models that have problems to describe the comportment at low shear rate region.

Hence, this work applies the Giesekus model [5] which is a non-linear model for viscoelastic fluid. The Giesekus model requires three material parameters and is one of the most used differential constitutive relation to characterize the non-linear viscoelastic behavior [6].

Xanthan gum is used for the experimental test by using different concentration. The xanthan gum is a microbiological polysaccharide, produce by the fermentation of xanthomonas campestris [7]. Because of its properties as stabilizer, Xanthan is primarily used for emulsions, water-based formulations and foams in feed, cosmetics and medical industries since its finding in 1950. [8]

METHODOLOGY

System description

With the aim of simplify the research, the Xanthan solution with air bubbles was considered as a multiphase fluid where the xanthan was a non-Newtonian fluid, while the bubbles were modeled as a Newtonian fluid. The solution was supposed to be isothermal, immiscible and under steady flow conditions. The computational domain is represented in the "Fig. 1."

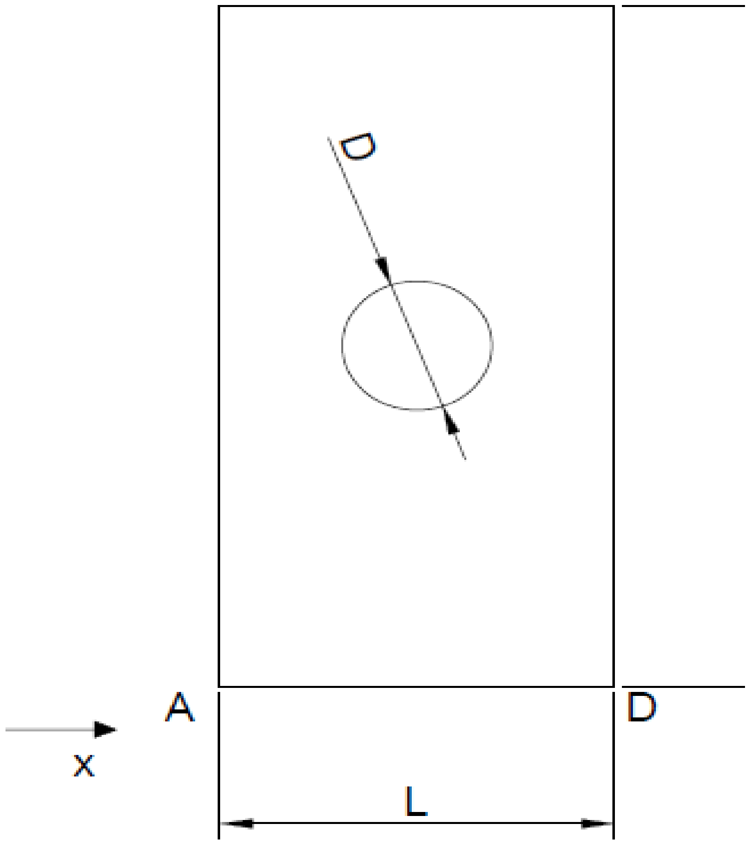


Figure 1: Schematic diagram for numerical simulation.

The Xanthan solution was prepared by dissolving 0.5%, of Xanthan in water. This procedure required a precision scale and a magnetic stirrer. The Xanthan solution was prepared at 20°C and mixed until the gum powder was completely dissolved into water.

The rheometer employed was a Discovery HR-2 rheometer from TA Instruments which was used to obtain the rheological properties of the Xanthan gum with a concentric cylinder geometry.

Two types of tests were performed: an amplitude sweep and steady flow tests both of which were taken at 20°C.

The VOF method

In this study, the volume of fluid (VOF) method was used for surface-tracking. VOF method is part of the Eulerian methods characterize for a mesh that could be either stationary or mobile. This method is based in Marker-and-cell (MAC) methods and use the fraction function C as the defined integral of fluids' characteristic function in the control volume. VOF method has different advantages as the maintenance of sharp interfaces through the surface compression approach, mass conservation without any reinitialization step and restriction of the volume fraction $0 \leq \Upsilon \leq 1$ [9].

Here, to distinguish each fluid, the Hamilton-Jacobi equation was used, expressed as

$$\Upsilon = \begin{Bmatrix} 1 Xanthan \\ 0 Airbubble \\ 0 < \Upsilon < 1 attheinterface \end{Bmatrix}$$

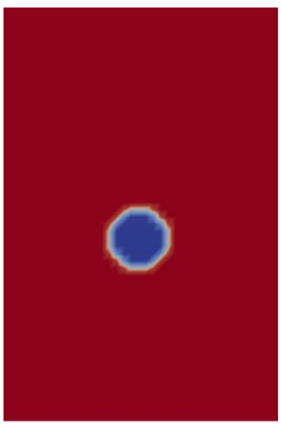


Figure 2: Blue corresponds to $\Upsilon = 0$ and red corresponds to $\Upsilon = 1$.

Governing equations

The governing equations are the equations of continuity (2) and the Navier-Stokes equation (3)

$$\nabla \cdot (u) = 0 \tag{2}$$

$$\frac{\partial(\rho u)}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \nabla \tau \tag{3}$$

Where u is the velocity vector, p the pressure, ρ the density of the fluid and τ the stress tensor. With the "Eq. (2)." and "Eq. (3)." is possible to describe the relation between the stress and deformation.

The stress tensor can be expressed in terms of the Newtonian solvent τ_s and the elastic polymeric τ_p:

$$\tau = \tau_s + \tau_p \tag{4}$$

$$\tau_s = 2\eta_s D \tag{5}$$

$$D = \frac{1}{2}(\nabla u + [\nabla u]^T) \tag{6}$$

Where η_s is the solvent viscosity and D is the deformation rate tensor.

The τ_p is a symmetric tensor obtained as the sum of the contribution of the individual relaxation modes:

$$\tau_p = \sum_{K=1}^{n} \tau_{p_K} \tag{7}$$

Constitutive equations of Giesekus model

The Giesekus model uses two constants: λ_1,and α, which correspond to the relaxation time and the mobility factor respectively. The Giesekus equation is written as:

$$\tau = \tau_s + \tau_p \tag{8}$$

$$\tau_s = -\eta_s{}' \tag{9}$$

$$\tau_p + \lambda_1 \tau_{p_{(1)}} - \alpha \frac{\lambda_1}{n_p}(\tau_p \cdot \tau_p) = -n_p{}' \tag{10}$$

First, the zero-shear rate viscosity was determined by a steady flow test at 20°C.

After the zero-shear rate viscosity was determined, the equations for storage (G') "Eq. (12)." and loss (G''), "Eq. (11)." modules were used in order to calculate the relaxation time (λ_1). The plots were made assuming an equivalency between the frequency, and the shear rate. [10]

$$G'' = n_0 w \frac{1 + \lambda_1 w^2}{1 + \lambda_1^2 w^2} \tag{11}$$

$$G' = n_0 w^2 \frac{(\lambda_1)}{1 + \lambda_1^2 w^2} \tag{12}$$

Boundary conditions

In the analysis, the following boundary conditions were used for velocity: slip at the walls, fixedValue at the top and the bottom with a uniform value of (0 0 0), and an empty condition at the front and back. The set-value for velocity is zero. The zero gradient condition was used for pressure and for the stress tensor at the remaining boundaries. "Fig. 3."

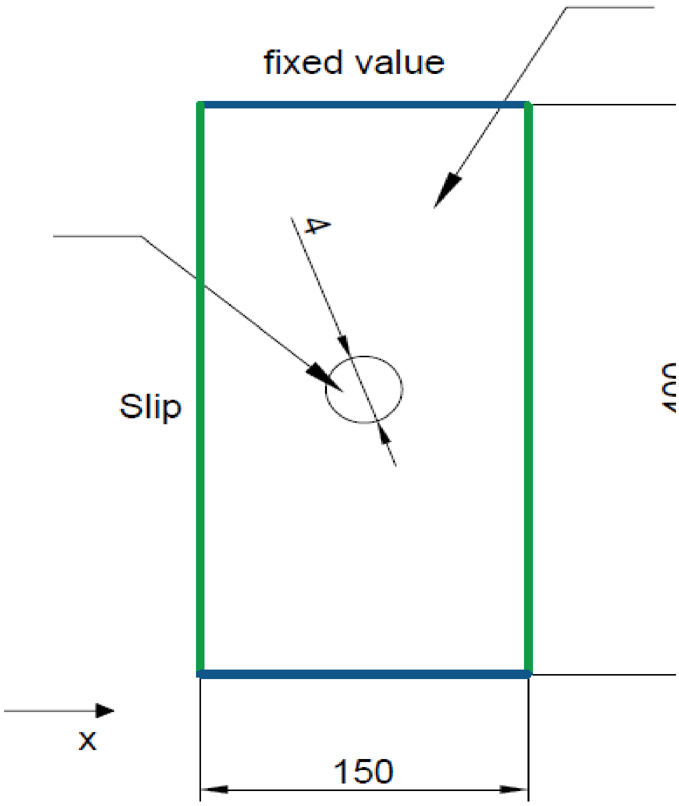


Figure 3: Schematic diagram of numerical simulation.

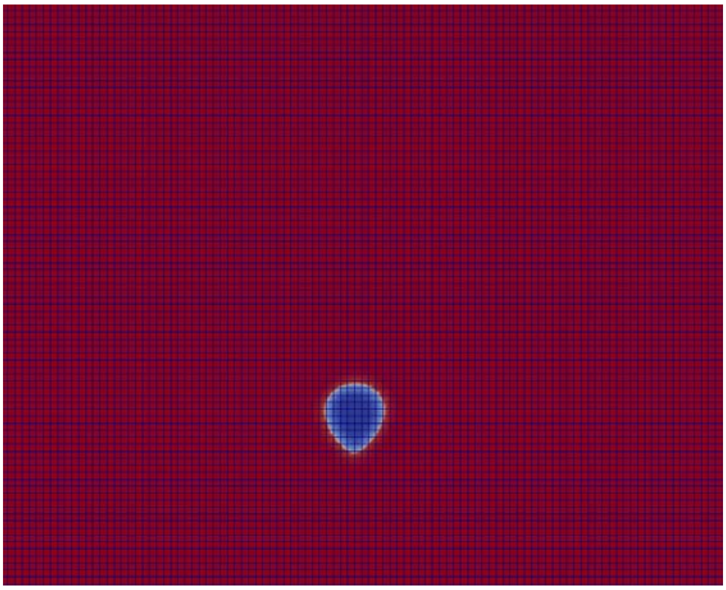


Figure 4: Computational grid

The mesh has 150 divisions in X-axis and 150 in Y-axis.

Numerical model

For the numerical model, the solver developed in the OpenFOAM software by Favero [11] was used. The Giesekus model is rearranged as:

$$\frac{1}{\lambda_k}\tau_{pk} + \tau_{p_k} - \frac{\alpha_k}{n_{pk}} * \left(\tau_{p_K} \cdot \tau_{p_K}\right) = \frac{-n_p}{\lambda_k} , \tag{13}$$

In OpenFOAM the “Eq. (13).” is represented as:

```
solve
(
    fvm::ddt(tauP) + fvm::div(phi, tauP)
    ==
    etaP / lambda * twoSymm( L ) +  twoSymm( C )
    - (alpha / etaP) * (tauP & tauP) -  fvm::Sp(1/lambda, tauP)
);
```

EXPERIMENTAL

The experiment was performed with an acrylic box that has a square section of 200 mm length and a height of 300 mm with the top open to the atmosphere. The box was under atmospheric pressure and at 20 ° C. It has a hole in the center of its bottom where a pipe of 3 mm was located. This tube was connected with a precision syringe pump that inserted air bubbles in the Xanthan solution. The surface tension of the solution is 7.2 x 10-2 N m-1 like water.

Besides the box and the pump, the images of rising bubbles were recorded using a single high-speed camera (CASIO EXILIM EX-FH20, Japan) which resolution was 1280 x 720 pixel and 30 fps.

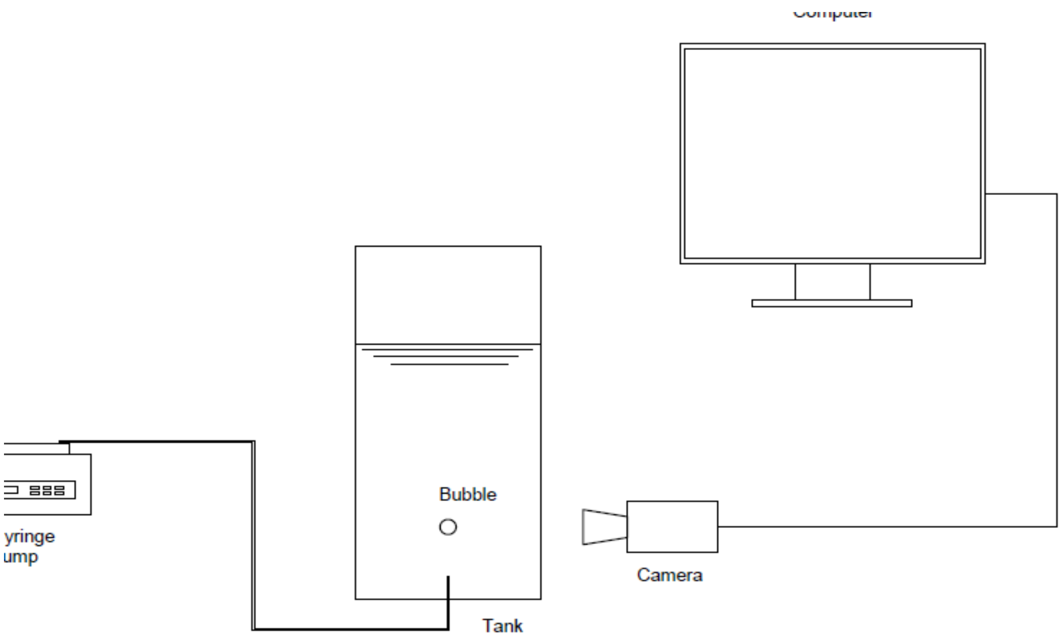
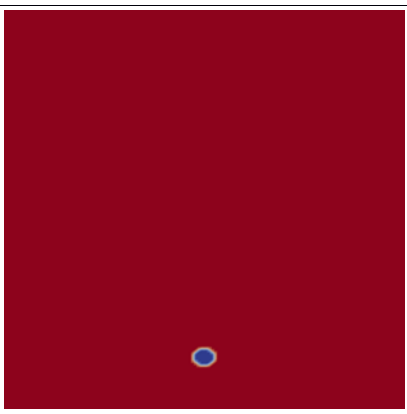
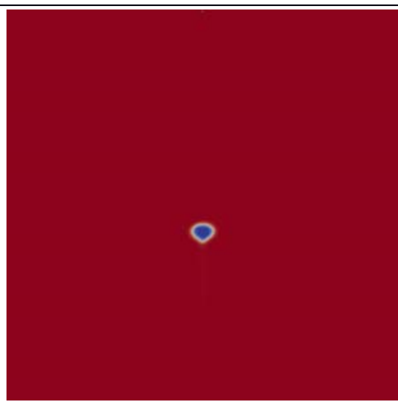
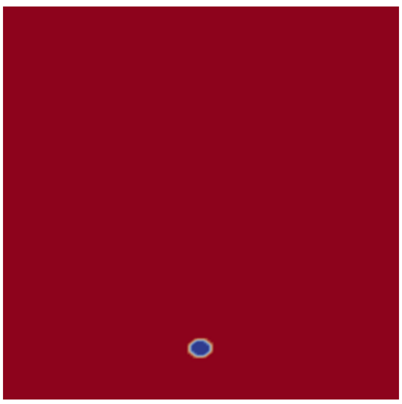
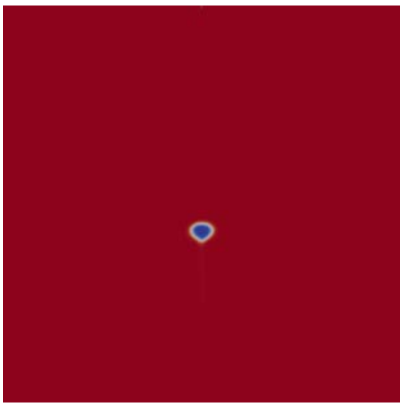


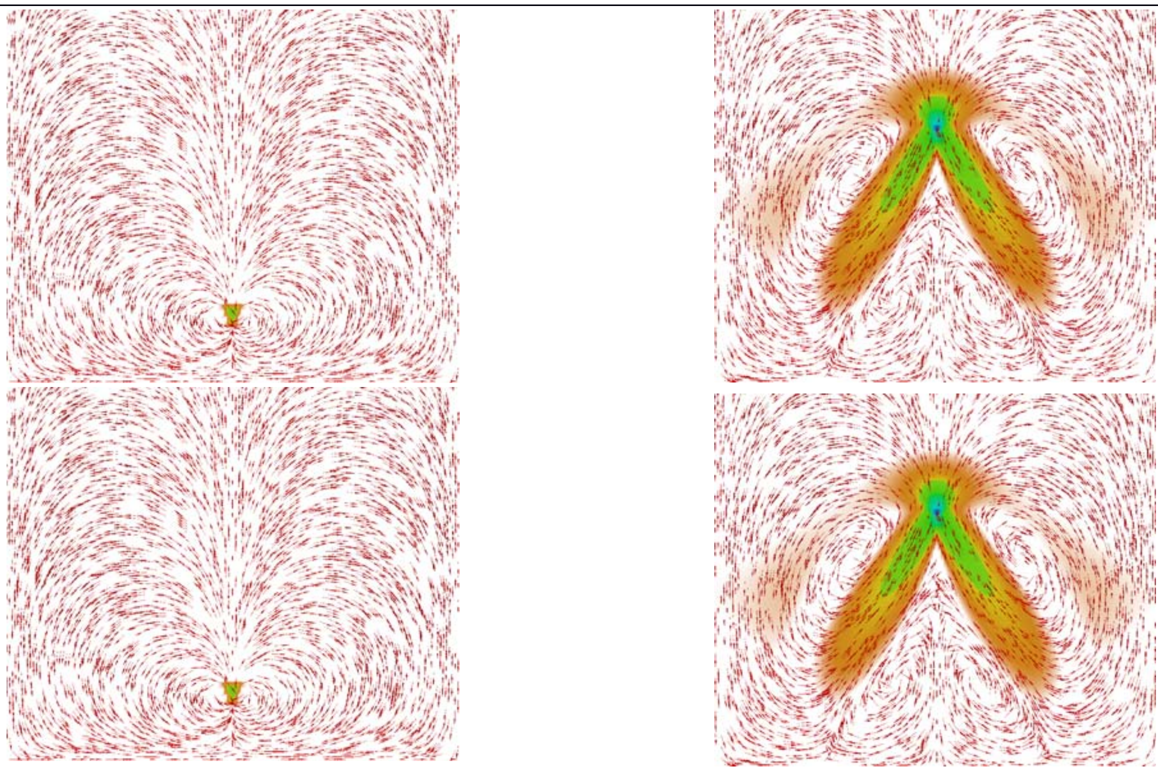
Figure 5: Schematic diagram of experimental setup.

RESULTS

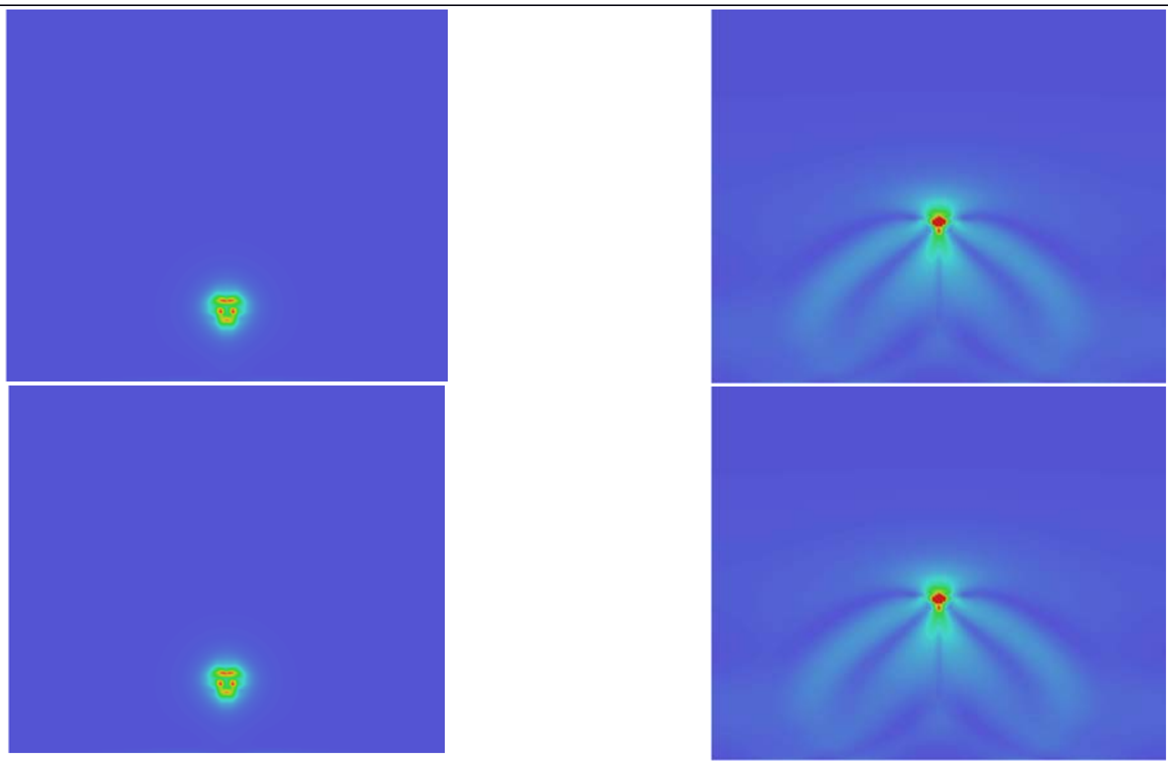
Simulation results

Table 1: The bubble shape and steady conditions given by the OpenFOAM software is compared in "Table 2." with the bubble shape and terminal steady conditions obtained with the experimental data.

t: 0 s	t: 10 s
Movement of a bubble rising in Xanthan gum	
	
	
Velocity field around a bubble rising	



Shear rate distribution and shape of a bubble rising



Shear stress at different times

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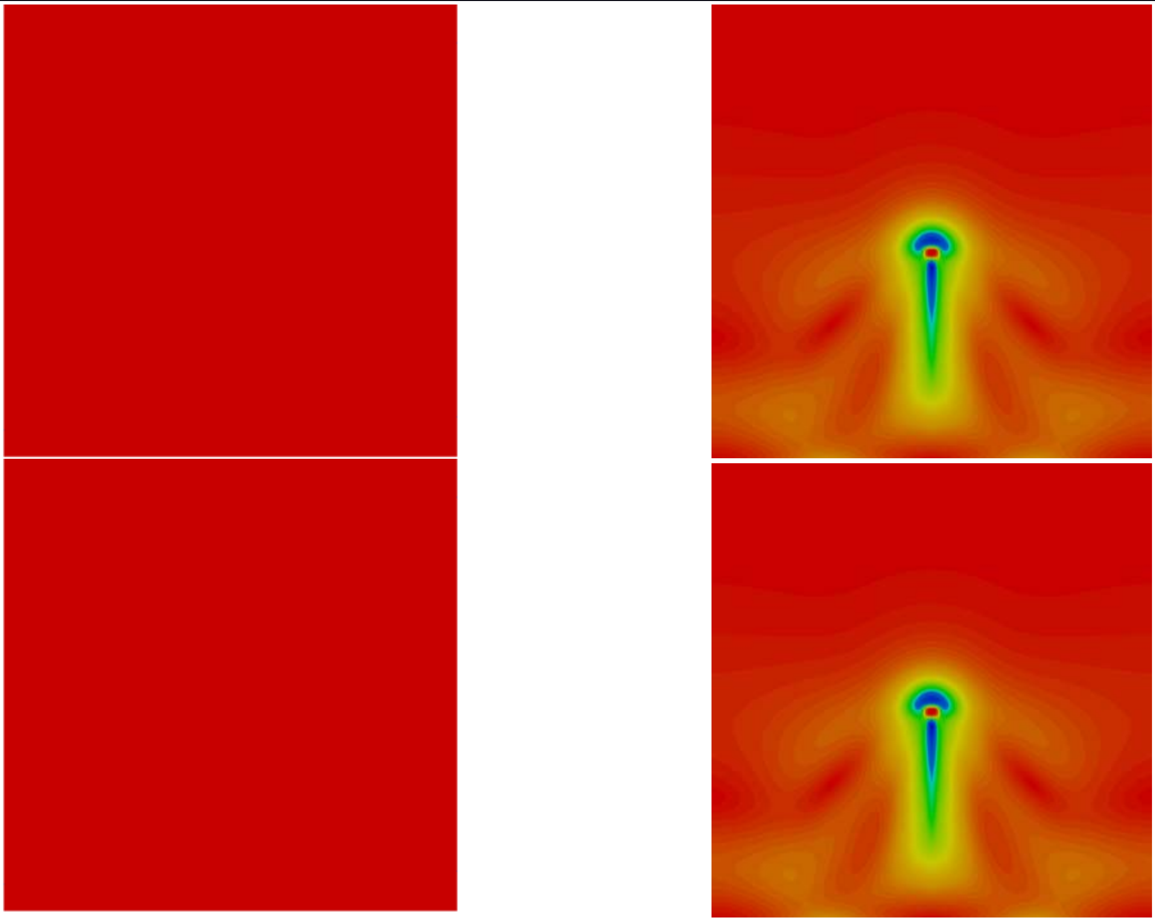
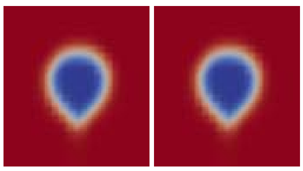
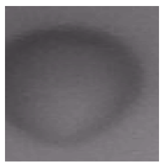
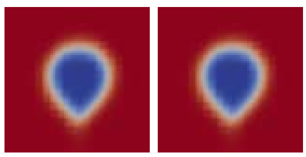
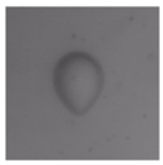
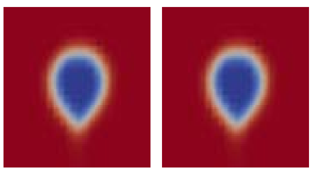


Table 2: Comparisons of bubble shapes observed in simulation and the experiment.

Time (s)	Simulation	Experiment
5		
7.5		
10		

To compare the results obtained in the simulation and experimentation is necessary to characterize the bubble. For this, we define a bubble acting under the influence of gravitational forces in a viscous fluid; this can be grouped in three different regimes: Spherical, ellipsoidal, and spherical cap as described Clift [12]. Three dimensionless numbers defined the regimen where the bubble belongs:

Bond number:

$$Bo = \frac{g\Delta\rho d_0^2}{\sigma}$$

Bond number is a dimensionless number define as the proportional ratio obtained between body forces (effective gravitational forces) and the surface tension.

Morton number:

$$Mo = \frac{g\Delta\rho n_l^2}{\sigma^3\rho_l^2}$$

The Morton number describes the properties of the surrounding fluid by using the viscosity, surface tension, gravity and density difference.

Reynolds number:

$$\mathfrak{R} = \frac{\rho_l U_t d_0}{n_l}$$

Reynolds number is a dimensionless number used to characterize the motion of the fluid, and we use this number to compare the simulation and the experiment.

“Eq. (14).”, “Eq. (15).” and “Eq. (16).” uses the following parameters: d_0 is the bubble diameter, ρ_l is liquid density, n_l is liquid viscosity, $\Delta\rho = \rho_l - \rho_g$ is density difference between continuous medium and the dispersed fluid, g is gravitational acceleration, U_t is the terminal velocity of the bubble and σ is the surface tension. In our example bubbles belongs to the ellipsoidal region.

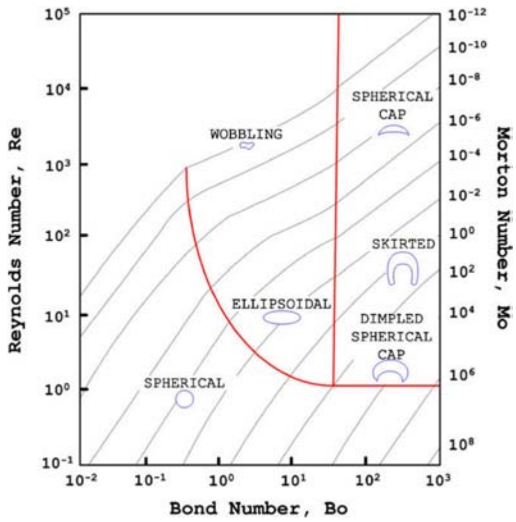


Figure 6: Shape regime map.

Ellipsoidal domain is a regime dominated by surface tension. This region has bubbles typically in the range of 1.3 to 6 mm, and the range for Bo number is 0.25 to 40. Terminal velocity is approached by the correlation suggested by Mendelson [13] based on wave theory:

$$U_t = \sqrt{\frac{2.14\sigma}{\rho_l d_0} + 0.505 g d_0}$$

The experimental data was presented in terms of Bond (Bo), Morton (Mo) (14) and Reynolds (Re) number. The evaluation is presented in “Table 3.”

Table 3: Comparisons between experimental and numerical results for a single bubble rising.

CONCENTRATION	BO	MOEXP	RECAL	REEXP	DEV%
0.5	2.17	5.08E-09	372.12	378.53	1.69

The comparison of the results obtained in the "Table 3." indicates a good agreement between the computational and experimental results. The employed model is valid for investigating the movement of the bubble at different concentration(16) laminar flow.

Rheology experiment

Xanthan gum as the majority of fluids is considered as a pseudoplastic (shear-thinning) fluid because its viscosity decreases when the strain rate increases. This behavior is showed in the “figure 7” and “figure 8.”

The necessary parameters for Giesekus model are detailed in “table 4”.

Table 4: Parameters for Giesekus model.

CONCENTRATION	NO (PA.S)	NL (M2/S)	NP (PA.S)	NS (PA.S)	λ (1/S)
0.5	82.213	0.00373	80.88	1.33	23.2

CONCLUSION

In the current research, the motion and behavior of air bubbles inside a non-Newtonian fluid are studied. The Giesekus model are used for numerical simulation. The numerical model is based in volume fluid method and the model equations are solved using the open-source OpenFOAM®, the non-newtonian library developed by Favero [xiii] was modified in order to use a multiphase solver, which is based in the interFoam solver.

The numerical model used is effective for this type of research. For instance predict their behavior, the results of the simulation are in line with those found in the literature and show agreement with those obtained experimentally.

Fluid viscosity increases as the concentration of Xanthan increases in the solution, affecting the velocity field of the bubble. The vortices generated around the bubble are the reason of the bubble deformation.

At higher concentrations, the velocity field is smaller and the Reynolds number decreases.

The domain should be much bigger to avoid the influence of the walls over the bubble and facilitate the convergence of the numerical model.

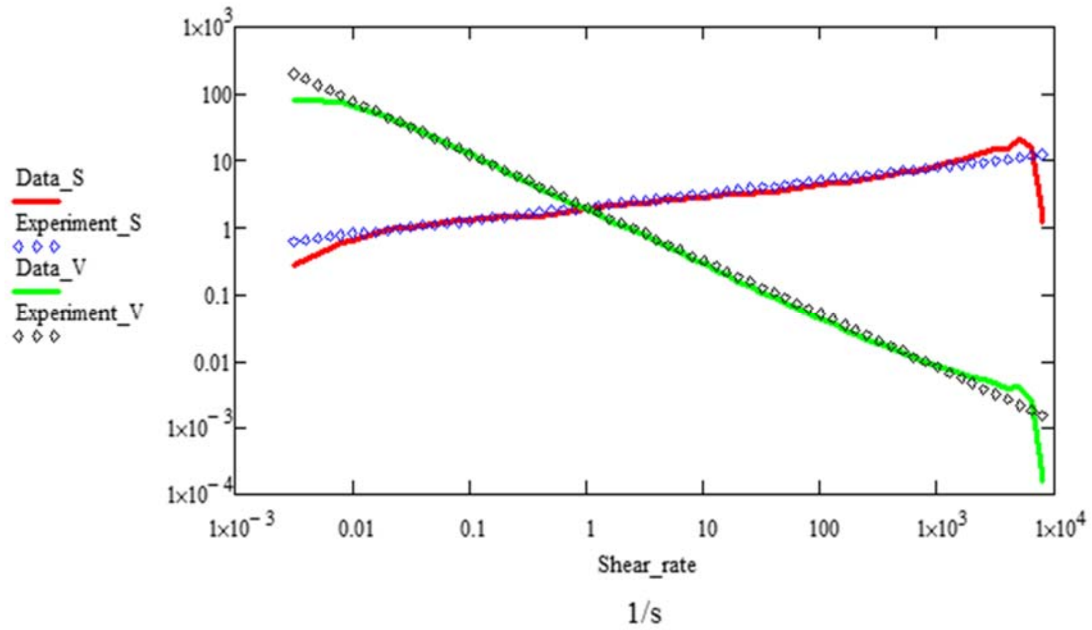


Figure 7: Comparison for steady flow test, concentration 0.5%, T = 20 °C.

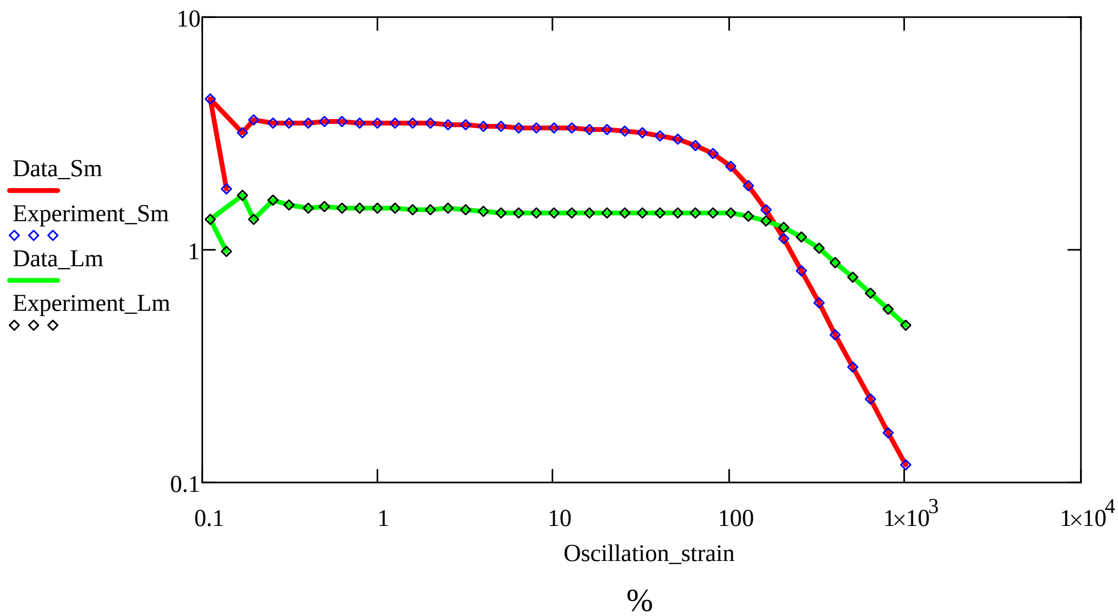


Figure 8: Comparison for the Amplitude sweep test, concentration 0.5%, T = 20 °C.

NOMENCLATURE

Notation

⍰	Phase from the Hamilton-Jacobi equation
u	Velocity vector
p	Pressure
ρ	Density
τ	Stress tensor
s	Solvent
p	Polymeric
n_p	Viscosity polymeric
n_s	Viscosity solvent
n_l	Cinematic viscosity
D	Deformation rate tensor
τ_p	Symmetric tensor
k	Consistency coefficient
n	Flow behavior index
λ	Relaxation time
α	Mobility factor
G'	Storage module
G''	Loss module
n_0	Zero-shear rate viscosity
w	Frequency
⍰́	Shear rate
Bo	Bond number
Mo	Morton number
$\Re$	Reynolds number
d_0	Bubble diameter
l	Liquid
g	Gas
$\Delta\rho$	Density difference
U_t	Terminal velocity
g	Gravitational acceleration
σ	Surface tension

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