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Simulation of Flamboyant Gums (Power Fluid) with the Lattice Boltzmann Method

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Abstract

From results obtained in the rheological characterization of a 4% dispersion of flamboyant gum with the HaakeRT20 viscometer, for different conditions of pH = 3.0 and 9.0, temperature 5˚C, 25˚C and 45˚C, the data of the rheological behavior of the gum dispersions were fitted to the power law model. To understand and predict the behavior of this gum, a model of Lattice Boltzmann D2Q9 was developed for the behavior, in addition to simulations for the conditions handled in the experiments performed with the HaakeRT20 viscometer.

Keywords

Lattice Boltzmann, Power Law Fluids, Shear Stress, Shear Rate Flamboyant Gums

1. Introduction

Gums or hydrocolloids are polysaccharides derived from plants, among which are guar, carob, gum Arabic from Acacia trees, the pectin of the citrus peel and the apple pulp. In the case of carrageenan and alginates which are extracted from marine algae, xanthan gum is produced by microbial fermentation [1].

Polysaccharides are used in many industrial processes such as thickeners, gelling agents, emulsifiers, adherents, etc. Its high molecular weight and the interactions between the polymer chains allow altering rheological properties such as viscosity when dissolved or dispersed [2] [3].

Rheology relates the behavior of materials when subjected to forces and deformations. These concepts are of great importance in rheological evaluations. The application areas are also extremely wide and diverse and require an important contribution of Engineers with extensive experience, although the Chemical and Process Engineers, by their role in the handling and processing of complex materials (such as foams, suspensions, emulsions, molten polymers and solutions, etc.), have a huge interest in this subject [4] [5].

There are factors that can influence the rheological properties such as, variety, composition, temperature, instrumental techniques among others.

The rheometer or viscometer is used to measure the rheological properties of fluids under the principle of resistance to flow by the action of a known force or stress produced by a known amount of flow. Between the viscometers used to measurement the properties, are the capillaries and the descending ball, in the case of rheometers, the rotary and oscillatory rheometer is the more used. Commonly in the rotational rheometers, the controlled rate and controlled stress approach are used. In the first approach, the material under study is placed between two plates, one of them is rotated at a fixed speed and the other plate measures the torsional force. In the second approach, the situation is reversed [6].

There are investigations to know the rheological properties of solutions of guar gum, xanthan and alginate with the addition of salep for different concentrations, using the power law model [7].

Other investigations to evaluate the rheological properties for food hydrocolloids (carrageenan, pectin, gelatin, starch and xanthan) using a rotational viscometer for different concentrations and temperatures. Finding that mainly the model that was most adjusted to most of the experiments was the power model, and to describe the effect of temperature the Arrhenius model was used. To evaluate the effect of the concentration on the apparent viscosity we used the power, exponential and polynomial model [8].

The effect of calcium salt and pH on the rheological properties of the solutions of mixtures of xantham-carboxymethylcellulose has also been investigated. The gum solutions in all proportions showed a behavior to the Herschel-Bulkley model. In their research they found that the addition of salt and the decrease in pH cause an apparent reduction in viscosity [9].

Other studies focus on the rheological properties of the exudate of bitter almond gum (BAG) at different shear rates, concentrations, temperatures and pH in the presence of several salts. The rheological data was adjusted with the Power law model. It was found that the apparent viscosity of the BAG solutions increased with the increase in gum concentrations and decreased with the increasing shear rate at a specific temperature. The salts caused a reduction in viscosity. All the treatments had significant effects on the rheological parameters [10].

Our investigations were based on Flamboyant seeds (*Delonix regia*), which were harvested from trees in the city of Cuernavaca, Morelos, Mexico. The flamboyant's gum (FG) was extracted according to Corzo-Rios, *et al.*, 2014 [11] with small modifications. The seeds of flamboyant were hydrated in distilled water (1:15 w/v) at 70˚C for 12 h for extraction of endosperm. The endosperm in water suspension (4:1 v/w) was prepared and blended for 5.0 min., for to obtain a small particle size and a homogeneous dispersion. Then this dispersion was heated to 50˚C under constant agitation for 30 min. It was then filtered sequentially through 50 (300 mm) and 100 mesh (147 mm) to separate the fibrous particles. The FG was precipitated with ethanol (700 g/L) in 3:1 v/v proportion, dried at 55˚C for 24 h in a vacuum oven, and milled to a 60 mesh (250 mm) size.

Subsequently, a rheological characterization of a 4% dispersion of flamboyant gum was carried out with the HaakeRT20 viscometer equipment, for different conditions of pH = 3.0 and 9.0 and temperatures 5.0˚C, 25˚C and 45˚C. Obtaining that the behavior found corresponds to a non-Newtonian fluid that was adjusted to that of the Power law.

The Lattice Boltzmann Method has been presented in many investigations as an alternative to address problems concerning computational fluid dynamics, which has proven to be an effective tool in the past two decades.

In works concerning the application of rheology, the droplet generation in Newtonian and non-Newtonian fluid in T-junction and cross-junction microchannels was simulated by the Lattice Boltzmann method. The results revealed that it is necessary to take into account non-Newtonian rheology instead of the simple assumption of Newtonian fluid in numerical simulations [12].

They have also been investigated the effects of capillary number, viscosity ratio, gravitational acceleration, wettability, geometry, and non-Newtonian rheology property on finger pattern using the Lattice Boltzmann Method. The results provide an understanding of the viscous fingering phenomenon and confirm that the Lattice Boltzmann Method is an effective tool to investigate the immiscible displacement in complex geometries, as well as the non-Newtonian multiphase fluid flow behavior problems [13].

The LBM model with color-gradient has been used to simulate immiscible two-phase flows with power-law rheology. The deformation of a Newtonian droplet in a power law matrix subject to a shear flow, and the influence of power-law index, number capillary, wall confinement, and viscosity ratio. In addition to investigating the effect of non-Newtonian rheology on the droplet breakup under different confinements, and the results of droplet breakup in Newtonian systems are also shown for comparison with available in the literature data [14].

The velocity profiles of Newtonian and non-Newtonian fluids in microchannels have been investigated by the micro-particle image velocimetry technique (micro-PIV). Polyacrylamide aqueous solutions with different concentrations were used as non-Newtonian fluids. The comparison of the experimentally measured velocity profiles with the use of micro-PIV with the Lattice Boltzmann simulation and an approximate solution, showed acceptable results, which could be an alternative to the use of rheometers [15].

In this work, an LBM D2Q9 was developed, in the case of a power fluid, in addition to performing computational experiments for the pH and temperature conditions handled in the experiments done with the Haake RT20 viscometer, with the purpose of predicting the behavior of a flamboyant gum with the LBM.

2. Equations Constitutive of the Movement of Fluids

Two of the most important equations in fluid mechanics are continuity and momentum. The first is the basic principle of the movement of fluids and requires that the mass be conserved, which is given by

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \boldsymbol{u} = 0 \tag{1}$$

In Equation (1), ρ is the density and $\boldsymbol{u}$ is the velocity of the fluid. The second refers to the movement of the fluid, as well as the forces that produce these movements

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}\right) = -\nabla \cdot \overline{\overline{\tau}} - \nabla P + \rho \boldsymbol{g} \tag{2}$$

In the case of a Newtonian fluid, the ratio of the shear stress $\tau_{\alpha\beta}$ and the strain rate tensor $\dot{e}_{\alpha\beta}$ is given by the following relationship

$$\tau_{\alpha\beta} = 2\mu \dot{e}_{\alpha\beta}; \quad \dot{e}_{\alpha\beta} = \frac{1}{2}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right) \tag{3}$$

In this relation, the viscosity μ does not depend on the $\dot{e}_{\alpha\beta}$, since μ remains constant. Incorporating this relation in Equation (2), we obtain the Navier Stokes equation

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}\right) = \mu \nabla^2 \boldsymbol{u} - \nabla P + \rho \boldsymbol{g} \tag{4}$$

For a non-Newtonian fluid, the power or model Ostwald of Waele is used, in which, the ratio of $\tau_{\alpha\beta}$ and $\dot{e}_{\alpha\beta}$ is given by

$$\tau_{\alpha\beta} = 2\mu_{eff} \dot{e}_{\alpha\beta}; \quad \mu_{eff} = k\dot{e}^{n-1}; \quad \dot{e} = \sqrt{\dot{e}_{\alpha\beta}\dot{e}_{\alpha\beta}} \tag{5}$$

In Equation (5), μ_{eff} is the effective viscosity, k and n are the rheological parameters corresponding to the consistency index and the fluid behavior index respectively. For the case of n = 1.0, it is a Newtonian fluid. If n < 1.0, it corresponds to a pseudoplastic liquid, in which, its effective viscosity decreases with $\dot{e}_{\alpha\beta}$. If n > 1.0, corresponds to a dilatant liquid, in these, the effective viscosity increases with $\dot{e}_{\alpha\beta}$ [16].

3. The Lattice Boltzmann Model

This method evaluates the evolution of the distribution function of particle $f_i = (\boldsymbol{x}, t)$ by means of the Boltzmann equation discretized in a lattice. That is the probability of finding a particle with velocity $\boldsymbol{e}_i$ at position $\boldsymbol{x}$ and time t. The method can be summarized in two stages, the first is the advance of the particles to the next lattice site along the directions of motion for each time step Δt. The second stage is to simulate the collisions of the particles. The two mentioned stages can be described through Boltzmann's discrete equation as

$$f_i\left(\boldsymbol{x}+\boldsymbol{e}_i, t+1\right)-f_i(\boldsymbol{x}, t)=-\Omega_i \tag{6}$$

The collision term Ω_i that appears on the right side of Equation (6), can be replaced by

$$f_i\left(\boldsymbol{x}+\boldsymbol{e}_i, t+1\right)-f_i(\boldsymbol{x}, t)=-\frac{1}{\tau}\left[f_i(\boldsymbol{x}, t)-f_i^{eq}(\boldsymbol{x}, t)\right] \tag{7}$$

This simplification is known as the BGK approach (Bhatnagar-Gross-Krook). The rate of change referred to the equilibrium is $1/\tau$, which is the inverse of the relaxation time.

The macroscopic variables can be calculated in a direct way from the values of the distribution function as

$$\begin{aligned} \rho(\boldsymbol{x}, t) &= \sum_{i=1}^{n} f_i(\boldsymbol{x}, t) \\ \boldsymbol{u}(\boldsymbol{x}, t) &= \frac{1}{\rho(\boldsymbol{x}, t)} \sum_{i=1}^{n} f_i(\boldsymbol{x}, t) \boldsymbol{e}_i \end{aligned} \tag{8}$$

In the case of a Newtonian fluid, the relation of the kinematic viscosity and the relaxation time is given by $\upsilon = 1/3(\tau - 1/2)$.

One of the contributions of the method presented in this work involves a modification of the LBGK presented by Aharonov and Rothman [17], N. Rakotomalala [18], E. Boek [16], and S. P. Sullivan [19], for non-Newtonian fluids (Ostwald-de-Waele), which consists in proposing the relaxation time τ contained in Equation (7), as a function of the apparent viscosity which, in turn, involves the rheological parameters n y k so that [20]

$$\tau=\frac{1}{2}+3k(2\dot{e})^{n-1} \tag{9}$$

4. Simulation of Shear-Thinning Fluids with the Lattice Boltzmann Method (LBM)

In this work two types of boundaries were used, the "bounce-back" in the walls to ensure that the speeds in these are zero, and the periodic boundary conditions, in which the nodes located in the border will have their neighboring nodes in the opposite border, with a lattice size of 80 × 80. The values of "n" used were 0.2, 0.3, 0.4, 0.5, 0.6 and 0.7, with "K" values of 6.5×10^{-5}, 9.0×10^{-5}, 9.0×10^{-5}, 9.0×10^{-5}, 6.5×10^{-3} and 6.5×10^{-3} respectively. The steady state was reached after 90,000 steps of time.

The validation of the LBM was performed using the analytical solution of the plane Poiseuille flow, in dimensionless form for a power fluid

$$\frac{\boldsymbol{u}}{\langle \boldsymbol{u} \rangle}=\frac{(A)\left[1-\left(\frac{B-y}{C}\right)^{\frac{1}{n}+1}\right]}{A+\frac{1}{(C)^{\frac{1}{n}+1}}\left(\frac{n}{2n+1}\right)\left[-(B)^{\frac{1}{n}+2}-(C)^{\frac{1}{n}+2}\right]} \tag{10}$$

In Equation (10), $\langle \boldsymbol{u} \rangle$ is the average speed, A, B and C are constants related to the flow dimensions between two plates.

The comparison of the analytical velocity profiles Equation (10) and those performed with the LBM showed a relative error rate between both velocity profiles of less than 0.8%.

Simulation of Pseudoplastic Fluids with the Lattice Boltzmann Method with Experimental Data of Flamboyant Gums

In this work, the results obtained from the rheological characterization of flamboyant gum were used. The equipment used for these characterizations was the HaakeRT20 Viscometer, obtaining the conditions, as well as the results presented in Table 1.

In Figure 1 and Figure 2 the graphs of the shear stress vs shear rate, obtained with the experimental values with the flamboyant gum are presented.

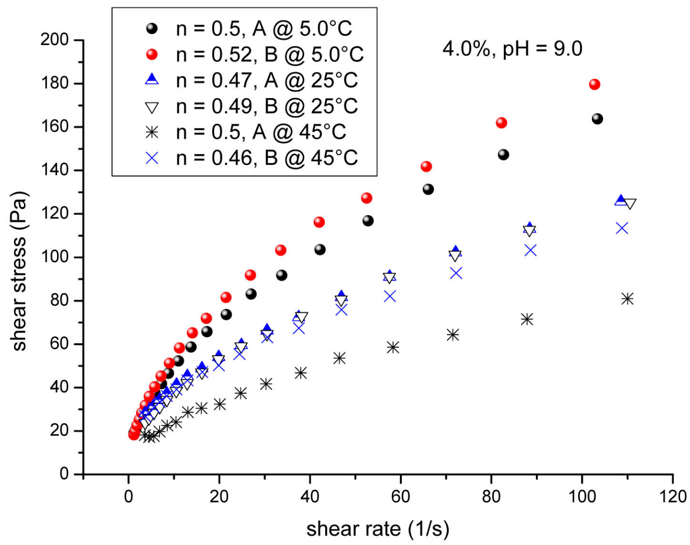


Figure 1. Flow graph for flamboyantgum, 4.0%, pH = 9.0.

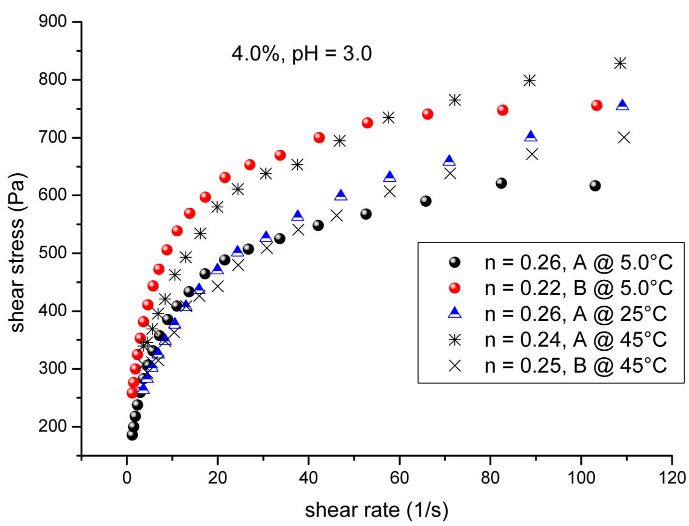


Figure 2. Flow graph for flamboyantgum, 4.0%, pH = 3.0.

Table 1. Experimental data obtained for a flamboyant gum obtained in a HaakeRT20 Viscometer. n = dimensionless and k = Pa·s^n.

Flamboyant gum, 4.0%, pH = 9.0 @ 5.0˚C				Flamboyant gum, 4.0%, pH = 3.0 @ 5.0˚C			
Sample A		Sample B		Sample A		Sample B	
n = 0.5	k = 16.06	n = 0.52	k = 16.32	n = 0.26	k = 201.59	n = 0.22	k = 286.51
Flamboyant gum, 4.0%, pH = 9.0 @ 25˚C				**Flamboyant gum, 4.0%, pH = 3.0 @ 25˚C**			
Sample A		**Sample B**		**Sample A**		**Sample B**	
n = 0.4708	k = 13.8158	n = 0.4961	k = 12.0731	n = 0.2653	k = 203.1150	n = 0.2345	k = 287.1152
Flamboyant gum, 4.0%, pH = 9.0 @ 45˚C				**Flamboyant gum, 4.0%, pH = 3.0 @ 45˚C**			
Sample A		**Sample B**		**Sample A**		**Sample B**	
n = 0.5	k = 7.84	n = 0.46	k = 13.47	n = 0.24	k = 264.18	n = 0.25	k = 212.78

In **Figure 1**, the results of the experiments are plotted for flamboyant gum conditions with a concentration of 4.0% of a pH = 9.0 and three different temperatures 5.0˚C, 25˚C and 45˚C, for two samples in each of the cases. For these conditions, it can be observed that the shear stresses decrease as the temperatures increase, as has been reported by other researchers for different types of gums [21] [22] [23].

In **Figure 2**, the results are presented at pH = 3.0, maintaining the conditions presented in the results obtained in **Figure 1**. It is observed that the effect of pH affects the behavior of the curves, because unlike the results obtained previously, at this pH value (3) little influence of the temperature is seen with shear stresses especially at speed values of shear less than 100 s^{-1}. In addition, it can be seen that the increase in shear stress is very pronounced which produces higher values of consistency index in the samples with pH = 3.0 than at pH = 9.0, which makes it difficult to determine the rheological behavior at higher shear rates at 100 s^{-1}.

An important aspect in the simulation of real systems is the correct transformation of units; that is, conversion of physical units to lattice units and vice versa. To do this, conversions were made of the experimental values of k_{phys} that have physical units with respect to the grid units k_{LB}, using the velocity of physical light and Lattice Boltzmann of 340.3 m/s and $\sqrt{1/3}$ respectively [24].

In **Table 2**, the results are presented for all samples of flamboyant gum.

In **Figure 3**, we present the comparison of velocity profiles for simulations with the LBM with those obtained with the analytical solution, considering the values reported in **Table 2**. The relative errors between the graphs were lower than 1.02%.

The shear stress and the shear rate were obtained through the analytical solution, with the simulations of the LBM and compared with the experimental values obtained with the HaakeRT20 viscometer. **Figure 4** shows the results obtained.

Figure 4 shows the comparison of the shear stress vs normalized shear rate of the analytical solution, Lattice Boltzmann with experimental values of flamboyant

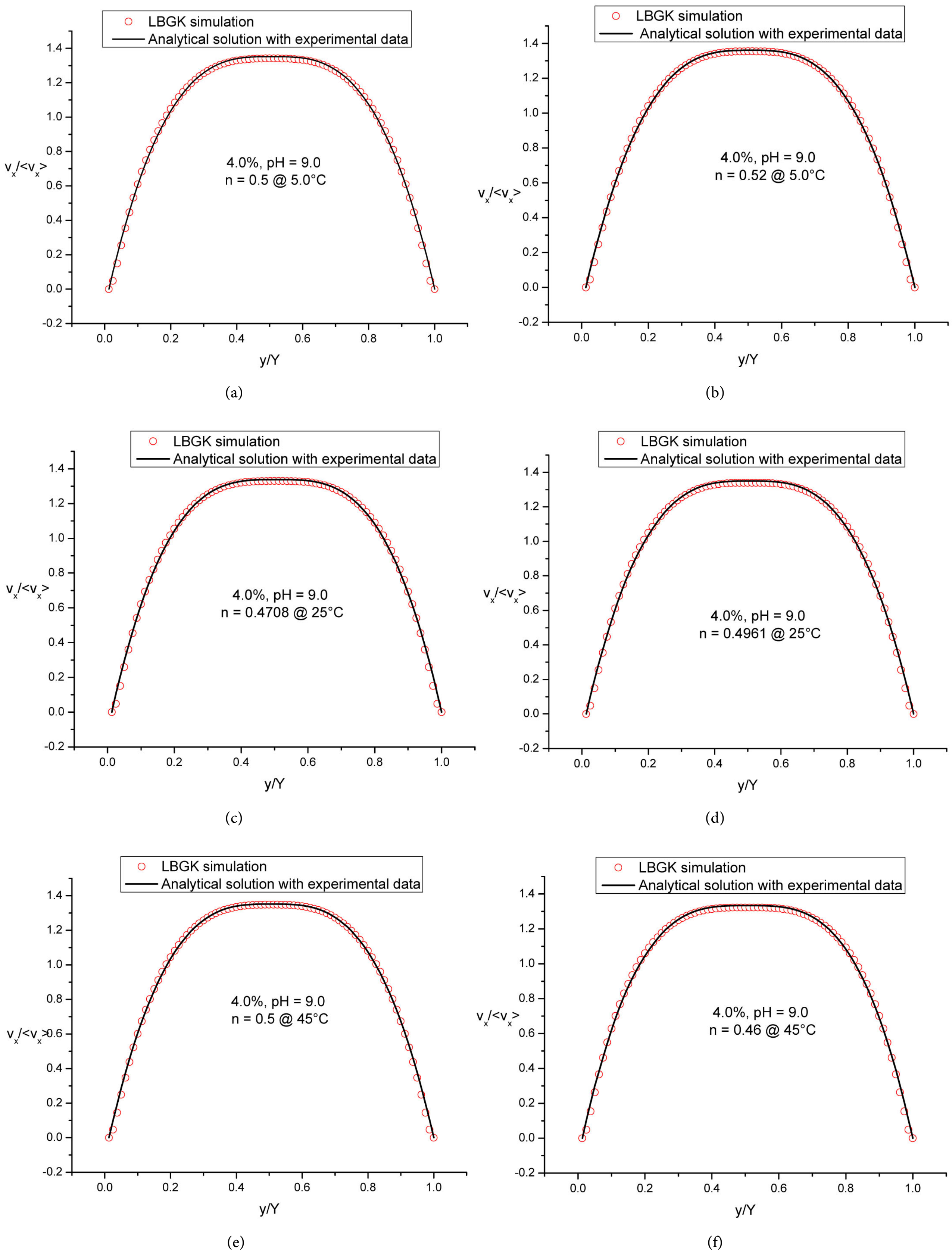
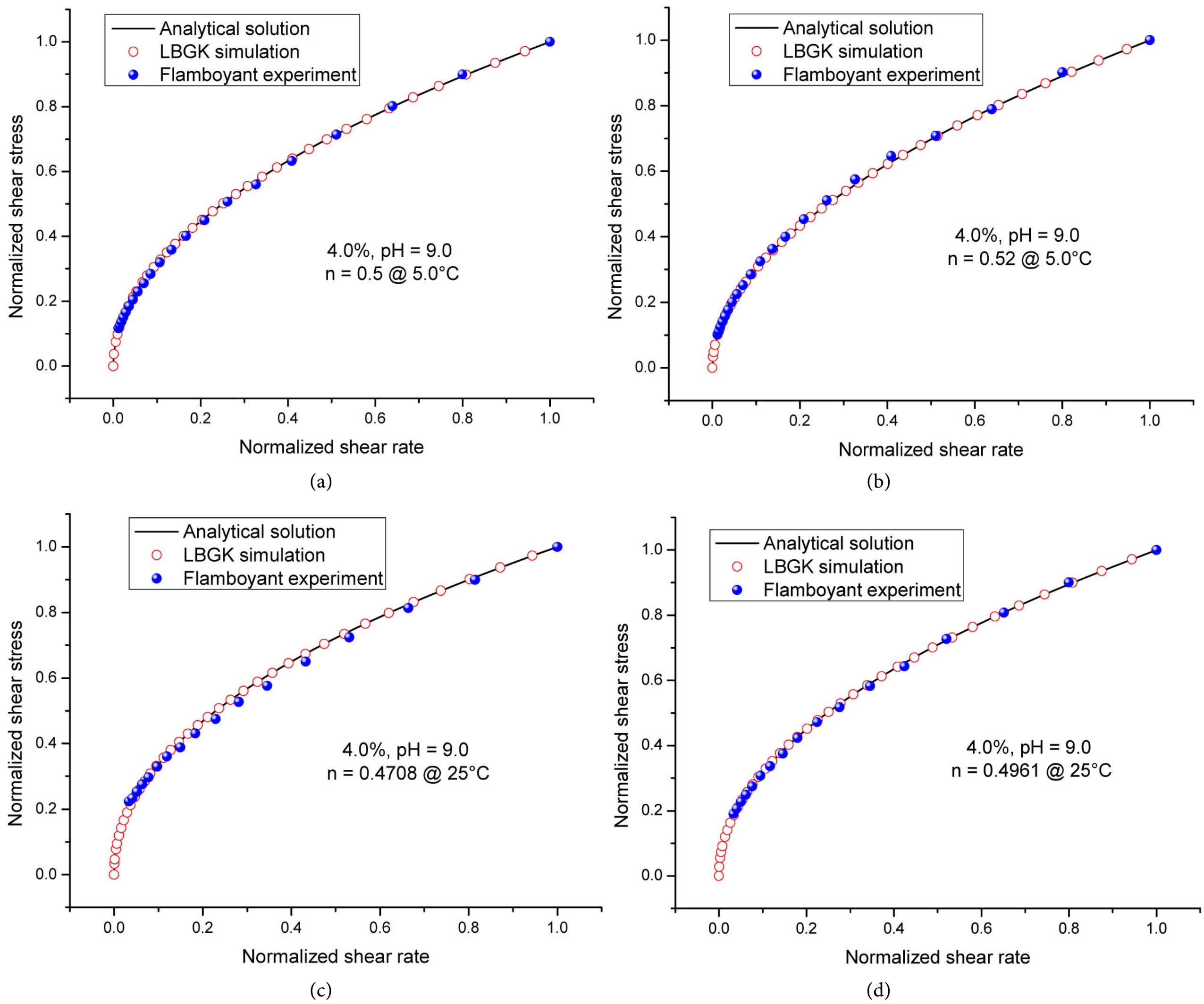
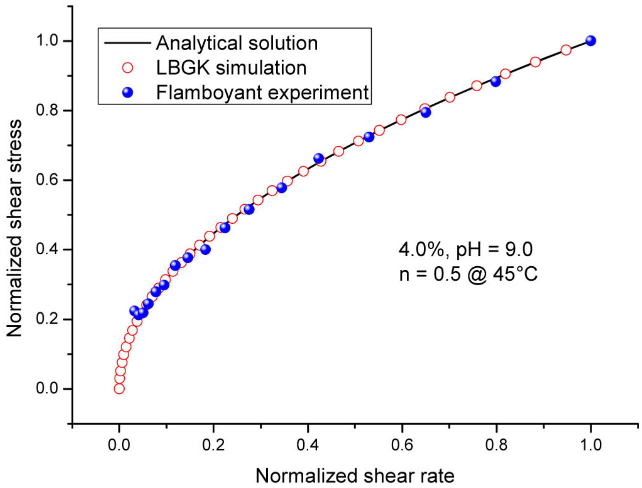


Figure 3. Comparison of velocity profiles with Lattice Boltzmann vs analytical solution, using the values in **Table 2**.

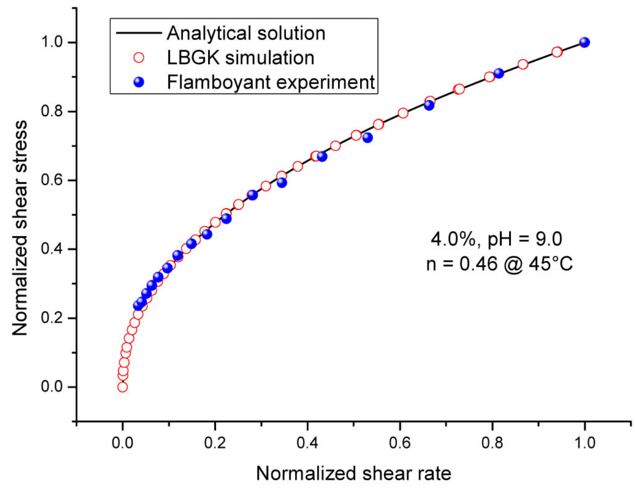
Table 2. Consistency index values in physical and lattice units (u.r).

	Sample	n	k_{phys} (Pa·s^n)	k_{LB} (u.r)
Flamboyant gum, 4.0%, pH = 9.0 @ 5.0˚C	A	0.50	16.06	8.1486×10^{-5}
	B	0.52	16.32	1.0186×10^{-5}
Flamboyant gum, 4.0%, pH = 9.0 @ 25˚C	A	0.47	13.82	5.1807×10^{-5}
	B	0.49	12.07	5.8830×10^{-5}
Flamboyant gum, 4.0%, pH = 9.0 @ 45˚C	A	0.50	7.84	3.9780×10^{-5}
	B	0.46	13.47	4.5165×10^{-5}
Flamboyant gum, 4.0%, pH = 3.0 @ 5˚C	A	0.26	201.59	8.5197×10^{-05}
	B	0.22	286.51	8.0020×10^{-05}
Flamboyant gum, 4.0%, pH = 3.0 @ 25˚C	A	0.27	203.12	9.0685×10^{-05}
	B	0.23	287.12	9.3181×10^{-05}
Flamboyant gum, 4.0%, pH = 3.0 @ 45˚C	A	0.24	264.18	9.0763×10^{-05}
	B	0.25	212.78	8.1080×10^{-05}

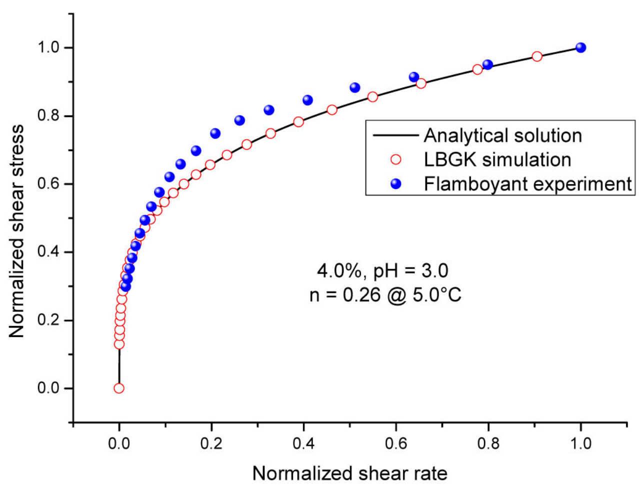



Analytical solution
LBGK simulation
Flamboyant experiment
4.0%, pH = 9.0
n = 0.5 @ 45°C
Normalized shear stress
Normalized shear rate

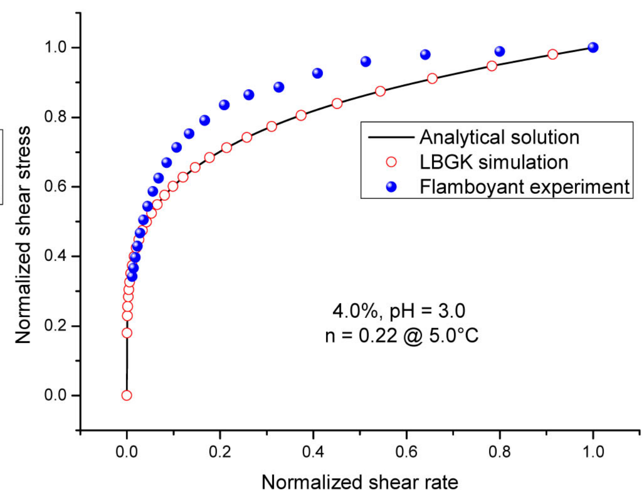
(e)


Analytical solution
LBGK simulation
Flamboyant experiment
4.0%, pH = 9.0
n = 0.46 @ 45°C
Normalized shear stress
Normalized shear rate

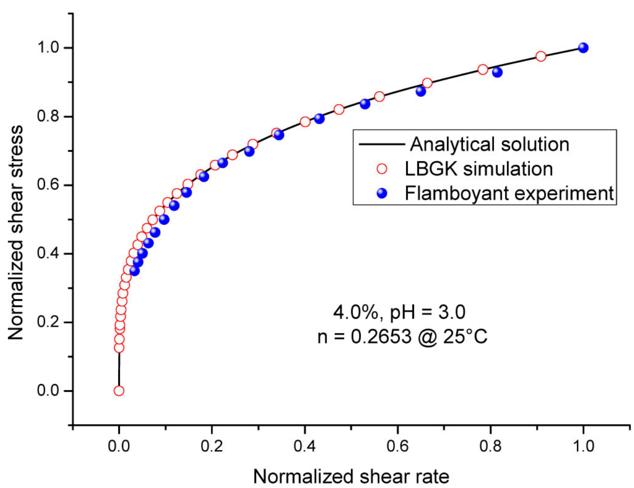
(f)


Analytical solution
LBGK simulation
Flamboyant experiment
4.0%, pH = 3.0
n = 0.26 @ 5.0°C
Normalized shear stress
Normalized shear rate

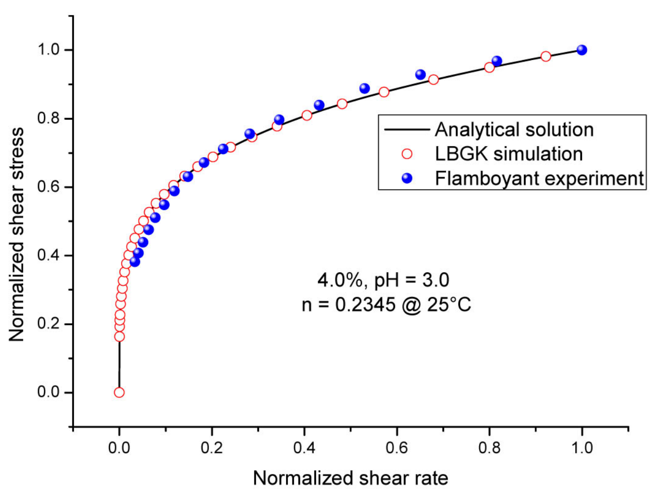
(g)


Analytical solution
LBGK simulation
Flamboyant experiment
4.0%, pH = 3.0
n = 0.22 @ 5.0°C
Normalized shear stress
Normalized shear rate

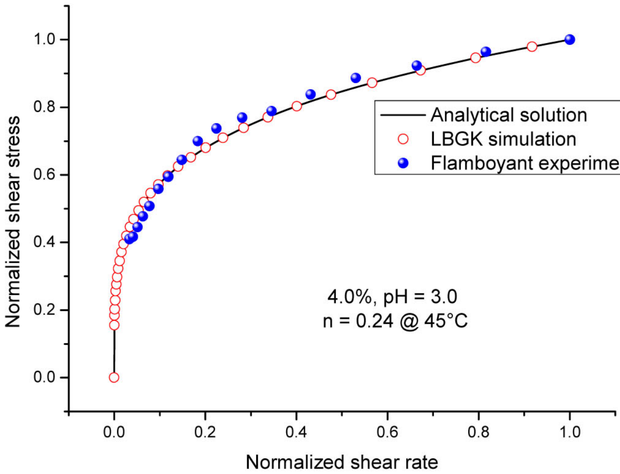
(h)


Analytical solution
LBGK simulation
Flamboyant experiment
4.0%, pH = 3.0
n = 0.2653 @ 25°C
Normalized shear stress
Normalized shear rate

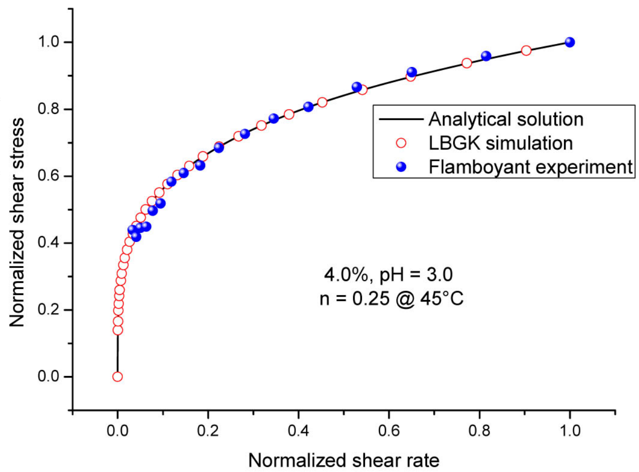
(i)


Analytical solution
LBGK simulation
Flamboyant experiment
4.0%, pH = 3.0
n = 0.2345 @ 25°C
Normalized shear stress
Normalized shear rate

(j)



(k)



(l)

Figure 4. Shear stress vs normalized shear rate with analytical solution, Lattice Boltzmann and with experimental values, presented in Table 2.

gum. The approximations are acceptable for the case of Figures 4(a)-(f), with the conditions of pH = 9.0, for the temperatures of 5.0˚C, 25˚C and 45˚C. However, for Figure 4(g) and Figure 4(h), in which the pH was decreased to 3.0 for a temperature of 5.0˚C, there is a departure from the experimental data with respect to the simulations with LBM and the analytical solutions. In the case of the temperature increase of 25˚C and 45˚C, the tendency is remarkably corrected, as shown in Figures 4(i)-(l).

5. Conclusions

A rheological characterization of the flamboyant gum was performed with the HaakeRT20 viscometer, for different conditions of pH = 3.0 and 9.0, temperature 5.0˚C, 25˚C and 45˚C, and it was found that this gum exhibited a behavior of power law of shear thinning type. The experimental data were compared with analytical solutions and with simulations carried out with the Lattice Boltzmann Method, which showed acceptable results, except for values of pH = 3.0 and temperature of 5.0˚C where differences can be observed between the 2 samples.

The Lattice Boltzmann Method, turns out to be an alternative to the conventional methods of computational fluid mechanics, in addition to presenting facility in terms of implementation and programming. The technique promises to be a predictive tool in the area of rheology.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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