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An Overview of Numerical Methods for non-Newtonian Flows

Martina Bašić

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KVALIFIKACIJSKI DOKTORSKI ISPIT

Pregled numeričkih metoda korištenih za simulacije strujanja ne-Newtonovskih fluida

Martina Bašić

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Nomenclature

Latin

d number of dimensions (2 or 3)

D Lagrangian derivative

$\boldsymbol{F}_{ext}$ external acceleration vector, usually gravitational acceleration

g gravitational constant

p pressure

t time instant

$\boldsymbol{u}$ velocity vector

Greek

$\Delta\alpha$ angle

δx displacement of fluid volume in the x direction

$\eta(\dot{\gamma})$ apparent viscosity

λ_1 relaxation time

λ_2 retardation time

μ fluid dynamic viscosity

μ_0 fluid dynamic viscosity at zero shear rate

μ_∞ fluid dynamic viscosity at infinite shear rate

ρ fluid density

$\boldsymbol{\tau}$ stress tensor

τ_0 yield shear stress

ν fluid kinematic viscosity

Abbreviations

2D	Two–dimensional
3D	Three–dimensional
BEM	Boundary Element Method
BC	Boundary condition\mathrm{D} Lagrangian derivative
CFL	Courant–Friederich–Lewy
CFD	Computational Fluid Dynamics
FDM	Finite Differences Method
FEM	Finite Element Method
FSI	Fluid–Structure Interaction
FVM	Finite Volume Method
FPM	Finite Pointset Method
GFDM	Generalized Finite Difference Method
MPS	Moving Particle Semi-Implicit method
NSE	Navier-Stokes Equations
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
PFEM	Particle Finite Element Method
SPH	Smoothed Particle Hydrodynamics
TVP	Thixotropic viscoplastic
VOF	Volume of Fluid

1 Introduction

The study of deformation and flow is known as rheology. Professor Eugene Bingham introduced the term in 1920 [1]. Rheology has evolved into a complex, multidisciplinary, and rapidly expanding area of research since then. It focuses on the movement of matter, including liquid and gaseous states as well as soft solids. Soft solids are solids that exhibit plastic flow deformation when subjected to applied force. The liquid and gas states studied in this branch of physics differ from other fluids and gases in that they lack a single coefficient of viscosity for a given temperature, i.e. they do not obey Newton's viscosity experiment law. Non-Newtonian fluids are type of fluids whose viscosity varies with strain rate, implying that the viscous stress within the fluid is not linear. The viscous stress tensor and shear rate change during the flow process. When compared to Newtonian fluids, the movement of non-Newtonian fluids is more complex and exhibits different flow characteristics. Microstructure developed in these fluids are complex, and they are being studied and described.

By relating stress to strain rate, we can describe the behavior of non-Newtonian fluids. They are classified into several groups and subgroups based on their physical properties. Some are very different, for example, shear-thinning viscosity can be reduced by stirring, shaking, or any other type of mechanical agitation. Those are for example: ketchup, yogurt, and acrylic paints. There are also thixotropic fluids, meaning that the relative velocity between the layers of fluid causes a reduction in viscosity. Some other materials exhibit the opposite behavior, known as rheopecty, in which viscosity increases due to relative fluid movement. They are also known as shear-thickening fluids or dilatant fluids.

Non-Newtonian fluids are important and can be found in industrial processes as well as in nature. For example, paint in chemical processing industry, plastics processing industry, slurries and muds in mining industry, blood, lymph fluid, cell fluid in biomedical flows, milk, chocolate, and edible oil in food industry. Non-Newtonian fluids exhibit viscous properties on a regular basis, and it is important for the designer or engineer to be familiar with the flow behaviour of such fluids, in order to identify the fluid physical properties, and how to use these properties to predict flow behavior in industrial process.

The behavior of foods, beverages, paints, and medications during processing is an important factor to consider. Non-Newtonian fluids are found in food processing where their character can alter the texture, flavor, and appearance of the product. Therefore,

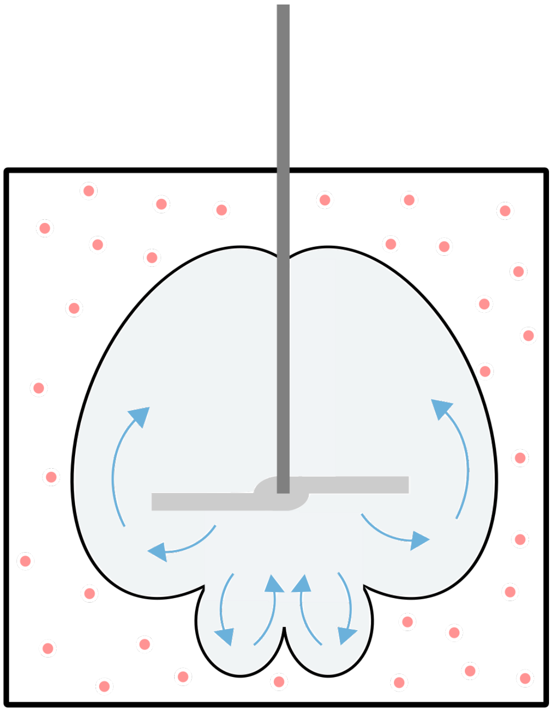

Figure 1.1: Representation of a non-Newtonian fluid moving around an impeller. Red dots represent the stagnant fluid area around the cavern. The size of the cavern is determined by the impeller type and torque.

maintaining delicate cell structure is critical in the food industry, as well as in paint, and pharmaceutical industries. Typical problem for such industries is mixing problem shown in Figure 1.1. Viscosity exists in all liquids and soft solids, and because food and medication processing is all about moving goods through systems by applying force to them, viscosity is a crucial aspect in the design and operation of such industrial processes. Shear forces that are result of relative motion between layers of the fluid have impact on the system design as well. The shear force acts in the direction that is parallel along the pump and tube surfaces, and resistance to such forces is proportional to the viscosity and smoothness of the interior pipe surface. The viscosity, pressure and temperature of the fluid inside the system affect the relative velocity of fluid particles i.e. the fluid or soft solid can move eather faster or slower. When processed, non-Newtonian fluids respond to shear stress and shear rate in a variety of ways. Some become thicker, i.e. their viscosity increases with increasing shear rate (cornstratch water combination), whereas others get less viscous (blood, ketchup, lotions ect.). Shear-sensitive fluids (shampoo, egg whites, ketchup) must be handled delicately throughout the production in order to maintain product quality. Since the system have impact on product integrity, it is important to determine the pump speed, pressure generated by pump, flow rates, pipe diameters, pipe roughness ect. By determining the shear sensitivity and viscosity of the product it is possible to maximize process efficiency. For example, viscosity influences how long it takes to distribute a product for packing. As a result, a process intended to optimize flow

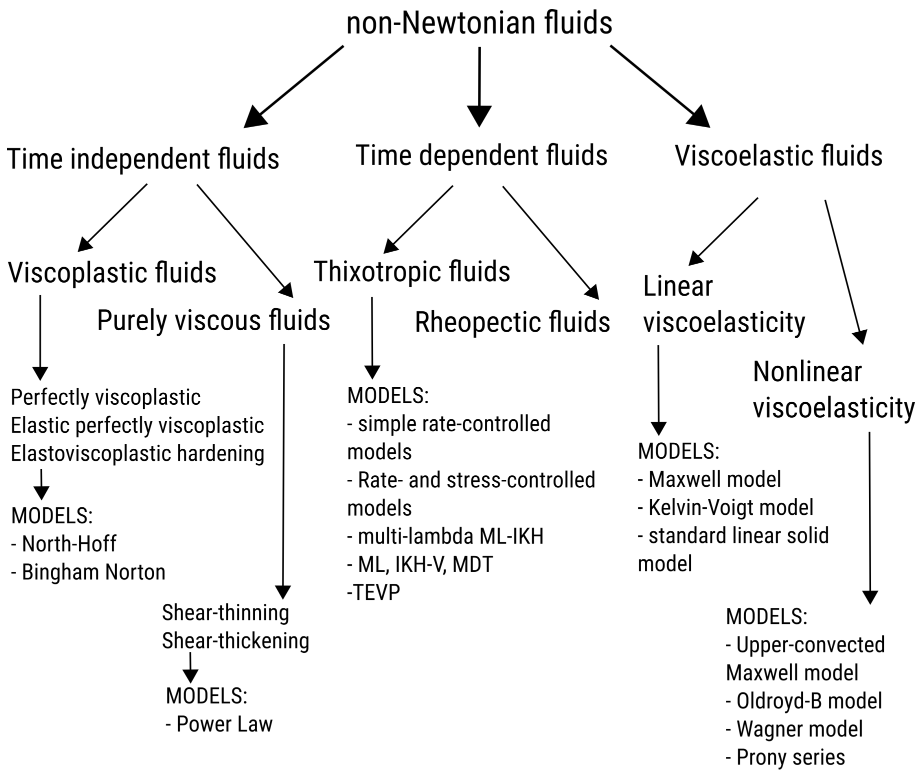

Figure 1.2: Non-Newtonian fluid classification and rheological models.

optimizes efficiency.

The most common issue that viscosity and shear sensitivity cause in industrial processes is excessive power consumption and the likelihood of product degradation. As a result, rheological testing and investigation include flow studies at different pressures and temperatures.

Non-Newtonian fluids are divided into three main types: time independent fluids, time dependent fluids, and viscoelastic fluids as can be seen in Figure 1.2.

1.1 Time independent fluids

Time independent fluids can be subdivided in two gropus:

I. Viscoplastic fluids,

II. Purely viscous fluids,

These two subgroups of time-independent fluids are explained below.

1.1.1 Viscoplastic fluids

Viscoplastic fluids act as solids until the yield value is exceeded, and when this happens they start to flow. The plastic deformation of a viscoplastic fluid is determined by the rate at which a load is applied. Toothpaste is an example of a viscoplastic fluid. When a viscoplastic fluid is squeezed, the pressure gradient drives the flow. After applying a certain amount of pressure to the tube, the toothpaste is extruded. The velocity in the center is uniform, and the flow is plug-like.

There are three rheological models of viscoplastic fluids. Perfectly viscoplastic solid (North-Hoff model), Elastic perfectly viscoplastic solid (Bingham-Norton model), Elasto-viscoplastic hardening solid. Bingham fluids are a significant class of viscoplastic fluids. Bingham material modeling is important for industrials because many materials behave like Bingham fluids (e.g. mayonnaise, ketchup, pastes, slurries, toothpaste, foams, oils, ceramics, emulsions, fresh concrete etc.), [2]. Bingham fluids have a linear character, constant viscosity, and constant yield stress. When the Bingham model starts to flow, it behaves like a Newtonian fluid. The Bingham model is used in mud flow calculations for drilling engineering since it only has two parameters: yield stress and plastic viscosity. Inter-particle bonding in the fluid must be broken in drilling by exceeding a certain shear stress limit. Until then, the fluid will resist to flow. Once the fluid begins to flow, the shear stress and shear rate respect a linear relationship between them. This assists the drilling fluid in suspending the solids and cuttings that are present in the fluid when the circulation stops. This model is widely used due to its simplicity and ability to estimate pressure loss in turbulent flow.

The theory of viscoplasticity is useful in the estimation of permanent deformations, the prediction of plastic failure of structures, the investigation of stability, automobile crash simulations, high temperature systems such as turbines and engines, e.g. a power plant, dynamic problems, and systems subjected to high strain rates.

1.1.2 Purely viscous fluids

The two main types of purely viscous fluids are pseudo-plastic or shear-thinning fluids and dilatant or shear-thickening fluids. All of these fluids lack the linear dependence of shear stress and shear strain rate that is characteristic of Newtonian fluids. The most commonly used model for purely viscous fluids is the so called Power Law model.

The viscosity of shear-thinning fluids decreases as the shear rate increases. This shear-thinning behavior is typical for ketchup, mayonnaise, whipped cream, biological fluids, quicksand, nail polish, modern paints, nearly all polymer melts, polymer solutions, and other materials. The wipped cream is a good example of how to describe the behavior of such a flow. Because of the low viscosity at a high flow rate, the cream exits the pipe bag nozzle smoothly, but it can still be taken into the spoon without dripping or spilling. The increased viscosity helps with its firmness. Shear-thickening fluids are the opposite of shear-thinning fluids. Their viscosity increases as the shear rate increases.

They have a particular ability to convert from liquid to solid with applied load. They are not often found as natural materials or fluids, although mixed water and sand can act as one. Standing in the wet sand will cause the legs to sink, but running over it, the mixture of a sand and water will act as a solid. Typical substance for these so-called thickening fluids is the 2:1 solution of corn-starch in water. The mixture, by stirring, is getting harder, and by throwing a heavy object on it, the object is going to bounce back, and the liquid phase is turn into a solid. After a while, it'll return to the liquid phase.

The application of shear-thickening fluids can be found in the body armor. Since the b2.3ody armours just made of kevlar have three main drawbacks: they are stiff, heavy and do not protect the extremities. Therefore, shear-thickening fluids are impregnated in kevlar. Silica particles in the ethylene glycol form impregnated in kevlar results in similar flexibility as regular kevlar, but the armour gets hardened when shot.

1.2 Time dependent fluids

Time Dependent Fluids are divided as into the following groups::

I. Thixotropic fluids,

II. Rheopectic fluids.

Under shear stress, the behavior of time-dependent fluids differs. Shear stress decreases monotonically for thixotropic fluids and decreases for rheopectic fluids for a constant shear rate. Rheopectic fluids can be sometimes confused with shear-thickening fluids. The distinction between these two is in the viscosity. The value of viscosity is time-dependent in rheopectic materials and increases with applied stress, while the value of viscosity of the shear-thickening materials increases only with an increase in stress. This type of viscosity is known as time-dependent viscosity.

Thixotropy is a shear-thinning property that is time dependent. Fluids that are thick in static conditions will begin to flow over time as a result of being shaken, agitated, or stressed in any way. Furthermore, they require a certain amount of time to reach a more viscous state. After the initial agitation has stopped, some fluids will instantly return to a thick gel state (e.g. ketchup), while others will take longer to return to the original state. Thixotropy arises as a result of the time required for particles or structured solutes to organize. After applying stress for a period of time, anti-thixotropic or rheopectic fluids exhibit an increase in viscosity. They are less researched because they do not appear frequently in nature and in industrial processes. Thixotropic viscoplastic (TVP) or ideal thixotropic models are modelled with simple rate-controlled model, Rate- and stress-controlled models. Models with multiple structural parameters as multi-lambda ML-IKH model, ML, IKH-V, MDT model and TEVP models.

Thixotropic fluids are found in foods (ketchup and yogurt), clay, cytoplasm and the ground substance in human body, drilling fluids, grease, printing ink, margarine, and polymer melts. Therefore they are widely used in the chemical and food industries. Thixotropic fluids are also significant in structural and geotechnical engineering, and they are the subject of extensive research. Contrary to thixotropic fluids, rheopectic fluids are extremely uncommon. Quicksand behaves as thixotropic fluid in the shear-thinning form; at first, it appears to be a solid, but by stepping into it, it becomes more viscous, and anything that applies stress sinks faster. Gypsum paste as well as cream is an example of a substance that exhibits rheopecty, because it becomes stiff only after prolonged beating. Some rheological phenomena, such as yielding, hysteresis in shear-rate ramps, the effect of rest time, and viscosity bifurcation, are accompanied by thixotrophy.

1.3 Viscoelastic fluids

A viscoelastic fluid can exist both as a solid and a fluid. Viscoelastic materials deform elastically, or elastically and plastically when they are subjected to a state of stress (pizza dough). The viscoelastic fluid material deforms elastically when the external stress is less than the yield stress value. When the external stress exceeds the yield stress, the stress-strain relationship can be either linear or non-linear. As a result, elastic or elastic and plastic deformations are possible. The elastic deformation disappears when the stress is removed, but the plastic deformation remains. If the material is under constant stress, it will deform indefinitely if it is a fluid and asymptotically if it is a solid. Fluids continue to deform under constant stress with increase in strain. This phenomena is called creep. If a material behaves elastically, the stresses may be constant when it is suddenly deformed and held in a fixed deformed state. If the material is fluid-like, the stress may decrease with time toward an isotropic state of stress, or toward an asymptotic limit anisotropic state of stress if the material is solid-like. This is referred to as stress-relaxation phenomena which is time-dependent decrease in stress under a constant strain. The creep and stress relaxation phenomena are known as viscoelastic phenomena because they are responses of viscoelastic materials to internal friction or viscous effects in the material itself. Viscoelastic properties are responsible for damping and energy dissipation when a material is subjected to dynamic loading. Depending on the stress-strain rate of a material hysteresis loop is observed. When a load is applied and removed from a viscoelastic fluid, energy is dissipated, whilst purely elastic materials do not exhibit energy loss. The observed hysteresis defines a loop with an area equal to the energy lost during the loading cycle. Sound propagation in liquids and gases is also an elastic response. Fluids are thus viscous and elastic in general, and their reaction is viscoelastic. On the other hand, the elastic deformations are very small in comparison to the viscous deformations.

Viscoelastic materials such as molten glass, metals, rubbers, and syntethic polymers are researched and used in a variety of industrial applications. Constitutive models for linear viscoelasticity include the Maxwell model, the Kelvin-Voigt model, the standard linear solid model, and the Burgers model. They are used to estimate the behavior of a material under various loading conditions. Nonlinear constitutive models for viscoelasticity are the second-order fluid, Upper-convected Maxwell model, Oldroyd-B model, Wagner model and Prony series. Nonlinear models describe some of the phenomena that fluids exhibit, as well as time-dependent behavior.

Although the stresses in both viscoelastic and thixotropic fluids are affected by their previous deformation experience, viscoelastic fluids are distinguished by elasticity, while thixotropic fluids are distinguished by the slow time dependency of their viscosity or yield stress.

2 Physics of viscosity

Rheological behaviours can be expressed mathematically through relations in constitutive equations. The physical quantities that influence the behaviour of non-Newtonian fluids are applied stress (τ) and deformation (γ). As a result, the following section discusses fundamental knowledge of viscosity, stress, and strain.

Viscosity is defined as resistance to fluid motion (i.e. continual deformation). The higher the viscosity of the fluid, the more resistance it will have against the flow and the more difficult it will be to travel or be transported from one location to another. For example, honey is such a viscous fluid that it sips through a spoon very slowly when removed from the jar. This is primarily due to the high viscosity, which indicates that there is a lot of tension in the surface, implying that there are a lot of forces acting on it. This means that the movement of the molecules is extremely slow. Water is another example of a low-viscosity fluid, because it flows easily and instantly.

It is important to understand where does the viscosity come from, and how does the fluid move.

Figure 2.1 depicts two plates with some sort of fluid between them. The bottom plate is a solid and static base plate, while the top plate is moving to the right by some force F. Fluids of any type, liquid or gas, with visible molecules, can be used. The fluid will not move all at once with the moving plate. One must keep in mind that molecules in fluids are not as tightly bound together as they are in solids. When the molecules are moved, they will try to adhere to the surfaces. The molecules closest to the surface will move with the velocity of the surface, followed by molecules in the lower layers. In the end, the plate will move, but the fluid will be displaced in infinitesimal layers and with infinitesimal height. The layers closest to the moving surface will move much faster than the layers at the bottom. As a result, the velocity will have a parabolic profile for Newtonian fluids. This is how viscosity is defined. The same is true for water in a pipe. Water near the walls will tend to adhere to the wall, and the highest velocity will be in the center of the pipe, because we have the least resistance closer to the center.

In a more formal sense, viscosity can be described as a contribution to shear stress. Shear stress is caused by transverse planes moving past each other. The infinitesimal change in shear stress is expressed as a change in force over a change in fluid area. The infinitesimal change in shear stress is expressed as follows:

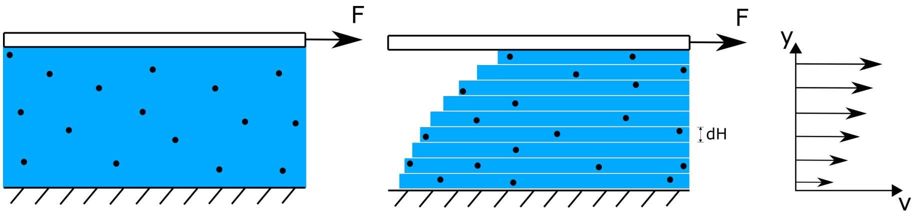

Figure 2.1: Definition of viscosity in simple shear flow.

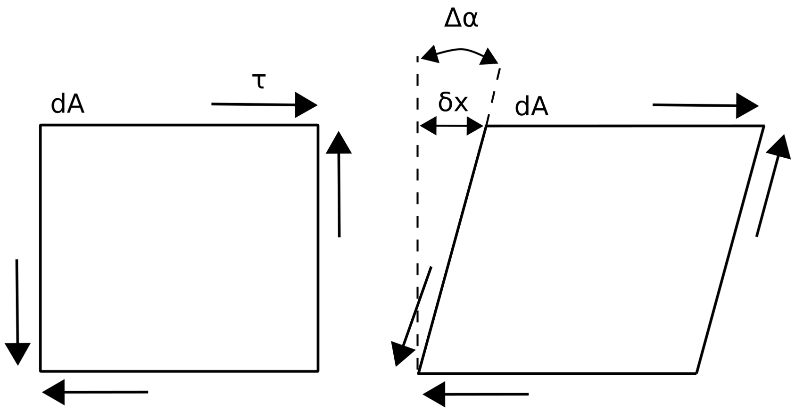

Figure 2.2: The change in fluid element in short period of time defines shear strain.

$$\tau = lim \frac{\Delta F}{\Delta A} = \frac{\mathrm{d}F}{\mathrm{d}A}, \tag{2.1}$$

where dF represents the change in the force and dA the change in the area of the fluid.

Because of the effects of stress on the small portion of fluid volume in Figure 2.2, displacement of fluid volume in the x direction δx will result in angle $\Delta\alpha$, which defines shear strain. The assumption is that the angle is very small, allowing the use of the following approximation:

$$\Delta\alpha \approx tan\Delta\alpha = \frac{\delta x}{\Delta y}. \tag{2.2}$$

Another relationship can be observed as a result of shear strain definition. The distance δx is dependent on infinitesimal velocity, and when the δx between the layers changes, the velocity changes as well, and this happens over a specific time interval. The expression is written as follows:

$$\Delta u \Delta t = \delta x, \tag{2.3}$$

and by rearranging equation (2.3) we get the following derived expression:

$$\frac{\Delta\alpha}{\Delta t} = \frac{\Delta u}{\Delta y}, \tag{2.4}$$

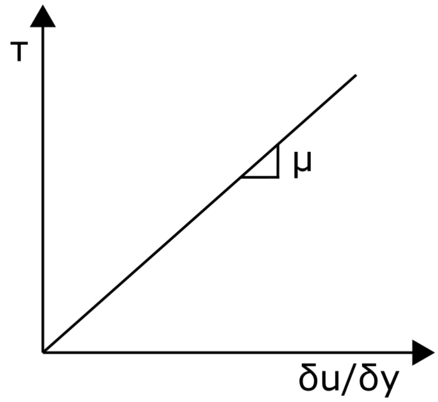

Figure 2.3: Newtonian fluid.

and if Δt $\rightarrow$ 0 the expression is given:

$$\frac{\delta \alpha}{\delta t} = \frac{\delta u}{\delta y}. \tag{2.5}$$

The shear stress can be described by the dynamic viscosity using terms from above. The following is a definition of shear stress:

$$\tau = \mu \frac{\delta u}{\delta y} = \mu \dot{\gamma} = \tau(\dot{\gamma}), \tag{2.6}$$

where letter μ represents the dynamic viscosity and has units of $\frac{\mathrm{N \cdot s}}{\mathrm{m}^2} = \mathrm{Pa}\ s$. The other type of viscosity is the kinematic viscosity. Kinematic viscosity is defined as the ratio of dynamic viscosity to fluid density:

$$\nu = \frac{\mu}{\rho}, \tag{2.7}$$

which has units of $\frac{\mathrm{m}^2}{\mathrm{s}}$.

When the shear stress is plotted against the velocity profile or the velocity gradient, a straight line for the Newtonian fluid should be visible, as shown in Figure 2.3. The gradient of plotted shear stress against velocity profile will be dynamic viscosity μ.

This is referred to as a Newtonian fluid because it adheres to the small angle assumptions on shear strain, which is also known as Newton's law of viscosity. These relationships are not strictly followed by non-Newtonian fluids. The curves observed in such cases are non-linear, and the viscosity will not be represented by these equations. It's going to be a lot more difficult. The constitutive equation for most non-Newtonian fluid in simple shear flow is known as the viscosity function or apparent viscosity $\eta(\dot{\gamma})$ and is defined as follows:

$$\eta(\dot{\gamma}) = \frac{\tau}{\dot{\gamma}}. \tag{2.8}$$

The apparent viscosity of a Newtonian fluid is constant and equal to the fluid's Newtonian viscosity, while the apparent viscosity of a non-Newtonian fluid depends on the shear rate. The SI unit for apparent viscosity is Pa·s. From Eq. 2.8 shear stress is defined as:

$$\tau = \eta(\dot{\gamma})\dot{\gamma}. \tag{2.9}$$

The properties that may affect viscosity are:

I. viscosity changes with respect to the temperature according to the type of fluid,

II. viscosity changes to a certain extent with the pressure,

III. viscosity changes with respect to the time.

It has been found empirically that the viscosity tends to fall with rise of the temperature. For liquid state it can be described with Andrade's equation as follows:

$$\mu = Be^{c/T}, \tag{2.10}$$

where B and c are constants. In the case of the gas state, there is the empirical Sutherland equation found through experiment:

$$\mu = \frac{BT^{3/2}}{T + C}, \tag{2.11}$$

where B and c are arbitrary constants. These empirical equations have been found through experiments.

Pressure causes an increase in viscosity of a liquid. Almost all liquids solidify when subjected to high pressure. Under extremely high pressure, even water can solidify. The viscosity of a gas, on the other hand, is nearly independent of pressure. It is only affected by extremely low or extremely high pressure. The viscosity of an ideal gas is sed to only be affected by the temperature.

As it was explained in Section 2, the viscosity of some of the fluids varies over time. Fluids are classified as thixotropic or rheopectic based on whether their viscosity decreases or increases over time.

The Deborah number (De) is a dimensionless number used to describe the flow's fluidity. It describes the material's flow under specific conditions. It is defined as a ratio of the time needed for fluid to adjust to applied stress and a time scale of the experiment or a computer simulation:

$$De = \frac{t_c}{t_p}, \tag{2.12}$$

where t_c denotes the relaxation time and t_p denotes the observation time, which is normally taken to be the process's time scale. A small De number identifies a material with a fluid-like behavior, while a high De number suggests a solid-like behavior, i.e. a solid-like material may flow if given enough time, or a fluid-like material may act solid if deformed quickly enough.

3 Mathematical model

3.1 Governing equations

The Navier–Stokes equations (NSE) in vector form for the incompressible fluid flow are described and solved. The conservation of momentum and mass is given as follows:

$$\frac{\mathrm{D}(\rho \boldsymbol{u})}{\mathrm{D}t} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \boldsymbol{F}_{ext}, \tag{3.1}$$

$$\nabla \cdot \boldsymbol{u} = 0, \tag{3.2}$$

where the advective derivative is expressed as $\mathrm{D}/\mathrm{D}t$, the velocity vector as $\boldsymbol{u}$, the fluid density as ρ, the fluid pressure as p, the stress tensor as $\boldsymbol{\tau}$, and $\boldsymbol{F}_{ext}$ as the vector of external forces. It is not explicitly shown, but Eqs. (3.1) and (3.2) imply temporal and spatial dependency. The stress tensor $\boldsymbol{\tau}$ is identified for an incompressible fluid as:

$$\boldsymbol{\tau} = 2\,\mu\,(\boldsymbol{E})\;\boldsymbol{E}, \tag{3.3}$$

where μ is the fluid's dynamic viscosity, and $\boldsymbol{E}$ is the strain rate defined as:

$$\boldsymbol{E} = \frac{1}{2}\left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right), \tag{3.4}$$

where $\nabla \boldsymbol{u}$ indicates the velocity-gradient tensor of the flowing material. The shear rate is defined as:

$$\dot{\gamma} = \sqrt{2\boldsymbol{E} : \boldsymbol{E}^T}, \tag{3.5}$$

where the colon (or double-dot) operator is defined as $\boldsymbol{E} : \boldsymbol{E}^T \equiv trace(\boldsymbol{E}\boldsymbol{E}^T)$, and *trace* represents the sum of the matrix diagonal elements.

3.1.1 Time independent models

Conditions under which Newtonian and non-Newtonian flows are obtained are very much different. Consequently, modeling methods become diverse. Some of the frequently used mathematical models of non-Newtonian fluids are listed and explained in the text below.

Power Law model

Power Law is a widely used and mathematically simple model that can approximately simulate the behavior of a non-Newtonian fluid. In this generalized model for purely viscous fluids shear stress tensor is calculated as:

$$\boldsymbol{\tau} = k\,|\dot{\gamma}|^{n-1}\,\dot{\gamma}, \tag{3.6}$$

the model is defined by the effective viscosity as a function of the shear rate as follows:

$$\mu\left(|\dot{\gamma}|\right) = \mu_0\,|\dot{\gamma}|^{n-1}, \tag{3.7}$$

where μ_0 represents the flow consistency index, and n is the flow behavior index. Depending on the flow-behavior index n, it can mathematically model three types of fluids. For $n < 1$, the effective viscosity decreases with increase of shear rate, i.e. it describes shear-thinning fluid. For $n > 1$, the model describes a shear-thickening fluid, and $n = 1$ describes a Newtonian fluid. The zero-shear viscosity is approached at very low shear rates, while the infinite shear viscosity is approached at very high shear rates.

Cross Power Law model

The Cross Power Law model has four parameters for the entire shear rate range, with the effective viscosity expressed as follows:

$$\mu\left(|\dot{\gamma}|\right) = \mu_\infty + \frac{(\mu_0 - \mu_\infty)}{1 + (m \cdot \dot{\gamma})^n}, \tag{3.8}$$

where μ_0 is viscosity at zero shear rate, μ_∞ is viscosity at infinite shear rate, n is the flow index and m is the amount of time in s required for linear behavior to change to a Power Law.

Bird Carreau model

Bird Carreau is a four parameter model that is valid for the entire range of shear rates. When there are significant deviations from the Power Law model, such as at very high and very low shear rates, it is necessary to incorporate the values of viscosity at zero and at infinite shear rate. At high and low shear rate values the Carreau fluid behaves as a Newtonian fluid. The effective viscosity is defined by the following equation:

$$\mu\left(|\dot{\gamma}|\right) = \mu_\infty + (\mu_0 - \mu_\infty) \times \left[1 + (k \cdot \dot{\gamma})^a\right]^{(n-1)/a}, \tag{3.9}$$

where a is set to the default value of 2. It denotes the transition from linear character to Power Law. μ_0 is viscosity at zero shear rate, μ_∞ is viscosity at infinite shear rate, k is the relaxation time in seconds s and n is power index.

Herschel-Bulkley model

Herschel-Bulkley model also belongs to the group of generalized models of a non-Newtonian fluid. In this model stress-strain relationship is non-linear and it is defined by shear stress tenzor and effective viscosity equation as follows:

$$\boldsymbol{\tau} = \tau_0 + k\left|\dot{\gamma}\right|^n, \tag{3.10}$$

$$\mu\left(\left|\dot{\gamma}\right|\right) = min(\mu_0, \frac{\tau_0}{\left|\dot{\gamma}\right|} + k \cdot \left|\dot{\gamma}\right|^{n-1}, \tag{3.11}$$

where μ_0 is viscosity at zero shear rate, τ_0 is the yield shear stress, k is the consistency and n is the flow index. If the $\tau < \tau_0$ the Hershel-Bulkley fluid will behave as a solid, and based on the value of flow behavior index the fluid shows shear-thinning character for $0 < n < 1$, Newtonian character for $n = 1$ and $\tau_0 = 0$, and shear-thickening character for $n > 1$.

Bingham model

The Bingham model [1, 3] is also a widely used viscoplastic non-Newtonian model. This viscoplastic model is commonly used in engineering because of its mathematical simplicity, i.e. it is a two-parameter model. It is used in food, drilling, oil and gas, chemical and many other industries as the majority of industrial fluids comply with Bingham law.

According to the [4] 3D model, the stress tensor is calculated as:

$$\boldsymbol{\tau} = \left[\mu_\infty + \frac{\tau_0}{\left|\dot{\gamma}\right|}\left(1 - e^{-m\left|\dot{\gamma}\right|}\right)\right]\dot{\gamma}, \tag{3.12}$$

where τ_0 is the yield stress, $\mu_\infty$is the dynamic viscosity at infinite shear rate and m is the regularization parameter. The effective viscosity is calculated using the following expression:

$$\mu\left(\left|\dot{\gamma}\right|\right) = \mu_\infty + \frac{\tau_0}{\left|\dot{\gamma}\right|}\left(1 - e^{-m\left|\dot{\gamma}\right|}\right). \tag{3.13}$$

Casson model

The Casson model as a rheological model that is used to describe viscoelastic flow. It is expressed in accordance with the Papanastasiou [4] regularization:

$$\boldsymbol{\tau} = \left[\sqrt{\mu}_\infty + \sqrt{\frac{\tau_0}{|\dot{\gamma}|}}\left(1 - e^{-\sqrt{m|\dot{\gamma}|}}\right)\right]^2 \dot{\gamma}, \tag{3.14}$$

where τ_0 is the yield stress, μ_∞ is the dynamic viscosity at infinite shear rate and m is the regularization parameter. The effective viscosity is obtained as follows:

$$\mu\left(|\dot{\gamma}|\right) = \left[\sqrt{\mu}_\infty + \sqrt{\frac{\tau_0}{|\dot{\gamma}|}}\left(1 - e^{-\sqrt{m|\dot{\gamma}|}}\right)\right]^2. \tag{3.15}$$

3.1.2 Time dependent models

Time dependent fluids are harder to model since shear stress τ changes with respect to time. Shear stress τ increases or decrease monotonically with constant shear rate $\dot{\gamma}$ and constant temperature. Initial properties are recovered some time after the shear rate has returned to zero. A thixotropic fluids experience hysteresis loop. Examples of these fluids are drilling fluids, grease, printing ink, margarine, and some polymer melts.

Oldroyd-B model

The Oldroyd-B model was introduced by James G. Oldroyd and is named after him ([5]). It is a time dependent model that can describe viscoelastic flow. For a fluid, the stress tensor is calculated from the following equation:

$$\boldsymbol{\tau} + \lambda_1 \overset{\triangledown}{\boldsymbol{\tau}} = 2\mu_0 \left[\boldsymbol{E} + \lambda_2 \boldsymbol{E}\right], \tag{3.16}$$

where μ_0 is total dynamic viscosity composed of solvent dynamic viscosity μ_s and polymer viscosity μ_p, λ_1 is the relaxation time, λ_2 is the retardation constant defined as follows:

$$\lambda_2 = \frac{\mu_s}{\mu_0}\lambda_1. \tag{3.17}$$

The upper-convected time derivative of a tensor, $\overset{\triangledown}{\mathbf{A}}$, is expressed as follows:

$$\overset{\triangledown}{\mathbf{A}} = \frac{\mathrm{D}\mathbf{A}}{\mathrm{D}t} - \mathbf{A} \cdot \nabla\mathbf{u} - \left(\nabla\mathbf{u}\right)^{\mathrm{T}} \cdot \mathbf{A}. \tag{3.18}$$

The shear-stress tensor can be split into the Newtonian solvent stress τ_s and the extra stress τ_p as follows:

$$\boldsymbol{\tau} = \boldsymbol{\tau}_s + \boldsymbol{\tau}_p, \tag{3.19}$$

where the solvent stress is defined as:

$$\boldsymbol{\tau}_s = \mu_s \dot{\gamma}, \tag{3.20}$$

and the extra stress is defined using the expression:

$$\boldsymbol{\tau}_p + \lambda_1 \overset{\nabla}{\boldsymbol{\tau}}_p = \mu_p \dot{\gamma}. \tag{3.21}$$

eXtended Pom-Pom (XPP) model

This numerical model was created for a significant class of polymeric flows defined by the Pom-Pom constitutive equation. The model was initially not applicable to free surface flow problems. McLeish and Larson [6] were the first to propose the model and was applied by Inkson [7]. The single-equation eXtended Pom-Pom (XPP) is given as follows:

$$f(\lambda, \boldsymbol{\tau})\boldsymbol{\tau} + \lambda_1 \overset{\nabla}{\tau} + G_0(f(\lambda, \boldsymbol{\tau}) - 1)\mathrm{I} + \frac{\alpha}{G_0}(\boldsymbol{\tau} \cdot \boldsymbol{\tau}) = 2\mu_P \mathbf{E}, \tag{3.22}$$

where $\boldsymbol{\tau}$ is the polymeric tensor, and the function $f(\lambda, \boldsymbol{\tau})$ is defined as:

$$f(\lambda, \boldsymbol{\tau}) = 2\frac{\lambda_1}{\lambda_2} e^{Q_0(\lambda-1)}(1 - \frac{1}{\lambda}) + \frac{1}{\lambda^2}\left[1 - \frac{\alpha}{3G_0^2} tr(\boldsymbol{\tau} \cdot \boldsymbol{\tau})\right], \tag{3.23}$$

and λ is the backbone stretch, which is specified as follows:

$$\lambda = \sqrt{1 + \frac{1}{3G_0} tr(\boldsymbol{\lambda})}. \tag{3.24}$$

The temporal constants of this model are λ_1 and λ_2 being, respectively, the orientation and backbone stretch relaxation times, Q is the number of arms at the backbone extremity of the Pom-Pom molecule, $QQ_0 = 2$, and G_0 is the linear relaxation modulus.

4 Numerical methods

4.1 Past Research Overview

The Boundary Element Method (BEM) is used in microfluidic pumping of non-Newtonian blood flow in combination with immersed boundary-lattice Boltzmann method (IB-LBM) Ren et al. [8]. The results of the calculations in the porous cavity show that BEM can be used effectively to solve transport phenomena in a saturated porous medium Jecl et al. [9, 10]. Florez et al. [11] used the BEM method to solve non-Newtonian flow in multi-domain problem that included viscous dissipation, temperature dependent viscosity, and natural convection. The multi-domain technique is a method of domain partitioning that divides the domain into smaller parts. Included effects brought numerical results closer to experimental results. Giraldo et al. [12] tracked motion and deformation of shear-thinning drop suspended in a Newtonian circular Couette flow (flow of a viscous fluid between two surfaces) with BEM method. The apparent viscosity was modeled wit Power Law model. The results revealed that non-Newtonian drops had larger deformations than Newtonian drops due to a general decrease in viscosity. The value of the local viscosities was discovered to be strongly dependent not only on the velocity field created by the internal cylinder's motion, but also on the surface tension forces.

Eldabe et al. [13] investigated non-Newtonian Casson fluid with magnetohydrodynamics (MHD) boundary layer flow on a moving wedge with heat and mass transfer. Consideration is given to the effects of thermal diffusion and diffusion thermo with an induced magnetic field. ODFs are solved by using FDM. This approximate numerical solution was found to be in good agreement with the analytical solution. Malkus et al. [14] investigated plane slow flow of a Maxwell fluid over a transverse slot. The FDM and FEM methods were used to obtain the results. FDM uses the differential form of the constitutive equation, whereas FEM uses the integral form. The two methods yield different results, especially at low De numbers. Extrapolation of the results to mesh with infinitesimally small spacing, on the other hand, reveals good overall agreement between the two methods. Sankar et al. [15] developed computational model to investigate the effects of a magnetic field in a pulsatile blood flow through narrow arteries with mild stenosis. The blood was treated as a Casson fluid. The simplified nonlinear partial differential equation is solved using FDM. Velocity is obtained with explicit finite-difference scheme. It is discovered that the velocity and flow rate drop as the Hartmann number increases, whereas the opposite pattern is observed for the wall shear stress and longitudinal impedance.

The Finite Element Method (FEM) was used to investigate mostly viscoplastic flows. In the 1980s, viscoelastic fluids were challenging to simulate due to loss of convergence. Fortina et al. [16] investigated numercial schemes for high De numbers. The problem of the convergence loss has tried to be resolved by using upwinding schemes. The simulations were done by decoupling the velocity and stress. The method had drawbacks and the authors suggested the use of better iterative schemes. Szady et al. [17] introduced a new discrete elastic-viscous-split-stress EVSS-G/FEM method which increases numerical stability compared to the original EVSS/FEM method. The results are obtained by simulating the steady-state flow in an eccentric rotating cylinder and a flow through a tube with wavy walls and square array. The authors report that any instabilities in the results came either by the finite element approximation or the time integration method, that is why they used implicit time integration method. They have proved that with the EVSS-G/FEM method calculations are stable for De $>$ 100, while simulations with EVSS/FEM are unstable even for De $>$ 5. Grillet et al. [18] in their study used mixed (DEVSS/hp-SUPG) FEM in order to simulate the effect of fluid elasticity and stress distribution in lid-driven cavity flow. They have treated idealized Taylor's corner, i.e. corner singularities by leaking a small amount of fluid which allowed convergence of the solution. Kren et al. [19] derived basic continuity and Navier-Stokes equations for Newtonian fluid with use of special constitutive equations for viscosity in order to solve the non-Newtonian fluid flow. The spatial discretization is conducted by employing the FEM method. The method is tested in the total knee replacement by modeling the synovial fluid flow. The method yielded decoupled solutions for fluid flow with deformations. Convection in a square cavity with the Bingham model without regularization was tested in the work of Huligol et al. [20]. The FEM method with the operator-splitting method was used to solve the flow with differently heated vertical sides of the cavity. The yielded and unyielded zones of the flow were found to be easily obtainable.

The Finite Volume Method (FVM) is used in viscoelastic fluid flows. Nefyotou et al. [21] research the non-Newtonian flow effects using generalized Newtonian constitutive equations using the Finite Volume Method (FVM). The FVM solver scheme caused the use of the pressure-correction method in combination with the SIMPLE algorithm. The convective term was calculated by using the third-order accuracy QUICK differencing scheme. In this way, numerical diffusion effects have been avoided. The lid-driven cavity flow is performed for Newtonian and non-Newtonian flows using the viscous models Power Law and Quemada, and viscoplastic models modified Bingham and Casson. The paper investigates the non-dimensional impact of non-Newtonian models and the shear-thickening or shear-thinning characteristics of the fluid. Zou et al. [22] incorporated the

Latice Boltzmann method (LBM) with the FVM and proposed an integration scheme for incompressible viscoelastic fluid flow. The novel scheme has the reliability and scalability of LBM and retains the precision and generality of the FVM. The findings are consistent with empirical and numerical results of other FVM schemes. De et al. [23] simulated unsteady viscoelastic fluid with FENE-P model on the 3D porous medium employing FVM with staggered grid. Boundary conditions were applied using a second-order immersed boundary method (IBM) which had previously been used only for Newtonian fluids. Simulations were conducted for De number up to 2.0 and low Reynolds number ($Re = 0.01$) although the cost of the simulation was high De et al. [24] researched creeping flow of a viscoelastic fluid through a porous 3D medium using FVM-IBM. Increased resistance of flow was associated with an increase in De number. A topology analysis of the flow was performed and it was found that most mechanical energy was dissipated in shear-dominated regions, even at increased viscoelasticity.

In Lagrangian methods, and therefore in Particle Finite Element Method (PFEM), the convective term is not included in the momentum equation, so there is no need for numerical stabilization. But the incompressibility constraint still requires the treatment of stabilized numerical methods. In addition, when large deformations are expected, the Lagrangian approach is more preferable instead of fixed mesh methods. Salazar et al. [25] used the PFEM to model the fluid-structure interaction for landslides. Landslides generate impulse waves, and due to the uncertain kinematics of the mobilized material, it is difficult to calculate fluid-solid interactions. Application of the method was presented through case studies and actual full-scale measurements where the method provides a good risk analysis that can be used to estimate future full-scale events. Celigueta et al.[26] presented the procedure for coupling the FEM for Eulerian and paticle FEM (PFEM) for Lagrangian flows with the discrete element method (DEM). The PFEM-DEM method calculates the drag force on fluid particles for non-Newtonian fluid by predicting the terminal velocity. The method treats non-spherical particles as spherical for contact force calculation, but corrects the drag force in terms of the particle shape. The technique is tested for the cuttings transport process (hole-cleaning) full of circulating fluids, which is common in the drilling industry. The method is useful for analyzing the motion in the vertical drill cuttings and can be applied to the non-vertical positions of the wellbore drilling operations. Cremonesi et al. [27] did a number of tests on Newtonian and non-Newtonian fluids in order to validate PFEM method. The method is based on a Lagrangian formulation of the Navier-Stokes equations with an explicit finite-element approach for weakly compressible fluids. The Bingham dam-break test showed good agreement with the experimental results. Larese [28] has introduced a stabilized mixed PFEM for the calculation of non-Newtonian viscoplastic flows. The Bingham model with variable yield threshold in combination with the Mohr-Coulomb resistance criterion was used to analyze the deformation of granular non-cohesive material. The Bingham model has been tested on benchmarks, but does not adequately describe the behavior of the granular slope. The introduced variable yield-threshold does not have a mesh-size limitation, and yet it adequately describes materials with internal friction angles below 45°. Franci and Zhang [29] simulated free-surface Bingham fluids using the Lagrangian approach. Two- and three-dimensional simulations are done using the PFEM, and solid structures are simulated by employing FEM. Franci and Zhang [29] showed a lot of tests including a 3D fresh concrete slump problem. In particular, this test is the most widely accepted tool for measuring cement consistency at the work site, as viscometers are not accepted when it comes to ongoing construction. Della Vecchia et al. [30] investigated Bingham fluids, specifically the rheological characteristics of water-soil mixtures on the dam-break tests. The numerical analysis examined the viscosity and yield stress of the Bingham model based on the CFD-PFEM parametric studies. Since the yield stress and viscosity could not be recognized separately from the position of the evolving liquefied mass in the experiment, these parameters were attempted to be identified with PFEM simulations. They are obtained by monitoring the evolving aspect ratio of the flow mass or fluid pressure on a rigid obstacle. The results of the PFEM revealed linearity between researched parameters.

The Smoothed Particle Hydrodynamics (SPH) method is widely used for a variety of fluid flow simulations Monghan et al. [31]. It is a Lagrangian and meshless method, suitable for simulating large deformations of solids and fluid flow, and therefore, it has been researched since its first publications Gingold et al. [32], Lucy et al. [33]. Researchers and scientists have been developing the SPH method, solvers and models according to the type of flow, although its traditionally formulation suffers from an inaccurate pressure field Xenakis et al. [34]. The SPH has also been applied to non-Newtonian problems including viscoelastic transient free-surface flows, such as mud and molding flows Fanf et al. and Shao et al. [35, 36], while Hossein et al. [37] presented a GPU implementation of the method to achieve better performance. Shao and Lo et al. [36] simulated a dam-break problem and discussed flow features of Newtonian and non-Newtonian flows. The simulations are conducted with the use of truly Incompressible SPH (ISPH) scheme for simulate divergence-free free surface flows. Its advantage lies in the ease of tracking the free surface using the similar procedure employed in the the moving particle semi-implicit (MPS) method. The findings correlated well with the experiments. Fan et al. [38] developed a matrix free, implicit SPH solver for highly viscous non-Newtonian flows that contain high-pressure areas. The standard, explicit SPH method was not feasible due to the need for a very small time step to achieve a stable simulation. Artificial force is created between the particles in order to stabilize the system, i.e. to prevent the tensile instability. With the modified Power Law model used, the method turned out to be suitable for simulating the flow of polymer fluids in the molding process. Zhu et al. [39] in his paper assessed how well the plastic viscosity can be determined using the SPH approach. Papanastasiou's [4] Bingham constitutive model was implemented into the SPH model and

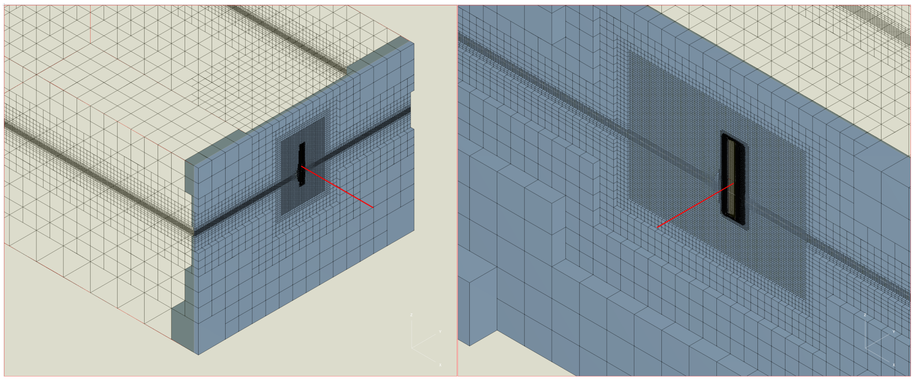

Figure 4.1: A example of an unstructured volume mesh prepared for a FVM simulation.

tested against the results of published data. The study determined adequacy of the vane rheometer to assess rheological properties. They concluded that higher Bingham number values are responsible for larger sizes of unyielded materials in the inner blade region. Xu et al. [40] advanced the SPH approach to 3D non-Newtonian flows with complex free-surface shapes. The viscosity is calculated using the Casson model. Artificial stress-term is inserted into the momentum equation to prevent tensile instability, which leads to clustering of particles and non-physical defects in fluid stretching. Three complex engineering processes were simulated as non-Newtonian free surface flows, including a droplet-impact problem. The shear thinning behavior was found to be visible in all cases and the developed SPH algorithm was stable, reasonably accurate and consistent with the published results. Xenakis et al. [34] used a diffusion-based ISPH method to describe free-surface flows. The approach has been developed to solve inelastic non-Newtonian flows by introducing a new viscous term that is more suitable for such flows. The novel approach was validated by comparison with analytical and experimental results.

4.2 Classification of numerical methods

4.2.1 Mesh-based methods

Mesh-based methods require a discretization of space in the form of subdivisions, which make a grid or a mesh. The mesh can contain complex topology, i.e. connectivity graphs between elements, and it can be locally refined where needed. An example of an a volumetric mesh for the FVM is shown in Figure 4.1. Popular mesh-based methods are listed below, and their characteristics are briefly described.

Boundary element method (BEM)

The boundary element method (BEM) is a fully equipped numerical technique for solving integral partial differential equations. Instead of using the entire space defined by the partial differential equation, the boundary element method attempts to fit the boundary values into the integral equation using the given boundary conditions. The integral equation can be used in the post-processing phase to directly compute the numerical solution at any desired point on the domain's boundary. As a result, the BEM disretizes the boundary and it is unsolvable for homogeneous and non-linear problems. It is more appropriate for domains that are infinite or semi-infinite.

Finite difference method (FDM)

The finite difference method (FDM) is a numerical technique for approximating differential equations. The FDM technique in a simple way solves linear or nonlinear ordinary differential equations (ODEs) or partial differential equations (PDEs). The method uses finite differences to replace derivatives in a differential equation. Then it converts them into a system of linear equations that matrix algebra can solve. The algebraic equations that result are solved, and an approximate solution is obtained. The domain must be structured in order to to yield accurate derivatives and therefore produce. Simple forms of FDM are inapplicable in unstructured domains, and mesh refining worsens conditioning. Generalized FDM, on the other hand, can be applied to complicated domains in a mesh-free manner, which is explained below.

Finite element method (FEM)

The finite element method (FEM) solves differential equations in two or three space variables numerically. The method is capable of dealing with complex domains. Space discretization divides large systems into smaller parts, known as finite elements. Finite elements accurately represent the complex geometry, and they can include dissimilar material properties. They are building the object's mesh, which represents the numerical domain used for calculations with a finite number of elements. The FEM formulation of the boundary value problem yields an algebraic equation system. Over the entire domain, the unknown function is approximated. Simple equations representing finite elements are combined to form a large system of equations that models the entire problem. In this manner, an easy representation of the total solution is obtained, as well as the capture of local effects. When the domain is discretized with many elements, conditioning issues arise. The FEM is more difficult and time-consuming to implement than the FDM. Both FEM and FDM struggle with large-scale problems and sparse matrices.

Particle Finite Element Method (PFEM)

Particle Finite Element Method (PFEM) models complex multidisciplinary engineering problems by combining Lagrangian particles and FEM. It is a tool for resolving multi-physics problems in evolving domains. The PFEM discretizes the physical domain with a mesh, and the governing PDEs are solved using the standard FEM method. The mesh nodes move according to the equation of motion when the fully Lagrangian approach is used. They behave like particles, and each particle has its own set of mathematical and physical properties. Mesh distortion is a common problem for mesh-based Lagrangian solvers, and it is usually resolved by creating a new mesh when the old one is too distorted. By keeping the nodes of a previous mesh fixed, PFEM avoids remapping from one mesh to another.

Finite volume method (FVM)

The finite volume method (FVM) is numerical method that solves PDEs. FVM is based on the mass conservation equations, described using fluxes. The concept of dividing a domain into finite volumes or cells is similar to that of the FEM. The conservation law is implemented in such a way that mass that enters the cell must exit the cell on the other side. In other words, the divergence term in volume integral is converted to surface integral using the divergence theorem. These termes represent fluxes at the surface of each finite volume cell. The method is suitable for unstructured meshes. The FVM can be compared with FDM in terms of using approximate derivatives in node points and with FEM by creating local approximations in order to get the global result.

Immersed boundary method (IBM)

The immersed boundary method (IBM) is approach for simulating fluid-structure interaction (FSI). It was first used to study blood flow through heart valves. The method solves coupled equations of motion for an elastic incompressible structure in a viscous and compressible fluid environment. It solves incompressible NS equations in particular. Delta function kernel equations describe the interaction of structure and fluid. The idea is that when the structure moves and deforms, there will be deformation that will push the structure to its preferred position, and the fluid near the structure will feel those effects. Similarly, when the fluid is moving, the structure needs to move at that same fluid velocity as well.

The method employs two distinct grids. The first grid represents the fluid and is known as the Eulerian frame or grid. There are no individual fluid particles floating around; there are positions that are throwing down a velocity probe and measuring the fluid velocity at

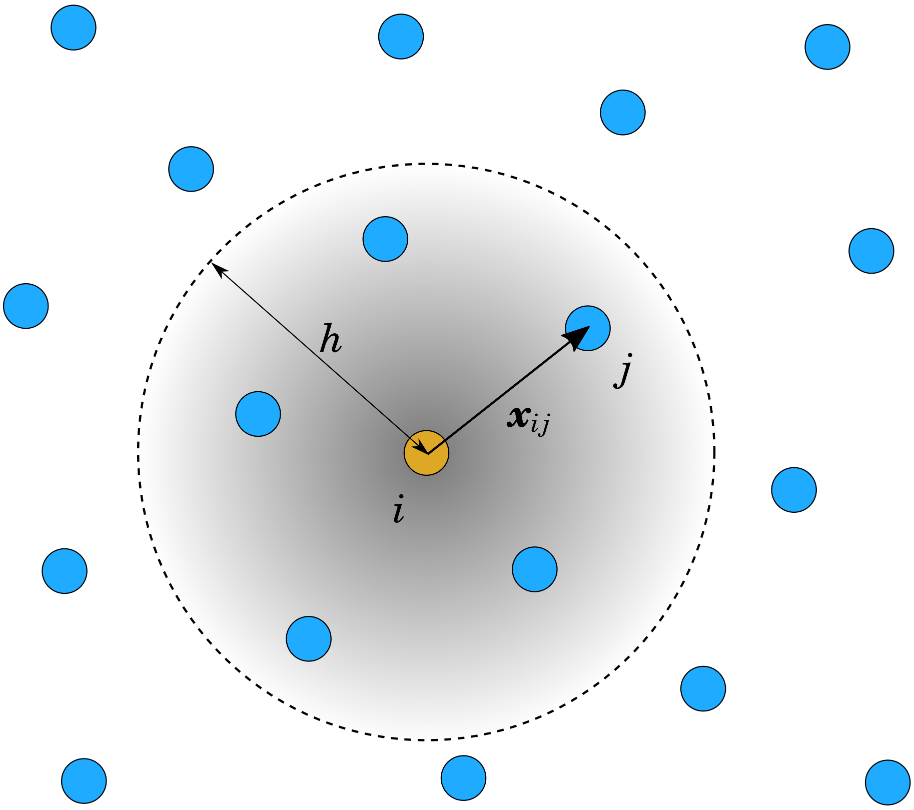

Figure 4.2: A representation of meshless discretization as a point cloud.

these positions through the simulation. There is, on the other hand, an actual immersed boundary or Lagrangian frame. That structure is deformable and has some physical material properties. Both grids are stacked on top of each other and communicate using differential equations as described below. Fiber models are material properties that can be implemented in a variety of ways. The fiber models are those that makes this method powerful.

4.2.2 Meshless Methods

Instead of discretizing space by finite volumes or finite elements, meshless methods discretize space as point clouds. The chunk of fluid volume is represented by a particle, while a point describes the state of fluid without the volume information. An example how the point cloud can replace the mesh discretization is shown in Figure 4.2.

Smoothed Particle Hydrodynamics (SPH) methods

Smoothed Particle Hydrodynamics (SPH) is a particle-based simulation method for solid mechanics and fluid flows. It can be used to calculate free surface flows or large boundary displacements. The continuum is defined as a cloud of discrete particles each with its own set of properties. The SPH defines the continuum description as an interpolation problem. The continuum field can be reconstructed by interpolating the scattered data. SPH represents particles in 2D and 3D using a Gaussian-like function. The end result is a smooth particle representation. It was thus given the name "smoothed" particle hydrodynamic. The Gaussian-like function is also known as the kernel function. It is possible to achieve a constant and continuous function by stacking particles together. Essentially, in the SPH, any type of PDE, such as conservation law, is transformed into an integral equation. After that, the kernel estimate provides an approximation for predicting field variables at discrete points. Changing the kernel functions and smoothing length can have an effect on the results as well as particle distribution along the axis. Furthermore, particle distribution affects the gradient. Due to the lack of mesh, the calculation and implementation procedures are simplified, and the code can be fully parallelized.

Moving Particle Semi-Implicit (MPS) methods

The Moving Particle Semi-Implicit (MPS) method is a Lagrangian method for free-surface incompressible flows. By solving NSE in a Lagrangian framework, fluid can be represented by particles whose motion is calculated by a kernel function based on interaction with neighboring cells. To divide each time step into prediction and correction steps, the fractional step method is used. The method is a derivative of the SPH method and was created to address the shortcomings of the SPH method for liquids and free-surface problems. The MPS is similar to SPH in that it provides approximation of the strong form of PDEs. The MPS employs simplified differential operators. The method employs local weighting in the absence of a kernel gradient. Basic SPH is used for compressible fluids, whereas weakly compressible SPH is used for liquid problems where the density is relatively constant. The kernel used in MPS is more of an asymptotic function than a smooth function like in SPH. Which of the following is a more natural description of particle-particle interaction. Because this is a semi-implicit method, the solution differs from SPH, which is a fully explicit method.

Generalized Finite Difference Method (GFDM)

The FDM contributed significantly to the generalized finite difference method (GFDM). In contrast to FDM, which requires the creation of an orthogonal grid, GFDM can be applied to an irregular set of points. It only requires the node coordinates. The method is applicable to any type of continuously changing domain geometry and can properly handle boundary conditions. The GFDM employs interpolation based on the Taylor series expansion and weighted least-squares fitting. In the method, it is critical to determine the effects of the weighting function, radius of influence, and stability parameters on time-dependent problems. Higher order approximations can be used to control the precision of the GFDM. Any physical or geometrical nonlinearity that occurs has no effect on the algorithm.

Finite Pointset Method (FPM)

The finite pointset method (FPM) is a numerical method used in continuum mechanics. FPM is a strong formulation that models PDS through direct operator approximation. For the FPM, the moving least squares (MLS) method is used and developed. In FPM, the fluid is represented by a collection of sampling points with local properties such as the pressure and velocity. This method differs from the others in that it allows for the use of a mixed Lagrangian-Eulerian approach. The points can move in a Lagrangian manner along with the flow or they can be fixed while the flow passes by them (Eulerian approach). In the Lagrangian approach, points can be added or removed to maintain the specified density. Smoothing length is commonly used to specify density. If increased accuracy is required, points could also be added in the Eulerian approach. The neighbor points are not fixed in either approach and are determined at each time step. The FPM, like most of mesh-free methods, can handle complex and/or time-evolving geometries and moving phase boundaries without additional computational effort. However, in order to produce good results, the points must cover the entire domain area. The points are not allowed to have gaps between them, which means that each point must have a certain number of neighbors and cannot cluster.

4.3 Open challenges

There are open challenges that have to be considered before introducing a novel methodology for non-Newtonian flows. The present methodology can further be improved in several directions. Some of the proposed improvements related to numerical features and physical modeling are listed below.

- Pressure and velocity are implicitly calculated in the methods that produce accurate results. The majority of these methods are mesh-based and Eulerian in nature, but they must deal with frameworks constrained by non-linear convective terms. Moreover, the CFL number requires good mesh quality and small time-step values for these methods to remain stable and accurate. The most well-known mesh methods are FEM and FVM. Besides the CFL and convective term, other open challenges are related to mesh-deformation issues and interface advection.
- A Lagrangian description of the flow, on the other hand, is natural description in which points move with the flow and do not require modelling of the convective term.

These methods can be more efficient and can deal with larger time-step values. Although the NSE lack of a convective term makes this type of flow description appealing to be solved implicitly, most Lagranigan methods are solved in the explicit manner. A method that efficiently and accurately describes flow in a Lagrangian manner and implicitly solves velocity and pressure is an open challenge. The PFEM method combines the Lagrangian and implicit methods well, but it still relies on the generated mesh. GFDM methods, on the other hand, can be implemented in the fully Lagrangian context but rely heavily on operators that are relatively slow.

- Having a Lagrangian method that is fully implicit and mesh-free would be a significant improvement. In theory, that method should produce accurate results, and it would be faster than traditional mesh-based Eulerian implicit methods but slower than Lagrangian explicit methods. At the same time, larger time-step could be used, resulting in a negligible loss of speed due to implicit solving pressure and velocity. This type of method could also be used to solve FSI problems with large deformations of the structure in any type of flow.
- Non-Newtonian flows with variable viscosity, as well as the governing equations that describe these multi-character flows, are major issues in industrial processes that require special attention. Processes that include mixing products with non-Newtonian character are still unsolved. Since viscosity resists to fluid motion, the motion created by the mixer impeller leaves portion of a tank unmixed. For shear-thinning and shear-thikening fluids the apparent viscosity is proportional to rotational speed. Time-independent fluids are influenced by shear rate applied to them, while time-dependent fluids change viscosity not only with shear rate, but also during and after the applied shear stress. The problem arrises much more when mixing process creates non-Newtonian fluid (start with low viscosity and ends with high viscosity). Powder adittion and emulsification can also be an issue.

5 Conclusions and Future Work

The problem of defining the character of viscosity that arises as a result of the complex physics described in Section 2 is a significant problem for a wide and diverse range of industrial processes. Food, mining and minerals, pharmaceuticals, paper processing, and other products in the form of pastes, slurries, concentrated solid suspensions, or emulsions are most common examples. The experimental and numerical methods listed above provide only a limited understanding of non-Newtonian flows. There are no tools for evaluating the viscosity and flow of complex fluids in industrial processes that are both computationally efficient and reliable. Therefore, new procedures for improving simulation and description of non-Newtonian fluid flow are necessary.

The advantages of a new meshless numerical methodology for single–phase incompressible flow that combines the benefits of mesh and mesh free methods would be numerous. Mesh-based Eulerian methods mostly use accurate solving schemes, but due to the CFL law, they require small time-step values. They have difficulty of reproducing free-surface flows, especially when large deformations are expected, i.e. they require complex techniques for free-surface tracking or capturing. For these reasons, building a convenient mesh is a time-consuming process that demands highly qualified engineer with experience. Mesh-free methods do not suffer from mesh-deformation issues, but they mostly solve the flow in the explicit context. Therefore, they mostly have difficulty reaching higher order of accuracy and using large time steps, i.e. they are not fully using advantages of Lagrangian description of flow.

The objective of the future work is to introduce a method for simulation of non-Newtonian fluids, which combines advantages of the meshless and Lagrangian methods, such as SPH and MPS, with the advantages of implicit schemes, that are mostly utilized by FVM and FEM. The novel methodology should rely on second-order consistent operators. The scheme will solve the generalized Navier-Stokes equations (NSE) using the split-step approach, where the pressure and the velocity is solved implicitly. After obtaining the pressure and velocity fields, the method should rely on Lagrangian advection which is shown to enable large time steps. Another benefits of such method would be its ease and speed of setting up the simulation, while getting accurate results. The simulations could be processed in short amount of time without need of expert engineer who would have complex background knowledge in numerical and mathematical modeling. The benefits combined could result in a faster decision-making process in the industry.

Abstract

Non-Newtonian fluids are a type of fluid whose viscosity varies with strain rate. Their movement is more complex and exhibits different flow characteristics from Newtonian flows. They are classified into several groups and subgroups based on their physical properties. Non-Newtonian fluids are important and can be found in industrial processes as well as in nature. The behavior of foods, beverages, paints, and medications during processing is an important factor to consider. Viscosity is a crucial aspect in design and operation of such industrial processes. The viscosity, pressure and temperature of the fluid inside the system affect the relative velocity of fluid particles. By determining the shear sensitivity and viscosity of the product, it is possible to maximize efficiency of the process. One way to determine the rheological behavior of a specific fluid or soft solid in an industrial process is through rheological experiments and measurements, while another is through numerical simulation of the entire industrial process. Today, having reliable simulations of the overall process is essential for efficient process design. In order to use numerical simulations, a good mathematical description of the flow as well as a numerical model of viscosity change are required. The paper provides an overview of non-Newtonian fluids, along with a review of fluids, a review of numerical methods and mathematical formulation is presented. A fully implicit scheme with the Lagrangian description of the flow and variable viscosity will be introduced in future work in order to avoid disadvantages of Eulerian mesh-based methods.

Keywords: non-Newtonian fluids, variable viscosity, Lagrangian flow, meshless method, implicit solver

Sažetak

Ne-Newtonovski fluidi su fluidi čija viskoznost nije konstantna, tj. promjenjiva je s brzinom deformacije fluida. Iz tog razloga tečenje je kompleksno i doživljava razne promjene unutar samog toka. Takvi fluidi su stoga podjeljeni u grupe prema njihovim fizikalnim karakteristikama. Ne-Newtonovski fluidi mogu biti nađeni u prirodi, ali su i bitan dio industrijskih procesa. Na ponašanje hrane, pića, boja, lakova i ljekova u procesu proizvodnje najviše utječe promjenjiva viskoznost ne-Newtonovskog fluida koja se treba uzeti u obzir. Viskoznost te tlak i temperatura unutar procesa utječu na relativnu brzinu kretanja fluida. Utvrđivanjem viskoznosti i osjetljivosti fluida na naprezanje moguće je optimirati proizvodni proces. Jedan način za utvrđivanje reoloških karakteristika i ponašanja fluida u procesu proizvodnje je utvrđivanje ponašanja fluida putem mjerenja i eksperimenta. Drugi način je modeliranje cjelokupnog proizvodnog procesa i numeričko predviđanje ponašanja fluida. U današnje vrijeme, modeliranje proizvodnog procesa je ključno za poboljšanje efikasnosti proizvodnje. Kako bi simulacije procesa bile vjerodostojne, matematički opis toka i numerika koja rješava takve tokove mora biti pouzdana. Ovaj rad daje pregled ne-Newtonovskih fluida, matematičkog modela i numeričkih metoda koje su do sada korištene u opisu ne-Newtonovskih fluida. U budućem radu očekuje se unaprijeđenje bezmrežne numeričke metode s Lagrangeovim opisom toka, uvođenje implicitnog solvera i varijabilne viskoznosti kako bi se izbjegli nedostatci metoda koje koriste Eulerov pristup i zahtjevaju izradu mreže.

Ključne riječi: ne-Newtonovski fluidi, varijabilna viskoznost, Lagrangeov tok, bezmrežne metode, implicitni solver

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