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ZERO-LEAKAGE SEALING SYSTEMS OPERATING IN LONG-TERM CONTACT WITH STORABLE ROCKET PROPELLANTS

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Abstract

The reliability of sealing systems in spacecrafts is crucial for the success of modern space exploration missions. Indeed, ensuring a leak-tight component subject to extreme conditions and aggressive fluids remains a significant engineering challenge. This research aims to understand and characterize micro-leakage flows of such systems. The Lattice Boltzmann Method is employed to simulate fluid flow through microchannels formed at the interface of the valve and valve seat. To use this method, the numerical generation of a 3D rough surface based on Gaussian distribution models, is generated to be fed as boundary conditions to the numerical solver.

1. Introduction

As expressed by the European Commission, the new era of "Space 4.0" [1] has begun. This era is characterized by an increasing number of participants and the arrival of innovative technologies, which together drive an increased demand for access to space. This can be shown by the growing number of launches per year, as shown by the U.S. International Trade Commission [2]. Despite major advances in rocket technology, some incidents show that complete reliability continues to be a work-in-progress [3-4].

A key factor in the performance and safety of modern launch systems is component resilience, particularly in valves, which are critical for controlling fluid flow. These components remain a major concern in all modern launchers as many incident reports [5] show valve malfunctions leading to disastrous consequences. The reliability of sealing systems in spacecrafts is crucial for the success of modern space exploration missions. Failures in these systems, such as the recent valve issues in Boeing's Starliner capsule [6], highlights the challenges faced in maintaining effective seals under severe working conditions. Indeed, ensuring a leak-tight component subject to cryogenic temperatures, steep temperature gardients and aggressive fluids remains a significant engineering challenge.

The aim of this research is to understand and characterize micro-leakage flows of such sealing systems. In the microscale, resolving Navier-Stokes equations may not be computationally tractable due to parameters such as density, speed and pressure no longer being continuous, additionally at such scales the no slip boundary conditions no longer hold and correction factors must be accounted for. To bypass this, the Lattice Boltzmann Method (LBM) is employed to simulate fluid flow through microchannels formed at the interface of the valve and valve seat. The distribution and size of these channels are directly dependent on the surface finish of both materials in contact. This method utilizes a probabilistic approach to simulate the behavior of particles on a discrete lattice. At each time step, the method evolves the particle distribution functions according to collision and streaming processes. These distribution functions represent the probability of finding a particle with a given velocity at a specific location, and their evolution tends toward equilibrium, capturing fluid dynamics behaviors [7].

To use this method, the numerical generation of a 3D rough surface based on Gaussian distribution models, which describe quite accurately real-world surfaces, is generated to be fed as boundary conditions to the numerical solver. Study of micro-mechanics and experimental tests results are used to determine the channel height, a crucial parameter for the simulation. This effective height is then fed into the LBM solver to compute the interfacial leakage flow under different operating conditions.

If the LBM-simulated leakage rates deviate from experimental results, further analysis will be conducted to account for alternative leakage pathways, such as the flow through porous media caused by material heterogeneities or seal

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defects. By combining surface roughness modeling, effective gap height determination and fluid dynamics simulations with experimental validation, this research develops a comprehensive framework for predicting and mitigating interfacial leakages. To investigate these micro-leakage flows in a realistic setting, a case study based on representative valve geometries and surface roughness parameters is considered.

2. Methodolody

As stated earlier, the goal of this research is to improve the understanding of fluid behavior in leakage flows, especially within valve systems, and to develop accurate prediction models. Leakage can arise from two mechanisms: flow through porous media and interfacial leakage. In this work, the focus is placed on interfacial leakage, which occurs when fluid escapes through microscopic channels formed between peaks of two sealing surfaces in contact.

Even the smoothest machined surfaces, which feel perfectly flat to the touch, reveal a rugged landscape of peaks and valleys under sufficient magnification. The resulting leakage can be extremely small, on the order of 10^{-2} µg/s in real aerospace applications [8], hence the name micro-leakage flows.

To model such flows accurately, it is important to identify the correct physical regime in which they occur. A key parameter for this is the Knudsen number (Kn), defined as the ratio of the mean free path of the gas molecules λ to a characteristic length scale L of the system:

$$Kn = \frac{\lambda}{L} \tag{1}$$

The mean free path represents the average distance a molecule travels before colliding with another molecule [9]. When Kn≪1, molecular collisions dominate and the gas can be treated as a continuous medium, allowing the use of classical Navier–Stokes equations (NSE). However, the behavior of the flow depends strongly on the value of this dimensionless number [10]:

- Kn < 0.001: Continuum regime – no-slip boundary conditions apply
- 0.001 < Kn < 0.1: Slip flow regime – velocity slip and temperature jump occur at boundaries
- 0.1 < Kn < 10: Transition regime – continuum assumptions break down
- Kn > 10: Free molecular regime – molecular interactions with walls dominate

By estimating the mean free path of the molecules as stated in [11] (see eq. (2) below where R is the perfect gas constant, T the temperature, d the molecular diameter of the considered gas (helium in this case), N_A Avogadro's number and P the fluid pressure), Kn falls within the range 0.01-0.1, placing the flow in the slip regime. Because of this (amongst other reasons), the LBM is chosen as the simulation method.

$$\lambda = \frac{RT}{\sqrt{2}\pi d^2 N_A P} \tag{2}$$

LBM is particularly well-suited not only because of its compatibility for flow fields of this magnitude, but also due to its computational efficiency. Unlike conventional CFD programs based on NSE which involve solving partial differential equations (with implicit non-local schemes), LBM is an explicit, local, and highly parallelizable method making it significantly faster [12, 13].

The LBM is a fluid simulation approach that takes a different path from traditional CFD methods. Indeed, instead of solving the NSE directly, it models fluid behaviour using particle distribution functions that will evolve through streaming and collision steps on a discrete lattice. This method is built on the Boltzmann equation [12], which gives it a solid physical basis and can be linked back to the macroscopic conservation laws of fluid mechanics. Another great advantage is that it is particularly well-suited for problems involving complex boundary conditions [14]. In the current case study, where the interaction between two rough surfaces is studied, LBM is thus well suited. The method is

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second-order accurate for weakly compressible flows and performs well as long as Mach numbers remain low [12, 15], otherwise the method must be adapted to compressible flows.

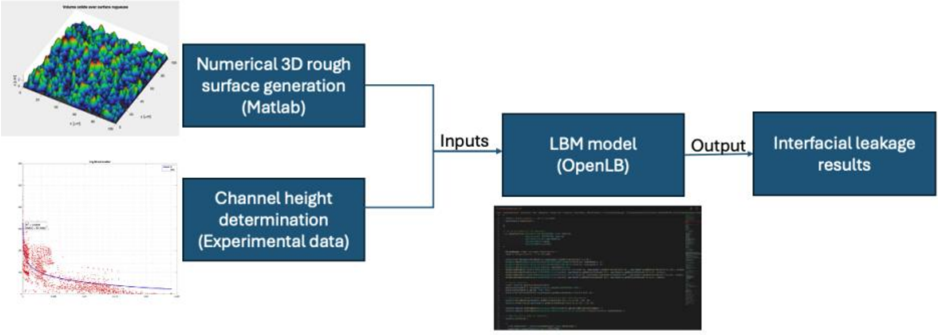

Figure 1: Workflow

To be able to use the LBM for leakage flow simulations, two inputs need to be fed to the solver. On one hand the boundary conditions, thus a model representing the channels through which the flow will pass is needed and on the other hand, the determination of the channel height, crucial parameter to have a good representation of the physical problem. A scheme of the workflow is presented in figure 1.

2.1 Rough surface interaction

Today it is well known that surfaces, whatever the finish state, are never truly flat. Indeed, any surface under sufficient magnification will show peaks and valleys or in other terms, a certain amount of rugosity, this causes the real area of contact to be extremely small when compared to the apparent area of contact [16]. This was not so clear in the scientific community before the 1900's. The work of Hertz in 1882 is considered to be the beginning of classical contact mechanics. Hertz established that the contact between curved surfaces did not occur over a single point but rather over a small surface, which increases with increasing load. Even though he considered his models to be perfectly smooth flat surfaces, and he did not introduce the notion of roughness in his studies, his theory was the foundation for later works on more realistic models considering the rugosity of surfaces [17].

The calculation of the true area of contact and its variation with load is very difficult to estimate and it is not until the late 1950's that the scientific understanding of surface asperities began to be more apparent. One of the key figures are Bowden and Tabor on their work "The friction and Lubrication of solids" in 1950 where they showed that the force of static friction between two sliding bodies is strongly dependent on the true area of contact. This was a milestone in the study of contact mechanics which led to the asperity contact theory of friction [18] giving theoretical sense to Amonton's empirical law of friction which states that the friction force is directly proportional to the applied load and independent of the apparent area of contact [19].

Another model, still used to this day is Archard's model. It is based on the theory of asperity contacts and gives a simple formulation to sliding wear. He states that the wear volume is proportional to the normal force, the sliding distance and inversely proportional to the hardness of the softer of contact partners [20]. It was assumed in previous models that the real area of contact between two surfaces is determined by the plastic deformation of their highest asperities, leading to the result that the real area of contact is directly proportional to the load and independent of the apparent area (as stated by Amonton empirical law). However, Archard pointed out that plastic deformation might hold true for the first few traversals of one body with respect to the other but this could not be the case when two surfaces in contact undergo thousands of repeated sliding cycles, as is the case in many applications, and that asperities should reach a steady state where only elastic deformation is involved. Thus, Archard showed that contrary to previous ideas, the true area of contact could be proportional to the load even under elastic deformation. [16]. Note that in its model, Archard assumed all asperities to be of hemispherical shape with a constant radius [21].

GreenWood and Williamson's (GW) study published in 1966 was yet another advancement in the field of tribology. In their work, GW assume that asperities have the same spherical radius, at least near their summit and that their height vary randomly. Even though this radii assumption might not be true, the effect is very small as the influences of greater and smaller radii largely cancel each other out [16]. Furthermore, they assume that asperities interact independently from each other, meaning the local deformation of an asperity won't affect the neighboring asperities. They also stated that only a small proportion of the area of contact is plastic and that overall properties will be close to that of elastic theory. During their work, they also developed an instrument capable of measuring surface topography and were able to plot graphs of surfaces which allowed them to lead a series of experiments to determine the height distribution of representative surfaces. They found that in accordance to results reported by Bickel in 1963, many surfaces have a height distribution that follows a Gaussian curve [16]. This study's modeling of contact between two rough surfaces is founded on their work.

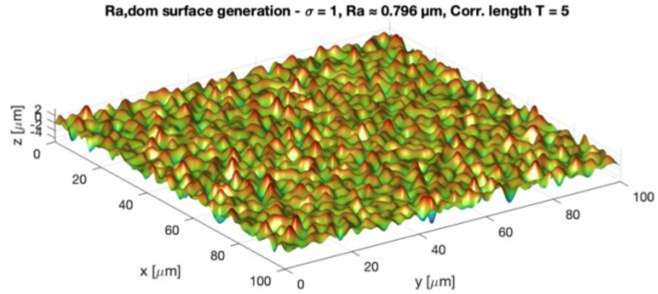

Figure 2: Random gaussian distribution of asperity heights

To be able to use the LBM, it is mandatory to give as input to the algorithm the boundary conditions which will determine the channels through which the gas will flow. According to micro contact mechanics, it is almost impossible to simulate the interaction between two rough surfaces. However, the interaction between a rough surface and a smooth plane will be considered, which represents well physical problems in many cases [21]. The surface represented in figure 2 follows thus a Gaussian random distribution of asperity heights. There are two main parameters to modelize this surface, the standard deviation of surface heights σ and the correlation length T. The standard deviation will give an indication on the asperity height distribution while the correlation length will characterize the peak density. The targeted rugosity of the surface will be the combined rugosity of the two surfaces in contact as defined in equation (3) where R_a is the absolute average roughness. As a result, the numerically produced surface should represent the characteristics of both studied surfaces.

$$R_{a\ comb} = \sqrt{{R_{a1}}^2 + {R_{a2}}^2} \tag{3}$$

2.2 Effective gap height

The numerical solver needs as input the boundary conditions of the problem. As the rough surface generation has already been discussed, what remains is the determination of the effective gap height h, which represents the distance separating the mean planes of both surfaces. This parameter is extremely difficult to measure, and in the present case, where a single rough surface is created to represent both surface characteristics, it becomes more of a theoretical construct than a physically measurable quantity. It would be ideal to find a dimensionless expression of h as a function of the contact pressure, thus allowing to estimate, under a single curve, the channel height for any material pair in contact for a given load. The non-dimensional process will be explained later.

$$h = (\frac{9F^2}{16R^*E^{*2}})^{1/3} \tag{4}$$

The effective gap height parameter could be computed in different ways depending on the assumptions made. For example, in the simplest case, it could be the deformation resulting from the contact of two idealized asperities. Using Hertz's contact theory [22], the approach can be justified by modeling asperities as hemispherical tips. In this context,

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the effective gap height would correspond to the deformation between two curved bodies under load, as given by Hertz's formula (see equation 4, where h is the deformation of the asperities, F the applied normal force, $R^*$and $E^*$are respestively the effective radii and young's modulus of both materials, their expression can be seen in equations 5. and 6; υ_i are poisson's ratio of each material). This approach provides a rational basis for estimating the contact-induced deformation between asperities, thereby allowing an approximate but physically grounded determination of the initial gap.

$$\frac{1}{E^*} = \frac{1-{\upsilon_1}^2}{E_1} + \frac{1-{\upsilon_2}^2}{E_2} \tag{5}$$

$$\frac{1}{R^*} = \frac{1}{R_1} + \frac{1}{R_2} \tag{6}$$

Another way could consist of computing this height through finite element analysis (FEA) as has been done in [23]. However, for this method to be precise enough it should require precise models for the program. Meaning that stress-strain curves in tension, compression of different samples would be required. Since joints are typically made from polymeric materials rather than pure, single-structure compounds, its mechanical behaviour can vary depending on factors such as molecular weight distribution, processing conditions, and degree of crystallinity. As a result, defining a unique or exact stress–strain curve for polymers is challenging and experimental characterization is often required for each specific formulation or application, this path was thus discarded.

Safran Aero Booster (SAB) realised in the early 2000's a test campaign whose aim was to increase their understanding on surface topology and seal tightness. Through tests and a semi-empirical model, it is possible to compute a theoretical gap height, which might be able to represent the parameter needed for the LBM simulations. This model incorporates one equation for each type of flow encountered (molecular, laminar and turbulent) and one equation giving the combined flow. The semi-empirical model's equations are not given here due to confidentiality purposes, but the parameters implied are stated here under [8]:

- Q_t, Q_l, Q_m are the turbulent, laminar, molecular and total computed flows
- C_d is an empirical parameter considering energy losses in turbulent flows
- $W, L \ and \ H_i$ are geometrical parameters of the channels
- $P_1$and P_2 are upstream and downstream pressures
- R is the ideal gas constant
- T is the temperature of the flow
- M is the molar mass of the gas
- γ is the heat capacity ratio

This model gives, for fixed working conditions, the leakage flows through some channels for any type of flow. Making use of the equations of this semi-empirical model provided by SAB one can thus get the total leakage flow as a function of the gap height (all other parameters are either known or measured). It is then possible to invert the resulting equation and get the channel gap height as a function of the leakage flow. As the measured leakage flow depends itself on the contact pressure between the surfaces, which is also known, a graph of the channel gap height as a function of the contact pressure can be drawn. Each test, depending on the conditions, will yield a different set of data points. It is now of interest to find parameters by which the dimensionless process will take place. It is expected that the rugosity of surfaces and the mechanical properties of the materials will be of influence for this parameter, thus the dimensionless channel height h^* and contact pressure P^* were chose to be computed as follows:

$$h^* = \frac{h}{R_{a\ comb}} \tag{12}$$

$$P^* = \frac{P}{E^*} \tag{13}$$

$R_{a\ comb}$ and E^* are given respectively in equations 3 and 5. This dimensionless height can then be normalized to 1 by dividing by the maximum reached value. SAB's tests have been made on flat-flat geometries and cone-sphere geometries. For the time being, only flat-flat sealing tests have been considered. By putting all the data sets into a single graph and plotting the best fitting curve, following a logarithmic distribution the graph shown in figure 3 is obtained where the correlation factor between the two parameters can be seen as is equal to 0.63.

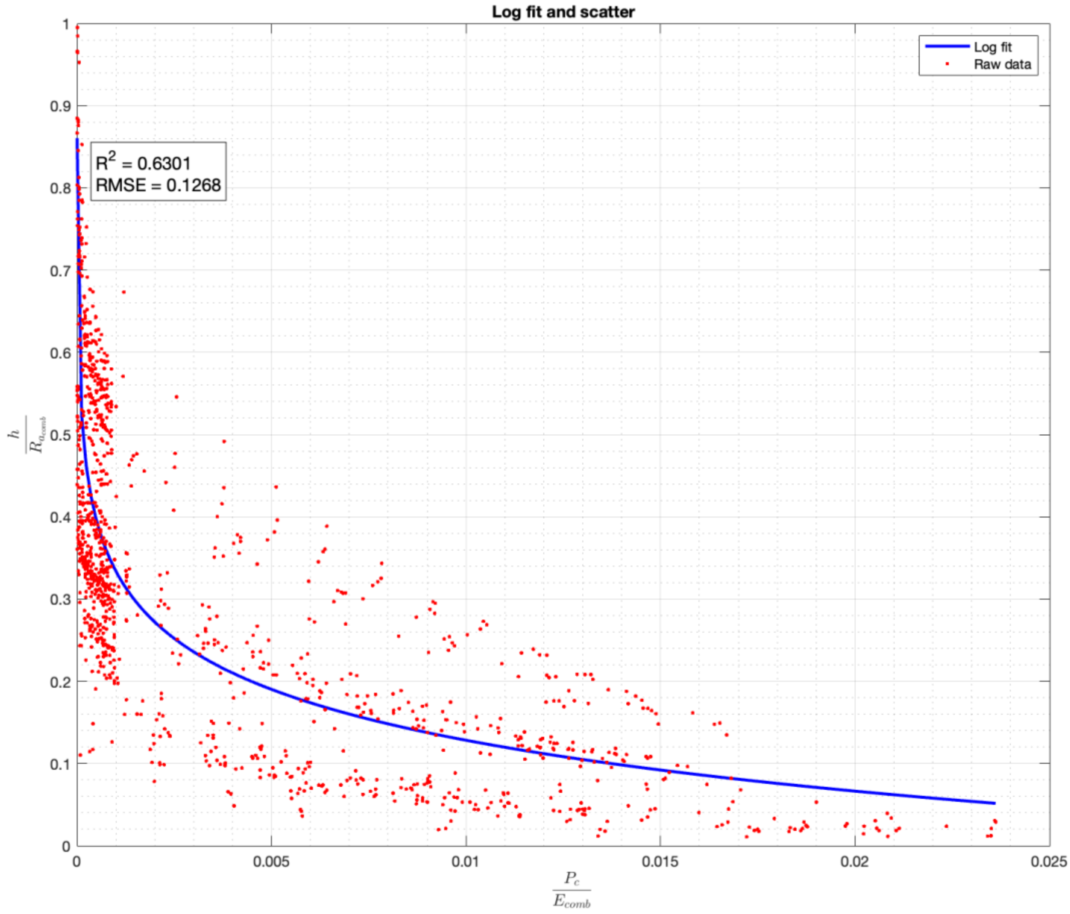

Figure 3: Experimental data points and best logarithmic fitting curve

2.3 Flow simulation

As stated earlier, for the flow simulation, it is the OpenLB software that will be chosen. As stated on their website, “The OpenLB project provides a C++ package for the implementation of lattice Boltzmann methods that is general enough to address a vast range of transport problems, e.g. in computational fluid dynamics. The source code is publicly available and constructed in a well readable, modular way. This enables for a fast implementation of both academic and advanced engineering applications. It is also easily extensible to include new physical models.” [24].

Since no simulation has yet converged and the models in use may still require refinement, a detailed explanation is not provided at this stage. However, a thorough description will be included in the forthcoming phases of this study.

3. Results

At this stage, no simulation has yet successfully converged, as this part of the project is still in its early development phase and requires further refinement. However, significant progress has already been made on the numerical setup. In particular, the implementation of boundary conditions within the OpenLB solver has been successfully achieved, allowing the system to correctly interpret the physical limits of the problem.

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The resulting computational domain is shown in Figure 4. The blue “mountains” represent the fluid domain, the region where gas flow will be simulated once the solver is set correctly. This visualization confirms that the geometry has been properly integrated into the simulation framework. While no flow behavior can be analyzed at this point, these early results provide a solid foundation for the upcoming simulation and validation steps.

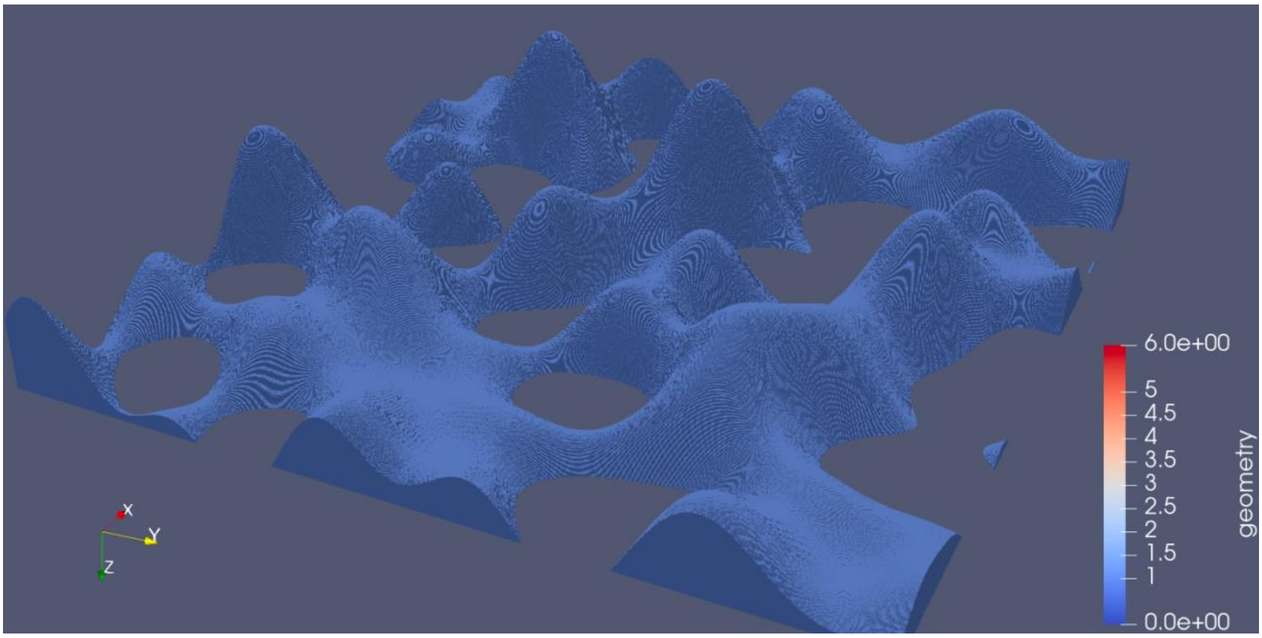

Figure 4 – View of the generated fluid domain in ParaView

4. Conclusions

This work represents the first step of a wider doctoral research project focused on modeling leakage flows in rocket valve systems using the Lattice Boltzmann Method (LBM). Although the method has been set up and preliminary models have been implemented, no simulation has yet fully converged. The current models are still being tested and require further refinement before any detailed analysis or interpretation can be made. For this reason, no in-depth results have been presented at this stage.

Nevertheless, this initial phase is crucial, as it establishes the framework upon which the rest of the research will build. The choice of LBM offers promising potential, especially in dealing with the complex geometries and micro-flows behaviors expected in valve leakage flows. The next phase of the project will focus on achieving stable and validated simulations, improving physical modeling (maybe a more advanced rough surface representation based on measured data), and comparing numerical outcomes with experimental or reference data.

In the long term, the goal is to develop a reliable simulation that can help better understand leakage mechanisms in valves (and even other domains), and eventually contribute to the design of these critical components.

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