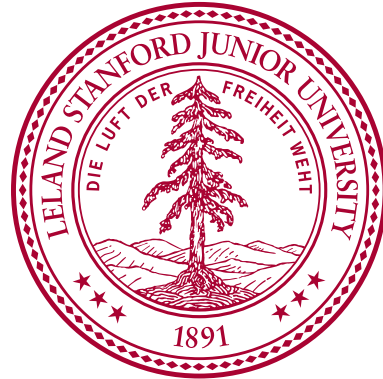




**Politecnico
di Torino**



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Multiscale modeling and performance assessment of TPMS-based heat pipe wicks for thermal management

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Abstract

The growing demand for high-performance thermal management in aerospace and electronics systems has renewed interest in passive two-phase heat transport devices such as heat pipes. The design of the porous wick structure is a critical factor governing heat pipe performance, as it controls both capillary pumping and conductive heat transfer. Triply periodic minimal surface (TPMS) structures have recently emerged as promising wick candidates owing to their tunable topology, high surface-area-to-volume ratio, and compatibility with advanced manufacturing techniques. However, validated numerical methodologies for the estimation of their effective hydraulic properties remain limited in the literature.

In this work, a multiscale modeling framework is developed to characterize the hydraulic permeability and effective pore radius of three TPMS topologies—Diamond, Gyroid, and Primitive—over a range of unit-cell sizes and porosities. Permeability is computed by solving the closure problem obtained through the homogenization of the pore-scale Stokes’ equations, yielding the effective permeability tensor of each unit cell. The homogenized model is validated against direct pore-scale numerical simulations, with relative errors below 5% for all investigated cases. The effective pore radius is estimated through an energy-based approach and validated using three-dimensional drainage simulations. Both models are further cross-validated against results available in the literature.

The resulting hydraulic parameters are then employed to evaluate the capillary performance of TPMS-based wicks and to perform device-scale simulations in COMSOL Multiphysics. In particular, a TPMS wick is compared against a conventional grooved heat-pipe design. For a unit-cell size of $775\ \mu\text{m}$ and a porosity of 80%, the Primitive topology exhibits a performance index 125% higher than the benchmark configuration, increasing the predicted capillary limit from $51\ \text{W}$ to $115\ \text{W}$. These results highlight the potential of TPMS-based wick structures for next-generation heat pipe applications and demonstrate the effectiveness of multiscale modeling as a design and characterization tool for advanced porous media.

To my father, who showed me how to care and love for others, to work hard, and to smile even when there is nothing to smile for. I am sure he would be proud of everything I have accomplished and hope, one day, to become the Man he once was...

A mio padre, che mi ha insegnato ad amare gli altri e a prendersene cura, a lavorare duro e a sorridere anche quando sorridere è l'ultima cosa che vorresti fare. Sono certo che sarebbe orgoglioso di tutto ciò che ho realizzato e spero, un giorno, di diventare l'Uomo che lui è stato...

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Prato, 2026

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1 Introduction

In the fifty years since their invention by German physicist Werner Jacobi in 1949 [1], integrated circuits have undergone a rapid development that has led these small chips made from silicon-based semiconductor materials to be implemented in virtually every electronic device being used today. The rate of development of modern integrated circuits is well described by Moore's Law, a semi-empirical relationship that tells us that the complexity of a microcircuit (measured, for example, in terms of the number of transistors) doubles every 18 months, or quadruples every 4 years [2]. At the same time, new technologies are pushing towards the miniaturization of these microcircuits to make them easier to integrate into various systems. This combination of increasing number of transistors and reduction in chip size has resulted in an increased power generation and a higher heat flux density [3], as shown in the graph in figure 1.

Today, thermal power per unit area can span from around $1 \text{ MW}/\text{m}^2$ for microcircuits used in servers, up to $5 - 10 \text{ MW}/\text{m}^2$ for phased array radar applications [3]. Furthermore, with the advent of artificial intelligence, the problem of thermal dissipation of these devices has become one of the bottlenecks that could slow down their development; this can happen for two reasons: on one hand, microprocessors are particularly susceptible to localized overheating phenomena, known as "hot spots", and therefore require adequate cooling to function properly; on the other, data centers used for training artificial intelligence are highly energy-intensive, given the amount of data they must process 24/7, 365 days a year. According to some estimations, data centers currently consume around 3% of the global energy consumption, and this figure is expected to rise to around 4% by 2030. For comparison, a large data center consumes an average of 20 to 50 MWh per year, which is enough energy to power approximately 37,000 homes over the same period of time [4]. Much of this energy, around 40%, is spent on refrigeration for these systems, so investing in the development of new thermal control technologies will be essential to ensure the sustainable and long-lasting use of technologies such as artificial intelligence.

What has just been discussed is just one example of how the need for new methods of dissipating and managing excess heat produced by various systems is one of the main engineering challenges that will have to be faced in the future. Obviously, the information technology (IT) sector is not the only one requiring elaborate thermal control systems: in the aeronautical and space sectors, heat flow management also represents a primary design challenge, which can determine the success or failure of a mission. In that sense, research carried out by the aerospace sector has accelerated the technological progress of thermal management (TM) systems like few other engineering fields have done.

A spacecraft, for instance, must be designed for highly hostile environments, in which the thermal gradients due to solar radiation are such that they can cause, in a few seconds, a temperature variation of hundreds of degrees on the same surface. Not only that, since

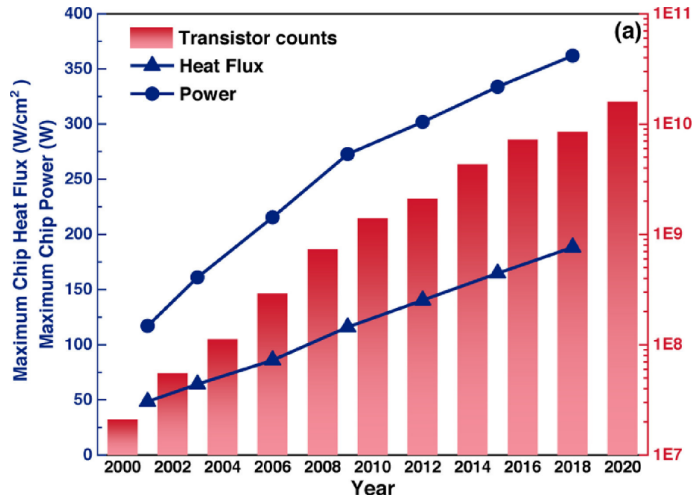


Figure 1: Number of transistors and heat flux increase through the years for integrated circuits. Picture taken from [5].

every extra gram during the launch phases of a spacecraft has a significant cost, these systems must be extremely light¹.

Another example where a thermal control system is essential is the cooling of the leading edge of hypersonic aircraft, an area where the heat being generated by aerodynamic actions can cause structural and/or auxiliary systems malfunctions. We therefore understand how, in cases like the ones just described, the feasibility of the project is closely linked to the management of the thermal loads expected during the mission.

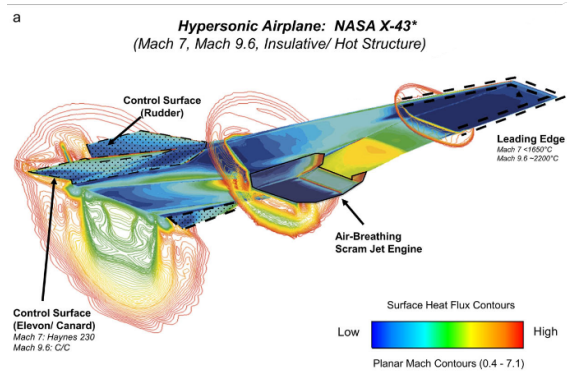


Figure 2: Heat fluxes on a hypersonic aircraft. Picture taken from [7].

From the examples given, we can therefore understand how the study of new thermal

¹Launching with SpaceX's Falcon 9, the "cheapest" launcher available today, costs around 1500 \$/kg [6]

management techniques and the evolution of existing ones can bring direct benefits to numerous engineering fields, including aerospace, IT and many others.

1.1 Thermal control system

Every aerospace component is designed to operate within a well-defined temperature range throughout the duration of the mission. Temperature variations on a spacecraft are determined by how much heat is absorbed, generated, stored, and dissipated by the spacecraft [8]. The system temperature can be maintained within the range determined during the design phase by ensuring that the heat flow out of the spacecraft equals the heat flow in; the thermal control system (TCS) is responsible for ensuring this balance.

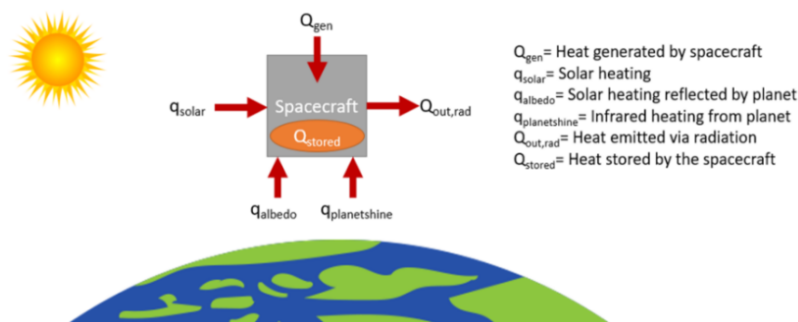


Figure 3: Thermal balance on a spacecraft. Picture taken from [9].

1.2 Thermal control solutions

Thermal control solutions can generally be divided into two categories:

- Passive control techniques
- Active control techniques

1.2.1 Passive control techniques

Passive control uses materials, devices, paints, coatings, and surface finishes to ensure the correct temperature ranges. Passive control systems have the great advantage of not requiring any type of moving mechanism or working fluid to operate, and are therefore very simple and inexpensive. The positioning of the various components and the selection of the geometric configuration can also be considered passive thermal control techniques. On the other hand, these devices do not guarantee high levels of heat flow control and therefore cannot be used for missions where the spacecraft is subject to significant heat exchange.

Some examples of passive thermal control techniques are:

- Insulation blankets (e.g. Multi-Layer Insulation)
- Radiative fins
- Solar screens
- Phase change materials
- Paints, liners e surface finishes

Altering the spacecraft's attitude can also be used as a passive thermal control technique.

1.2.2 Active control techniques

When the heat loads that needs to be dissipated of are high, it is necessary to use active thermal control systems, that is, more complex and expensive systems that use active components, such as moving parts or fluids, to guarantee a wider range of manageable power.

Some examples of active thermal control devices are:

- Electric heaters/coolers
- Heat exchangers
- Heat pipes
- Fluid loops
- Cryogenic coolers

Among the various methods listed, we will focus on heat pipes, which are active devices that exploit the latent heat of vaporization of a liquid to remove heat from the source.

2 Heat Pipes

The first heat pipe was invented by Gaugler in 1944 [10], but it was not until 1963 that Grover et al. [11], from the Los Alamos Scientific Laboratory, used this technology in an engineering application and that the term "heat pipe" was first coined.

A heat pipe can simply be seen as a self-contained structure which achieves very high thermal conductance by means of two-phase fluid flow with capillary circulation, to use the way that Cotter put it [12].

The first heat pipe application in microgravity was implemented in 1967, in the same laboratory where it was invented, demonstrating that this device could be used for space thermal management applications. After that, many new types of heat pipes were invented to solve any kind of problem, both on space and on earth, and the state of the art for heat pipe's manufacturing and operation was set.

2.1 Working principles

A heat pipe is basically a closed container which has three main components: an external casing, a porous wick and a vapor chamber. Inside the heat pipe one can find only one working fluid which will be in the liquid phase inside the porous wick and in the gaseous phase in the vapor chamber. The main feature of a heat pipe, as stated before, is that, if properly designed, it can transport heat from a heat source to a heat sink with a very small temperature drop. These devices are, in fact, also called "heat transport-passive devices", where here passive means that they work without the need of any external energy input, as it will be explained later in more details.

Conceptually, a heat pipe can be divided in three sections: the "hot section", or evaporator, where heat is absorbed; on the opposite side there is the "cold section", or condenser, where heat is dissipated; between the two an adiabatic section, where the temperature is almost constant, can be found.

To understand the working principle of a heat pipe, one can simply follow the loop that the working fluid makes, as shown in figure 4: heat is absorbed in the evaporator by the liquid inside the porous wick, which evaporates and enters the vapor chamber. This hot vapor then travels to the opposite end of the heat pipe, to the cold section, where it condenses back inside the porous wick, thanks to the heat removal provided by the heat sink. The loop closes with the liquid that travels in opposite direction with respect to the vapor, and goes back to the evaporator section.

From what has been said, the primary driving force that causes the heat pipe to operate, is an externally applied heat load to the evaporator and a heat removal at the condenser [13]. What makes the heat pipe conduct heat with minimal temperature losses is the low pressure drop of the vapor flow between the evaporator and the condenser, making the boiling-condensing cycle basically isothermal.

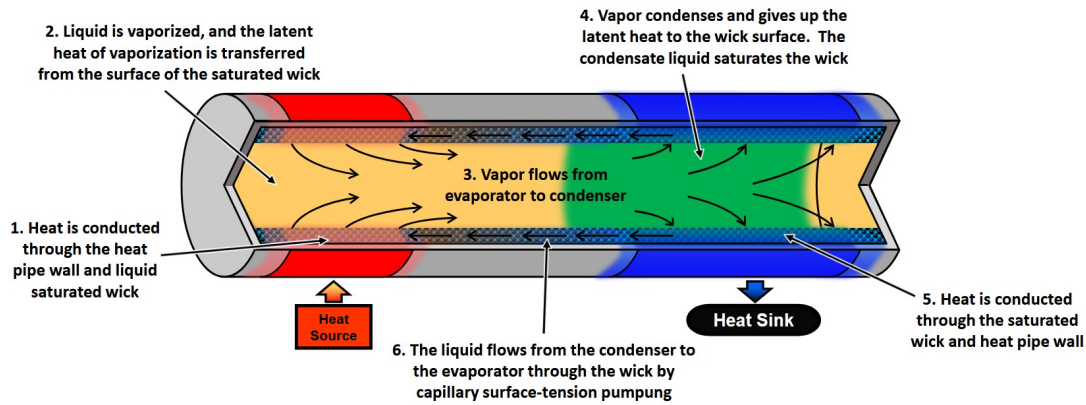


Figure 4: Heat pipe principle of operation. Picture taken from [13].

Another feature of the heat pipes is that they allow to transport great amount of heat, if compared to any other convective system, given the same temperature difference: they can do that thanks to the latent heat of vaporization of the working fluid, which is more than an order of magnitude larger than the sensible heat of any solid or fluid material. This latent heat is, in fact, the physical quantity that is being transported from the evaporator to the condenser. Heat pipes can thus be used to control very high heat flows with small lightweight structures and without the need of any external energy input, making them ideal for space applications.

2.2 Types of heat pipes and operating temperatures

There are many types of heat pipes, each one for a specific application. The main designs according to Faghri [14] are:

- Two-phase closed thermosyphon
- Capillary-driven heat pipe
- Annular heat pipe
- Vapor chamber
- Rotating heat pipe
- Gas loaded heat pipe
- Loop heat pipe

The most common design, and the one on which this research will be focused on, is the capillary-driven heat pipe (conventional heat pipe). This device is ideal for transferring heat over long distances with very small temperature drop.

Heat pipes can also be classified based on their working temperature [15]:

- Cryogenic $\rightarrow 0\text{ K} \div 150\text{ K}$
- Low temperature $\rightarrow 150\text{ K} \div 750\text{ K}$
- High temperature $\rightarrow \text{from } 750\text{ K} \div 3000\text{ K}$

The main difference from cryogenic, low temperature and high temperature heat pipes is in the working fluid being used: usually elemental or simple organic compounds are used in the cryogenic range, mainly polar molecules or halocarbons in the low temperature range, and liquid metals in the high temperature range. We will come back to the working fluid selection later on.

Now let us explain in more details the physical aspects of how heat pipes work.

2.3 Working physics of heat pipes

A heat pipe, in its simplest form, is composed by a sealed container, a wick and a suitable working fluid which in thermodynamic equilibrium with its own vapor. When heat is applied to the evaporator, a slight change in temperature of the fluid occurs, allowing for part of the liquid to evaporate, and, since we are in saturation conditions, this temperature difference results in a difference in vapor pressure which causes the vapor to flow from the evaporator section to the condenser section, where heat is removed and turns back to the liquid phase. At steady state operations, the amount of heat absorbed at the evaporator (hot side) is equal to the one released at the condenser (cold side), as the conservation of energy requires.

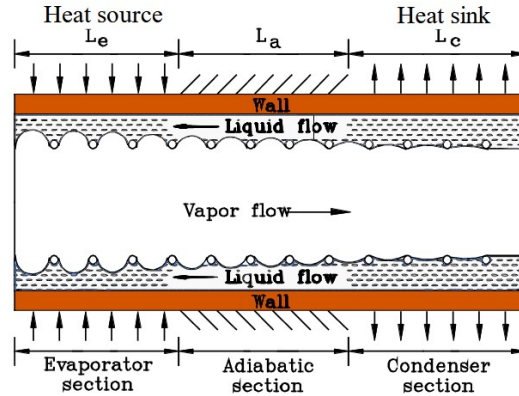


Figure 5: Working principle of a heat pipe. Picture taken from [14].

As it can be seen in figure 5, as the liquid evaporates, the liquid-vapor interface recedes somewhat in the pores of the wick. The curvature of the interface being generated is not equal along the axial length of the heat pipe, in fact, on the condenser side, this meniscus is almost flat; this difference in the radius of curvature of the liquid-vapor interface is what generates a net pressure difference in the liquid phase which translates in the capillary pumping action that the wick provides.

In the same figure, we can see that the heat pipe also presents an adiabatic section between the evaporator and the condenser: as the name suggest, this section is characterized by no heat exchange with the environment and the temperature will thus be constant in this section.

As it should already be clear, heat pipes operate through the coupled action of capillary-driven fluid flow and heat-transfer processes. Capillary forces provide the pressure difference required to recirculate the working fluid, while heat-transfer processes govern the exchange of heat between the heat pipe and its surroundings.

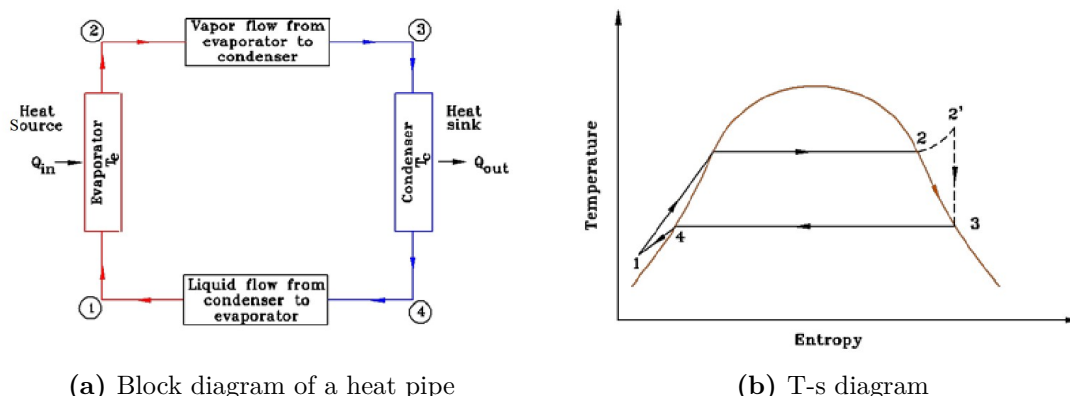


Figure 6: Thermodynamic cycle of a heat pipe. Picture taken from [14].

Since there is a mass of fluid that moves at a certain velocity inside the heat pipe, who is providing the work needed to make this motion happen? Given that the internal thermodynamical workings of a heat pipe are based on the First and Second Laws of thermodynamics, the answer to this question should be clear: work is internally generated thanks to the curved menisci and consumed in overcoming hydrodynamic losses, making the net work exchanged with the environment equal to zero. Specifically, the energy conversion occurs during the phase change across the curved liquid-vapor interface, where heat is converted in mechanical energy and a pressure head appears. The curvature of the liquid-vapor interface automatically adjusts in such a way that the work of the system, that is the capillary pumping, is just enough to win the pressure losses [15].

One last thing that can be derived from the Second Law is that the ΔT from the hot and

cold side can never be equal to zero, and thus, an isothermal heat pipe is not possible. Now, let us focus on the physics behind the generation of a curved liquid-vapor interface.

2.3.1 Liquid-vapor interface

Along the length of the heat pipe the pressure difference between the liquid and vapor phases is a function of the x coordinate (parallel to the axis of the heat pipe). This, in turn, causes the interface to curve by a certain amount and the pressure difference between the two phases to increase going from the condenser to the evaporator.

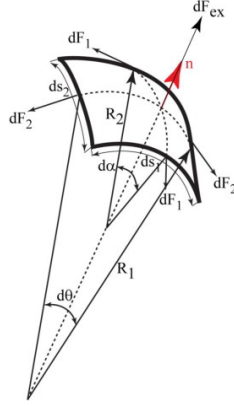


Figure 7: Curvature radii of a meniscus. Picture taken from [16].

The pressure generated by the surface tension is guided by the Young-Laplace equation and can be expressed as a function of the surface tension of the liquid and the curvature radius of the interface:

$$\Delta P_i(x) = \sigma \left(\frac{1}{R_1(x)} + \frac{1}{R_2(x)} \right) \quad (1)$$

where σ is the surface tension of the liquid while R_1 and R_2 are the two curvature radii of the liquid-vapor interface.

The surface tension is an intra-molecular force that is generated by the difference in the forces pulling the water molecules on the utmost layer of a liquid volume. This molecules will experience a greater pull from other water molecules compared to the pulling forces applied by air molecules, making the surface of the liquid curved. The surface tension is a property of the liquid

The contact angle is the angle formed by the surface tangent of the liquid-vapor interface and the tangent of the solid-liquid interface at the point of intersection. It can be evaluated via experimental testing.

Thanks to this ΔP_i , the pressure balance between liquid and vapor phases is maintained at every x coordinate.

The concaveness of the interface also gives an indication over on which side the pressure is greater: the pressure will be higher for the fluid on the concave side of the meniscus. Going back to eq. (1), we can simplify it by assuming a spherical liquid-vapor interface. Note that this assumption holds as long as the capillary length scale l_{cap} is smaller than the capillary radius.

The capillary length scale is defined as follows:

$$l_{cap} = \sqrt{\frac{\sigma}{\rho g}} \quad (2)$$

where ρ is the density of the liquid and g is the acceleration of gravity.

With some basic trigonometry one can find the simplified equation for the pressure drop in the following form:

$$\Delta P_i(x) = \frac{2\sigma \cos \theta}{r} \quad (3)$$

where θ is the liquid-solid contact angle and r is the radius of curvature of the liquid-vapor interface.

Another observation that is interesting to note is that, since the interfacial pressure ΔP_i is only determined by the aforementioned curvature, the only purpose of the porous wick is to generate this curved interfaces. In fact, wick properties such as pore size and contact angle, only influence the upper limit of the ΔP_i [15]. This upper limit is what we have previously referred to as capillary pressure. We are now going to focus on this upper limit.

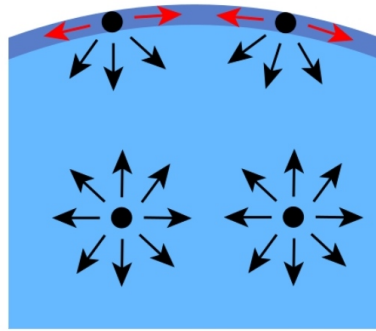
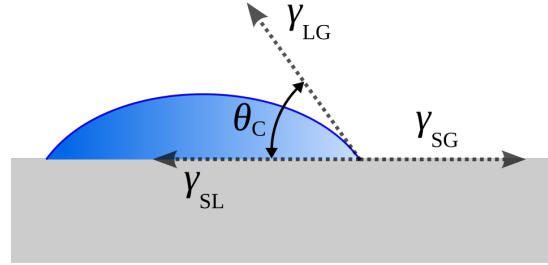


Diagram of the cohesive forces on molecules of a liquid

(a) Intramolecular surfaces



(b) Contact angle

Figure 8: Surface tension and contact angle.

2.3.2 Capillary pressure

As it has already been stated, the capillary pressure, or capillary pumping head, is the maximum achievable pressure difference by a certain wick:

$$\Delta P_c = \Delta P_i|_{max} = \frac{2\sigma \cos \theta}{r_{eff}} \quad (4)$$

where r_{eff} is the effective pore radius of the wick.

The r_{eff} parameter is a geometric property of the wick, and it can be viewed as the radius of a capillary tube that would be able to generate a capillary pressure equivalent to the one generated by the porous medium. It is used to collapse the geometric complexity of the porous structure into a single representative length scale that controls the pumping force. From the equation above it can be seen how the maximum capillary driving force that can be generated is limited by the geometry of the wick itself: the liquid-vapor interface's receding inside the porous wick is bounded by the pores' shape. During normal operations, if the heat pipe is properly designed, the capillary pressure generated by the wick will be lower than the maximum achievable. When the maximum capillary pressure is reached, the heat pipe incurs in what is called the "capillary limit".

2.3.3 Capillary limit

During on-design operations, the pressure gain given by the capillary pumping should equal the losses in both liquid and vapor to allow the rate of circulation of the fluid to adjust itself based on working conditions. The pressure losses that the working fluid encounters during its path are due to body forces (gravity or other accelerations) and viscous and dynamic flow.

Usually, this pressure drop is divided into the three different components [13]:

- Pressure drop in the vapor flow, ΔP_v
- Pressure drop in the liquid flow, ΔP_l
- Gravitational head, ΔP_g

To ensure proper circulation, the capillary pumping head must be greater than the total pressure drop:

$$\Delta P_c \geq \Delta P_v + \Delta P_l + \Delta P_g \quad (5)$$

If this condition is not satisfied, the heat pipe is said to have reached its capillary limit. Under this condition, the capillary pressure generated by the wick is no longer sufficient to sustain the required fluid circulation. As a result, the evaporation rate exceeds the rate at which liquid is returned to the evaporator, leading to liquid depletion in the evaporator section. This may cause local dry-out and the formation of hot spots, resulting in a significant degradation of the heat pipe performance. Consequently, the maximum heat

transport capability of the heat pipe is ultimately limited by the performance of the wick structure.

2.3.4 Other heat transport limits

The capillary limit is the most common limit that is reached under normal heat pipe operations, but many other factor could reduce the maximum heat-absorbing capabilities of the heat pipe.

For instance, other limits are:

- Viscous limit
- Boiling limit
- Entrainment limit
- Sonic limit

The viscous limit is typically reached when the working temperatures are very low, making the viscous resistance encountered by the vapor flow very high due to an increase in density and vapour pressure.

The boiling limit happens when the heat flux provided at the evaporator is high enough to cause the nucleation of bubbles inside the porous wick, creating hot spots by a reduction in the liquid-solid heat transfer surface area. Excessive boiling may lead to dry-out. This limit can be more restricting than the capillary limit when non-metallic working fluids are used at high operating temperatures.

The entrainment limit is reached when high velocity vapor flows are present in the vapor chamber. Normally, for low relative velocities, the shear forces that are generated at the liquid-vapor interface are low and contribute only to pressure losses through viscous actions. If the velocity is high enough, an instability of the liquid surface could cause the vapor to uptake a small part of liquid mass, which will be entrained in the vapor. This mass will be removed from the mass being pumped back to the evaporator, reducing the amount of heat that the heat pipe can absorb.

Finally, we have the sonic limit when the vapor reaches the sonic conditions when moving from the evaporator to the condenser. In fact, the channel that the vapor moves through can be seen as a convergent-divergent nozzle [14], as shown in figure 9. As with any other fluid dynamic flow, the sonic conditions can only be reached in the throat of this channel and once they are reached, a further increase in the heat input can not translate into a higher vapor mass flow rate and we say that the flow is choked.

These are just the most common factors that limit the heat transfer capability of a heat pipe, but many other may take place (vapor pressure limit, frozen startup limit, condenser heat transfer limit, vapor continuum limit, flooding limit [14]).

Now that we understand the principle of working of heat pipes, we can focus on the most important component of these devices, that is, the wick.

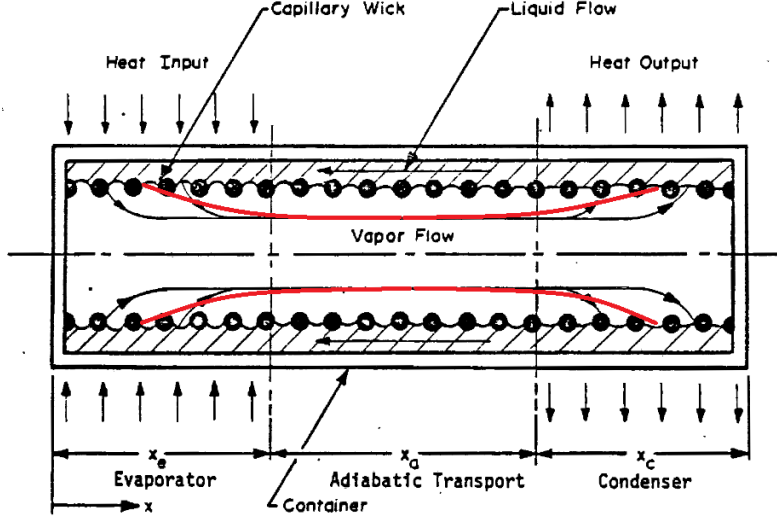


Figure 9: Convergence-divergence channel for the vapor flow (in red).

2.4 Heat pipe's wick

From what has been said in the previous sections, the wick is the medium via which liquid is recirculated from the condenser to the evaporator section, and it needs to do it by generating the highest possible capillary pumping head and the minimum pressure losses. For this exact reason, a wick has to satisfy two contrasting demands: provision of a flow path with low resistance for the condensate, which requires an open porous structure with high permeability and a small pore size of the wick, for high capillary pumping pressure [17]. The performance of a wick thus depend on two main parameters: permeability (K) and effective pore size (r_{eff}). The latter has already been introduced before, we will now talk about permeability.

Permeability, typically indicated with the letter K , can simply be viewed as a parameter that describes the relationship between pressure drop and mass transport through porous media, and is therefore a key parameter to evaluate the performance of porous wicks like the ones that can be found in heat pipes. The unit measure of permeability is square meters, and it can be measured experimentally with different methods, such as the forced flow test or the rate-of-rise test (which can also be used to measure the effective capillary radius) [18]. On a more theoretical level, permeability is a proportionality constant that appears in the Darcy's Law and relates the velocity of the (laminar) flow to the pressure drop:

$$v = \frac{K \Delta P}{\mu L} \longrightarrow K = \frac{v \mu L}{\Delta P} \quad (6)$$

where v is the velocity magnitude, ΔP is the pressure drop along the length L of the porous media and μ is the dynamic viscosity of the fluid.

From the correlation given by Darcy, which is valid only if the inertial terms of the fluid flow can be neglected (i.e. when $Re \ll 1$), we see that for a given velocity of the flow, if the permeability of the media increases the pressure drop decreases, and vice versa. Even though the permeability of a porous medium is typically considered as a scalar value, since the direction of the fluid is known in most cases, there are certain applications where the porous structure is anisotropic and thus the permeability takes the form of a tensor. We will come back to this particular case later.

From what it has been said, it should be clear that a properly-designed wick, that allows the heat pipe to have good fluid circulation and thus absorb and transfer great amount of thermal power, should have high permeability K (to reduce the pressure drop and thus the pressure losses of the liquid flow ΔP_l) and a high effective capillary radius r_{eff} (to increase the capillary pumping head ΔP_c). Basically, the first requirement moves the operating point away from the capillary limit, whereas the second requirement increases the capillary limit. The issue with this design requirements is that the most commonly used wicks in the industry can not respect both of them, but can only optimize for one, to the detriment of the other. The reason for this is that higher permeabilities can be obtained only with smaller pore radii. This limit can be bypassed using non-conventional wicks.

Heat pipe's wicks can be classified according to the regularity of their internal structure:

- Homogeneous wicks
- Composite wicks

2.4.1 Homogeneous wicks

Homogeneous wicks are porous structures whose properties are uniform in all directions. As previously discussed, these wicks cannot simultaneously maximize both permeability, K , and effective pore radius, r_{eff} ; therefore, their performance is generally lower than that of more advanced wick structures. On the other hand, they are simpler to design and manufacture, easier to prototype, and suitable for a wider range of applications.

The most commonly used types of homogeneous wicks are [14]:

- Screen mesh
- Sintered metal
- Axial grooves

Screen mesh wicks are the simplest type of wicks that can be used in heat pipes and consist of a metal or cloth fabric held by tension inside the heat pipe. This type of wicks generate medium-high capillary pressure heads but suffer from low permeability. The sintered metal wicks can be manufactured by packing small metal spheres or particles, with sizes that range from few microns to tens of microns, and then heating them until they are sintered to each other and to the heat pipe's wall. This second type of wick can be used for applications

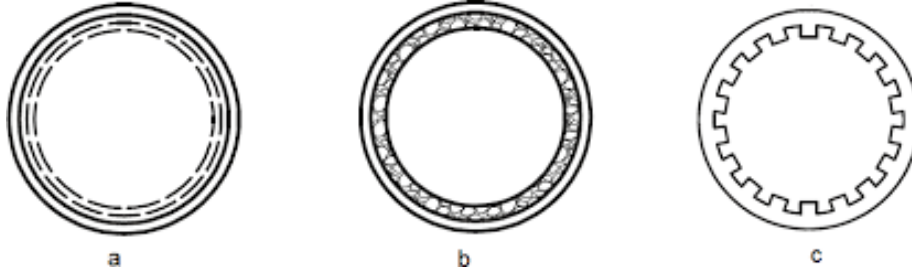


Figure 10: Mesh (a), sintered (b) and grooved (c) wicks.

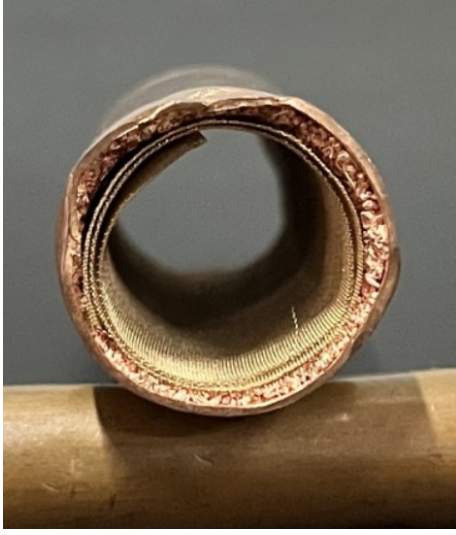
where high capillary pumping is needed, given the small effective pore radius of the structure, and where low permeability is not an issue. The last type of homogeneous wicks, the axial grooves one, can be produced via extrusion or broaching and is the wick with the highest permeability and, thus, the lowest capillary pressure head [19]. The axial grooves wick is one of the most commonly used wicks for space applications, since in microgravity there is basically no gravimetric head that work against the fluid flow, and thus the capillary pressure head only needs to win the pressure drop caused by viscous forces.

For those applications where high permeability and high capillary pumping are needed, homogeneous wicks may not be able to satisfy the requirements. In such cases, composite wicks may be more well suited.

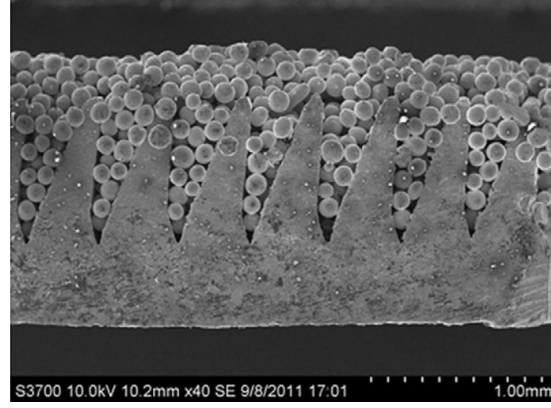
2.4.2 Composite wicks

Composite wicks enable the designer of the heat pipe to have both small pores at the liquid-vapor interface to generate higher capillary pumping and larger pores inside the wick to allow for higher permeability. Usually, these type of wicks are made by combination of homogeneous wicks. For instance, the simplest way to obtain a composite wick is to use two different screen meshes, one with finer pores at the liquid-vapor interface, and one with larger pores inside the wick. Another type of composite wick can be obtained by combining the axial groove one with the screen mesh on top of it, allowing for a smoother passage for the fluid flow (higher permeability) and a decent capillary pumping head (small effective pore radius). Many other combinations are proposed in literature to obtain composite wicks, for example, Chavhan et al. [20] analyzed the hydraulic performances of a sintered-screen mesh wick, obtaining a 13.31% lower thermal resistance compared to a sintered wick, whereas Deng et al. [21] studied a wick obtain by the composition of an axial grooves and a sintered wicks, showing a 20% increase in capillary performances compared, again, to a sintered wick.

Composite wicks have the great advantage of being customizable, based on the application, to obtain the maximum performances of the heat pipe. The downsides of a more complex porous structure are the higher costs of manufacturing, especially for long heat pipes, and the lower reliability.



(a) Screen mesh combined with sintered wick



(b) Grooved combined with sintered wick

Figure 11: Examples of composite wicks.

Building upon the concept of composite wicks, new manufacturing technologies, such as additive manufacturing, allow the fabrication of complex metal structures that could be used to create porous wicks that maximize both permeability and capillary pumping.

2.4.3 Additively manufactured wicks

Recent advancements in metal 3D printing techniques are allowing to build new types of structures, characterized by greater design freedom and small-scale features when compared with other manufacturing techniques [22]. Additive manufacturing (AM) allows to design complex topologies, with smooth curvatures, high surface-to-volume ratios and highly connected pores structures, features that are key in the design of any type of heat exchanger device, especially for a heat pipe's wick. Another great advantage of 3D metal printing is that, not only does it allow to obtain structures that cannot be obtained with traditional manufacturing techniques, but it also allows to obtain them with a significantly lower number of components, and therefore, a significantly lower complexity.

Even though not a lot of research on 3D printed wicks for heat pipes has been done, some studies can be found on this topic, with promising results. A review of heat transfer devices based on AM was proposed by Jafari and Wits [23]. They also proposed, a capillary performance analysis for 3D-printed metal wick structures for heat pipe applications [22]. Esarte et al. [24] presented a 3D-printed wick for loop heat pipes. Ang et al. published a pore-scale simulation of additively-manufactured wicks based on X-Ray tomography [25]. Sobhani et al. [26] presented a case study, in collaboration with NASA, for grooved ceramic

heat pipes for space applications. Finally, Zhao et al. [27] proposed a performance analysis of an additive manufactured structure for loop heat pipes, based on triply periodic minimal surface (TPMS).

Let us briefly talk about the manufacturing processes that can be used to build a 3D printed porous wick. The most suited AM technique used for producing porous structures characterized by small features is the power bed fusion (PBF) technique, which can be further divided into two other major techniques:

- selective laser melting (SLM), which uses a high-intensity laser to melt the metal powder;
- electron beam melting (EBM), which uses an electron beam instead.

Of the two, the first one, SLM, is the most used one to build complex structures like the ones that we are going to study, thanks to the quality of the printed product. SLM working principle is based on a system of mirrors used to precisely orient the direction of a laser beam which is used to melt the first layer of powder metal, following the designed path, as shown in figure 12. After having selectively melted the first layer of metal, another layer of powder is pushed on the previous one, and the process is repeated [28]. Layer by layer, the overall rough geometry is obtained and can be passed to post-processing.

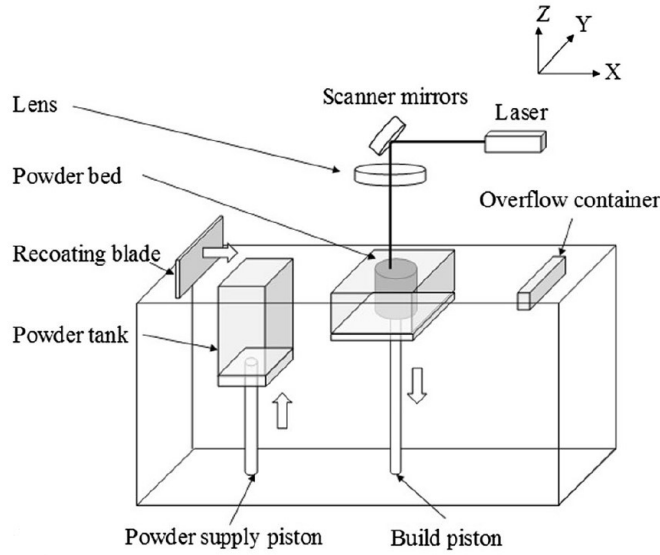


Figure 12: SLM scheme.

Given the nature of the manufacturing process, it goes without saying that the quality of the final print improves inversely with the size of the laser beam and the thickness of each layer being melted. A smaller beam and a small thickness of each layer allows for finer

details to be produced.

With the current technologies, the smallest geometric feature that can be printed with commercially available 3D printers is in the order of the tens of microns. For instance, the M1 Cusing SLM 3D printer, produced by Concept Laser, has a minimum layer thickness of $20 \mu m$ and a laser focus diameter of $50 \mu m$, with energy source of $200 \div 400 W$ [28]. Even lower feature sizes will be obtainable in the near future thanks to new 3D printing technologies that will allow greater design freedom.

2.5 Working fluid selection

Depending on the application, each heat pipe will have its particular temperature range in which it needs to operate. To make sure that the heat pipe works properly, the designer must choose a working fluid that is suited to work in that temperature range.

The fluids that can be used for the various temperature ranges are shown in figure 13.

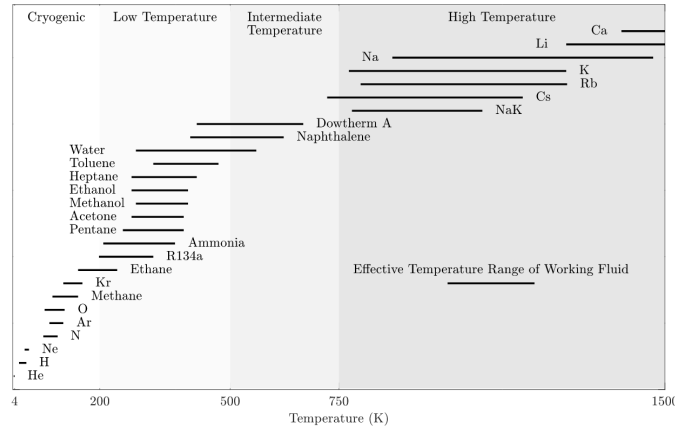


Figure 13: Working fluids for each temperature range. Picture taken from [29].

A parameter that is often used to decide which fluid is the best for the particular application is the following merit number:

$$M = \frac{\rho_l \sigma_l h_{lv}}{\mu_l} \quad (7)$$

where ρ_l is the density of the fluid, σ_l is the surface tension, h_{lv} is the latent heat of vaporization and μ_l is the dynamic viscosity, all evaluated at the working temperature of the heat pipe. This merit number is essentially the ratio between the positive and negative properties of the fluid concerning thermal transport, and it is used to rank fluids based on their heat transport capacity. Figure 14 shows the merit number as a function of temperature for different working fluids.

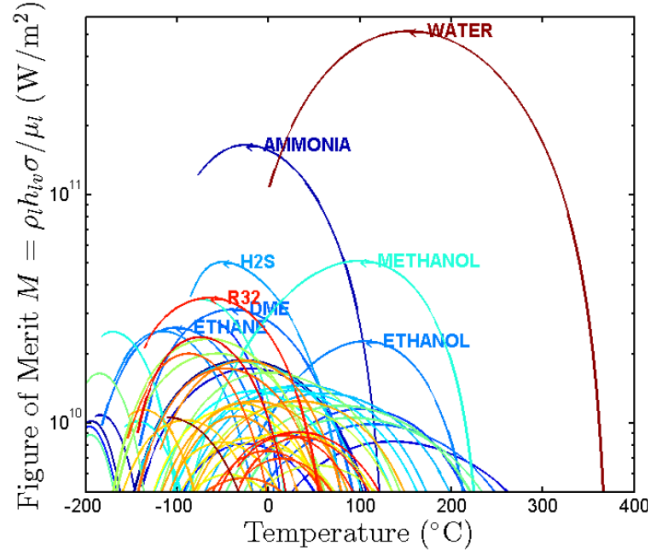


Figure 14: Merit number for different working fluids. Picture taken from [30].

Another thing that needs to be considered when deciding which fluid to use is the compatibility with the structural material of the heat pipe. Longevity of a heat pipe can be assured by selecting a container, a wick and welding materials that are compatible with one another and with the working fluid of interest. For instance, the structural material used for the casing and wick of the heat pipe may be soluble in the working fluid at the operating temperature, or it may even catalyze the decomposition of the working fluid at the expected operating temperature [14].

These are the most commonly used combinations of working fluid and material:

- Low temperature: Ammonia/Aluminum, Ethanol/Copper, Water/Copper;
- Intermediate temperature: Mercury/Stainless Steel;
- High temperature: Lithium/Superalloys;

We will come back to talking about working fluid and material selection when discussing device scale simulations in section 7.4.1. Finally, the material selection also needs to account for the manufacturing process being used, which is especially true for additive manufacturing.

3 Triply periodic minimal surfaces

First introduced by Hermann Schwarz and his student E.R. Neovius in the 1880s [31], triply periodic minimal surface (TPMS) represent a family of zero-thickness periodic surfaces formed by points in space that satisfy an implicit function equation.

These structures exhibit striking similarities to biological tissues found in nature and are for this reason, called "bio-mimetic". For instance, the microstructure of the wings of some species of butterfly resemble a type of TPMS structure [32]. These bio-mimetic properties contribute to the increasing interest and popularity of TPMS structures, given that they were optimized by millions of years of genetic evolution.

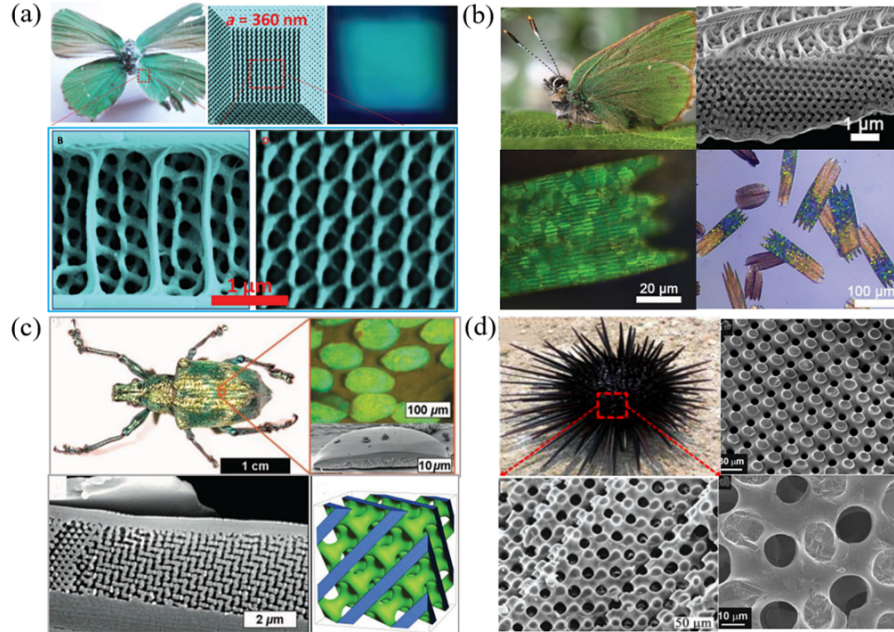


Figure 15: Example of TPMS structure that can be found in nature. Picture taken from [32].

The simplest way to create a TPMS structure is to use the level-set implicit equations derived from the Fourier series, which can be written in the generic following form:

$$F(X, Y, Z) = C \quad (8)$$

where $X = 2\pi x/l_x$, $Y = 2\pi y/l_y$, $Z = 2\pi z/l_z$, and x, y, z are spatial coordinates, l is the length of a unit cell, and C is a constant.

The family of known TPMSs is very large, in figure 16 are represented the most commonly used ones and their relative periodic cellular arrays, whereas in table 1 are summarized the level surface expressions that define the surface geometry of these structures. Once the single unit cell is created, the whole lattice structure can be generated by extending by periodicity the single unit cell.

Mathematically, these structures present several interesting properties that make them appealing for many different engineering applications: they present a zero-mean curvature at each point, first and second order continuity and a controllable geometric morphology. Moreover, they possess high specific surface area, low flow resistance, superior strength and stiffness and excellent thermal performances, making them ideal form thermal management applications [32], as shown in Figure 17.

In figure 17 are also shown the two different families of TPMS structure that exist: *Sheet* and *Network*. *Sheet* TPMS are obtained by thickening the implicit surface to obtain a wall that divides the volume into two separate domains; to define them we need to specify unit cell size, mid-plane offset and wall thickness. With *Network* TPMS the implicit surface is used to divide the volume into an empty domain and a solid domain, thus they only need the unit cell size and mid-plane offset to be completely defined. For instance, the structures shown in figure 16 are all in the *Network* family.

In this study, we will focus our attention only on three *Network* TPMS: Diamond, Gyroid and Primitive.

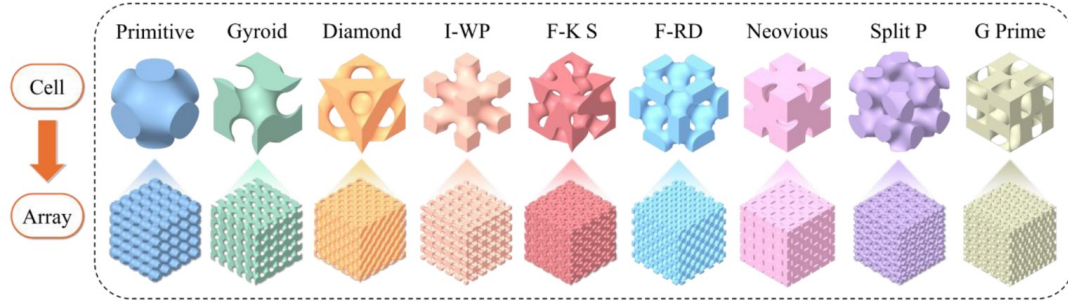


Figure 16: TPMS unit cells and relative periodic arrays. Picture taken from [27].

3.1 TPMS for thermal management applications

Most of the research that has been done on TPMS for thermal applications has been published in the past 5 years or so, due to the fact that previously additive manufacturing technologies were not mature enough to produce these type of structures, which are characterized by small features, with the required level of details [32].

One of the first characterization of TPMS structures for heat transfer applications was carried out by Li et al. [33], where they simulated a bio-inspired heat exchanger based

TPMS Type	Level Surface Expression $f(x, y, z) + t = C$
Primitive	$\cos\left(\frac{2\pi}{l}x\right) + \cos\left(\frac{2\pi}{l}y\right) + \cos\left(\frac{2\pi}{l}z\right) + t = C$
Gyroid	$\sin\left(\frac{2\pi}{l}x\right) \cos\left(\frac{2\pi}{l}y\right) + \sin\left(\frac{2\pi}{l}y\right) \cos\left(\frac{2\pi}{l}z\right) + \sin\left(\frac{2\pi}{l}z\right) \cos\left(\frac{2\pi}{l}x\right) + t = C$
Diamond	$\sin\left(\frac{2\pi}{l}x\right) \sin\left(\frac{2\pi}{l}y\right) \sin\left(\frac{2\pi}{l}z\right) + \sin\left(\frac{2\pi}{l}x\right) \cos\left(\frac{2\pi}{l}y\right) \cos\left(\frac{2\pi}{l}z\right) + \cos\left(\frac{2\pi}{l}x\right) \sin\left(\frac{2\pi}{l}y\right) \cos\left(\frac{2\pi}{l}z\right) + \cos\left(\frac{2\pi}{l}x\right) \cos\left(\frac{2\pi}{l}y\right) \sin\left(\frac{2\pi}{l}z\right) + t = C$
I-WP	$2\left(\cos\left(\frac{2\pi}{l}x\right) \cos\left(\frac{2\pi}{l}y\right) + \cos\left(\frac{2\pi}{l}y\right) \cos\left(\frac{2\pi}{l}z\right) + \cos\left(\frac{2\pi}{l}z\right) \cos\left(\frac{2\pi}{l}x\right)\right) - \left(\cos\left(\frac{4\pi}{l}x\right) + \cos\left(\frac{4\pi}{l}y\right) + \cos\left(\frac{4\pi}{l}z\right)\right) + t = C$
F-K S	$\cos\left(\frac{4\pi}{l}x\right) \sin\left(\frac{2\pi}{l}y\right) \cos\left(\frac{2\pi}{l}z\right) + \cos\left(\frac{2\pi}{l}x\right) \cos\left(\frac{4\pi}{l}y\right) \sin\left(\frac{2\pi}{l}z\right) + \sin\left(\frac{2\pi}{l}x\right) \cos\left(\frac{2\pi}{l}y\right) \cos\left(\frac{4\pi}{l}z\right) + t = C$
F-RD	$-4\left(\cos\left(\frac{2\pi}{l}x\right) \cos\left(\frac{2\pi}{l}y\right) \cos\left(\frac{2\pi}{l}z\right)\right) - \left(\cos\left(\frac{4\pi}{l}x\right) \cos\left(\frac{4\pi}{l}y\right) + \cos\left(\frac{4\pi}{l}y\right) \cos\left(\frac{4\pi}{l}z\right) + \cos\left(\frac{4\pi}{l}z\right) \cos\left(\frac{4\pi}{l}x\right)\right) + t = C$
Neovius	$3\left(\cos\left(\frac{2\pi}{l}x\right) + \cos\left(\frac{2\pi}{l}y\right) + \cos\left(\frac{2\pi}{l}z\right)\right) + 4\cos\left(\frac{2\pi}{l}x\right) \cos\left(\frac{2\pi}{l}y\right) \cos\left(\frac{2\pi}{l}z\right) + t = C$
Split P	$1.1\left(\sin\left(\frac{4\pi}{l}x\right) \sin\left(\frac{2\pi}{l}y\right) \cos\left(\frac{2\pi}{l}z\right) + \sin\left(\frac{4\pi}{l}y\right) \sin\left(\frac{2\pi}{l}x\right) \cos\left(\frac{2\pi}{l}z\right) + \sin\left(\frac{4\pi}{l}z\right) \sin\left(\frac{2\pi}{l}y\right) \cos\left(\frac{2\pi}{l}x\right) - 0.2\left(\cos\left(\frac{4\pi}{l}x\right) \cos\left(\frac{4\pi}{l}y\right) + \cos\left(\frac{4\pi}{l}y\right) \cos\left(\frac{4\pi}{l}z\right) + \cos\left(\frac{4\pi}{l}z\right) \cos\left(\frac{4\pi}{l}x\right)\right) - 0.4\left(\cos\left(\frac{4\pi}{l}x\right) + \cos\left(\frac{4\pi}{l}y\right) + \cos\left(\frac{4\pi}{l}z\right)\right) + t = C$
G Prime	$\sin\left(\frac{4\pi}{l}x\right) \cos\left(\frac{2\pi}{l}y\right) \sin\left(\frac{2\pi}{l}z\right) + \sin\left(\frac{4\pi}{l}y\right) \cos\left(\frac{2\pi}{l}z\right) \sin\left(\frac{2\pi}{l}x\right) + \sin\left(\frac{4\pi}{l}z\right) \cos\left(\frac{2\pi}{l}x\right) \sin\left(\frac{2\pi}{l}y\right) + 0.32 + t = C$

Table 1: Level surface expressions of TPMS lattice structures

on triply periodic minimal surface for supercritical CO₂ cycles. An improvement of the overall thermal performance (through a variable called performance evaluation coefficient) of 15 – 100% and the Nusselt number of 16 – 120% were estimated, for a given pumping power, when compared with a printed circuit heat exchanger. Reynolds et al. [34], simulated using computational fluid dynamics (CFD) tools a 3D printed TPMS-based structure to evaluate its thermo-fluid dynamical performances when used as a bi-liquid heat exchanger, demonstrating an overall increase in the Nusselt number of 13% for a given pumping power, as compared to a straight tube heat exchanger. More recently, TPMS structures have been researched for heat pipes applications. Zhao et al. [27] studied the hydraulic and thermal performance of many TPMS structures for loop heat pipe wicks, demonstrating a 16% improvement of the heat transfer coefficient, with respect to a more typical 3D printed structure. They also developed a novel hybrid TPMS structure, obtained by the superposition of classical lattices, that can be topologically optimized based on the application. Finally, Ma et al. [35] measured the hydraulic performances, in terms of permeability and effective pore radius, of three different sintered TPMS structures: Gyroid, Diamond and Primitive. Of the three, the Gyroid has demonstrated to be the most

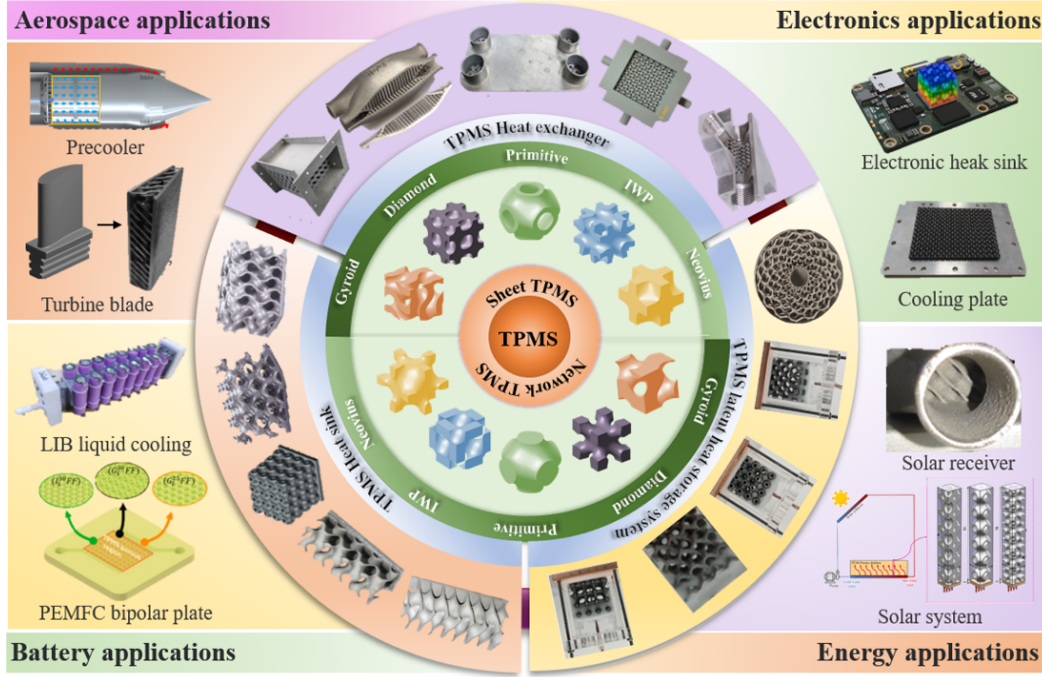


Figure 17: Applications of TPMS. Picture taken from [32].

promising one to be utilized for high-performance, lightweight and highly interconnected heat pipe structures.

Even though the papers that have already been published suggest promising results, literature on this topic remains scarce and a lot of research and development, in terms of both numerical characterization and data collection, still needs to be done to allow these new topologies to have a significant impact on the industry. The objective of this thesis is twofold: first, to demonstrate that TPMS-based structures can significantly enhance the performance of heat pipes for space applications; second, to show that, by interpreting these structures through a multiscale framework, it is possible to substantially reduce computational costs while enabling more efficient design optimization.

3.2 TPMS manufacturing process

Given the topological complexity of TPMS structures, the only viable way to manufacture them is via additive manufacturing.

As for porous wicks (Section 2.4.3), selective laser melting is the go-to technique to manufacture these types of structures. The SLM printing process is shown in figure 19.

First, the geometry is created inside a CAD software by defining the level-set functions, then the CAD model is sliced into layers and passed to the 3D printing machine. Inside the

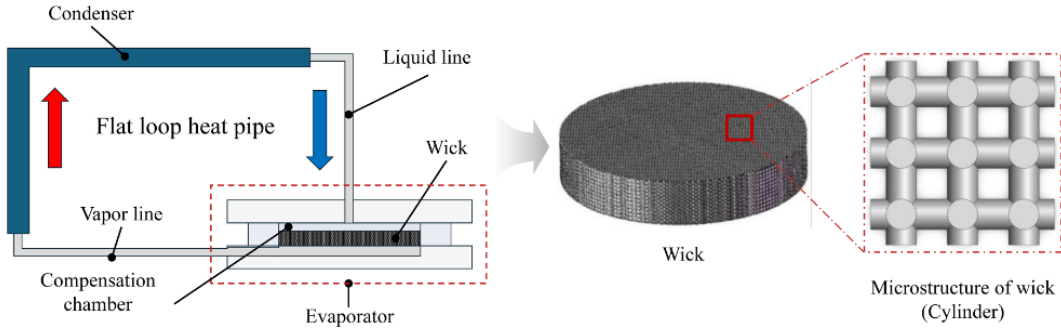


Figure 18: Loop heat pipe with a lattice structure. Picture taken from [27].

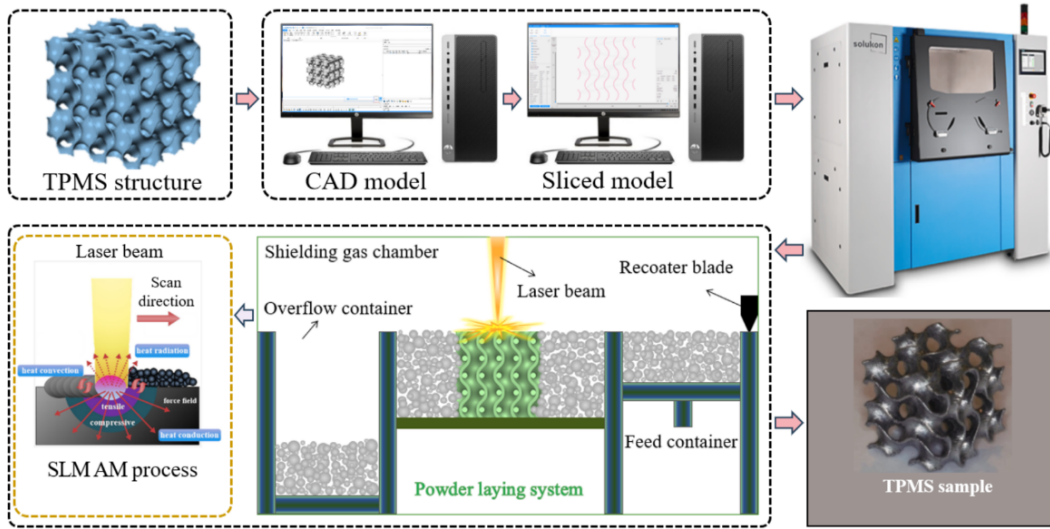


Figure 19: SLM manufacturing workflow to obtain a Gyroid TPMS structure. Picture taken from [32].

machine, a metal powder is melted layer-by-layer via a high energy laser beam. To prevent oxidation of the fused metal after melting has occurred, it is essential to shield it from the oxygen-rich atmosphere by using an inert gas (Argon is typically used). Finally, the 3D printed geometry is removed from the surrounding powder and the final geometry is thus obtained.

Like all AM processes, SLM is inherently complex, posing significant challenges in achieving the desired forming quality and geometry accuracy. The quality of the 3D printing process directly affects the thermal-hydraulic performances of the structure.

For thermal management applications, ideally one would like to use specific materials with high thermal conductivity, strength and compatibility with the working fluid. Having

said that, AM works better with certain types of materials, and does not work at all with others; for this reason, the range of materials to choose from is limited. Typically, materials like Al-Si alloys, pure copper, stainless steel, and Inconel alloy are the most suited for selective laser melting.

Parts obtained via 3D printing will almost always have some types of internal defects. The most common ones are pores generated due to a lack of fusion, caused by insufficient laser energy input, and "keyhole" pores, which arise when the energy density of the laser is too high. Both types of defects are shown in Figure 20.

Thanks to computer tomography (CT) techniques, these internal defects can easily be identified and evaluated.

Beyond internal defects, AM also generates surface imperfections and geometric deviations from the designed model. These include: sticking powder, overhang and "staircases" effect (shown in Figure 21).

Geometrical parameters such as porosity, wall thickness and pore size can end up being very different from what was predicted prior to the manufacturing of the TPMS, generating uncertainties on the performance evaluation of said structures.

For instance, previous studies [36, 37] have shown how the porosity of the final 3D printed structure can deviate from the design value from 5% up to 12%. These manufacturing imperfections greatly affect the thermal-hydraulic behavior of TPMS structures. Specifically, geometric deviation and surface roughness generated by the low-quality 3D printing, can increase flow resistance, disrupt flow uniformity and even lead to blockages [38]. These defects can lead to errors in the evaluation of the pressure drop with the "ideal" geometry up to almost 70% [39], causing high uncertainty in the numerical results.

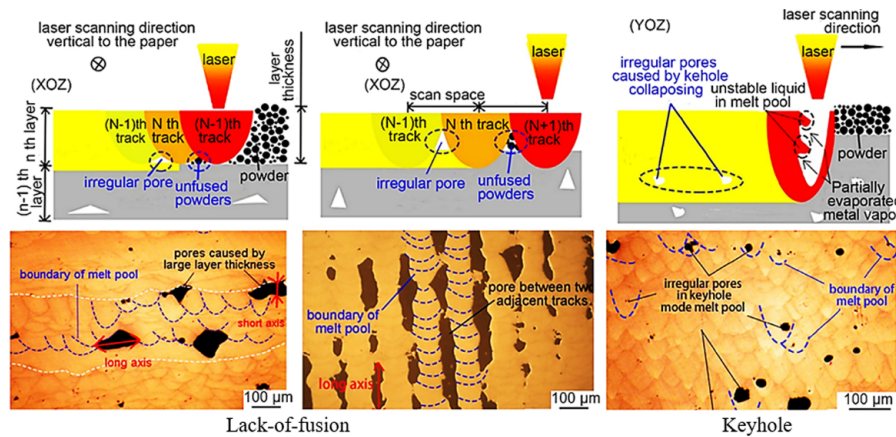


Figure 20: Lack of fusion and keyhole internal defects. Picture taken from [32].

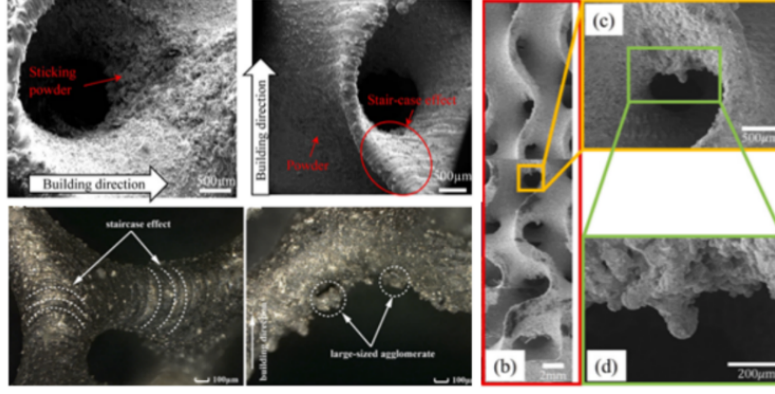


Figure 21: Sticking powder, staircase and over-hanging effects. Picture taken from [32].

3.3 Numerical simulation of lattice structures

One of the main drawbacks of TPMS structures in thermal applications is the complexity of their numerical simulations. The intricate and tortuous flow passages, the geometrical complexity of the structures, and the large number of unit cells typically required all contribute to the difficulty of mesh generation and model setup, as it will be discussed in Section 5. Nevertheless, in many thermal management applications, the Reynolds number remains sufficiently low for the flow to stay in the laminar regime, thereby simplifying the numerical solution and eliminating the need for turbulence modeling.

4 Multiscale modeling

Due to the complexity of the real-world, basically all physical phenomena have some sort of multiscale nature. In fact, to use the way Weinan E put it "It is not an easy task to think of a situation that does not involute any multiscale characters" [40]. That is, a behavior characterized by a certain macro-scale effect that is caused by micro-scale interactions (or vice versa). This hierarchical nature of physics is what makes it both so difficult to understand and astonishing at the same time.

One of the most explicit example of multiscale behavior that we can think of is pressure: pressure is the averaged effect of the collisions of fluid molecules, which in turn are regulated by molecular dynamics interactions, as shown in figure 22. In this example, pressure is the macro-scale effect of the micro-scale behavior of molecules.

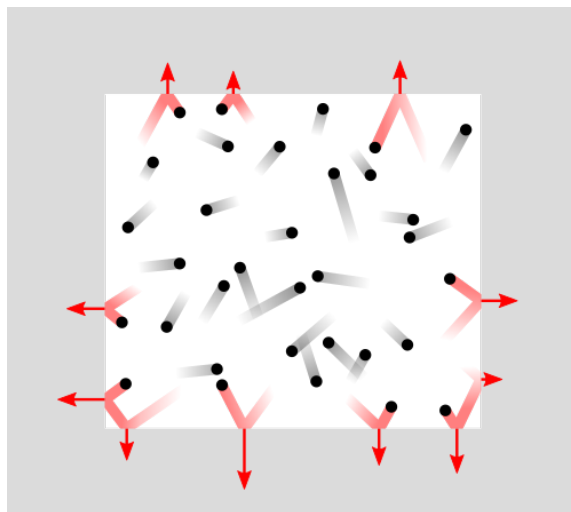


Figure 22: Pressure as a macro-scale effect of micro-scale collisions.

As was recognized by Dirac [41], every physical process that arises in applied sciences and engineering could be modeled accurately with quantum mechanics, which is the fundamental physics theory describing matter and energy at the atomic and subatomic levels. For instance, in the previous example, we could use quantum mechanics equations to determine the exact kinetic energy of every fluid molecule and then obtain the law of motion of each particle and thus the force exerted on each collision with a solid body; by averaging these forces we would obtain the exact pressure in every point of the domain. It is easy to understand why this modeling process would be far to inefficient computationally wise, given the great mathematical complexity of quantum mechanics principles, making this approach impossible to use them in any engineering application. At the same time,

modeling only the greatest scale that we are interested in could lead to results that are not accurate enough. For instance, another way to calculate the pressure of a gas inside a solid container would be to use the ideal gas equations, which is certainly easier to apply, but may lead to errors in the results that may be too high for certain applications.

The objective is to determine effective constitutive relationships and material properties directly from the underlying physics and microstructure, rather than relying solely on experimental characterization or empirical correlations. By coupling models operating at different scales, it is possible to derive the macroscopic behavior from microscopic physical mechanisms, thereby combining the computational efficiency of continuum-scale models with the predictive accuracy of detailed microscale simulations [40].

The idea behind multiscale modeling is certainly not new, in fact it has been used for example by Warshel and Levitt in 1976 to obtain the quantum mechanics-molecular mechanics (QM-MM) approach in chemistry [42] and by Car and Parrinello in 1985 [43] to arrive to the Car-Parrinello molecular dynamics method.

What has sparked a new interest in recent years on multiscale modeling is the recognition that such philosophy can be helpful in all areas of science and engineering, and is not limited to chemistry or material science like it was previously thought [40].

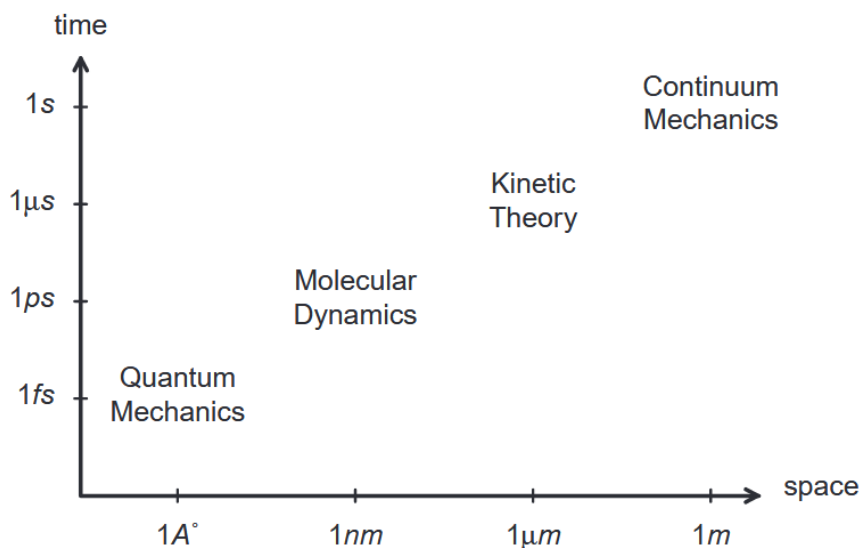


Figure 23: Commonly used models of physics at different scales.

The nature of transport phenomena in porous media is inherently multiscale, and can thus be modeled at different scales [44]. In the study of flow at a system scale, macro-scale models are usually preferred to micro-scale ones due to their computational efficiency. In fact, porous media is characterized by high heterogeneity and complex flow path that make pore-scale simulations (i.e. solving the Navier-Stokes equations at the scale of the pores)

Gases, plasmas	Liquids	Solids
Gas dynamics	Hydrodynamics	Elasticity models
MHD	(Navier-Stokes)	Plasticity models
		Dislocation dynamics
Kinetic theory	Kinetic theory	
	Brownian dynamics	Kinetic Monte Carlo
Particle models	Molecular dynamics	Molecular dynamics
Quantum mechanics	Quantum mechanics	Quantum mechanics

Figure 24: The multi-physics hierarchy.

too expensive, making them suitable only for domains that are too small to generate useful predictions at system scale. The idea behind multiscale models for transport in porous media is to bridge the gap between micro and macro scales by deriving an "upscaled" model starting from equations defined at the pore-scale that we assume are exact.

This theoretical process, that we call upscaling, has two major benefits [45]:

1. it rigorously tracks the hypothesis and approximations entailed in any given macro-scale model;
2. it establishes a quantitative connection between pore-scale topology and effective parameters that goes beyond pure parametric fitting;

The first point may not seem that relevant for practical engineering applications, but indeed it allows the practitioner to ensure that the macro-scale model obtained is predictive and accurate within certain applicability conditions. With the term "predictive" here we mean that the approximation error of the upscaled model compared to the averaged pore-scale solution is bounded by the upscaling error. An example applied to porous structure of the predictability is given in section 5.3.1. We note that an upscaled model may be accurate without being predictive when the accuracy cannot be *a priori* guaranteed; this usually happens when we try to apply the upscaled model outside the applicability regime. Being able to predict the error of the model *a priori* is really relevant to achieve a purely predictive understanding of macro-scale models (in contrast to model fitting).

The second consideration is equally important, since it helps the engineer to predict the effects that changes at the pore-scale have on the device scale.

This, for instance, opens the possibility of controlling system response by engineering micro-scale topology [44]. We now understand why multiscale models can be a useful mathematical tool at our disposal, let us now go into more details on how to apply an upscaling method to obtain macro-scale equations for fluid flow in porous media.

The number of upscaling techniques is quite vast and each one has its advantages and drawbacks, below are listed just a few examples of the techniques that can be used [44]:

- Method of volume Averaging
- Hybrid Mixture Theory
- Thermodynamically Constrained Averaging Theory (TCAT)
- Homogenization Theory
- Renormalization Group Theory

Of all the methods listed, we are going to focus on homogenization theory for this study, since is the one that is the best suited for transport inside periodic porous media.

4.1 Homogenization Theory

Homogenization methods are used to study the asymptotic behavior of a boundary value problem (BVP) characterized by rapidly varying material properties or geometrical features. This situation naturally arises in porous media, where the presence of a heterogeneous microstructure introduces variations at a much smaller length scale than the characteristic dimensions of the macroscopic problem. As a result, the governing partial differential equation (PDE) exhibits rapidly oscillating coefficients associated with the local material and transport properties of the porous medium.

Homogenization theory is based on the hypothesis that the porous medium Ω , with characteristic dimensionless length scale equal to 1, can be represented microscopically by a collection of spatially periodic "unit cells" Y , each with characteristic length ε , such that the scale separation parameter

$$\varepsilon \ll 1. \tag{9}$$

In fact, this theory is also called periodic homogenization. From now on we will make the following assumptions:

- Periodic porous medium
- Newtonian fluid
- Incompressible flow
- $Re \ll 1$
- Porous medium saturated with a single-phase fluid

These assumptions are typically satisfied for the problem we are considering. Taking as reference figure 25, we consider a porous medium $\hat{\Omega}$ whose characteristic length is L . Here the "hat" symbol ($\hat{\cdot}$) indicates a dimensional quantity. As it has already been said, let us assume that the medium can be represented microscopically by a collection of spatially periodic unit cells $\hat{Y}$ with characteristic length l , such that:

$$\varepsilon = \frac{l}{L} \ll 1 \quad (10)$$

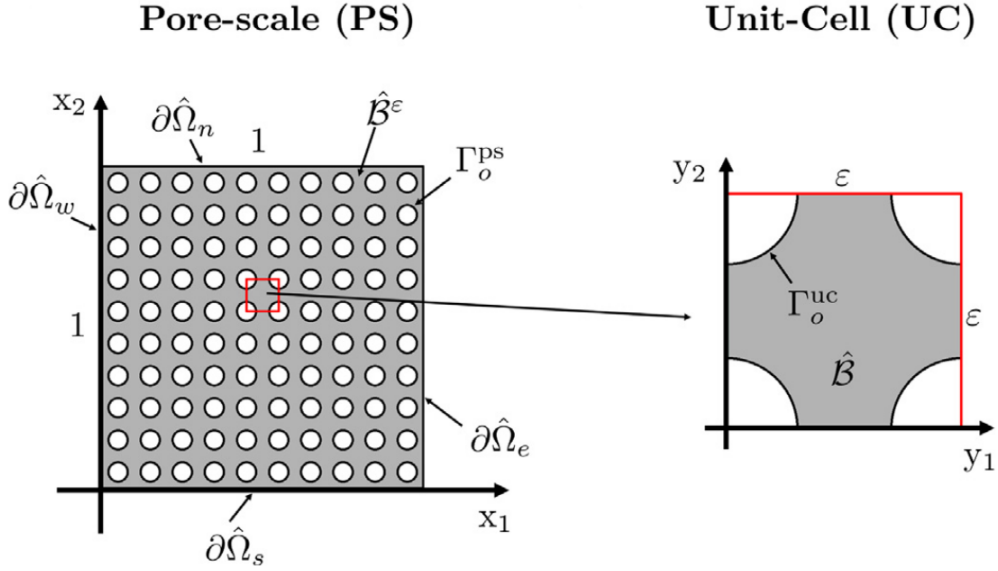


Figure 25: Pore-scale domain (left) and unit cell (right), where x and y are the macroscopic and microscopic coordinate systems, respectively. The gray region indicates fluid domain, and the white areas the solid domain. Picture taken from [46].

The unit cell $\hat{Y}$ consists of the pore space $\hat{B}$ and permeable solid matrix $\hat{G}$:

$$\hat{Y} = \hat{B} \cup \hat{G} \quad (11)$$

The pore space and solid matrix are separated by the smooth surface $\hat{\Gamma}$.

For the assumptions made, the pore space $\hat{B}$ of each unit cell $\hat{Y}$ form a multi-connected porespace domain:

$$\hat{B}^\varepsilon \subset \hat{\Omega} \quad (12)$$

where the ε apex indicates a parameter defined at the pore-scale.

The pore space domain $\hat{B}^\varepsilon$ is bounded by the smooth surface $\hat{\Gamma}^\varepsilon$. Thanks to the hypothesis that $Re \ll 1$ we can simplify the Navier-Stokes equations by neglecting the inertial terms in

the momentum balance equation, thus obtaining the Stokes' equations, which describe the flow field $\hat{\mathbf{u}} = (\hat{u}_1, \hat{u}_2, \hat{u}_3)$ of a creeping flow (i.e. a flow where inertial forces are assumed to be negligible in comparison to viscous forces).

Let us derive the Stokes' equations starting from the Navier-Stokes formulation.

4.1.1 Stokes equations

We start with conservation of mass, which can be written in the general form as:

$$\frac{\partial \hat{\rho}}{\partial \hat{t}} + \hat{\nabla} \cdot (\hat{\rho} \hat{\mathbf{u}}) = 0 \quad (13)$$

We now introduce the hypothesis of incompressible fluid:

$$\frac{D \hat{\rho}}{D \hat{t}} = 0 \mapsto \hat{\rho} \hat{\nabla} \cdot \hat{\mathbf{u}} = 0 \mapsto \hat{\nabla} \cdot \hat{\mathbf{u}} = 0 \quad (14)$$

Moving onto the momentum balance, it can be written as:

$$\hat{\rho} \frac{D \hat{\mathbf{u}}}{D \hat{t}} = \hat{\nabla} \cdot \boldsymbol{\sigma} + \hat{\rho} \hat{\mathbf{f}}_e \quad (15)$$

where $\boldsymbol{\sigma}_n = \boldsymbol{\sigma} \cdot \mathbf{n}$, $\boldsymbol{\sigma} = -\mathbf{P} \cdot \mathbf{n} + \boldsymbol{\tau}_n$.

With the hypothesis of Newtonian fluid, we can re-write the stress tensor so that it is proportional to the second derivative of the velocity:

$$\boldsymbol{\sigma} = -\nabla P + \nabla \cdot \boldsymbol{\tau} = -\nabla P + \mu \nabla^2 \mathbf{u} \quad (16)$$

By plugging it into equation (15) and by expanding the material derivative, we obtain:

$$\hat{\rho} \frac{\partial \hat{\mathbf{u}}}{\partial \hat{t}} + \hat{\nabla} \cdot (\hat{\rho} \hat{\mathbf{u}} \cdot \hat{\mathbf{u}}) + \hat{\nabla} \hat{p} - \hat{\mu} \hat{\nabla}^2 \hat{\mathbf{u}} = 0 \quad (17)$$

where $\hat{\mu}$ is the fluid dynamic viscosity and $\hat{p}$ is the pore-scale pressure.

Finally, we use the hypothesis that both the Reynolds number and the Reynolds transient number are very small when compared to 1²:

$$\begin{cases} Re = \frac{\rho U l}{\mu} \ll 1 \\ Re_t = \frac{l^2}{\mu T^*} \ll 1 \end{cases}$$

where U is a characteristic velocity and T^* a characteristic time.

With this assumption, the inertial and non-stationary terms inside the momentum equation become negligible, and we get the following set of equations:

$$\hat{\nabla} \cdot \hat{\mathbf{u}} = 0, \quad \hat{\mathbf{x}} \in \hat{B}^\varepsilon \quad (18a)$$

$$\mu \hat{\nabla}^2 \hat{\mathbf{u}} - \hat{\nabla} \hat{p} = 0, \quad \hat{\mathbf{x}} \in \hat{B}^\varepsilon \quad (18b)$$

$$\hat{\mathbf{u}} = 0, \quad \hat{\mathbf{x}} \in \hat{\Gamma}^\varepsilon \quad (18c)$$

²This assumption usually holds for the considered application (flow inside a heat pipe porous wick)

Equation (18a) is the continuity equation for an incompressible fluid, whereas equation (18b) is the momentum balance, and we can see how we only have the viscous term (and the driving force, i.e. the pressure gradient). We also need to impose the no-slip condition at the interface between the solid and the fluid Γ , this condition is given by equation (18c). This set of equations is defined at the pore-scale, which in our case is the microscopic scale. What we would like to do is to upscale these equations to obtain a new set which is now defined at the macroscopic scale. To do so we will use homogenization theory. Let us list the steps that one has to take to solve the flow using this framework:

1. If one starts with a real porous medium that is not periodic (not our case) the first step is to conceptualize it as a periodic structure made up of repeating unit cells of size ε ;
2. Derive the continuum scale equations from the pore-scale ones, via the process called upscaling;
3. Calculate the effective parameters (via the closure variables ³) and obtain a set of PDEs that can be numerically solved;
4. To obtain the numerical solution, start by solving the boundary value problem⁴ on the unit cell, calculate the closure variables, plug the closure variables into the effective coefficients and calculate them, then plug these effective coefficients in the continuum scale equations;

By following this procedure one can make sure that the model is fully consistent and the approximation error will be known *a priori* (if the equations are applied within the applicability conditions, which are also given by the procedure).

We will now apply the upscaling technique via asymptotic expansion to obtain the continuum scale equations.

4.2 Upscaling

Before applying the asymptotic expansion, we need to non-dimensionalize all the pore-scale equations that we have just obtained.

From now on all the non-dimensional quantities will be indicated without the hat symbol (" $\wedge$ ").

³A closure variable is a variable that can be obtained by solving a boundary value problem at the pore-scale and that is needed to solve the continuum equations

⁴A boundary value problem is a set of differential equations that is subject to boundary conditions. A solution of the BVP is a solution of both the differential equations and the boundary conditions

Let us start by non-dimensionalizing the physical quantities:

$$\begin{aligned}\mathbf{x} &= \frac{\hat{\mathbf{x}}}{L} \quad , \quad \mathbf{u} = \frac{\hat{\mathbf{u}}}{U} \quad , \quad p = \frac{\hat{p}l^2}{\hat{\mu}UL} \quad , \quad \nabla = L\hat{\nabla} \quad , \quad \nabla^2 = L^2\hat{\nabla}^2 \\ \mathbf{y} &= \frac{\hat{\mathbf{y}}}{l} \quad , \quad T_\alpha = \frac{\hat{T}_\alpha}{T_\alpha^r}\end{aligned}$$

where $\alpha = s, l$ indicates the domain on which the variable is being considered (s for the solid domain, l for liquid the liquid one) and r indicates a reference variables.

In this study we are using a two-scale asymptotic expansion, where the two scale parameters are $\mathbf{x}$, the macroscopic (or slow) variable and $\mathbf{y}$, the microscopic (or fast) variable.

We then plug these variables in the Stokes' equations:

$$\frac{1}{L}\nabla \cdot U\mathbf{u} = 0 \tag{19a}$$

$$\hat{\mu} \cdot \frac{U}{L^2}\nabla^2\mathbf{u} - \frac{1}{L} \cdot \frac{\hat{\mu}UL}{l^2}\nabla p = 0 \tag{19b}$$

By rearranging the terms we obtain the non-dimensionilized form of the Stokes' equations:

$$\nabla \cdot \mathbf{u} = 0 \tag{20a}$$

$$\varepsilon^2\nabla^2 \cdot \mathbf{u} - \nabla p = 0 \tag{20b}$$

We now consider the following power series expansion of velocity and pressure (both functions of fast and slow variables $\mathbf{y}$ and $\mathbf{x}$):

$$\mathbf{u} = u_0(x, y) + \varepsilon u_1(x, y) + \varepsilon^2 u_2(x, y) + \dots \tag{21a}$$

$$p = p_0(x, y) + \varepsilon p_1(x, y) + \varepsilon^2 p_2(x, y) + \dots \tag{21b}$$

We then start expanding the differential operators inside the Stokes' equations, considering the following chain rule:

$$\nabla_\varepsilon f = \nabla_x f + \frac{1}{\varepsilon}\nabla_y f \tag{22}$$

By superposing the velocity and pressure expansion (truncated at ε^1) into equations (20a) and (20b):

$$\varepsilon^2\nabla_x^2(u_0 + \varepsilon u_1) + 2\varepsilon\nabla_x\nabla_y(u_0 + \varepsilon u_1) + \nabla_y^2(u_0 + \varepsilon u_1) - \nabla_x(p_0 + \varepsilon p_1) - \frac{1}{\varepsilon}\nabla_y(p_0 + \varepsilon p_1) \simeq 0 \tag{23a}$$

$$\nabla_x(u_0 + \varepsilon u_1) + \frac{1}{\varepsilon}\nabla_y(u_0 + \varepsilon u_1) \simeq 0 \tag{23b}$$

Let us develop each term:

$$\varepsilon^2 \nabla_x^2 u_0 + \varepsilon^2 \nabla_x^2 u_1 + 2\varepsilon \nabla_x \nabla_y u_0 + 2\varepsilon^2 \nabla_x \nabla_y u_1 + \nabla_y^2 u_0 + \varepsilon \nabla_y^2 u_1 - \nabla_x p_0 - \varepsilon \nabla_x p_1 - \frac{1}{\varepsilon} \nabla_y p_0 - \nabla_y p_1 \simeq 0 \quad (24a)$$

$$\nabla_x u_0 + \varepsilon \nabla_x u_1 + \frac{1}{\varepsilon} \nabla_y u_0 + \nabla_y u_1 \simeq 0 \quad (24b)$$

Since we truncated the pressure and velocity at the second order, we expect an error in the order of $\mathcal{O}(\varepsilon^2)$, if that doesn't turn out to be the case, some other errors are adding up.

The last step is to collect like-power terms of ε :

$$\varepsilon^{-1}) \quad \nabla_y^2 p_0 = 0 \quad \Rightarrow \quad p_0 = p_0(x) \quad (25a)$$

$$\nabla_y u_0 = 0 \quad (25b)$$

$$\varepsilon^0) \quad \nabla_y^2 u_0 - \nabla_x p_0 - \nabla_y p_1 = 0 \quad (26a)$$

$$\nabla_x u_0 + \nabla_y u_1 = 0 \quad (26b)$$

$$\varepsilon^1) \quad 2\nabla_x \nabla_y u_0 + \nabla_y^2 u_1 - \nabla_x p_1 = 0 \quad (27a)$$

$$\nabla_x u_1 = 0 \quad (27b)$$

All equations are coupled together, in fact we say that we have a hierarchy of problems. To close the problem we need the constitutive relations (i.e. closure variables).

By combining equation (25b) and (26a), and the no-slip boundary condition, we obtain:

$$\nabla_y^2 u_0 - \nabla_x p_0 - \nabla_y p_1 = 0 \quad (28a)$$

$$\nabla_y u_0 = 0 \quad (28b)$$

$$u_0 = 0 \quad \text{on} \quad \Gamma_{sl} \quad (28c)$$

Note that u_0 and p_1 are defined at the pore-scale.

By collecting like-power of ε we have thus found a cascade of equations which can be iteratively solved if a closure, i.e. a relationship between the leading order and the higher order terms, is established [46].

To establish this relationship, we can observe that the problem is linear, thus we can assume that the solution can be found in the following form:

$$u_0(x, y) = -\mathbf{k}(y) \nabla_x p_0 \quad (29a)$$

$$p_1(x, y) = \mathbf{a}(y) \nabla_x p_0 + \tilde{p}(x, t) \quad (29b)$$

where p_0 can be proved to be a function of x only, $\mathbf{k}$ is a tensor and $\mathbf{a}$ is a vector. If we now plug this solution into equations (28), we obtain:

$$-\nabla_y^2 \mathbf{k} \nabla_x p_0 - \nabla_y \mathbf{a} \nabla_x p_0 - \nabla_x p_0 = 0 \quad (30a)$$

$$\nabla_y \mathbf{k} \nabla_x p_0 = 0 \quad (30b)$$

By factoring out the term $\nabla_x p_0$ from equation (30a), we can write:

$$\left(\nabla_y^2 \mathbf{k} + \nabla_y \mathbf{a} + \mathbf{I} \right) \nabla_x p_0 = 0 \quad (31a)$$

$$\nabla_y \mathbf{k} \nabla_x p_0 = 0 \quad (31b)$$

where $\mathbf{I}$ is the identity tensor.

Finally, thanks to scale separation, given by $\varepsilon \ll 1$, we can eliminate all the slow variable x dependencies:

$$\nabla_y^2 \mathbf{k} - \nabla_y \mathbf{a} + \mathbf{I} = 0 \quad (32a)$$

$$\nabla_y \mathbf{k} = 0 \quad (32b)$$

$$\mathbf{k} = 0 \quad \text{on} \quad \Gamma_{sl} \quad (32c)$$

$$\mathbf{k}, \mathbf{a} \quad \text{periodic in } \mathbf{y} \quad (32d)$$

We have found a new set of PDEs, that are defined at the pore-scale (they are a function of only y) that, if solved, allow us to find the closure variables $\mathbf{k}$ and $\mathbf{a}$, that is, the variables that contain the information of the microscopic scale and that allow us to separate it from the macroscopic scale. This set of PDEs is what we call "closure problem", since it is the problem that, if solved, allows to obtain the variables that close the modeling loop.

From the previous set of equations we can see another great advantage of the homogenization theory: it allows us to obtain the exact form of the upscaled equations for the problem we are trying to solve (Stokes' flow in this case). That goes in contrast with other techniques that, for example, try to generate a fitting curve to determine effective flow parameters, without deriving the equations that regulate the physic behind the particular flow. By looking at set (32) we can see that the form of the equations are very similar to the ones defined at the pore-scale. In fact, the closure problem obtained is composed of a Stokes-like equation, a continuity equation and a non-slip boundary condition that are characterized by different variables with different tensorial orders if compared to Stokes' equations, but that are formally combined into equations that, in the end, model the same physics. Even though it is not the general case that the upscaled equations have the same form of the micro-scale ones, for the closure problem of Stokes' flow it is generally true [46].

There is another constraint that needs to be added so that the closure problem is complete, that is, a time-independent global constraint on the spatial average of the closure variable $\mathbf{a}$:

$$\langle \mathbf{a} \rangle = \mathbf{0} \quad (33)$$

where the operator $\langle \cdot \rangle$ defines the volumetric average over the unit cell:

$$\langle \cdot \rangle = \frac{1}{|Y|} \int_{B(x)} \cdot \, dB \quad (34)$$

With this constraint we impose that the closure variable has zero mean over the unit cell and this guarantees the existence and the uniqueness of the closure problem solution [47]. It is worth noting that the objective of the closure problem is to predict the permeability tensor $\mathbf{K}$ and not to predict the details of the pressure and velocity fields [48]. In fact, the closure variables $\mathbf{a}$ and $\mathbf{k}$ are not physical quantities, but their direct evaluation allows for reconstruction of pore-scale velocity and pressure through (21).

The dimensionless permeability tensor is defined as the spatial average of the closure variable $\mathbf{k}$ over the unit cell:

$$\mathbf{K} = \langle \mathbf{k}(y) \rangle \quad (35)$$

It can be shown that $\mathbf{K}$ is a symmetric positive-definite tensor that depend only upon the geometry of the unit cell [49].

One last interesting fact is that equations (20) can be upscaled to Darcy's law as follows:

$$\langle \mathbf{u} \rangle = -\mathbf{K} \cdot \nabla p_0 \quad (36a)$$

$$\nabla \cdot \langle \mathbf{v} \rangle = 0 \quad (36b)$$

What is interesting about Darcy's law is that it was first derived experimentally by Darcy and then proven to have a rigorous mathematical derivation later on, via the application of the homogenization theory. We can thus say that Darcy's law provides an effective representation of the pore-scale Stokes' flow within errors of order $O(\varepsilon)$, as explained by Marušić-Paloka and Piatnitski [50].

Now that we have derived all the necessary upscaled equations, we can move on to solving them.

5 Numerical simulations

In this section we will focus on finding the solution of the previously defined equations for three different *Network* TPMS (shown in figure 26): Diamond, Gyroid and Primitive.

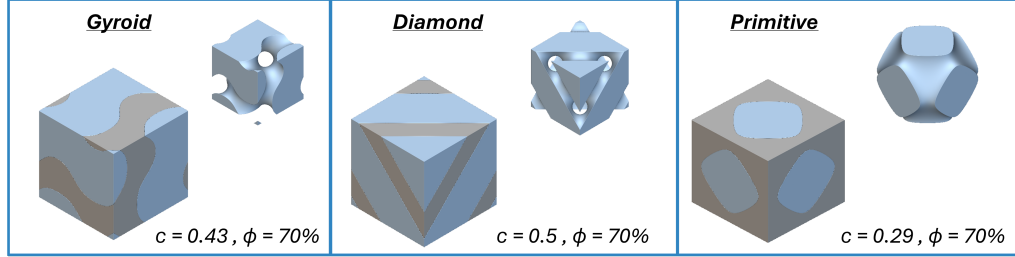


Figure 26: Unit cells being considered for this study. The solid domain is colored in grey and the fluid one in light blue. The c parameter is the mid-plane surface offset used to obtain the specific porosity ϕ (measured in mm).

The set of equations that we want to solve on the single unit cell is the following:

$$\nabla_y^2 \mathbf{k} - \nabla_y \mathbf{a} + \mathbf{I} = 0 \quad (37a)$$

$$\nabla_y \mathbf{k} = 0 \quad (37b)$$

$$\mathbf{k} = 0 \quad \text{on} \quad \Gamma_{sl} \quad (37c)$$

$$\langle \mathbf{a} \rangle = \mathbf{0} \quad (37d)$$

$$\mathbf{k}, \mathbf{a} \quad \text{periodic in } \mathbf{y} \quad (37e)$$

To solve this closure problem, we will use the finite element CFD software COMSOL Multiphysics.

This section will be structured as follows:

1. Description of the workflow for the geometry creation and fluid flow analysis
2. Solution of the closure problem
3. Results validation
4. Results comparison with literature

5.1 Workflow description

Let us first describe the workflow that will be used for all the simulations, starting from the creation of the geometry and up to the CFD analysis.

In figure 27 the general workflow used for the simulations is presented.

SIMULATION WORKFLOW

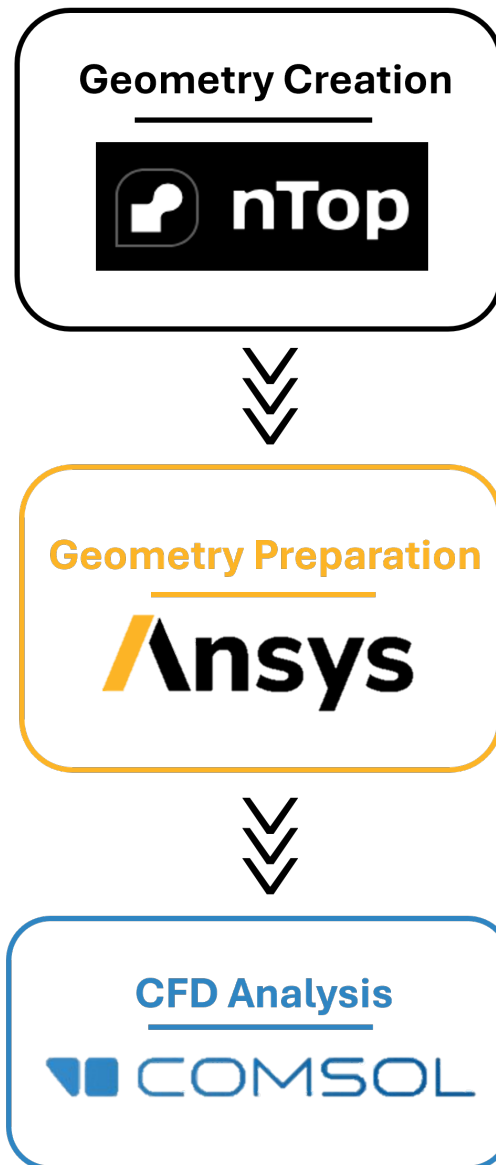


Figure 27: General workflow used for the simulations.

The three main software that we are going to use are:

- nTopology
- Ansys SpaceClaim
- COMSOL Multiphysics

The first one, nTopology, is a relatively new 3D modeling software that leverages implicit modeling⁵ to allow the user to create complex shapes and modify them easily, without breaking the model [51]. Given that the geometries that we want to generate are in fact based on implicit equations (see section 3), this software allows us to easily generate, parametrize and export them.

The steps to create and export a geometry in nTopology are the following:

1. Basic geometry creation and parametrization
2. Surface meshing to obtain an STL body
3. Export of the STL file

A representation of the various steps for the creation and export of a Diamond TPMS unit cell can be seen in figure 28. Note that the surface meshing phase is essential to obtain an exportable STL geometry. Basically, the purpose of surface meshing is to transform the virtual CAD body into a surface body made up of small bi-dimensional triangles. Given that you can not describe a curved surface using planar entities, there will always be an approximation error and, in this sense, the greater the amount of triangles used to approximate the CAD body, the closer the STL body will be to the ideal one.

Note that, during the geometry creation, the dimensions of the unit cell are increased by 1 mm in all directions to accommodate the fact that the exact unit cell will be later extracted using another software.

The second software being used is Ansys SpaceClaim, which is a solid CAD software that implements a lot of tools to manipulate STL bodies. In figure 29 are depicted all the steps needed to obtain the finalized geometry in Ansys SpaceClaim.

The workflow to obtain the finalized geometry is the following:

1. Import the raw STL body
2. Check if there is any error in the facets
3. Create a cube with dimensions equal to the unit cell size ($5 \times 5 \times 5$ mm in this case)

⁵Implicit modeling defines shapes and objects with mathematical functions, allowing to create complex shapes more easily and offering more flexibility and automation. This goes in contrast with explicit modeling where geometries are defined by precise coordinates and manual steps, offering higher control and precision but also suffering from a more rigid process.

4. Use the "*intersect facets*" tool to extract the final geometry
5. Scale the geometry as needed using the "*scale facets*" tool

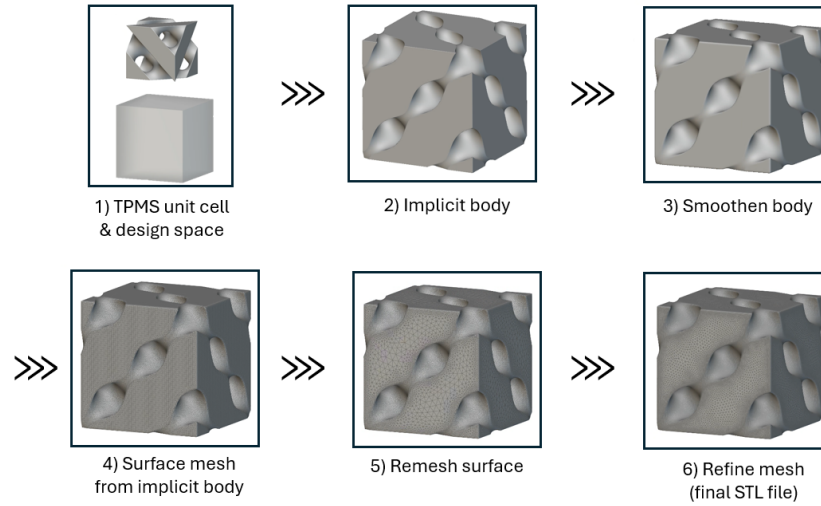


Figure 28: STL body creation in nTop.

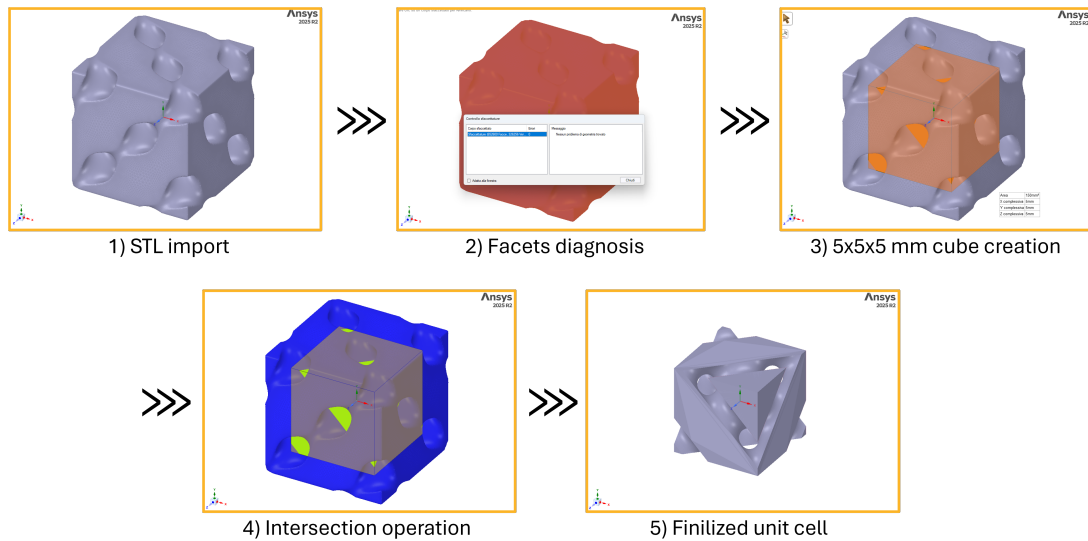


Figure 29: STL body preparation workflow in SpaceClaim.

Now that we have a finalized geometry, we can import it in COMSOL Multiphysics and start setting up the fluid model.

One great advantage that COMSOL has compared to other competitors is that it allows the user to easily define custom PDE problems that can be solved using a finite element approach. This is essential to solve the closure problem on the unit cell, as it will be shown later on in this section.

The model and simulation setup can be divided in the following steps (shown in figure 30):

1. Geometry import and conversion to solid body
2. Materials and equations setup
3. Meshing
4. Post-processing

We now have defined the general workflows that will be used to obtain the numerical results. These workflows will be adapted based on the simulation that will be done (e.g. the model equations used to find the solution of the closure problem will differ from the ones used to find the pore-scale solution).

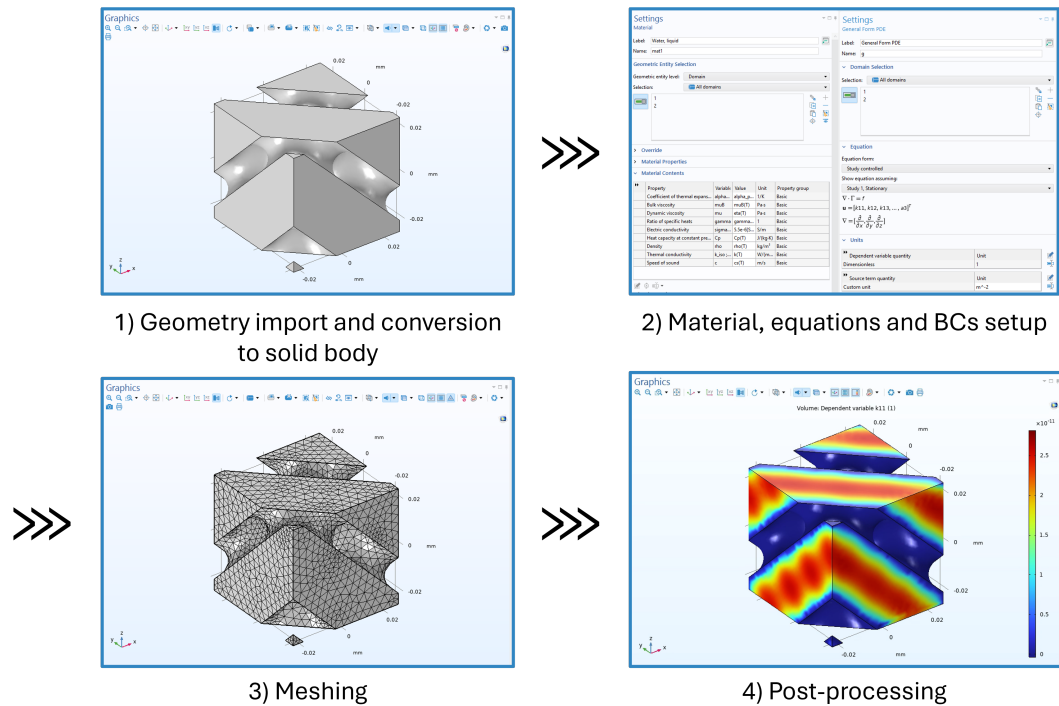


Figure 30: Model setup and simulation in COMSOL Multiphysics.

Next, we will focus first on the solution of the closure problem for three different topologies, then we will validate the results by solving the pore-scale equations (i.e. Stokes’

flow) on the same three topologies, and finally we will cross-verify the results with results found in literature. Specifically, we are going to cross-verify the results obtained from the simulations with the ones obtained in reference [27]. To make sure that the cross-verification makes sense, the unit cell sizes that we are going to consider for all the simulations need to be the same as the ones used in the paper ($50 \mu m$, $40 \mu m$, $30 \mu m$, $20 \mu m$, $10 \mu m$), assuming that if the results are congruent with these unit cell sizes, then they will also be for all the others, thus neglecting scaling effects. In figure 31 the numerical workflow is shown.

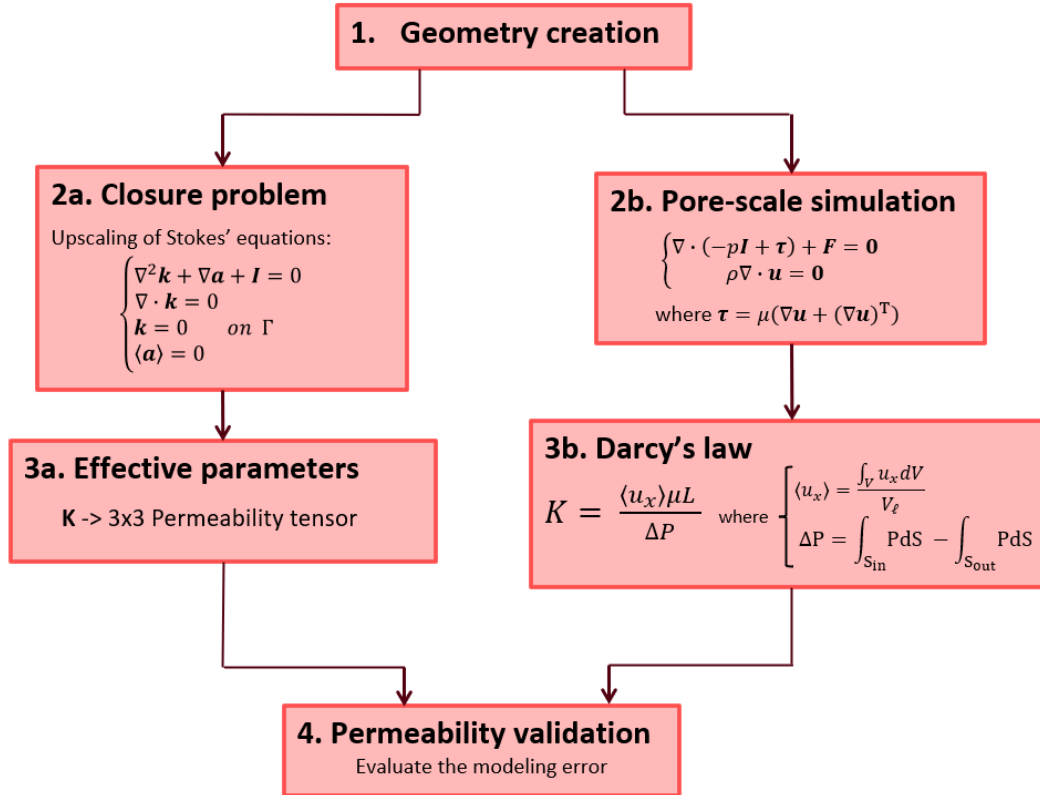


Figure 31: Numerical workflow.

5.2 Closure problem

The main objective of the analysis that will be conducted in this section is to solve the closure problem (see section 4.1). To do so, we first need to implement the boundary value problem into COMSOL, and we are going to do so by setting up the upscaled equations derived in the previous chapter.

5.2.1 Model setup

To set up the upscaled equations in COMSOL we use the "*General Form PDE*" interface, although the same results could be obtained using more general frameworks (e.g. *Weak Form PDE*).

The General Form PDE equation is the following:

$$e_a \frac{\partial^2 u}{\partial t^2} + d_a \frac{\partial u}{\partial t} + \nabla \cdot \Gamma = F \quad (38)$$

where u is the dependent variables field vector, e_a and d_a are the mass and damping coefficients respectively, Γ is the conservative flux vector and F is the source term vector. With this interface, one can implement into the model several physical phenomena by correctly defining the various parameters that have been previously introduced.

The first two terms from equation (38) can be neglected, since the study is stationary. We are left with the following equation:

$$\nabla \cdot \Gamma = F \quad (39)$$

By solving the boundary value problem we want to find the k and a tensorial quantities. That said, each component of both k (3x3 tensor) and a (3x1) vector will be associated to one element of the dependent variables field vector u .

We get the following resulting vector of dimensions 12x1:

$$\mathbf{u} = [k_{11}, k_{12}, k_{13}, k_{21}, k_{22}, k_{23}, k_{31}, k_{32}, k_{33}, a_1, a_2, a_3]^T \quad (40)$$

Note that COMSOL allows only for one vector field to be defined, that is why the component of both closure variables are appended to the same vector, instead of using two separate ones.

What we are trying to do is to replicate set (37) using equation (39). Being that the form of the equations is not exactly the same, we need to manipulate them first.

We can re-write equation (37b) and equation (37c) as follows:

$$\nabla \cdot \overbrace{\nabla \mathbf{k}}^{=\Gamma} = -\overbrace{\nabla \mathbf{a} - \mathbf{I}}^{=F} \quad (41a)$$

$$\underbrace{\nabla \mathbf{k}}_{=\Gamma} = \underbrace{0}_{=F} \quad (41b)$$

The conservative flux vector will be a 12x1 vector where every element is also a 3x1 vector composed of the partial derivatives of each dependent variable. The last 3 element of Γ will be 3x1 vectors composed of just the dependent variables (not derived).

An example of how the Γ vector would look like is shown below:

$$\mathbf{\Gamma}^T = \left[\begin{bmatrix} k_{11x} \\ k_{11y} \\ k_{11z} \end{bmatrix}^T \quad \begin{bmatrix} k_{12x} \\ k_{12y} \\ k_{12z} \end{bmatrix}^T \quad \begin{bmatrix} k_{13x} \\ k_{13y} \\ k_{13z} \end{bmatrix}^T \quad \dots \quad \dots \quad \dots \quad \begin{bmatrix} k_{11} \\ k_{12} \\ k_{13} \end{bmatrix}^T \quad \begin{bmatrix} k_{21} \\ k_{22} \\ k_{23} \end{bmatrix}^T \quad \begin{bmatrix} k_{31} \\ k_{32} \\ k_{33} \end{bmatrix}^T \right]^T \quad (42)$$

where we have used the following notation:

$$k_{ijx} = \frac{\partial k_{ij}}{\partial x}, \quad k_{ijy} = \frac{\partial k_{ij}}{\partial y}, \quad k_{ijz} = \frac{\partial k_{ij}}{\partial z}, \quad i, j = 1, 2, 3 \quad (43)$$

The source term vector will also be 12x1 and will be composed as follows:

$$\mathbf{F}^T = \begin{bmatrix} -a_{1x} - 1 \\ -a_{1y} \\ -a_{1z} \\ -a_{2x} \\ -a_{2y} - 1 \\ -a_{2z} \\ -a_{3x} \\ -a_{3y} \\ -a_{3z} - 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}^T \quad (44)$$

where the notation is similar to the previous one:

$$a_{ix} = \frac{\partial a_i}{\partial x}, \quad a_{iy} = \frac{\partial a_i}{\partial y}, \quad a_{iz} = \frac{\partial a_i}{\partial z} \quad i, j = 1, 2, 3 \quad (45)$$

The next step is to set up the boundary conditions, which will be:

- Dirichlet BC on the interior walls (no-slip boundary condition)
- Periodic BCs along the 3 main directions
- Global constraint to impose that the average of $\mathbf{a}$ is equal to zero in the unit cell

To apply the Dirichlet BC we can impose that the components of the $\mathbf{k}$ tensor are equal to zero along the internal walls of the unit cell, as prescribed by equation (37d). The boundaries to which the Dirichlet BC is applied to are shown in figure 32.

For what concerns the periodic BCs, the continuity of all the dependent variables is imposed on the three pair of opposing faces of the unit cells, as shown in figure 33.

Finally, the global constraint on $\mathbf{a}$ can be simply imposed by defining a global equation for each component of the vector:

$$\langle a_1 \rangle = \frac{\int_B a_1 dB}{V_B} = 0 \quad (46a)$$

$$\langle a_2 \rangle = \frac{\int_B a_2 dB}{V_B} = 0 \quad (46b)$$

$$\langle a_3 \rangle = \frac{\int_B a_3 dB}{V_B} = 0 \quad (46c)$$

Now that the physical model is correctly set up, we can move on to adding the material properties. We will only use water for the following simulations, to add its properties to the model, we can simply import them from the COMSOL material library. The fluid properties used for the simulation are presented in figure 34.

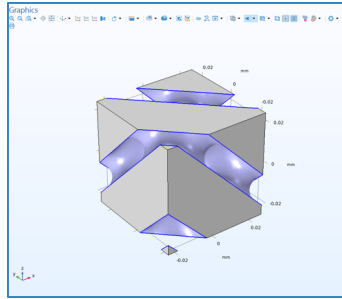
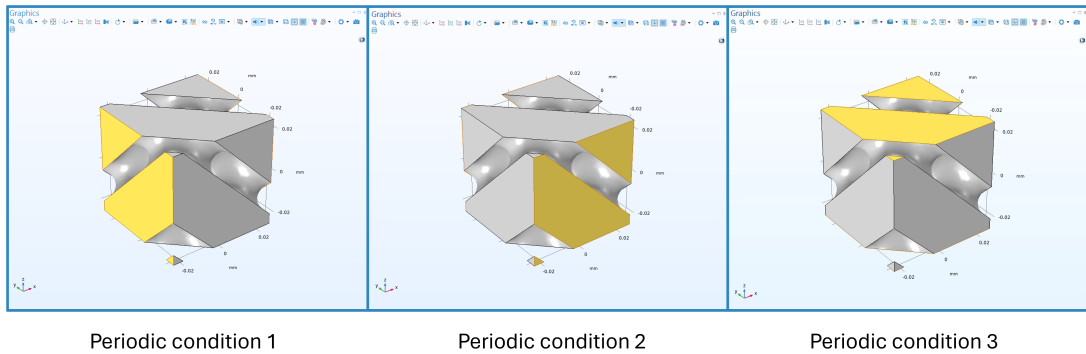


Figure 32: Boundaries to which the Dirichlet BC is applied.



Periodic condition 1

Periodic condition 2

Periodic condition 3

Figure 33: Periodic boundary conditions.

Property	Variable	Value	Unit
Coefficient of thermal expansion	alpha_is...	alpha_p(T)	1/K
Bulk viscosity	muB	muB(T)	Pa·s
Dynamic viscosity	mu	eta(T)	Pa·s
Ratio of specific heats	gamma	gamma_w(T)	1
Electric conductivity	sigma_is...	5.5e-6[S/m]	S/m
Heat capacity at constant pressure	Cp	Cp(T)	J/(kg·K)
Density	rho	rho(T)	kg/m ³
Thermal conductivity	k_iso ; kii...	k(T)	W/(m·K)
Speed of sound	c	cs(T)	m/s

Figure 34: Fluid properties used for the simulations.

5.2.2 Meshing

The last step before we can start simulating is to produce a high quality mesh.

COMSOL, like many other CFD software, divides the mesh creation process into multiple steps:

1. Set the element sizing
2. Create a surface mesh
3. Make the surface mesh on opposing periodic faces identical
4. Generate the final 3D mesh

COMSOL also allows the element size to be automatically set according to the selected physics, which in this case is fluid dynamics.

All 3D meshes used in this study are unstructured and composed of tetrahedral elements, generated using the "*Free Tetrahedral*" tool.

The sizing parameters and mesh settings are described in more details in the sensitivity analysis section (section 5.2.3).

Finally, note that no boundary layer inflation was added. Since the flow considered in this study is governed by the Stokes' equations, inertial effects are neglected and viscous effects dominate throughout the domain. Therefore, the flow does not develop thin inertial boundary layers as in high-Reynolds-number flows. The velocity gradients associated with the no-slip condition are instead resolved through the overall mesh refinement. Hence, dedicated inflation layers near the solid walls are not needed.

Figure 35 shows three meshes generated using three different element sizes.

The mesh generation process was repeated for all unit cell sizes and TPMS types. Table 2 reports the mesh statistics, including the number of elements, average element size, refinement ratio and mesh quality. The statistics are only reported for the $40\text{ }\mu\text{m}$ cell size because the sensitivity analysis was performed on this case only. Since the geometry and flow configuration are equivalent for the same TPMS at different unit cell sizes, the results of the sensitivity analysis can be assumed to be representative of the other unit cell sizes as well.

Once all the meshes have been created, the sensitivity analyses can be performed with the aim of determining the mesh convergence properties and establish the overall discretization error relative to the mesh element size.

5.2.3 Sensitivity analysis

To analyse the mesh convergence properties we use the Richardson extrapolation (RE) framework, outlined by the Fluids Engineering Division of ASME [52]. We use the RE method because it is very straightforward to apply, and it still remains one of the most

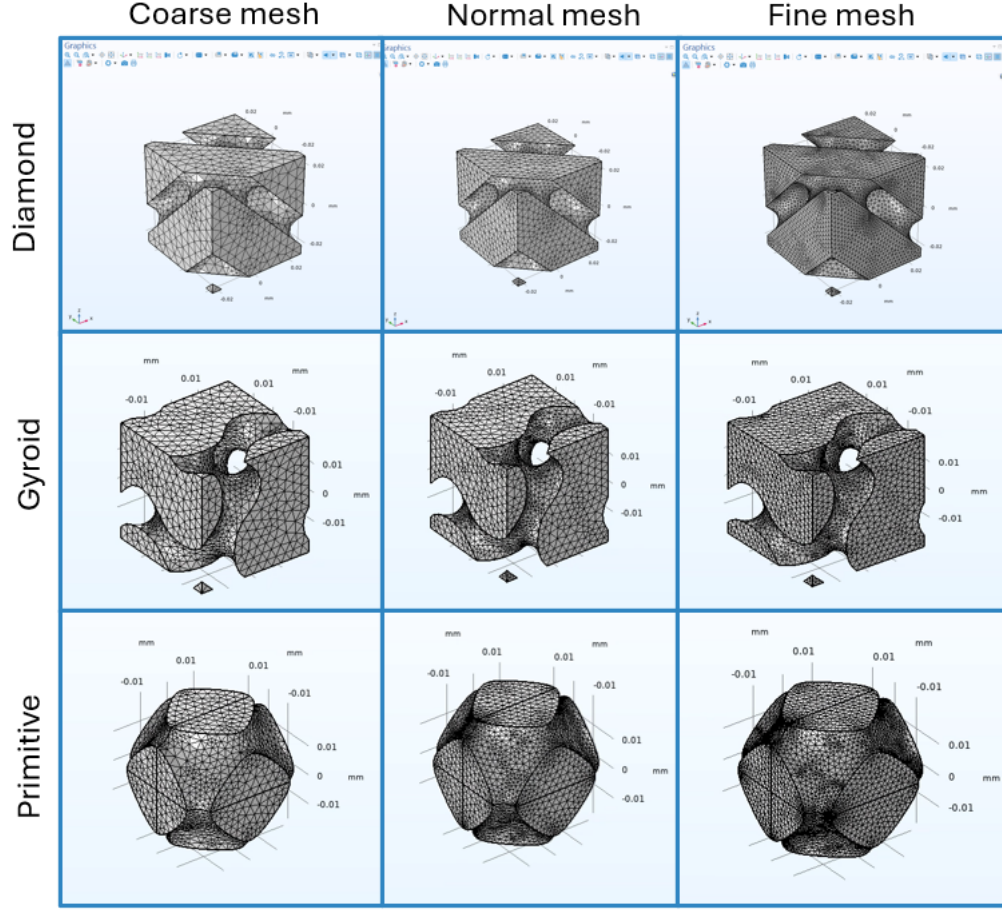


Figure 35: Different mesh sizing.

reliable methods available for the prediction of numerical uncertainty. The method can be divided into 5 steps:

1. Define a representative cell, mesh, or grid size h :

$$h = \left[\frac{1}{N} \sum_{i=1}^N (\Delta V_i) \right]^{1/3}$$

where ΔV_i is the volume of the i -th cell, and N is the total number of cells used for the computations.

2. Run simulations on three different sets of grids to determine a key variable important to the objective of the simulation (K in our case). The mesh refinement factor

$l = 40 \text{ } \mu\text{m}$				
	# Elements	Average size [mm]	Refinement ratio	Quality
Diamond	53488	$9.582e - 4$	—	0.660
	35776	$1.096e - 3$	1.14	0.664
	80379	$8.365e - 4$	1.14	0.662
Gyroid	16306	$1.397e - 3$	—	0.646
	32302	$1.113e - 3$	1.26	0.649
	63389	$8.886e - 4$	1.26	0.659
Primitive	27293	$1.179e - 3$	—	0.662
	57021	$9.225e - 4$	1.26	0.662
	113297	$7.338e - 4$	1.26	0.662

Table 2: Mesh statistics.

$r = h_{coarse}/h_{fine}$ should be greater than 1.3 to ensure accurate uncertainty estimations, based on experience [52].

- Let $h_1 < h_2 < h_3$ and $r_{21} = h_2/h_1$, $r_{32} = h_3/h_2$, we can calculate the apparent order p of the method using the following expression

$$p = \frac{1}{\ln(r_{21})} |\ln |\varepsilon_{32}/\varepsilon_{21}| + q(p)|$$

$$q(p) = \ln \left(\frac{r_{21}^p - s}{r_{32}^p - s} \right)$$

$$s = 1 \cdot \text{sgn}(\varepsilon_{32}/\varepsilon_{21})$$

where $\varepsilon_{32} = \phi_3 - \phi_2$, $\varepsilon_{21} = \phi_2 - \phi_1$, and ϕ_k denotes the solution on the k -th grid.

- Calculate the extrapolated values using

$$\phi_{ext}^{21} = (r_{21}^p \phi_1 - \phi_2)(r_{21}^p - 1)$$

$$\phi_{ext}^{32} = (r_{32}^p \phi_2 - \phi_3)(r_{32}^p - 1)$$

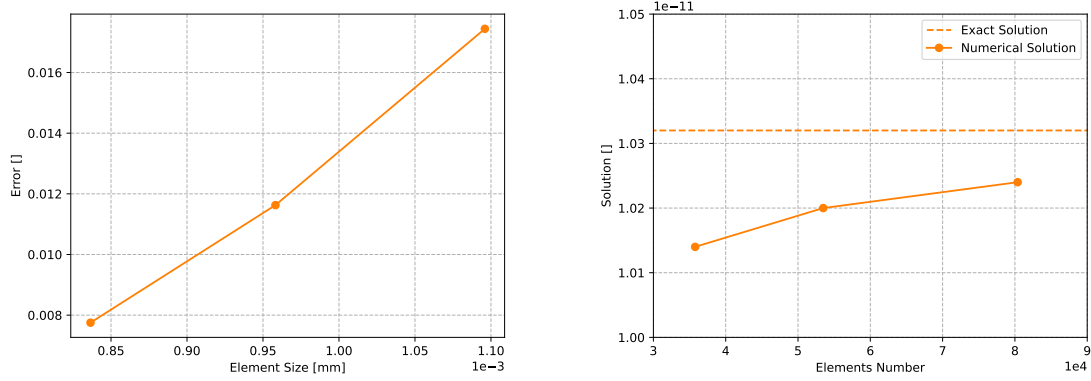
- Finally, calculate the following error estimates

$$e_a^{21} = \left| \frac{\phi_1 - \phi_2}{\phi_1} \right| \quad \text{Approximate relative error,}$$

$$e_{ext}^{21} = \left| \frac{\phi_{ext}^{12} - \phi_1}{\phi_{ext}^{12}} \right| \quad \text{Extrapolated relative error,}$$

$$GCI_{fine}^{21} = \frac{1.25e_a^{21}}{r_{21}^p - 1} \quad \text{Fine-Grid Convergence Index (GCI).}$$

The plots resulting from the RE convergence analysis of the three TPMS structures of unit cell size equal to $40 \mu m$ are shown in figures 36, 37 and 38.



(a) Relative error on the numerical solution as a function of mesh element size. (b) Numerical solution as a function of number of mesh elements.

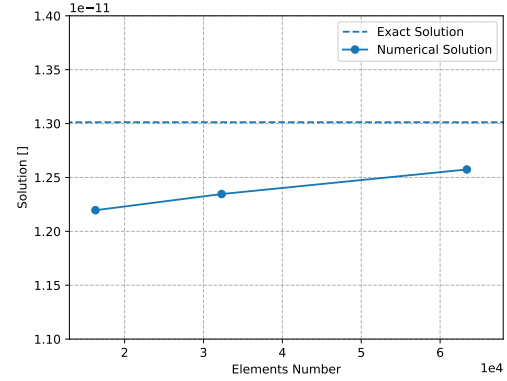
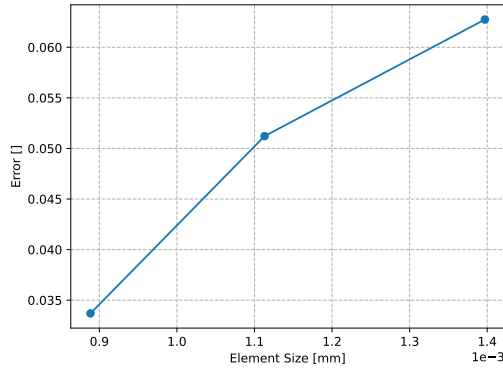
Figure 36: Sensitivity analysis results for the Diamond topology.

As it can be seen, for all three TPMS structures, the discretization error decreases monotonically with the mesh element size. At the same time, the solution, which for this analysis is the $i = 1, j = 1$ component of the permeability tensor obtained by solving the BVP, tends to exact theoretical solution.

In table 3, the convergence properties (i.e. order of convergence, refinement ratio and grid convergence index) are reported.

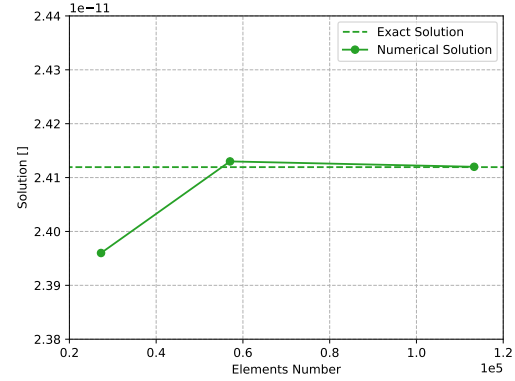
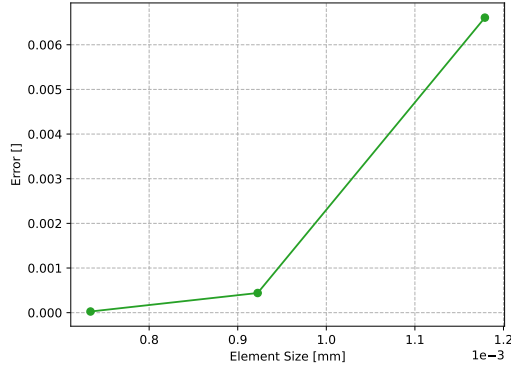
From these results we can confidently say that the discretization error is negligible and that we have reached the mesh convergence even with the intermediate mesh for all three TPMS unit cells. Thanks to this study, we can run all the simulations for the other unit cell sizes, namely $50 \mu m$, $30 \mu m$, $20 \mu m$, $10 \mu m$, knowing that the results obtained from these simulations will be accurate, reliable and independent of mesh elements size.

Now that we have established that the mesh convergence is guaranteed, we can run the simulations for the solution of the closure problem that will allow us to obtain the effective parameters and thus the permeability tensor.



(a) Relative error on the numerical solution as a function of mesh element size. (b) Numerical solution as a function of number of mesh elements.

Figure 37: Sensitivity analysis results for the Gyroid topology.



(a) Relative error on the numerical solution as a function of mesh element size. (b) Numerical solution as a function of number of mesh elements.

Figure 38: Sensitivity analysis results for the Primitive topology.

5.2.4 Simulation results

In this section we will analyse the plots obtained from the upscaled closure problem simulations. As it has already been said in section 4.2, the key results of the closure problem simulations are the effective parameters $\mathbf{k}$ and $\mathbf{a}$, a tensor and a vector, respectively. These effective parameters are the key variables of the homogenization theory that carry the information of the micro-scale all the way up to the macro or continuum scale, allowing the connection between the two. From the effective parameters, one can obtain physical

$l = 40 \text{ } \mu\text{m}$			
	$r_{21} = r_{32}$	p	GCI
Diamond	1.14	3.09	0.052
Gyroid	1.26	1.81	0.188
Primitive	1.26	12.26	0.020

Table 3: Mesh convergence

quantities, such as the permeability tensor $\mathbf{K}$, by simply integrating them over the unit cell volume.

Let us now plot the solutions of the 3D simulations for the effective parameter $\mathbf{k}$.

Note that the plots shown below represent the vector field of only one unit cell, but due to the fact that the medium is periodic, we can imagine to extend the same flow pattern to an infinite number of unit cells in the 3 cartesian directions.

Another fact that is important to address is related to the tensorial quantities that are being plotted: we are plotting the components of the effective parameter $\mathbf{k}$ but, given that these components can be translated directly to the permeability tensor components via a volume integration, we are going to discuss the results assuming that we are plotting the permeability components instead of the effective parameter ones.

Given what has been said, from figure 39, we can clearly see the symmetric nature of the permeability tensor $\mathbf{K}$, where the diagonal elements are related to the permeability in the 3 main directions, namely x for K_{11} , y for K_{22} and z for K_{33} . Permeability can simply be viewed as a quantity that determines how much a pressure gradient in a certain direction affects the velocity of the flow. For instance, the component K_{11} of the permeability tensor quantifies the effect that the pressure gradient in the x direction has on the velocity on the same x direction. With this in mind, we can understand the physical meaning of the off-diagonal terms of the permeability tensor: they represent the effect that the pressure gradient on a certain direction i has on the velocity field on a orthogonal direction j . For example, the component K_{12} quantifies the influence that gradients on the x direction have on flow in the y direction. We can thus say that the off-diagonal terms represent the directional coupling or anisotropy of the porous medium being studied. In general, it is common to have anisotropic porous media with symmetric permeability tensors, where the K_{ij} component equals the K_{ji} one.

Another interesting fact that can be noted from figure 39 is that the off-diagonal terms are very small when compared to the diagonal ones and that they can assume negative values. Physically this fact does not make sense, since that permeability must always be positive⁶. We can justify this incongruence by simply noting that the permeability tensor is positive-definite, and that we can always rotate the coordinate system to a specific

⁶Permeability relates the pressure gradient to the direction and intensity of the flow. For any non-zero pressure gradient vector, the energy dissipation is positive and the resulting flow will always have a component in the direction of decreasing pressure. A negative permeability would violate the 2nd law of thermodynamics.

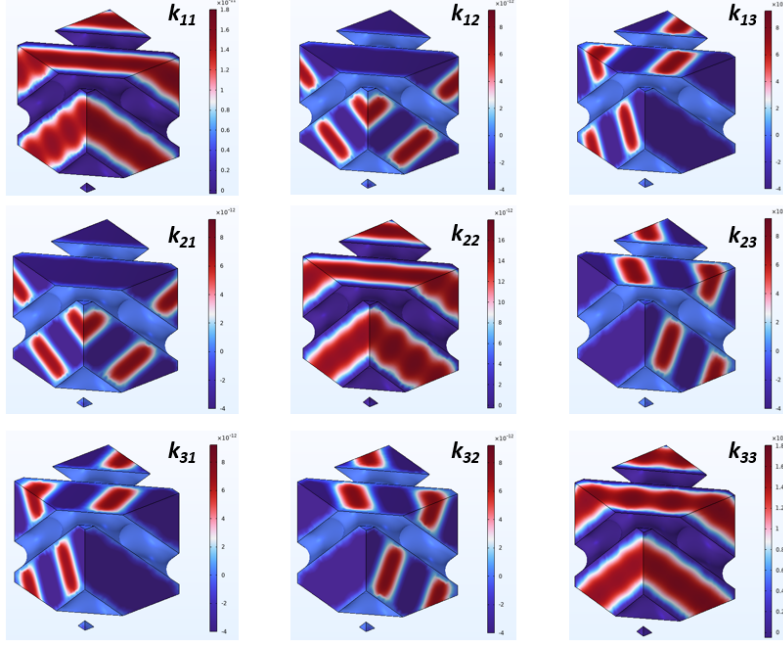


Figure 39: k field of the Diamond unit cell.

orientation (the principal axes) where all off-diagonal terms become zero, thus obtaining the principal permeability tensor. Given what has been said, we can see the negative values of the permeability in the off-diagonal terms as mathematical artifacts that can be solved simply by considering another coordinate system. Finally, note that the diagonal terms can not be negative, given that the tensor must be positively defined.

In figure 40 and figure 41 the permeability tensor components are plotted. By comparing the two figures we can clearly see how the two TPMS unit cells present a drastically different anisotropy, with the Gyroid unit cell having a high anisotropic behavior while the Primitive one being perfectly symmetric in all three directions.

To measure the anisotropy of a tensor, we can introduce two quantities:

$$AI = \frac{\max(K_{ii}) - \min(K_{ii})}{\text{mean}(K_{ii})} \quad \text{anisotropy index} \quad (47)$$

$$ODR = \frac{\max_{i \neq j} |K_{ij}|}{\text{mean}(K_{ii})} \quad \text{off-diagonal ratio} \quad (48)$$

We can plot these two indices for all three structures and for all the unit cell sizes being considered (figure 42). As expected, the Gyroid structure presents the highest level of anisotropy, followed by the Diamond one. The Primitive structure is, in all effect, symmetric. The slight variations on both the AI and ODR are due to numerical error related to the mesh creation process.

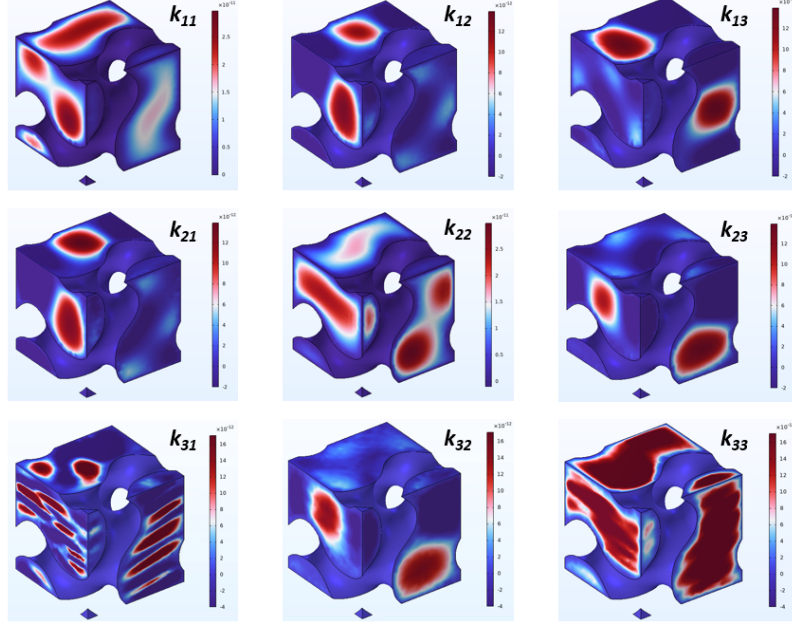


Figure 40: $\mathbf{k}$ field of the Gyroid unit cell.

In figure 43 can be found the values of all the components of the permeability tensors that will be later used for the model validation.

Now that we have completed the analysis of the $\mathbf{k}$ component of the solution of the closure problem, we can briefly talk about the $\mathbf{a}$ component. Physically, the components a_1 , a_2 and a_3 of the effective parameter $\mathbf{a}$ can be thought of as the local pressure associated with a flow field $\mathbf{k}$ driven by a pressure drop aligned with the three main directions x , y and z , respectively. In this specific study, we are not really interested in this parameter, given that it does not have a direct influence on the hydraulic performances of the porous structure at the macroscopic scale.

5.3 Darcy's flow

We have now completed the left branch of the workflow diagram in figure 31, having obtained the effective parameters and thus the permeability tensor.

The next logical step is to validate the upscaled model. To do so, we need to run pore-scale simulations on the same topologies treated in the previous section and then compare the results.

The parameter that will be used for the validation is the permeability in the x direction, which corresponds to the axial direction of the heat pipe.

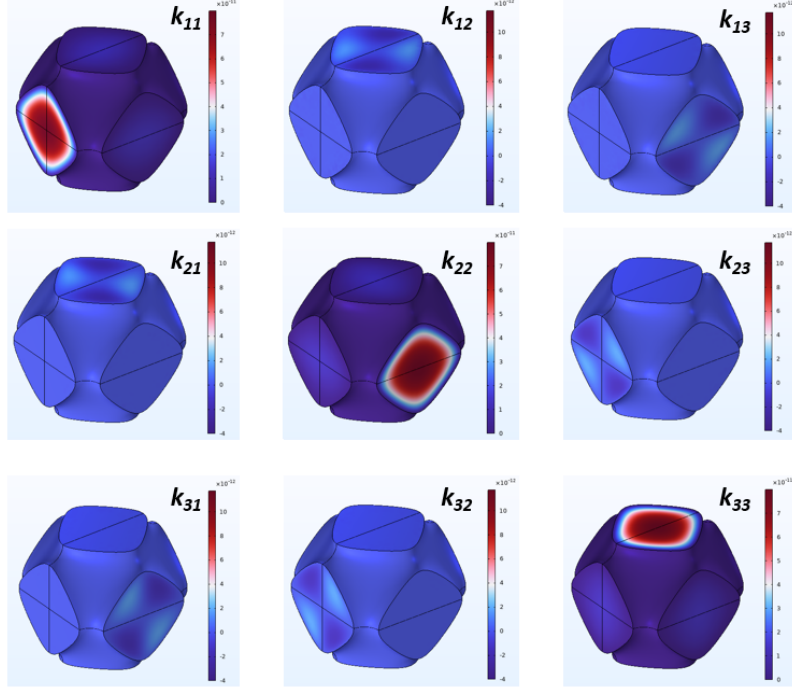
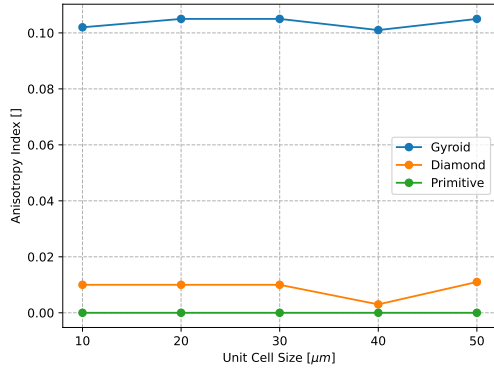
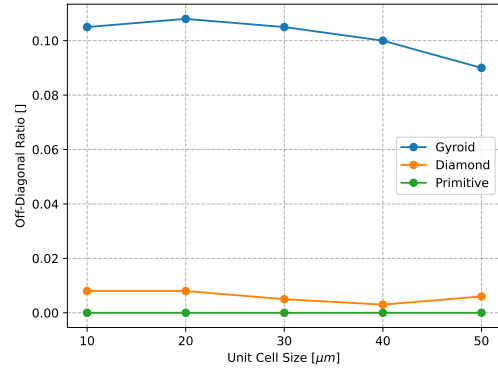


Figure 41: k field of the Primitive unit cell.



(a) AI for different unit cell sizes.



(b) ODR for different unit cell sizes.

Figure 42: AI and ODR for all unit cell sizes and structures.

Gyroid 50μm			Diamond 50μm			Primitive 50μm		
1,96E-11	6,09E-13	6,21E-13	1,59E-11	9,20E-14	4,83E-14	3,77E-11	-3,52E-16	-5,57E-16
6,09E-13	1,97E-11	5,97E-13	9,20E-14	1,57E-11	-5,19E-16	-3,52E-16	3,77E-11	-1,52E-16
1,83E-12	6,81E-13	2,18E-11	4,83E-14	-5,19E-16	1,58E-11	-5,57E-16	-1,52E-16	3,77E-11
Gyroid 40μm			Diamond 40μm			Primitive 40μm		
1,22E-11	4,75E-13	4,45E-13	1,02E-11	2,59E-14	1,05E-14	2,41E-11	1,04E-16	-1,41E-16
4,75E-13	1,22E-11	4,47E-13	2,59E-14	1,03E-11	1,61E-14	1,04E-16	2,41E-11	-6,22E-17
1,26E-12	5,41E-13	1,35E-11	1,05E-14	1,61E-14	1,02E-11	-1,41E-16	-6,22E-17	2,41E-11
Gyroid 30μm			Diamond 30μm			Primitive 30μm		
6,94E-12	2,33E-13	2,33E-13	5,70E-12	3,10E-14	2,44E-14	1,36E-11	-6,74E-17	-5,80E-17
2,33E-13	6,97E-12	2,26E-13	3,10E-14	5,64E-12	1,33E-15	-6,74E-17	1,36E-11	-1,91E-16
7,53E-13	2,74E-13	7,70E-12	2,44E-14	1,13E-15	5,70E-12	-5,80E-17	-1,91E-16	1,36E-11
Gyroid 20μm			Diamond 20μm			Primitive 20μm		
3,09E-12	1,03E-13	9,93E-14	2,53E-12	1,92E-14	4,54E-15	6,03E-12	6,78E-17	-1,08E-16
1,03E-13	3,09E-12	9,59E-14	1,92E-14	2,51E-12	-3,65E-15	6,78E-17	6,04E-12	-3,81E-17
3,45E-13	9,59E-14	3,43E-12	4,54E-15	-3,65E-15	2,53E-12	-1,08E-16	-3,81E-17	6,04E-12
Gyroid 10μm			Diamond 10μm			Primitive 10μm		
7,72E-13	2,57E-14	2,55E-14	6,32E-13	4,83E-15	1,07E-15	1,51E-12	6,51E-18	-8,80E-18
2,57E-14	7,73E-13	2,55E-14	4,83E-15	6,26E-13	-1,13E-15	6,51E-18	1,51E-12	-3,89E-18
8,42E-14	2,72E-14	8,54E-13	1,07E-15	-1,13E-15	6,32E-13	-8,80E-18	-3,89E-18	1,51E-12

Figure 43: Components of the various permeability tensors.

5.3.1 Model setup

Given that we are trying to validate a problem obtained from the upscaling of the Stokes' equations, the most natural thing to do is to validate the results by solving the Stokes' flow on the same topologies, and that is exactly what we are going to do.

The equation for the Stokes' problem have already been introduced in section 4.1.1, but let us re-write the equations one more time:

$$\nabla \cdot \mathbf{u} = \mathbf{0}, \quad \mathbf{x} \in B^\varepsilon \quad (49a)$$

$$\mu \nabla^2 \mathbf{u} - \nabla p = \mathbf{0}, \quad \mathbf{x} \in B^\varepsilon \quad (49b)$$

$$\mathbf{u} = \mathbf{0}, \quad \mathbf{x} \in \Gamma^\varepsilon \quad (49c)$$

To solve this set of PDEs we are going to use the stationary *Creeping Flow* model, which is preset in COMSOL.

Thanks to the homogenization theory framework, we know that the modeling error introduced with the upscaled equations should be bounded by the small scale parameter ε to the power of the truncation order of the asymptotic expansion. In our specific case, the two-scale asymptotic expansions for both velocity and pressure were truncated to the first order, meaning that the maximum modeling error that we can expect from comparing the results obtained from the upscaled equations with the ones obtained from the pore-scale

simulations, should be smaller than ε^1 . If that is not the case, then the upscaled equations obtained are not correct and the whole homogenization workflow must be repeated.

We know that the small scale parameter is defined as:

$$\varepsilon = \frac{l}{L} \quad (50)$$

Given this, we want to simulate the fluid flow on a domain that is large enough, compared to the unit cell size, to have an ε that is as small as possible. At the same time, we can not reduce too much ε because that would imply higher computational costs associated with the pore-scale simulations on a larger domain.

Given that, we are going to run the pore-scale simulations on domains of increasing length in the x direction, while keeping the unit cell size the same. This goes in contrast for what it is usually done for numerical validation of upscaled equations, where the macroscopic domain is kept the same size and what is reduced is the size of the unit cell [46]. Figure 44 shows the fluid domains that are being simulated for the same three topologies. From now on, all the resulting flow fields will be displayed only for the 3 unit cells fluid domain for convenience purposes.

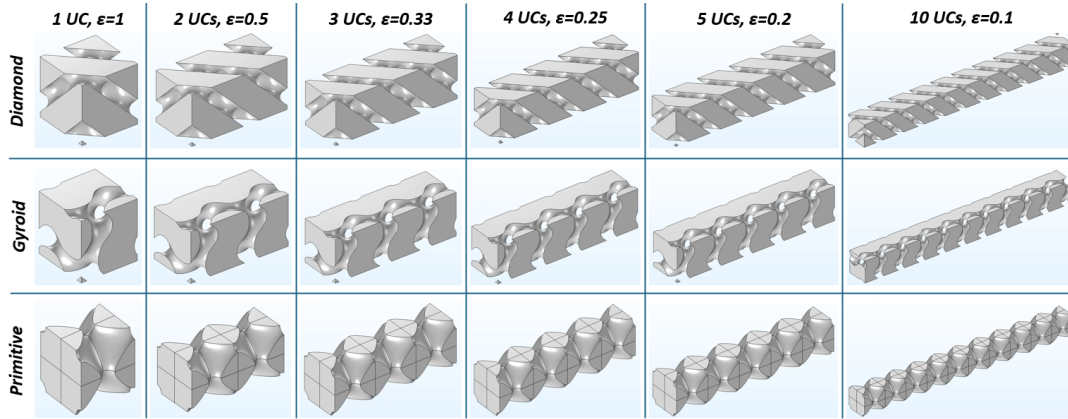


Figure 44: Fluid domains used for the pore-scale simulations.

Finally, we impose the following periodic boundary conditions on pressure, as shown in figure 45:

- $\Delta P \neq 0$ in x direction
- $\Delta P = 0$ in y and z directions

Note that, as long as we stay inside the Darcy's flow regime, the magnitude of the periodic pressure applied in the x direction is not relevant, given that in this regime the pressure drop is directly proportional to velocity (with permeability as the constant of

proportionality). To check if we are indeed inside the required regime, we will plot the values of the pressure drop per unit length as a function of velocity and check if the relationship is linear or not (see section 5.3.5)

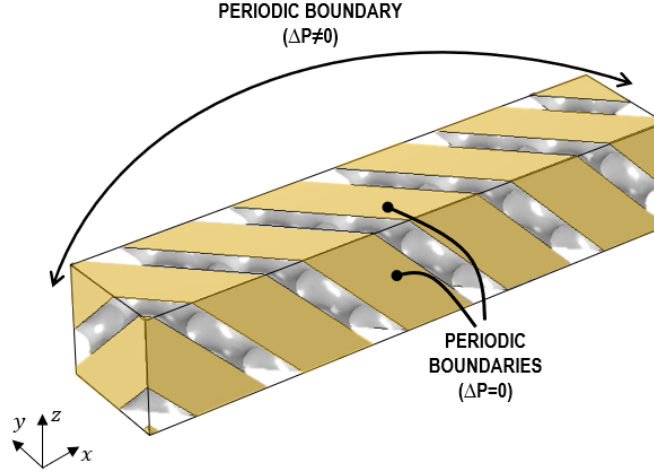


Figure 45: Periodic boundary conditions for the pore-scale simulations.

As for the closure problem, we apply the no-slip boundary condition to the liquid-solid interface, as shown in figure 46.

5.3.2 Solver

As it has already been said in the previous section, to solve the fluid flow we are going to use the *Creeping Flow* model setup of COMSOL. This template model can be used to simulate fluid flows at very low Reynolds numbers for which the inertial term in the Navier–Stokes equations can be neglected, which is exactly the case for Stokes’ flow. The following flow assumptions are made:

- Incompressible flow ($Re < 1$)
- Newtonian fluid
- Stationary

As for the discretization, we are going to use a P2-P1 scheme, which will now be explained in more details. This particular scheme, often used for solving Stokes and Navier-Stokes equations, uses second-order (quadratic) polynomial shape functions to solve for the fluid velocity field, and first-order (linear) shape functions to solve for the pressure field.

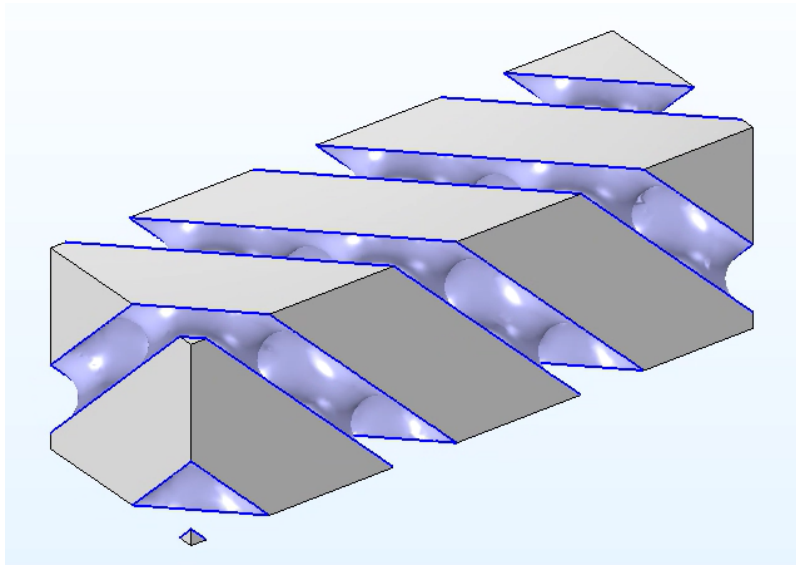


Figure 46: No-slip boundary condition.

This means that more nodes are used to approximate velocity as compared to the ones used to approximate pressure. For instance, edges and mid-points could be used for velocity and only vertices for pressure. A representation of the P2-P1 (Taylor-Hood) elements is shown in figure 47.

Using a discretization scheme with different polynomial order for velocity and pressure is essential when solving the so-called "saddle point" problems⁷: when solving this problems it is essential to ensure the Ladyzhenskaya-Babuska-Brezzi (LBB) condition, also known as the inf-sup stability condition. The LBB condition ensures that for every possible pressure field, there is a corresponding velocity field that "responds" to it. If this condition is not respected, the saddle point problem will not have a single, stable solution and spurious oscillation ("checkerboard" patterns) can appear in the pressure field. To avoid the generation of said instability, elements of different order must be used.

The downside of using P2-P1 elements is that the computational power needed to solve the flow will be higher, due to an increased number of DOF.

5.3.3 Meshing

The workflow used to mesh the fluid domains for the pore-scale simulations is the same as the one used for the closure problem discussed in section 5.2.2. The only difference is that now we need to mesh domains that are as much as 10 times larger than the ones meshed

⁷In linear algebra, a saddle point problem is a problem where the solution is maximum in one direction and minimum in another. The coefficients' matrix for these problems is partly positive and partly negative.

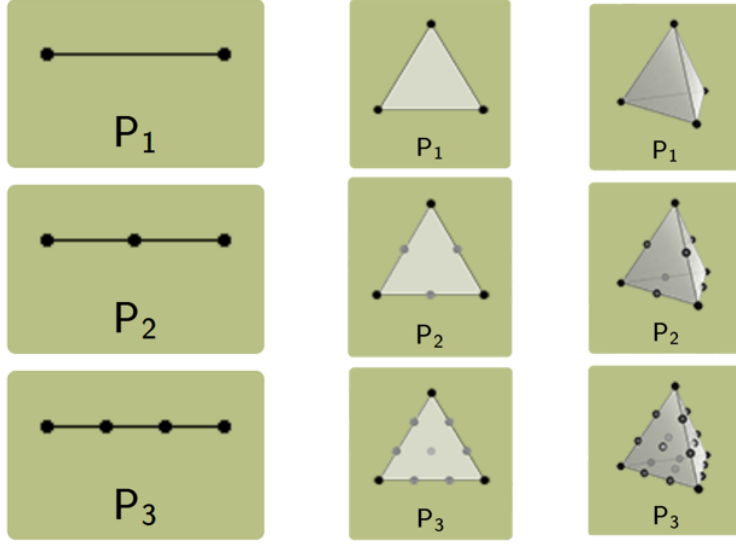


Figure 47: Finite elements types of the polynomial family for 1D, 2D and 3D (from left to right).

for the closure problem. Since we want to keep the same mesh element size, the simulations will be computationally more expensive, due to an increase in the number of mesh elements.

After the meshes have been generated, we can move on to the mesh convergence analysis. As it was the case for the closure problem simulations, we can run the RE for the three TPMS topologies considering only one unit cell size and one domain length, assuming that the flow configurations does not change, but it only gets scaled/extended. Given this, we will run the sensitivity analysis only on the $40\ \mu\text{m}$ unit cell size and only for the domains composed of three unit cells in the axial direction.

5.3.4 Sensitivity analysis

The procedure is exactly the same as the one explained in section 5.2.2. Here, we will only present the results of the analysis.

$l = 40\mu\text{m}, \# \text{ UCs} = 3$			
	$r_{21} = r_{32}$	p	GCI
Diamond	1.26	4.68	0.029
Gyroid	1.26	1.86	0.0536
Primitive	1.26	2.21	0.0005

Table 4: Mesh convergence.

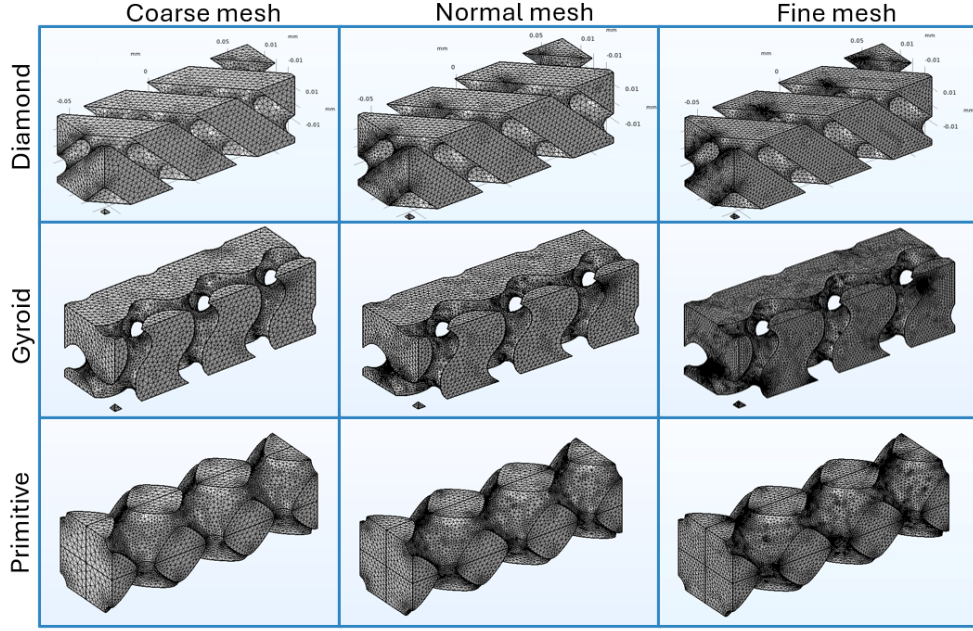
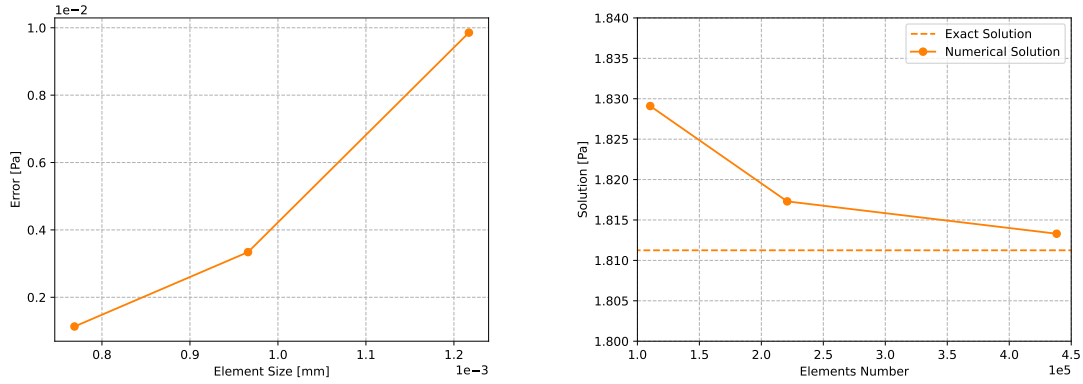


Figure 48: Meshes used for the pore-scale simulations.

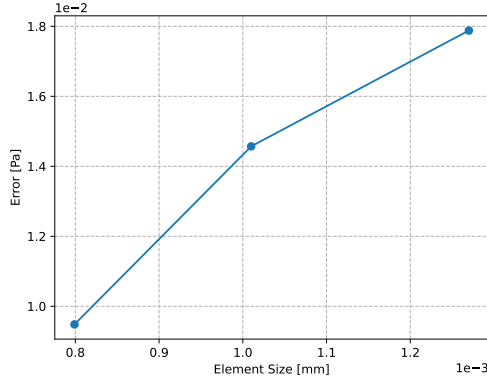


(a) Relative error on the numerical solution as a function of mesh element size. (b) Numerical solution as a function of number of mesh elements.

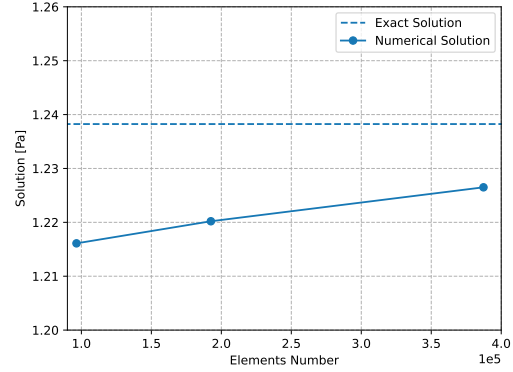
Figure 49: Sensitivity analysis results for the Diamond topology.

From figures 49, 50, 51 and table 4 we can clearly see that mesh convergence is reached for all three levels of refinements.

An even better estimation of the order of convergence and GCI could be obtained using an

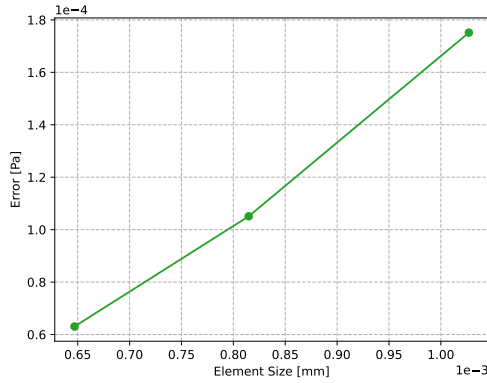


(a) Relative error on the numerical solution as a function of mesh element size.

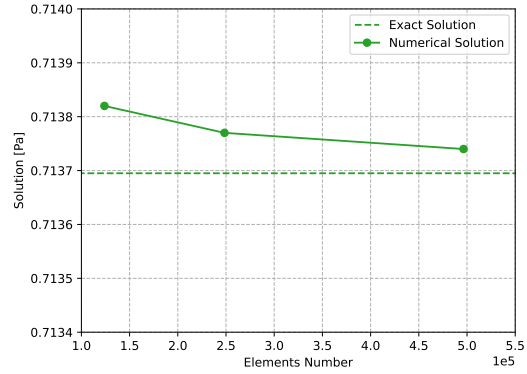


(b) Numerical solution as a function of number of mesh elements.

Figure 50: Sensitivity analysis results for the Gyroid topology.



(a) Relative error on the numerical solution as a function of mesh element size.



(b) Numerical solution as a function of number of mesh elements.

Figure 51: Sensitivity analysis results for the Primitive topology.

additional level of mesh refinement, but given the accuracy required for the present study, three levels are more than enough.

Let us now present the results (velocity and pressure fields) of the flow simulations obtained from the pore-scale study.

5.3.5 Simulation results

In this section we are going to discuss the results obtained from the solution of the Stokes' equations defined at the pore-scale. As previously said, only the plots for the three unit cells fluid domain will be shown for conciseness.

Let us start by plotting the velocity magnitude volume plots.

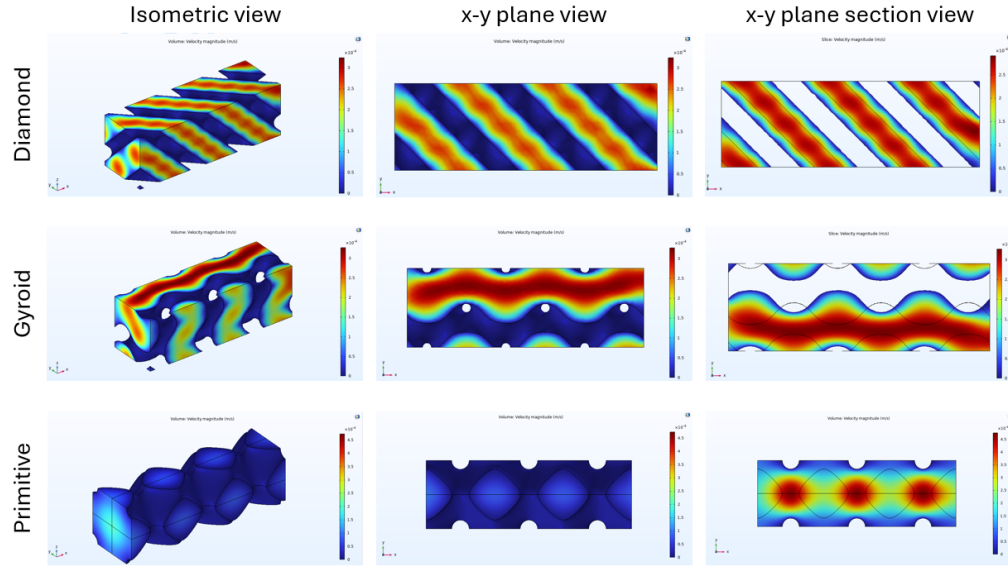


Figure 52: Velocity magnitude plots for the pore-scale simulations.

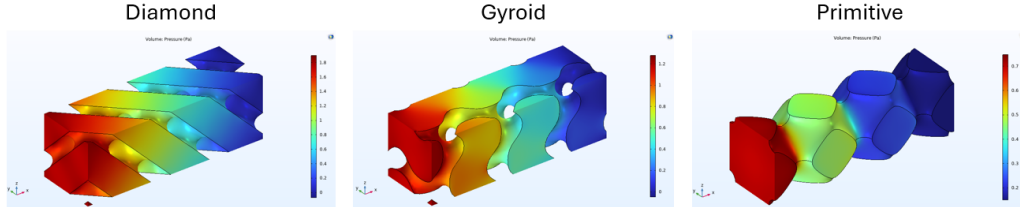


Figure 53: Pressure field plots for the pore-scale simulations.

To make sure that the assumption of Darcy's flow holds, we need to check that the pressure drop set as the periodic boundary condition on the inlet and outlet boundaries does not translate into a velocity (and thus a Reynolds number) which is outside the Darcy's regime. Figure 54 shows why it is important to stay inside this regime to make sure the mathematical derivations hold: one key step in the upscaling via homogenization workflow is that we assume a linear solution for the problem (see equation (29)). This assumption is valid as long as we are inside the Darcy's regime, where the relationship between flow

velocity and pressure drop per unit length is linear. To show that we are indeed inside the

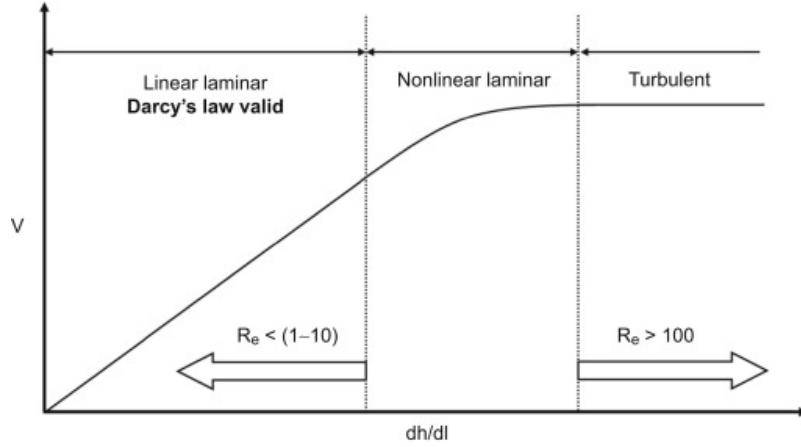


Figure 54: Various flow regimes.

Darcy's flow regime, we can plot the pressure drop per unit length as a function of the x velocity and check if the gradient of the curve obtained is constant or not. From figure 55 it can be seen that, indeed, we are inside the aforementioned regime for all three structures.

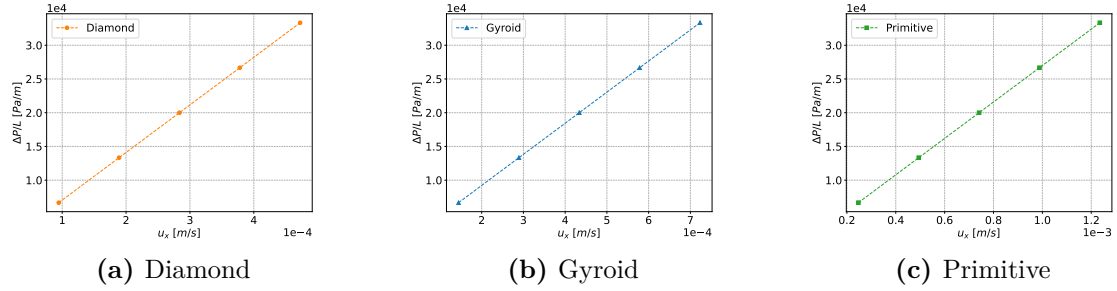


Figure 55: Check for the Darcy's regime.

The parameter that we want to estimate with this pore-scale simulations is the permeability. Specifically, we want to know the x component of the permeability tensor. To evaluate the permeability, we use Darcy's law:

$$K_x = \frac{\mu \langle u_x \rangle L}{\Delta P} \quad (51)$$

In this equation, u_x is the volume-averaged velocity over the whole fluid domain (figure 56):

$$\langle u_x \rangle = \frac{1}{V_l} \int_{V_l} u_x dV \quad (52)$$

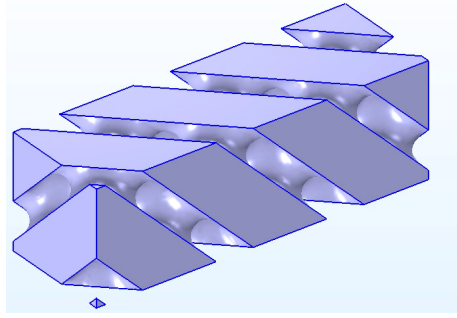


Figure 56: Integration volume for average velocity.

and ΔP is the imposed periodic pressure drop. In tables 5, 6 and 7 are reported the results of the pore-scale simulations for varying domain length and fixed unit cell size, which in this case was taken equal to $50 \mu m$. For all the simulations, the working fluid used is water ($\mu = 10^{-3} \frac{kg}{m \cdot s}$), as it was the case for the closure problem simulations. Note, however, that the working fluid used in these simulations is irrelevant for the results obtained, given that the permeability is a property of the structure that quantifies how easily a fluid can move through it, but does not depend on the fluid itself.

As expected, there is a linear relationship between pressure drop and velocity. The results also show how the permeability does not change with an increased domain length, indicating that with the periodic boundary conditions applied the boundary effects are negligible and do not appear to affect the results.

Diamond, $l = 50 \mu m$					
# UCs	$L [\mu m]$	$\Delta P [Pa]$	$u_x [m/s]$	$K_x [m^2]$	
1	50	0.5	$1.42e^{-4}$	$1.42e^{-11}$	
2	100	1	$1.42e^{-4}$	$1.42e^{-11}$	
3	150	1.5	$1.42e^{-4}$	$1.42e^{-11}$	
4	200	2	$1.42e^{-4}$	$1.42e^{-11}$	
5	250	2.5	$1.42e^{-4}$	$1.42e^{-11}$	
10	500	5	$1.42e^{-4}$	$1.42e^{-11}$	

Table 5: Pore-scale simulations results for the Diamond topology.

One last check that needs to be addressed to make sure that the simulations make physical sense is to see if permeability changes with inlet velocity. Given what has already been said, permeability should not change with the velocity of the fluid flow, since it is a property of the porous medium.

Figure 57 proves that permeability does not, in fact, change with the volume-averaged velocity. This result could have been obtained just by looking at tables 5, 6 or 7: velocity

Gyroid, $l = 50 \mu m$					
# UCs	$L [\mu m]$	$\Delta P [Pa]$	$u_x [m/s]$	$K_x [m^2]$	
1	50	0.5	$2.17e^{-4}$	$2.17e^{-11}$	
2	100	1	$2.17e^{-4}$	$2.17e^{-11}$	
3	150	1.5	$2.17e^{-4}$	$2.17e^{-11}$	
4	200	2	$2.17e^{-4}$	$2.17e^{-11}$	
5	250	2.5	$2.17e^{-4}$	$2.17e^{-11}$	
10	500	5	$2.17e^{-4}$	$2.17e^{-11}$	

Table 6: Pore-scale simulations results for the Gyroid topology.

Primitive, $l = 50 \mu m$					
# UCs	$L [\mu m]$	$\Delta P [Pa]$	$u_x [m/s]$	$K_x [m^2]$	
1	50	0.5	$3.75e^{-4}$	$3.75e^{-11}$	
2	100	1	$3.75e^{-4}$	$3.75e^{-11}$	
3	150	1.5	$3.75e^{-4}$	$3.75e^{-11}$	
4	200	2	$3.75e^{-4}$	$3.75e^{-11}$	
5	250	2.5	$3.75e^{-4}$	$3.75e^{-11}$	
10	500	5	$3.75e^{-4}$	$3.75e^{-11}$	

Table 7: Pore-scale simulations results for the Primitive topology.

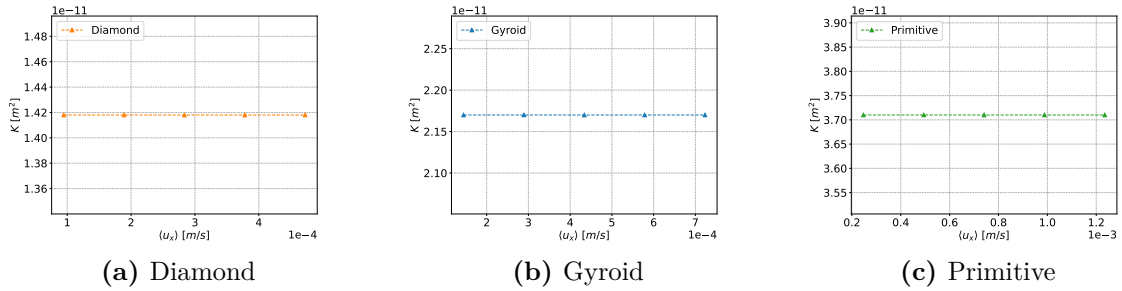


Figure 57: Permeability as a function of average flow velocity.

scales linearly with pressure drop and permeability is equal to the ratio between velocity and pressure drop (multiplied by two constants μ and L). If we want to double the velocity we would need to double the imposed pressure drop, which translates in a constant permeability.

5.4 Closure problem and pore-scale simulations comparison

Now that we solved both the closure problem and the pore-scale simulations, the last thing that is left to do is to compare the results and check if the relative error on permeability is

bounded by the small scale parameter ε or not. If it is, then the model is validated and the upscaled equations can be used to obtain the effective parameters for the device-scale simulations, otherwise, the upscaled equations do not model the physics of the problem correctly and the whole homogenization theory workflow needs to be reviewed to check for errors.

Before we can start comparing the results, we need to clarify the reasoning behind the choice of the fluid domain size on which we are solving the pore-scale equations. We already discussed how the homogenization framework tells us that, for the model to be validated, the error on the output parameters of the closure problem must be smaller than ε , which is defined as the ratio of the microscopic length scale l and the size of the macroscopic domain L . Given this definition, we understand how the maximum error that we can have depends on the overall size of the fluid domain that we are using to solve the pore-scale equations. For instance, if the macroscale length is only three times as large as the microscale one (i.e. $L = 3 \cdot l$), then the maximum allowable error will be $\varepsilon = 0.33$; an error this big would not be a good measure of the accuracy of the model we have built. This is exactly the reason why we are considering domains that are as much as 10 times larger than the single unit cell, because otherwise the validation step using the small scale parameter would be trivially satisfied.

Another important thing to note is that we are only considering a domain that is composed of $n \times 1 \times 1$ unit cells in the x , y and z direction, respectively. Ideally, we would like to use a domain of size $n \times n \times n$, but given that this would increase the size of the computational domain of 100 times (in the worst case) and that we are only interested in validating the x component of the permeability, we can assume that the boundary effects on the periodic faces normal to the y and z axis on the $n \times 1 \times 1$ domain can be neglected.

In figure 58 are plotted the permeability results for both the closure problem and the pore-scale simulations for the different domain lengths. Again, all the results are shown only for one unit cell size ($50 \mu m$ in this case) but they can be assumed valid for all the other unit cell sizes (as long as the Darcy's flow regime holds), given that the only difference is a scaling transformation.

To evaluate the relative error we use the following equation:

$$E_{rel} = \frac{|K_x^{PS} - K_{11}^{CP}|}{K_{11}^{CP}} \quad (53)$$

where the superscript PS stands for "pore-scale" and the superscript CP for "closure problem".

Tables 8, 9 and 10 summarize the final model validation.

From the last column of the three tables, it can be seen that the relative error is, for all the topologies and for all domain sizes, lower than the small scale parameter ε , confirming that the model is indeed valid.

Finally, let us plot the results of the previous tables in figure 59.

Now the upscaled model has been validated and can be used to retrieve the effective

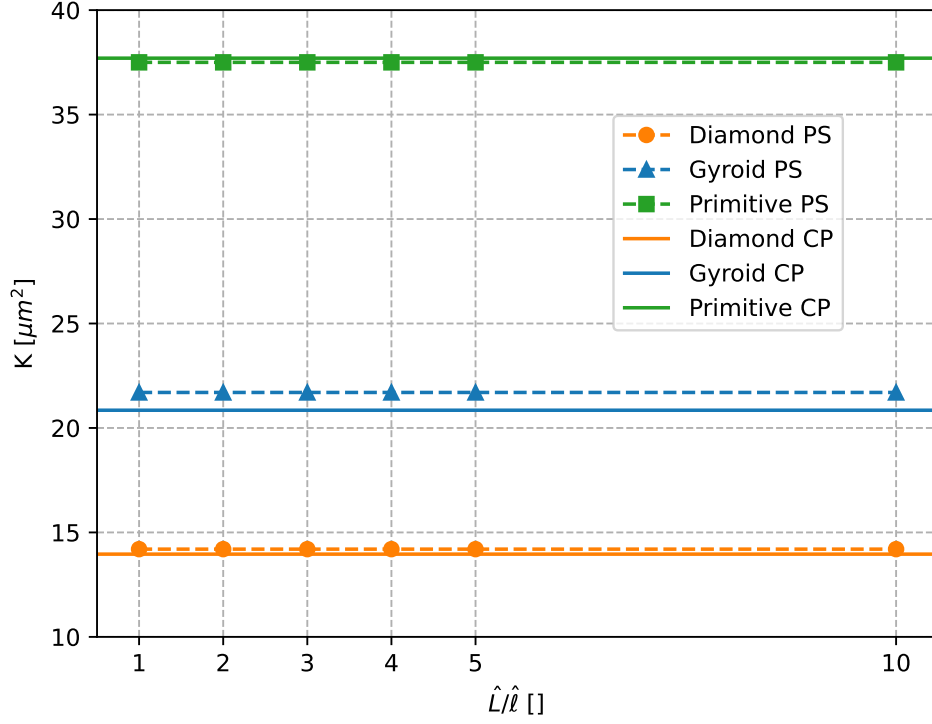


Figure 58: Permeability comparison between closure problem and pore-scale simulations.

Diamond, $l = 50 \mu m$				
# UCs	$K_x^{PS} [m^2]$	$K_{11}^{CP} [m^2]$	$\varepsilon [-]$	$E_{rel} [-]$
1	$1.42e^{-11}$	$1.40e^{-11}$	1	0.014
2	$1.42e^{-11}$	$1.40e^{-11}$	0.5	0.014
3	$1.42e^{-11}$	$1.40e^{-11}$	0.33	0.014
4	$1.42e^{-11}$	$1.40e^{-11}$	0.25	0.014
5	$1.42e^{-11}$	$1.40e^{-11}$	0.2	0.014
10	$1.42e^{-11}$	$1.40e^{-11}$	0.1	0.014

Table 8: Model validation results for the Diamond topology.

parameters, specifically permeability, for the device-scale simulations. One more check that can be done is to compare the results of all the simulations with results found in literature. That is precisely what we are going to do in the next section.

Gyroid, $l = 50 \mu m$				
# UCs	$K_x^{PS} [m^2]$	$K_{11}^{CP} [m^2]$	$\varepsilon []$	$E_{rel} []$
1	$2.17e^{-11}$	$2.08e^{-11}$	1	0.043
2	$2.17e^{-11}$	$2.08e^{-11}$	0.5	0.043
3	$2.17e^{-11}$	$2.08e^{-11}$	0.33	0.043
4	$2.17e^{-11}$	$2.08e^{-11}$	0.25	0.043
5	$2.16e^{-11}$	$2.08e^{-11}$	0.2	0.038
10	$2.15e^{-11}$	$2.08e^{-11}$	0.1	0.034

Table 9: Model validation results for the Gyroid topology.

Primitive, $l = 50 \mu m$				
# UCs	$K_x^{PS} [m^2]$	$K_{11}^{CP} [m^2]$	$\varepsilon []$	$E_{rel} []$
1	$3.75e^{-11}$	$3.77e^{-11}$	1	0.005
2	$3.75e^{-11}$	$3.77e^{-11}$	0.5	0.005
3	$3.75e^{-11}$	$3.77e^{-11}$	0.33	0.005
4	$3.75e^{-11}$	$3.77e^{-11}$	0.25	0.005
5	$3.75e^{-11}$	$3.77e^{-11}$	0.2	0.005
10	$3.75e^{-11}$	$3.77e^{-11}$	0.1	0.005

Table 10: Model validation results for the Primitive topology.

5.5 Cross verification with literature

To further verify that the results obtained for permeability are correct, we are going to compare them to the results obtained from Zhao et al. [27]. In particular, we are going to consider the plot in figure 60 that is presented in the paper.

From this plot, we are only interested in the "Diamond", "Gyroid" curves, since these are the TPMS structures used in this study. Note that even though the results for the Primitive structure are also present, the paper is considering a *Sheet* Primitive, whereas we are considering a *Network* Primitive (see section 3), thus we can not cross-verify the permeabilities for this topology. Nevertheless, the check on both Diamond and Gyroid should be sufficient to verify the validity of the pore-scale simulations.

Another thing that needs to be addressed is that we can not immediately compare the results because the way that the permeability is calculated in the paper differs slightly from the way used in this study. Specifically, in this study we are using the volume-averaged velocity to estimate the permeability, whereas in the paper the inlet velocity is used. The computational domain and boundary conditions also differs: Zhao et al. use a domain composed of 5 unit cells in the x direction with a cubic reservoir placed at the inlet to guarantee a fully-developed flow. For what concerns the BCs, they apply periodic BCs in the y and z directions, and a velocity inlet (with magnitude low enough to guarantee

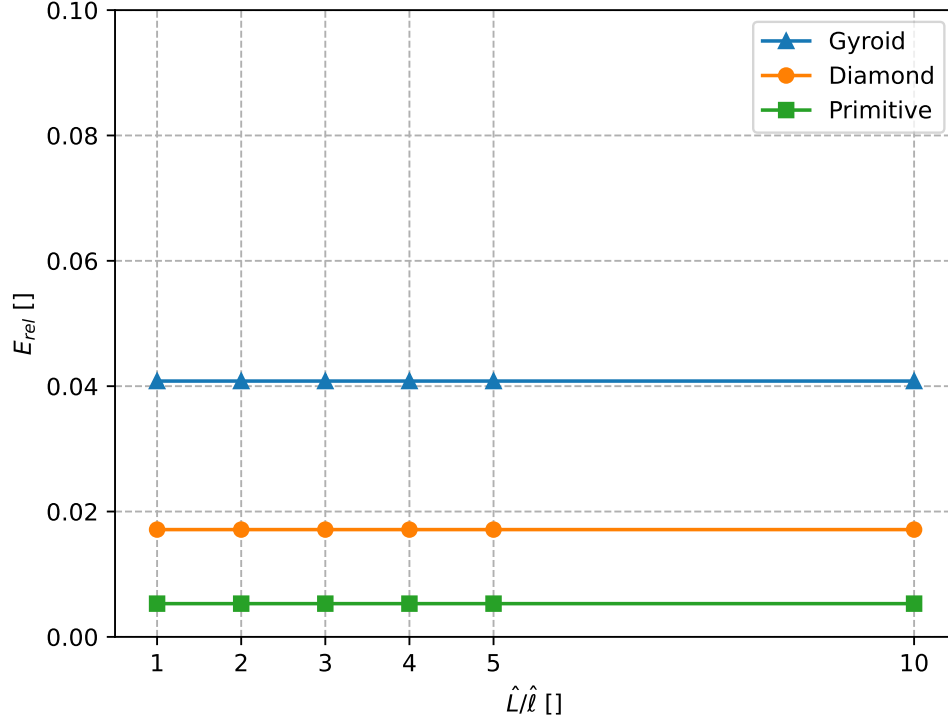


Figure 59: Relative error for varying domain size.

Darcy's flow) and pressure outlet.

The two different computational domains (for the Diamond topology) and boundary conditions are shown in figure 61.

The results for permeability obtained using this setup are plotted in figure 62.

As we can see from the plot in figure 62, the results match closely the ones obtained by Zhao et al. in [27].

Now that the final literature cross-verification is completed, we can move on to the effective pore radius estimation.

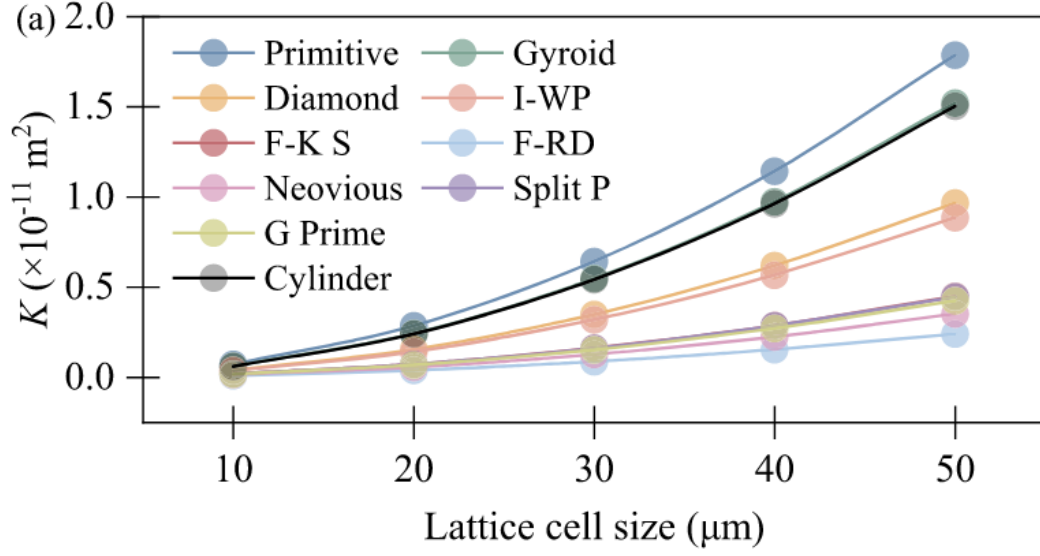


Figure 60: Cross-verification permeability values ([27]).

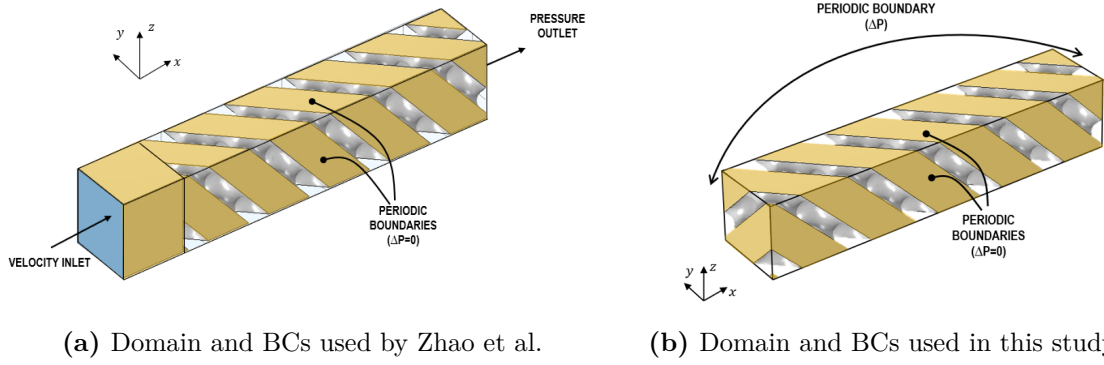


Figure 61: Comparison between the setup used in [27] and the one used in this study.

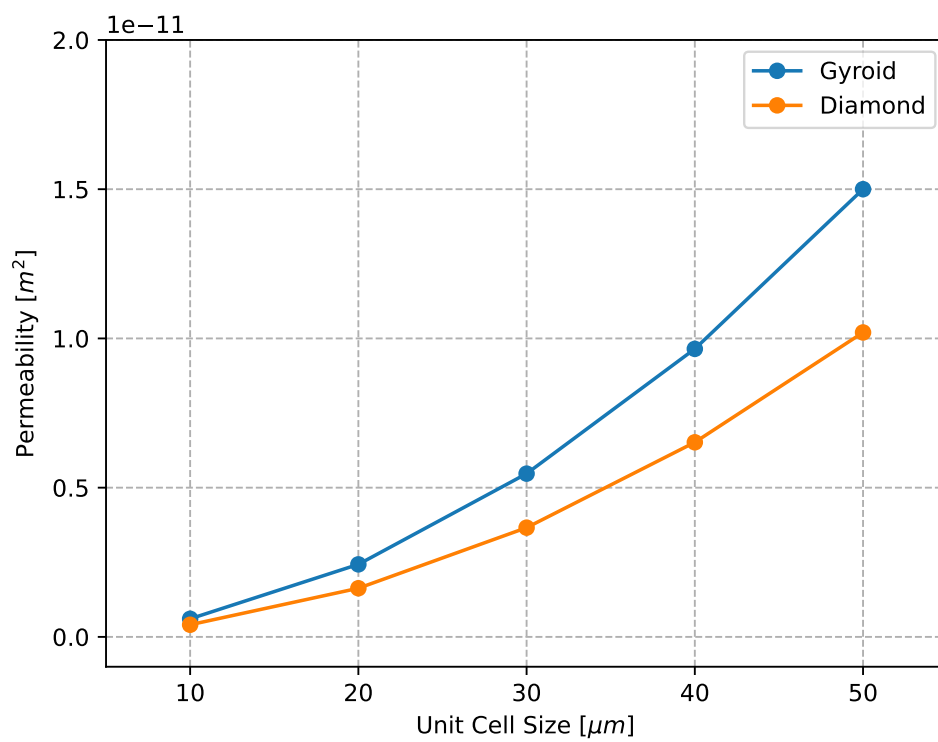


Figure 62: Permeability results obtained using the Zhao et al. computational setup.

6 Effective pore radius

In section 2.3.2 we discussed how the capillary pumping that the wick is able to provide depends on the effective pore radius:

$$\Delta P_c = \frac{2\sigma \cos \theta}{r_{eff}} \quad (54)$$

We already introduced the concept behind the effective pore radius in section 2.3.2. Conceptually, the idea behind this parameter is similar to the one of multi-scale modeling: we are lumping the effects generated by a complex, irregular structure into a single bulk parameter.

On this chapter, we are going to use different methods to evaluate the effective pore radius of the different TPMSs, starting with a thermodynamic approach.

6.1 Thermodynamic approach

The core idea behind this approach to evaluate r_{eff} , proposed by Rootare et al. [53], is that whenever a meniscus advances through a pore, two energy exchanges happen at the same time:

1. Capillary pressure performs mechanical work on the liquid
2. The interfacial free energy of the system changes due to the creation of liquid-solid interface and the disappearance of solid-vapor interface

At equilibrium, the mechanical work associated with capillary pressure balances the change in interfacial free energy.

To explain better how this energy balance enables to obtain the effective pore radius, let us start by considering a simple case of capillary rise inside a tube with constant diameter, shown in figure 63. Note that the shape of the structure considered is not relevant for this analysis, as it will be better explained later; we are considering a capillary tube just for clarity purposes. First, we evaluate the infinitesimal work done by the capillary pressure to advance the liquid-vapor interface by dl :

$$dW_p = \Delta P_c \cdot \overbrace{A \cdot dl}^{dV} \quad (55)$$

where A is the cross-section of the arbitrary porous structure and dV is the volume of fluid displaced.

In this particular case, A can simply be evaluated using the effective capillary radius, which for a tube of constant section is equal to the geometric radius:

$$A = \pi r_p^2 \quad (56)$$

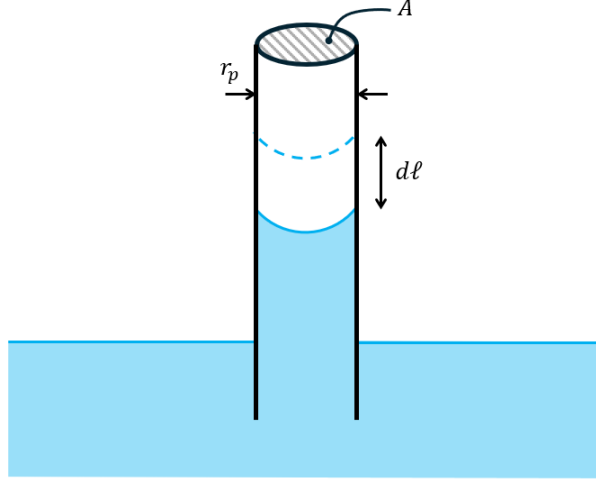


Figure 63: Liquid rise inside a capillary tube.

Then, we evaluate the change in surface energy due to the replacement of solid-vapor interface with solid-liquid interface:

$$dE_s = (\gamma_{SL} - \gamma_{SV}) \cdot \overbrace{2\pi r_p \cdot dl}^{dS} \quad (57)$$

where γ_{SL} and γ_{SV} are the solid-liquid and solid-vapor surface energies, respectively, and dS is the increment in wetted wall surface.

The difference in surface energies can be re-written using Young's equations:

$$\gamma_{SL} - \gamma_{SV} = \sigma \cos \theta \quad (58)$$

We then obtain:

$$dE_s = -\sigma \cos \theta \cdot 2\pi r_p \cdot dl \quad (59)$$

Note that the minus sign is needed because for wetting fluids ($\theta < 90^\circ$), which are the one we are going to consider, the system lowers its energy when the liquid front advances.

Finally, we impose the energy balance:

$$dW_p = dE_s \quad \rightarrow \quad \Delta P_c \cdot dV = -\sigma \cos \theta \cdot dS \quad (60)$$

By plugging in equation (54), we arrive at the following formulation for the effective pore radius:

$$\frac{2\sigma \cos \theta}{r_{eff}} = -\sigma \cos \theta \cdot dS \quad \rightarrow \quad r_{eff} = \frac{2dV}{dS} \quad (61)$$

Equation (61) tells us that the effective pore radius can simply be estimated once the volume and the wetted surface area are known, independently of the structure topology

and the working fluid considered. The factor 2 comes from the two principle curvatures of the liquid meniscus in the Young's equation.

An interesting aspect of this approach is that it is, in someways, coherent with the multi-scale approach that we used to evaluate permeability. In fact, the equation that we just found bridges the gap between the microscopic pore structure with the macroscopic thermodynamic behavior.

Since in section 6.3 we are going to compare the results with the experimental ones obtained by Ma et al. [35], the unit cell sizes and the porosities used for the estimation of r_{eff} are going to differ from the ones used in the previous sections. This, however, is not really an issue, given that the main scope of this research is to develop a rigorous numerical workflow that can be used to design 3D printed porous wicks for thermal management applications. The final step of this work will be to put everything together and design a wick for a specific test case application; in that case, we are going to stick to the same unit cell sizes and porosities for both the permeability and effective pore radius evaluation.

Given that, we are going to consider the same unit cell size of 1.6 mm for all three topologies, and the following porosities: 56.3% for the Diamond, 63.5% for the Gyroid and 70% for the Primitive.

Moreover, Ma et al. are using a *Sheet* Primitive topology, whereas we are using a *Network* one, similarly to what happened in the previous chapter. Thus, we are going to consider, only for the comparison, a *Sheet* Primitive topology, like the one shown in figure 64.

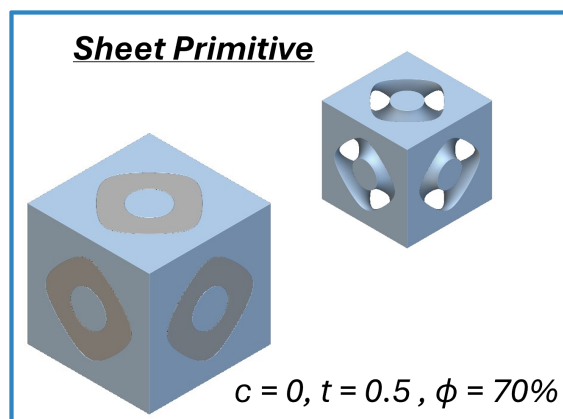


Figure 64: Primitive unit cell being considered for evaluating the effective pore radius. The solid domain is colored in grey and the fluid one in light blue. Here t is the wall thickness in mm , c mid-surface offset also in mm and ϕ the porosity.

To evaluate the fluid volume and the overall wetted surface, we are going to use COMSOL, since it gives us the tools to achieve this kind of task.

The analysis will be done on the single unit cells, but given the periodic nature of the lattice we are considering, the effective pore radius calculated will be the exact same for the whole

structure.

To evaluate the volume V , we can simply use the "*Volume Measurement*" tool in COMSOL (see figure 65).

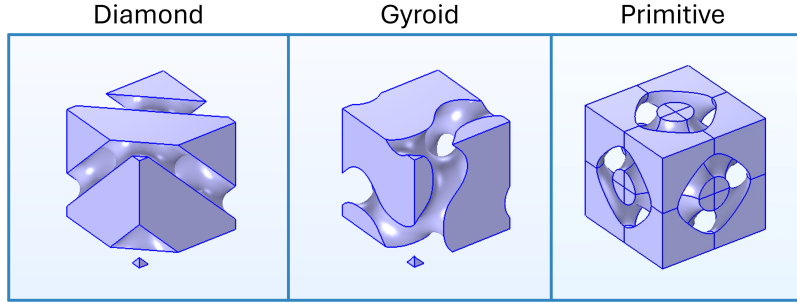


Figure 65: Fluid volume considered to evaluate the effective pore radius.

Similarly, we use the "*Surface Measurement*" tool to evaluate the area wetted by the fluid (see figure 66).

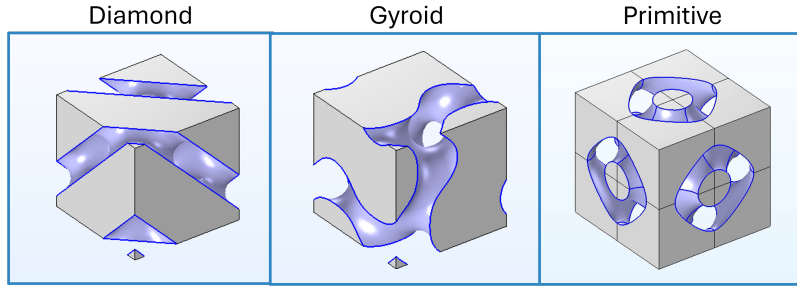


Figure 66: Wetted surface considered to evaluate the effective pore radius.

Table 11 summarizes the results obtained from this thermodynamic analysis.

$l = 1.6 \text{ mm}$				
UC	ϕ []	S [m^2]	V [m^3]	r_{eff} [m]
Diamond	0.563	$1.75e^{-5}$	$2.31e^{-9}$	$2.64e^{-4}$
Gyroid	0.635	$1.46e^{-5}$	$2.61e^{-9}$	$3.58e^{-4}$
Primitive	0.7	$1.13e^{-5}$	$2.68e^{-9}$	$4.74e^{-4}$

Table 11: Effective pore radius results from thermodynamic analysis.

The Primitive structure shows the highest effective pore radius, followed by the Gyroid and the Diamond structures. This was to be expected, since the permeabilities follow the same order.

To verify the results obtained with this method, we are going to use a completely different one, based on 3D image processing. After doing that, we are going to compare the results obtained with the two methods with the aforementioned experimental results.

6.2 Visual imaging approach

What we will try to do in this section is use *PoreSpy*, an open-source Python toolkit for quantitative image analysis of 3D porous media, to evaluate the effective pore radius of the three structures and then compare the results with the ones obtained in the previous section. In particular, we are going to run drainage simulations to obtain a pressure that is equivalent to the capillary one, and then use it to estimate r_{eff} . Before running this simulation though, we need to create an image stack that can be read by *PoreSpy*, to do that we are going to use another Python toolkit, called *vedo*.

The whole workflow looks like this:

1. Geometry creation in *nTop*
2. Binarization and slicing using *vedo*
3. Drainage simulation using *PoreSpy*
4. Effective pore radius evaluation

Starting with the first step, we create the lattice structures of size $3 \times 3 \times 5$ unit cells for all three topologies in *nTop* and export them as STL files. Note that, in this case, the size of the domain is dictated only by computational costs; ideally we would like to use a greater number of unit cells in all directions, but this turns out to be computationally expensive, so we will find a caveat to work around this issue, as it will be explained later. In figure 67 the three STL geometries generated can be seen.

For the second step we use *vedo*, another open-source Python toolkit for the geometrical analysis and manipulation of 3D objects, to first binarize and then slice the geometry. The output of this second step will be a *.tiff* file that can be read by *PoreSpy*. Let us explain into more details how the binarization and slicing works.

Binarization is the process through which *vedo* converts the continuous mesh surface into a discrete 3D voxel grid, where each voxel is either solid (1) or void (0), at a fixed resolution (0.025 mm/voxel in this case). To binarize an STL file, *vedo* starts by defining the bounding box of the mesh, i.e. the 3D volume that needs to be discretized. Then it creates a regular 3D grid over that bounding box; each voxel of the grid will be represented by a cube of size equal to 0.025 mm . The last step consist in the inside/outside classification of each voxel. To do so, *vedo* uses an internal ray tracing algorithm that works like this: the STL mesh is considered as a closed surface and for each voxel a ray is cast from its center; if this ray intersects an odd number of times the mesh boundary, then the voxel is considered inside the mesh and the boolean value of 1 is associated to it, if the number of intersections is

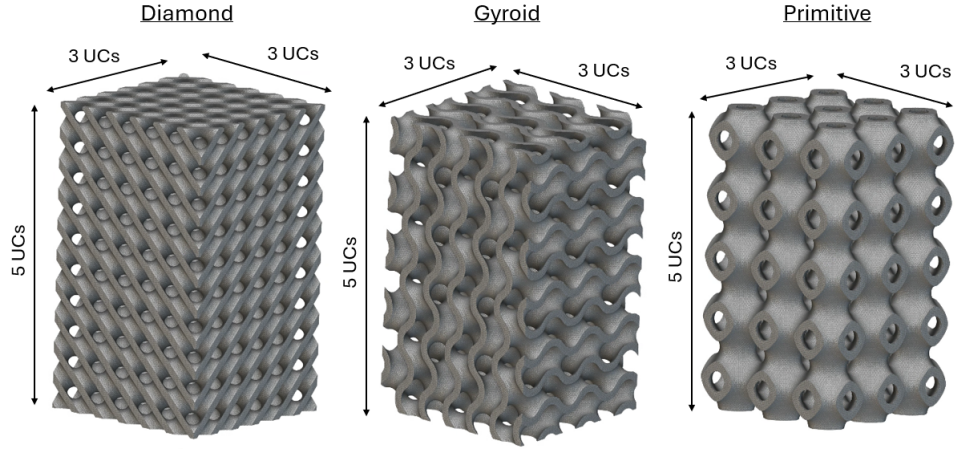


Figure 67: STL files generated for image analysis.

even, then the voxel is considered as being outside of the mesh and the boolean value of 0 is associated to it. This process is a trivial extension to the third dimension of the *Jordan Curve* theorem [54].

The output of the binarization is, basically, the same STL file approximated using cubic voxels, as shown in figure 68.

The binarized geometry is then reshaped into a ZYX NumPy array, scaled to 8-bit and saved as a multi-slice TIFF stack that can be imported in *PoreSpy*.

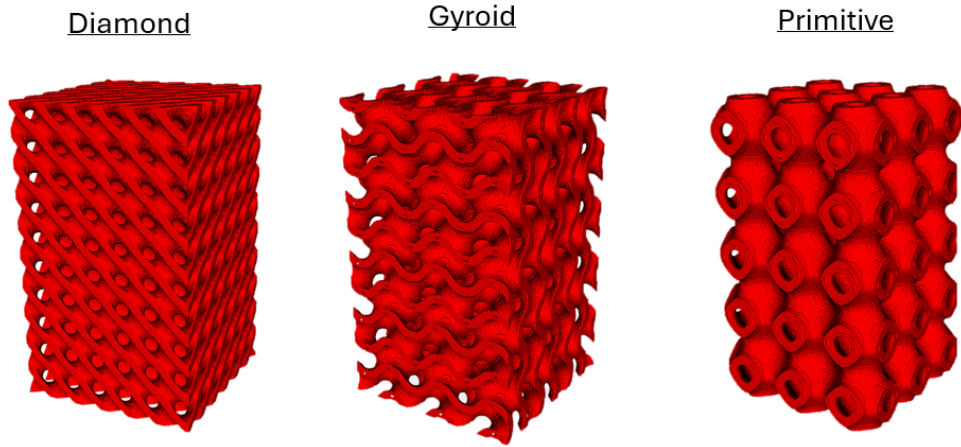


Figure 68: Binarized geometries.

The third step consists in the drainage simulation. Ideally, we would like to run an

imbibition analysis to simulate the capillary rise of the wetting phase inside the porous medium, similarly to what happens in a rate-of-rise test ⁸. Unfortunately, *PoreSpy* can not yet execute this kind of analyses, this is why we are running a drainage simulation.

Drainage is the process through which a non-wetting phase ($\theta > 90^\circ$) displaces a wetting phase ($\theta < 90^\circ$) out of the porous medium. If gravity is present, the non-wetting phase needs to win both the capillary forces generated by the liquid-solid interface and the gravitational head. The pressure at which the non-wetting phase forms a continuous path along the height of the porous medium is called "break-through pressure", see figure 69 for reference. The break-through pressure is the pressure that it is going to be used to obtain the effective pore radius from *PoreSpy*, as it will be now explained.

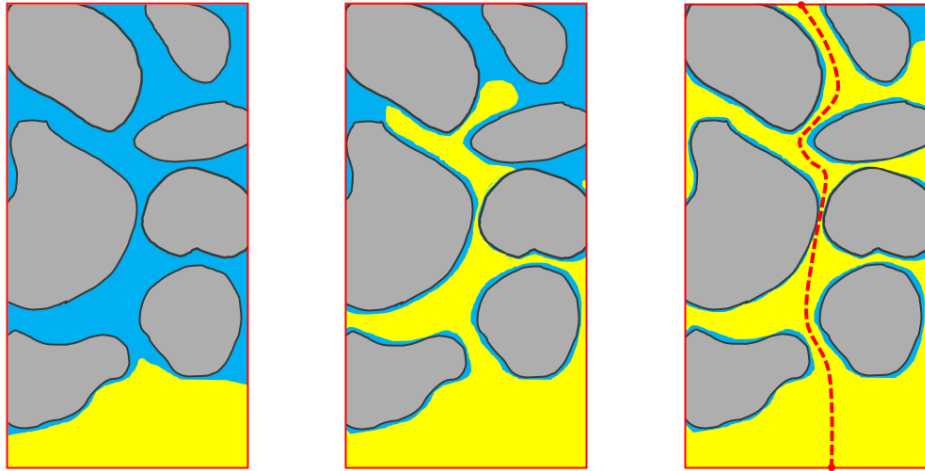


Figure 69: Drainage schematic with break-through of the non-wetting phase (dashed red line).

Let us break down the drainage analysis in the following steps:

1. Conversion of the void space in *True* boolean and the solid space in *False* boolean
2. Computation of the Euclidean distance transform dt to the nearest solid wall for each void voxel, thus obtaining the local inscribed sphere radius at each pore location

⁸Experiment used to characterize the effective pore radius of a porous structure by placing it in contact with a liquid reservoir and waiting for the capillary forces to draw in, upward against gravity, enough liquid to reach an equilibrium height. By measuring the head of the liquid one can retrieve the effective pore radius.

3. Application of the Young-Laplace equation for each voxel, converting the distance transform into a capillary entry pressure map; the pressure needed for a non-wetting fluid to invade a certain voxel is associated to it

$$P_c = \frac{-2\sigma \cos \theta}{dt \cdot (\text{voxel size})} \quad (62)$$

4. Gravity correction via the addition of a hydrostatic pressure to simulate the resistance of the wetting phase being pushed up

$$P_c^* = P_c + \Delta\rho \cdot g \cdot h \quad (63)$$

Figure 70 presents the three geometries already converted by *PoreSpy* into boolean values.

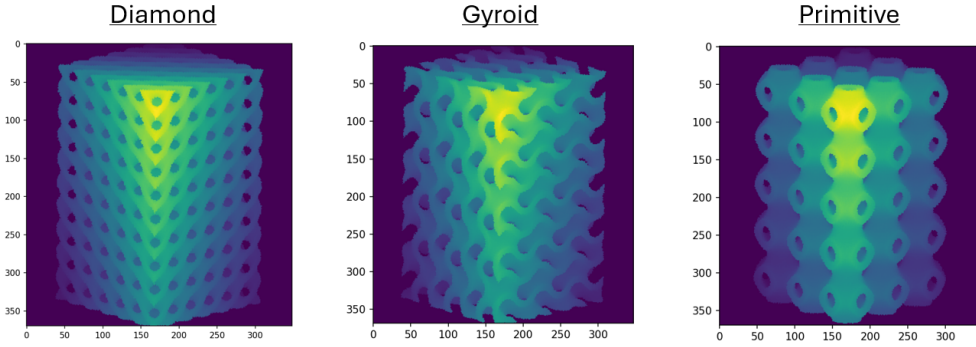


Figure 70: 3D geometries converted from the TIFF image stack into a boolean array for drainage simulations.

Before moving on to talk about the drainage simulation results we first need to explain the caveat that we were referring to previously. The computational domain is 5 unit cells (8 mm) tall, which means that the whole porous structure will be saturated with the non-wetting phase almost instantly, since the gravitational head is so small. On the other hand, we can not use a domain of greater size because it would be computationally too expensive. The work around that we can use is to multiply the hydrostatic pressure term by an intensification factor $k_h = 100$, so that the gravitational head will be so great that the non-wetting phase will need to reach high pressure to drain all the wetting phase, even if the porous structure is so short. Note that this does not change the final effective pore radius being calculated, and to understand why, we can look at the equation used to retrieve the effective pore radius from these simulations:

$$r_{eff} = \frac{2\sigma \cos \theta}{P_c^* - k_h \cdot \Delta\rho \cdot g \cdot h} \quad (64)$$

We are interested in the difference between the pressure applied to the non-wetting phase at the moment of break-through, $P_{c,break}^*$, and the magnified hydrostatic pressure term due to gravity, $k_h \cdot \Delta\rho \cdot g \cdot h$. This difference depends only on the porous structure topology and thus remains constant for varying k_h (true only if the structure is spatially uniform, i.e. it has same pore size everywhere⁹). The only reason why we are considering the magnification factor is to visually check at what iteration step of the drainage simulation we have the breakthrough and then gather the capillary pressure at that specific iteration to be used to calculate r_{eff} . Without multiplying by k_h , we would have a porous medium that is not saturated at iteration n and is completely saturated at iteration $n + 1$, we thus lose information about when the breakthrough happens.

We can now present the results of the drainage simulations, as seen in figure 71.

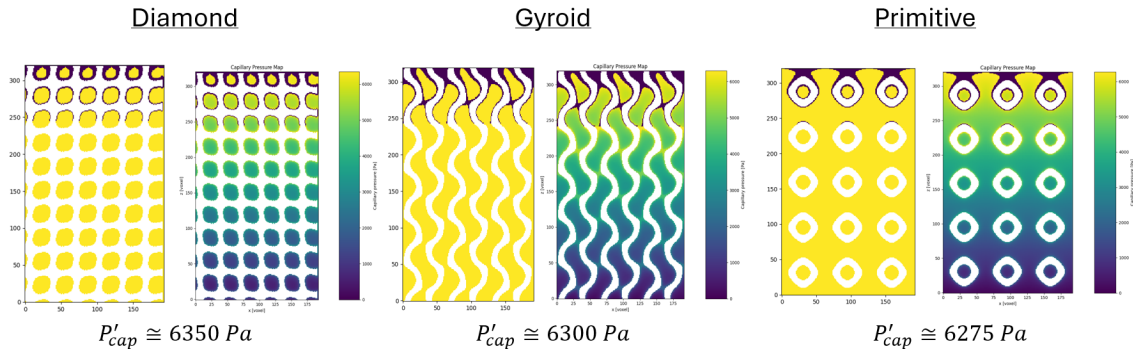


Figure 71: Results of the drainage simulation for the three TPMS. For each topology, the image on the left represents the saturation map, the one on the right the capillary pressure map.

The results are plotted only for the median sections of the 3D structures at the instant when we have breakthrough. For all plots, the solid phase is colored in white and the wetting phase in purple. For the saturation maps the yellow domain represents the non-wetting phase, whereas for the pressure map the gradient shows the zones of the domain that have been saturated at lower pressures in purple, and the one saturated at higher pressures in yellow.

Now, let us present the results of this analysis in terms of effective pore radius, calculated using equation (64). The fluid considered for the drainage simulation is Ammonia.

Finally, we can compare the results with the ones obtained in the previous section.

The results show great agreement, especially considering that we are using an image-based approach that does not take into account several physical phenomena, such as

⁹If the geometry is perfectly uniform, which is the case for a periodic lattice, then every horizontal cross-section has identical pore size distribution, there is no preferential invasion path and $P_{c,break}^*$ depends only on the topological property of the unit cell and is independent of k_h . The only effect that changing k_h has is the rescaling of the pressure axis.

$l = 1.6mm$			
UC	ϕ []	$P_{c,break}^*$ [Pa]	r_{eff} [m]
Diamond	0.563	6350	$2.67e^{-4}$
Gyroid	0.635	6325	$3.20e^{-4}$
Primitive	0.7	6275	$5.33e^{-4}$

Table 12: Effective pore radius results from drainage simulations.

$l = 1.6mm$			
UC	r_{eff}^{PS} [m]	r_{eff}^E [m]	E_{rel} []
Diamond	$2.67e^{-4}$	$2.64e^{-4}$	0.01
Gyroid	$3.20e^{-4}$	$3.58e^{-4}$	0.11
Primitive	$5.33e^{-4}$	$4.74e^{-4}$	0.12

Table 13: Results comparison between energy analysis and drainage simulation. Here the superscript *PS* stands for *PoreSpy* and refers to the results of the drainage simulations, whereas the superscript *E* stands for *Energy* and refers to the results of the energy analysis.

dynamic contact angle effects or the fluid-fluid interface dynamics, and works on a geometry discretized to a lower resolution from the ideal one. Despite this, the results are incredibly accurate, probably due to compensation errors.

The last step that is left is to compare the results of the energy analysis and the drainage simulation with experimental results found in literature.

6.3 Results validation

As previously mentioned, to validate the results obtained with the two methods, we are going to consider the ones obtained by Ma et al.[35]. In the paper the authors analyse the capillary performances, specifically permeability and effective pore radius, of a 3D printed TPMS wick for heat pipe applications. In particular, they compare the hydraulic properties of the three structures obtained via SLM using two different set of input laser energy densities during the manufacturing process. This lead to two sets of printed structures, one set having a higher level of details (the one manufactured using higher energy densities), which they called sample Group A, and the other set having a lower level of resolution (the one manufactured using higher energy densities), which was named sample Group B. Since we are using the results of the paper to validate the ones obtained for ideal structures and not 3D printed ones, we are only going to consider the hydraulic parameters obtained for group A, reason being that they are the ones relative to printed structures that are topologically closer to the ideal ones.

The plot presented by the authors that we are the most interested in is the one presented in figure 72, where the values of r_{eff} obtained through a rate-of-rise method are reported.

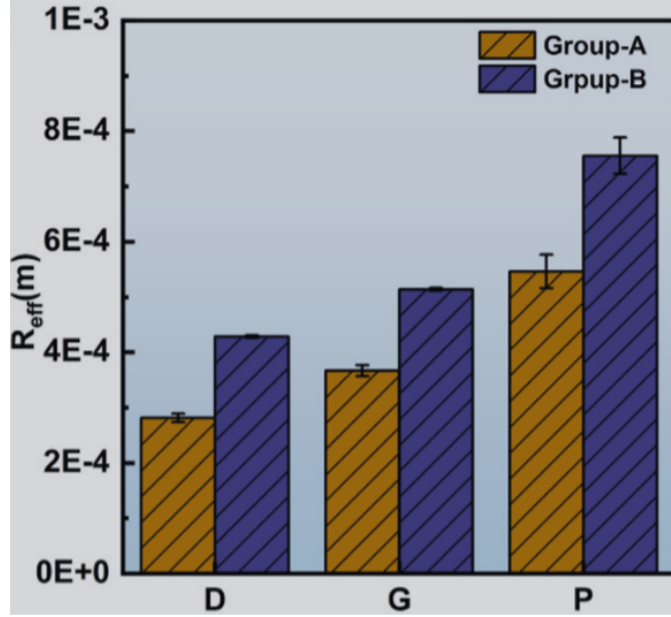


Figure 72: Results of the rate-of-rise test presented by Ma et al. [35].

In figure 72, the letters D , G and P , stand for *Diamond*, *Gyroid* and *Primitive*, which are the topologies being studied in the paper.

One thing that can be immediately noticed by looking at the plot is that the Primitive structure presents the higher r_{eff} , followed by the Gyroid and the Diamond, which is the same order obtained from the previous analyses. The only thing that is left to do is to retrieve the effective pore radius values from the graph and use them as comparison.

The results are reported in table 14.

$l = 1.6mm$			
UC	$r_{eff}^{PS} [m]$	$r_{eff}^E [m]$	r_{eff}^P
Diamond	$2.67e^{-4}$	$2.64e^{-4}$	$2.80e^{-4}$
Gyroid	$3.20e^{-4}$	$3.58e^{-4}$	$3.60e^{-4}$
Primitive	$5.33e^{-4}$	$4.74e^{-4}$	$5.50e^{-4}$

Table 14: Results comparison between energy analysis, drainage simulation and literature. Here the P superscript stands for *Paper*, indicating the values of r_{eff} retrieved from literature.

In figure 73, the histogram relative to the r_{eff} values obtained with the different methods is plotted.

We can see how the results from all three methods are close to one another, indicating

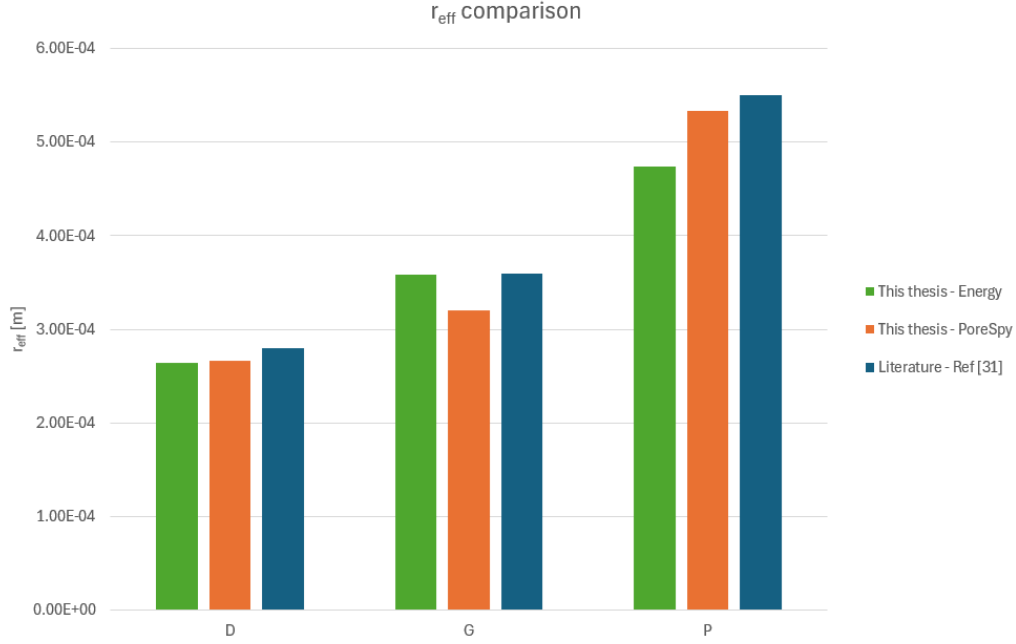


Figure 73: Histogram for r_{eff} comparison. In green we have the one obtained in this work using the energy approach, in orange we have the one obtained using the image-based approach, and in blue we have the values presented by Ma et al.[35].

good agreement between the two numerical approaches and the experimental results. Now that we have defined a way to numerically compute the effective pore radius, combined with the previous multi-scale approach to obtain permeability, we have a fully consistent numerical workflow that can be used to compute the hydraulic properties of an additively manufactured periodic porous medium. The last thing that is left to do is to apply this workflow to design and optimize the porous wick of a heat pipe as a whole. That is exactly the goal of the last chapter of this thesis.

7 Device-scale simulations

In this last chapter, we will take advantage of the homogenized properties obtained via the upscaling procedure and the effective pore radius estimation to run device-scale simulations. Specifically, we will consider an axisymmetric circular heat pipe where the casing is idealized as a circular tube with spherical end-caps. This geometry of the device will allow us to leverage both the axial and the bilateral symmetries to greatly reduce the computational costs needed to simulate the whole 3D domain, reducing the simulations to a bi-dimensional domain.

The elements that compose the heat pipe and the overall setup are shown in figure 74.

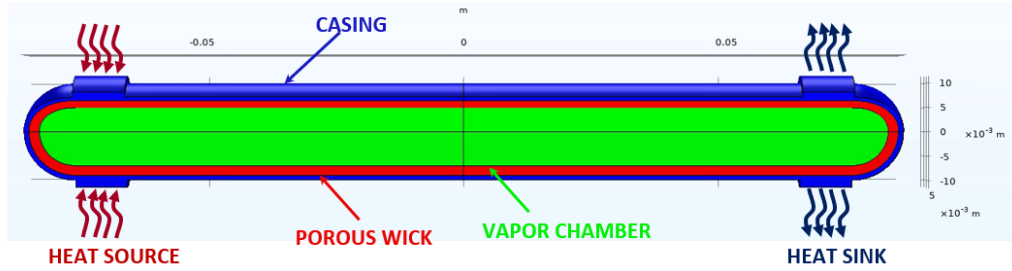


Figure 74: Main components of the heat pipe used for device-scale simulations.

It should be noted that the wick is assumed to remain fully saturated throughout the simulations. Consequently, the flow is modeled as a single-phase liquid flow and phase distribution effects are neglected. In practice, the heat input applied at the evaporator could lead to liquid depletion within the porous structure, resulting in the formation of vapor regions and a local reduction of the liquid saturation. Under sufficiently high heat loads, this phenomenon may eventually lead to dry-out.

To ensure the validity of the fully saturated assumption, preliminary calculations were performed to estimate the capillary limit of the wick. The geometries and operating conditions considered in this study were selected such that the imposed heat load remains below the predicted dry-out threshold. Therefore, liquid replenishment is expected to be sufficient to maintain full saturation of the porous structure, making single-phase description of the flow an appropriate approximation.

To compare the results of the TPMS-based heat pipe, we are going to take as reference a grooved-wick heat pipe found in literature and compare the key performance parameters of the latter with the ones of the former, making sure to set up the simulations so that the effects of the wick topology can be isolated, as it will be described in section 7.1.

The comparison will be subdivided in to two different steps:

1. First, we will analytically evaluate the ability of the wick to dissipate thermal power by defining a performance index (PI)
2. Then, we will run device-scale simulations in COMSOL for both the benchmark case and for the TPMS-based heat pipe with the highest PI

Note that the aim of the second step is not to run thorough device-scale simulations and prove that the TPMS-based heat pipe works better or worst than the grooved one, the aim is to simply show a practical application of how the parameters derived in previous chapters can effectively be used to simulate the whole device, and particularly how the flow in the porous medium can be approximated by considering it as a medium with homogenous properties. In fact, in chapter 4.2 we went from the pore-scale up to the macroscopic scale of the porous lattice, in this final step we go from the macro-scale up to the device-scale.

7.1 Benchmark heat pipe

The heat pipe taken as a benchmark can be found in the *HEAT PIPE DESIGN HANDBOOK* [15], in section "*SAMPLE A - FIXED CONDUCTANCE HEAT PIPE*".

The geometrical parameters, the working fluid and the properties of the wick for the benchmark case are all reported in table 15.

To isolate the effects of the wick on the overall device performances, which is the whole point of this analysis, we will only change the wick type (from grooved to TPMS) and its porosity. We could also change, for example, the thickness of the wick or the lengths of the evaporator and condenser, but this could lead to possible performances improvements not due to wick's effect but to geometrical changes.

For what concerns the TPMS-based wick, since we want to find an optimum configuration of unit cell size l and porosity ϕ , we will run a parametric analysis where we change the values of both parameters. In particular, we are going to consider the following combinations:

- 3 different topologies — Diamond, Gyroid, Primitive
- 3 different porosities — $\phi = [0.5, 0.7, 0.8]$
- 3 different unit cell sizes — $l = [775 \mu m, 387.5 \mu m, 193.75 \mu m]$

Note that the cell sizes that have been chosen are exactly equal, one half and one fourth of the wick thickness d , which is equal to $775 \mu m$.

Now that we have defined the parameters needed to run device-scale simulations, we can start comparing the performance index of all the structures. To do that, we will first write the equations for the limits introduced in sections 2.3.3 and 2.3.4.

BENCHMARK SETUP	
Wick type	Grooved
Wick material	Aluminum
Fluid	Ammonia
Heat pipe OD [mm]	5.85
Vapor core diameter [mm]	6.45
Internal diameter [mm]	8
Number of grooves [-]	35
Area per groove [mm ²]	0.3
Heat pipe length [mm]	1000
Evaporator length [mm]	80
Adiabatic length [mm]	80
Condenser length [mm]	840
Operative temperature [°C]	0 ÷ 40
Heat input [W]	15
Heat load at evaporator [W/m ²]	20404.5
$\Delta T_{\max}$ [K]	6
Wick thickness [mm]	0.775
Groove width [mm]	0.3875
Solid wall width [mm]	0.194
Φ [-]	0.67
Permeability [mm ²]	1.12×10^{-8}
Effective pore radius [m]	0.3875

Table 15: Grooved heat pipe used as benchmark (taken from Sample Problem A — Heat Pipe Design Handbook [15]).

7.2 Heat pipe operating limits

To derive the exact equations for each operating limit, we will reference the work done by Brouwer [30].

In the following list the equation for each operating limit can be found:

- Capillary limit

$$Q_c = \frac{2\sigma_l \rho_l h_{lv}}{\mu_l} \cdot \frac{A_w}{L_{eff}} \cdot \frac{K}{r_{eff}} \quad (65)$$

where h_{lv} is the latent heat of vaporization of the working fluid and A_w is the wetted cross-sectional area of the wick.

- Viscous limit

$$Q_v = \frac{\pi r_v^4 h_{lv} \rho_v P_v}{12 \mu_v L_{eff}} \quad (66)$$

where P_v is the vapor tension of the working fluid.

- Boiling limit

$$Q_b = \frac{4\pi L_e \lambda_{eff} T_v \sigma_l}{h_{lv} \rho_v \ln\left(\frac{r_i}{r_v}\right)} \cdot \left(\frac{1}{r_n} - \frac{1}{r_{eff}}\right) \quad (67)$$

where λ_{eff} is the effective conductivity of liquid and solid walls, T_v is the saturation temperature of the working fluid and r_n is the radius of the nucleation site.

- Sonic limit

$$Q_s = 0.474 \cdot A_v h_{lv} \cdot (\rho_v P_v)^{1/2} \quad (68)$$

- Entrainment limit

$$Q_e = A_v h_{lv} \cdot \left(\frac{\rho_v \sigma_l}{2r_{eff}}\right)^{1/2} \quad (69)$$

We will later use these equations to trace the maximum heat that can be dissipated in the evaporator as a function of the working temperature of the heat pipe.

7.3 Performance Index

The performance index can be simply defined by considering only the wick-related terms in equation (65) for the capillary limit:

$$PI = \frac{K \cdot r_{eff}}{A_w} \quad (70)$$

where K is the wick permeability, r_{eff} is the effective pore radius and A_w is the wetted cross-section of the wick.

We already now how to calculate K and r_{eff} , so let us briefly describe the process used to evaluate A_w .

To estimate the wetted cross-sectional area of the wick we simply use the "*Surface Measure*" tool in COMSOL to measure the area of multiple cross-sections, as shown in figure 75, and then estimate the average value for the whole unit cell. The number of cutting planes used is 30, even though in the figure only 3 planes are shown.

We now have all that is needed to evaluate the PI for all the wick types.

The performance index clearly asses the ability of the porous structure to transport liquid from the condenser back to the evaporator. A higher PI translates to a wick with better capillary performance.

In table 16 are reported the values of the performance parameters of the benchmark porous wick. These are the values that will be directly compared to the ones of the TPMS-based wicks.

Now let us do the same for the TPMS-based wicks, considering first a fixed porosity ($\phi = 0.7$).

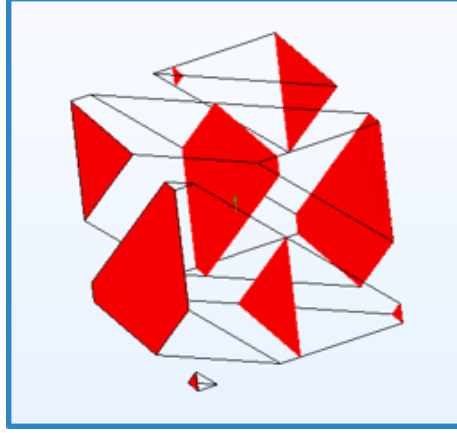


Figure 75: Example of cross-sections used to measure the A_w parameter.

Benchmark					
ϕ	K [m ²]	r_{eff} [m]	K/r_{eff} [m]	A_w [m ²]	PI [m ³]
0.67	1.12×10^{-8}	3.88×10^{-4}	2.89×10^{-5}	6.46×10^{-6}	1.87×10^{-10}

Table 16: Benchmark performance parameters.

In figures 76, 77, 78 and 79 the plots of the parameters listed in table 17 can be found. The red dashed line indicates the value of each parameter for the benchmark case.

From the results it is clear that even though the grooved wick presents a higher K/r_{eff} ratio than the TPMS-based wick in this configuration, the latter has a A_w high enough to compensate for the lower hydraulic performances. In the end, the grooved wick performs better than all the TPMS wicks configurations, except for the Primitive one with $l = 775 \mu\text{m}$. From these results, we see that higher unit cell sizes help the 3D printed wick perform better, this is why we are going to repeat the analysis by changing ϕ and fixing l at $775 \mu\text{m}$.

As we did previously, let us plot the results presented in the previous tables (figures 80, 81, 82 and 83).

From figures 80, 81, 82 and 83 it is clear how all three TPMS topologies present higher capillary performances for $l = 775 \mu\text{m}$ and $\phi = 0.8$ then the benchmark case. Specifically, the maximum PI improvements are 4.3% for the Diamond, 19.3% for the Gyroid and 125% for the Primitive. The great improvement for the Primitive structure can be attributed to the combination of a much higher permeability and wetted cross-section, which translate to lower flow tortuosity, and an effective pore radius that is still quite small.

This simple analysis already proves that these lattice structures can greatly improve the heat dissipation capabilities of thermal management systems such as heat pipes, even in their simplest form (i.e. without any type of topological optimization). To complete the study, we will now run device-scale simulations for the whole heat pipe, considering only

Diamond, $\phi = 0.7$					
l [m]	K [m ²]	r_{eff} [m]	K/r_{eff} [m]	A_w [m ²]	PI [m ³]
1.94×10^{-4}	2.37×10^{-10}	8.30×10^{-5}	2.86×10^{-6}	4.00×10^{-6}	1.14×10^{-11}
3.87×10^{-4}	9.50×10^{-10}	1.66×10^{-4}	5.72×10^{-6}	7.00×10^{-6}	4.01×10^{-11}
7.75×10^{-4}	3.80×10^{-9}	3.32×10^{-4}	1.14×10^{-5}	1.40×10^{-5}	1.60×10^{-10}

Gyroid, $\phi = 0.7$					
l [m]	K [m ²]	r_{eff} [m]	K/r_{eff} [m]	A_w [m ²]	PI [m ³]
1.94×10^{-4}	2.96×10^{-10}	9.40×10^{-5}	3.15×10^{-6}	3.00×10^{-6}	9.45×10^{-12}
3.88×10^{-4}	1.18×10^{-9}	1.87×10^{-4}	6.31×10^{-6}	7.00×10^{-6}	4.42×10^{-11}
7.75×10^{-4}	4.73×10^{-9}	3.73×10^{-4}	1.27×10^{-5}	1.30×10^{-5}	1.65×10^{-10}

Primitive, $\phi = 0.7$					
l [m]	K [m ²]	r_{eff} [m]	K/r_{eff} [m]	A_w [m ²]	PI [m ³]
1.94×10^{-4}	5.65×10^{-10}	1.26×10^{-4}	4.48×10^{-6}	3.00×10^{-6}	1.35×10^{-11}
3.88×10^{-4}	2.26×10^{-9}	2.52×10^{-4}	8.97×10^{-6}	7.00×10^{-6}	6.28×10^{-11}
7.75×10^{-4}	9.04×10^{-9}	5.05×10^{-4}	1.79×10^{-5}	1.30×10^{-5}	2.33×10^{-10}

Table 17: Permeability and performance index for TPMS structures at $\phi = 0.7$.

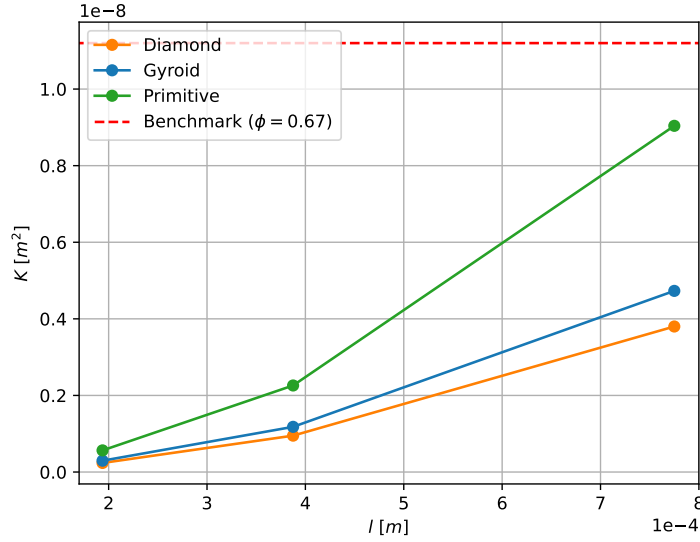


Figure 76: Permeability as a function of unit cell size ($\phi = 0.7$).

the benchmark wick and the Primitive one with $l = 775 \mu m$ and $\phi = 0.8$. Given that, let us now describe the general workflow used to set up the device-scale

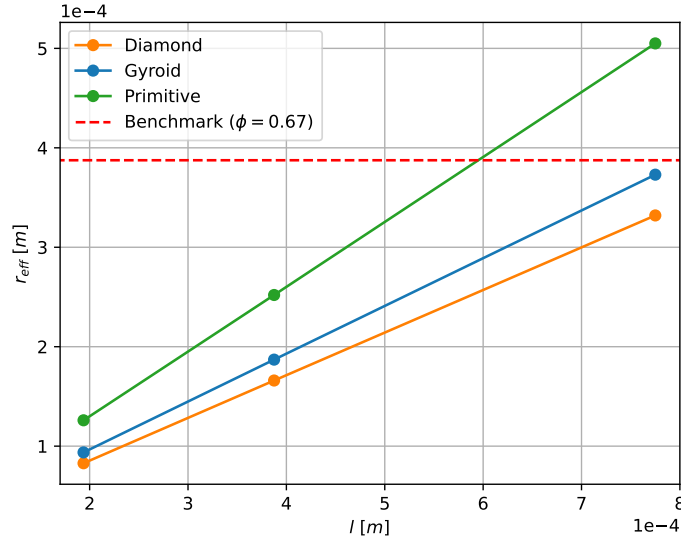


Figure 77: Effective pore radius as a function of unit cell size ($\phi = 0.7$).

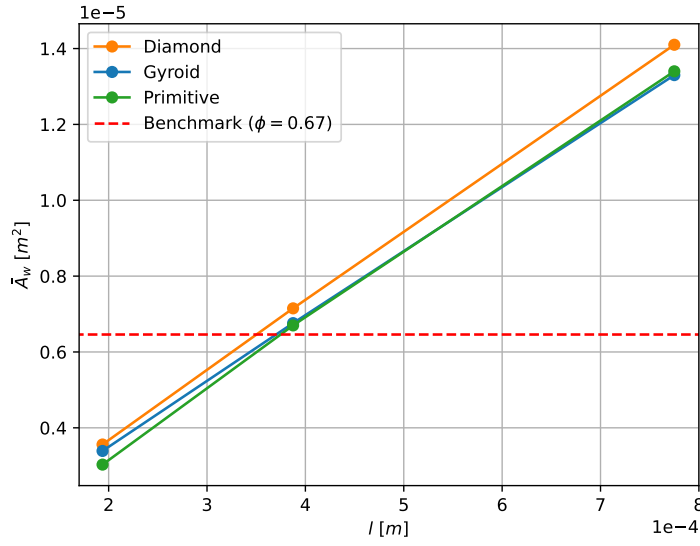
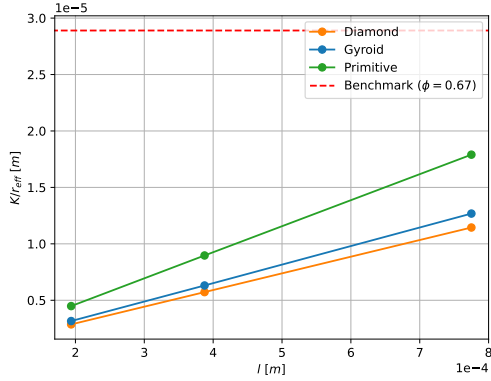
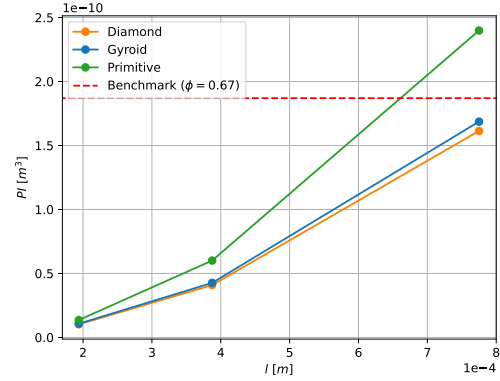


Figure 78: Wetted cross-section area as a function of unit cell size ($\phi = 0.7$).

simulations. Note that the COMSOL template model "*Heat Pipe with Accurate Liquid and Gas Properties*" [55] is going to be used to simplify the implementation and the results



(a) $K/r_{eff} = f(l)$ ($\phi = 0.7$)



(b) $PI = f(l)$ ($\phi = 0.7$)

Figure 79: Performance parameters as a function of unit cell size.

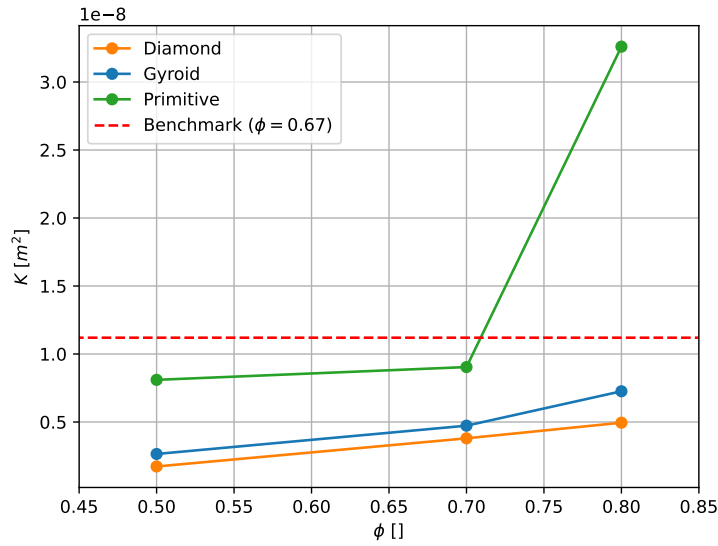


Figure 80: Permeability as a function of porosity ($l = 775 \mu m$).

analysis. The following workflow will be described at a high level, for more details on how to set up this model step-by-step, one can refer to the aforementioned tutorial.

Diamond, $l = 7.75 \times 10^{-4} \text{ m}$					
ϕ	$K \text{ [m}^2\text{]}$	$r_{\text{eff}} \text{ [m]}$	$K/r_{\text{eff}} \text{ [m]}$	$A_w \text{ [m}^2\text{]}$	$PI \text{ [m}^3\text{]}$
0.5	1.73×10^{-9}	2.08×10^{-4}	8.32×10^{-6}	1.00×10^{-5}	8.32×10^{-11}
0.7	3.80×10^{-9}	3.32×10^{-4}	1.14×10^{-5}	1.40×10^{-5}	1.60×10^{-10}
0.8	4.95×10^{-9}	4.07×10^{-4}	1.22×10^{-5}	1.60×10^{-5}	1.95×10^{-10}

Gyroid, $l = 7.75 \times 10^{-4} \text{ m}$					
ϕ	$K \text{ [m}^2\text{]}$	$r_{\text{eff}} \text{ [m]}$	$K/r_{\text{eff}} \text{ [m]}$	$A_w \text{ [m}^2\text{]}$	$PI \text{ [m}^3\text{]}$
0.5	2.65×10^{-9}	2.61×10^{-4}	1.02×10^{-5}	1.00×10^{-5}	1.02×10^{-10}
0.7	4.73×10^{-9}	3.73×10^{-4}	1.27×10^{-5}	1.30×10^{-5}	1.65×10^{-10}
0.8	7.26×10^{-9}	4.88×10^{-4}	1.49×10^{-5}	1.50×10^{-5}	2.23×10^{-10}

Primitive, $l = 7.75 \times 10^{-4} \text{ m}$					
ϕ	$K \text{ [m}^2\text{]}$	$r_{\text{eff}} \text{ [m]}$	$K/r_{\text{eff}} \text{ [m]}$	$A_w \text{ [m}^2\text{]}$	$PI \text{ [m}^3\text{]}$
0.5	8.10×10^{-9}	4.64×10^{-4}	1.75×10^{-5}	1.30×10^{-5}	2.27×10^{-10}
0.7	9.04×10^{-9}	5.05×10^{-4}	1.79×10^{-5}	1.30×10^{-5}	2.33×10^{-10}
0.8	3.26×10^{-8}	1.32×10^{-3}	2.47×10^{-5}	1.70×10^{-5}	4.20×10^{-10}

Table 18: Permeability and performance index for TPMS structures at $l = 7.75 \times 10^{-4} \text{ m}$.

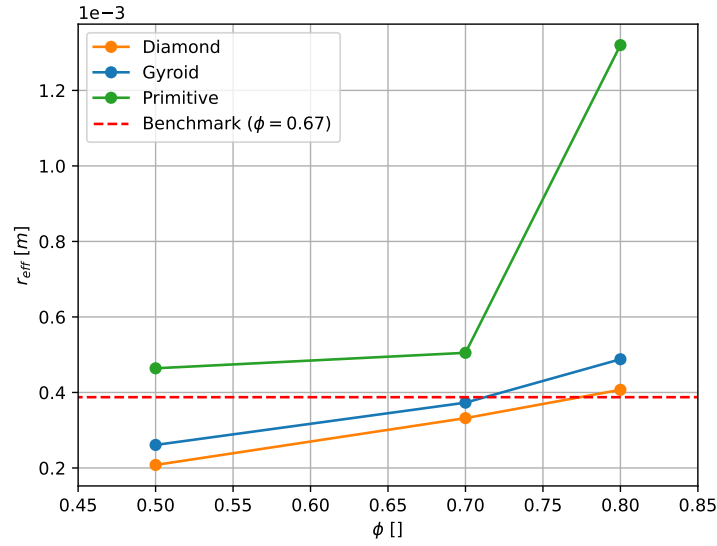


Figure 81: Effective pore radius as a function of porosity ($l = 775 \text{ }\mu\text{m}$).

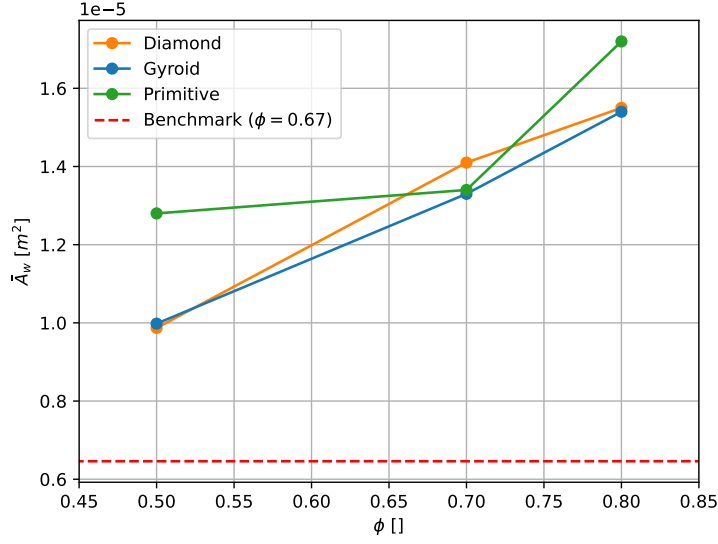
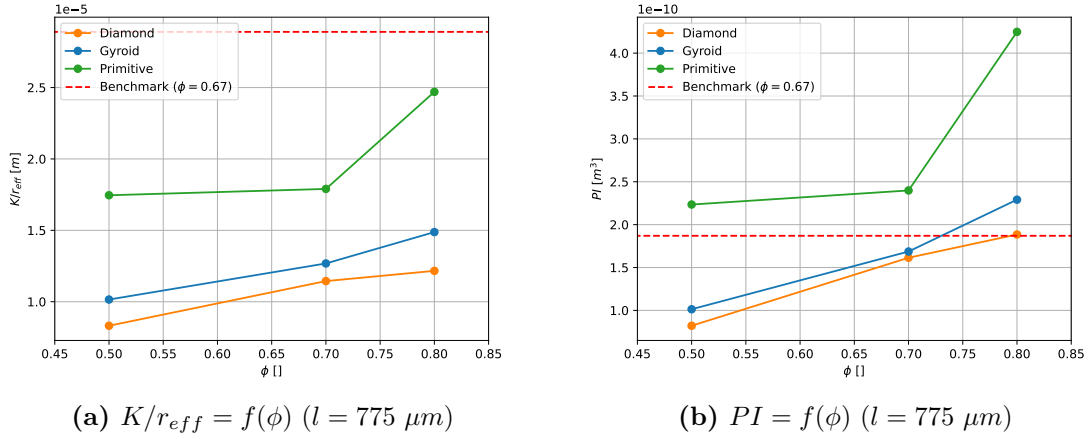


Figure 82: Wetted cross-section area as a function of porosity ($l = 775 \mu m$).



(a) $K/r_{eff} = f(\phi)$ ($l = 775 \mu m$)

(b) $PI = f(\phi)$ ($l = 775 \mu m$)

Figure 83: Performance parameters as a function of porosity.

7.4 Device-scale simulations workflow

In this section the general workflow used to run device-scale simulations will be described. In particular, we will consider:

- Geometry and working fluid setup

- Physics setup
- Mesh generation
- Numerical approach

7.4.1 Geometry and working fluid setup

As it has already been said, the heat pipe will be modeled leveraging the axial symmetry, to do that we will approximate the device as a cylinder with two spherical end-caps. The geometric parameters used are the ones listed in table 15. Figure 84 shows one half of the cross-section of the device, which will be mirrored and revolved around the central axis to obtain the 3D domain.

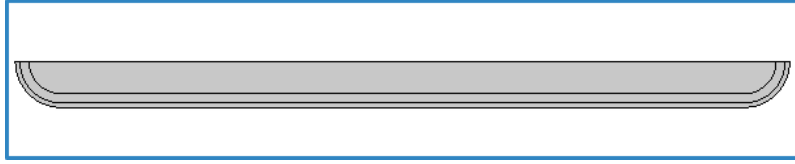


Figure 84: Device-scale geometry.

Note that, to allow a clear representation, the device shown in picture 84 is shorter than the actual one being tested.

From the same figure, the three components of the heat pipe (i.e. the external casing, the porous wick and the vapor chamber) can clearly be distinguished.

For what concerns the materials and working fluid used, we are simply going to take the ones from the benchmark. We will thus use aluminum for both the external casing and the porous wick and Ammonia (NH₃) as the working fluid. This is one of the most used combinations for heat pipes that work in the low temperatures range like the one we are considering.

The material properties for aluminum are reported in figure 85.

Since the working temperature range for this application is $0^{\circ}C \div 40^{\circ}C$, we can evaluate the merit number introduced in section 2.5 for NH₃ at the median temperature of $20^{\circ}C$:

$$M = \frac{\rho_l \sigma_l h_{lv}}{\mu_l} = 1.1 \cdot 10^{11} \frac{W}{m^2} \quad (71)$$

7.4.2 Physics setup

To simulate the fluid flow in the vapor chamber we are using the "*Laminar Flow*" template model, since the Reynolds number is low enough. The pressure inlet boundary considered for the vapor cavity will coincide with the interface between the porous wick and the cavity itself, as shown in figure 86. The reason for this boundary choice is that the vapor generated

»	Property	Value	Unit
☒	Heat capacity at constant pressure	900[J/(kg*K)]	J/(kg·K)
☒	Thermal conductivity	238[W/(m*K)]	W/(m·K)
☒	Density	2700[kg/m^3]	kg/m ³
	Relative permeability	1	1
	Electric conductivity	3.774e7[S/m]	S/m
	Relative permittivity	1	1
	Coefficient of thermal expansion	23e-6[1/K]	1/K
	Young's modulus	70[GPa]	Pa

Figure 85: Aluminum material properties.

inside the wick at the evaporator will translate into a positive mass flow rate that enters the vapor cavity, whereas at the condenser section the vapor that condenses back into the wick will be accounted for as a negative mass flow rate that exits the vapor domain.

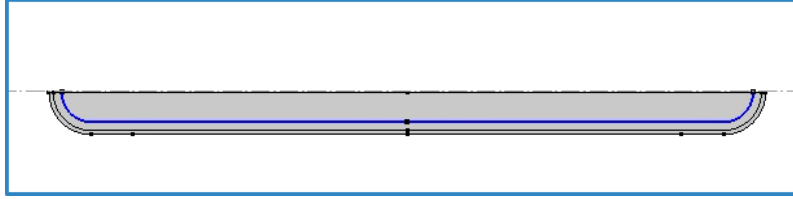


Figure 86: Vapor cavity inlet.

For the liquid flow in the porous medium we are instead going to use the "*Brinkman Equation*" template model with the "*Neglect inertial term (Stokes flow)*" option selected. This will ensure consistency between the results obtained via upscaling, where we considered $Re \ll 1$, and the current simulations.

In this case we are using a velocity inlet boundary condition placed on the same exact boundary used for the *Laminar Flow* model.

Finally, since we want to run a conjugate heat transfer (CHT) simulation, we also need to implement a coupled model for the fluid flow and heat transfer. To do that, we are going to use the "*Heat Transfer in Porous Media*" template model, which allow us to simulate heat transfer through porous media and account for the conduction and convection in the porous matrix's solid and open-pore phases. To correctly set up the model we first indicate which domains are the solid (external casing), the porous (wick) and the fluid (vapor) ones. Then, we set two separate heat fluxes boundary conditions, one with a positive heat flux at the heat source and one with a negative one at the condenser. The heat flux at the condenser will be the one associate to the convective heat transfer coefficient h of the cooling device we are using. We are going to take $h = 250 \text{ W/m}^2\text{K}$, which could be achieved via air cooling.

The final boundary condition that we set is a boundary heat source condition at the interface between the vapor cavity and the porous wick. This will enable us to account for the thermal energy being carried from the evaporating liquid into the vapor cavity and, vice versa, from the vapor cavity to the liquid in the condenser.

7.4.3 Mesh generation

To correctly model the physics of the problem, we use a combination of structured and unstructured mesh. In particular, we will use the unstructured triangular mesh in both the evaporator and the condenser, where we have vectorial fields, such as velocity and heat flux, that have components in many directions. The structured mesh will instead be used in the remaining domain (adiabatic section), where the main vector components are in the x and y directions. This mesh structures is the same for all three domains (vapor cavity, porous wick and solid casing).

To ensure that the gradients at the wall boundary and the wick-vapor cavity interface are correctly modeled, an inflation boundary layer mesh is added. Specifically, 8 layers were added.

Figure 87 shows the generated mesh at the evaporator (the one at the condenser is equal) with a zoom box on the transition between structured and unstructured mesh and the boundary layer inflation.

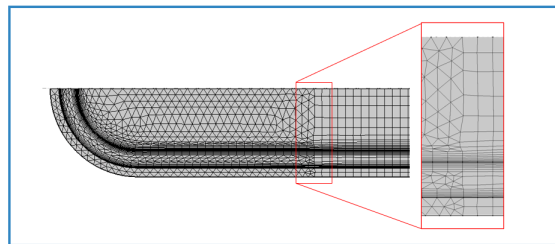


Figure 87: Generated mesh for device-scale simulations.

7.4.4 Numerical approach

Finally, let us briefly describe the numerical approach used to solve the equations.

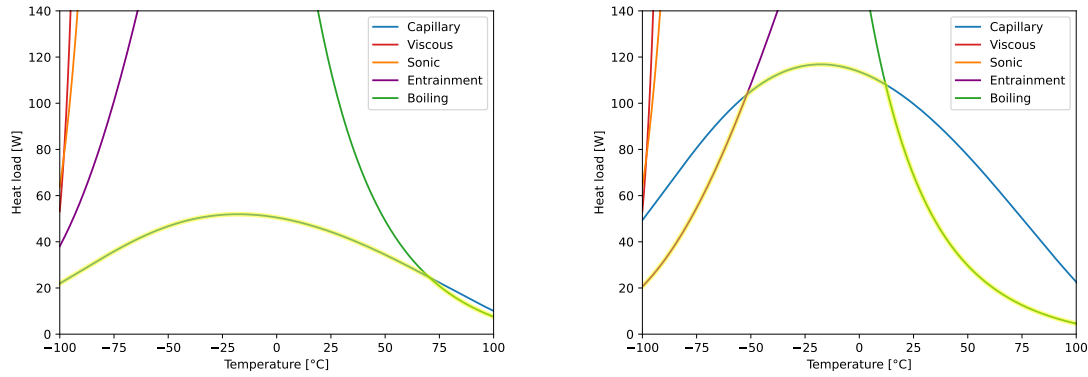
To improve the robustness and efficiency of the simulations, we will run two consecutive stationary solvers:

1. First we solve only the laminar flow in the vapor cavity and the heat transfer in porous media
2. Then we use the solution of the first step as initial values for the second one, for which we activate also the Brinkman model

By doing this, we solve the "hardest" physic, the Brinkman model, with an initial guess of the solution fields already close to the final one. This guarantees that the final solution of the fully-coupled nonlinear system converges in fewer iterations compared to a "cold start". For what concerns the discretizations used, we have P1-P1 elements for the laminar flow model (no inf-sup condition issues), P2-P1 elements for the flow in porous media model (inf-sup condition to be respected) and a linear discretization for the temperature field of the heat transfer in porous media model.

7.5 Results

We can immediately plot the heat pipe's limit by simply implementing the equations introduced in section 7.2 for both the benchmark (figure 88a) and the Primitive wick (figure 88b).



(a) Benchmark heat pipe operational range.

(b) Primitive heat pipe operational range.

Figure 88: Heat pipe's limits.

These results clearly show how the capillary performances of the device (often the bottleneck for maximum disposable heat) are greatly improved by using the TPMS-based wick. The maximum heat load goes from 51 W to 115 W, corresponding to an increment of 125%, equal to the increment in the PI, as expected.

From the same plots, we can also see how the limiting factors for the TPMS-based heat pipe are the entrainment limit for low working temperatures, the capillary limit for medium temperatures and the boiling limit for the higher temperature range. This was also to be expected given that we only improved the hydraulic performances of the wick that directly affect the capillary limit, without considering the other limiting factors. Nonetheless, the operational range of the Primitive-wick heat pipe is still far greater than the one of the grooved-wick heat pipe, proving that, at least for this specific application, 3D printed lattice structures such as the ones being considered in this study can greatly improve the device

performances (if correctly designed).

Now that we have completed this preliminary analysis, we can move on to the device-scale simulations results.

We will run a parametric sweep for the heat loads while maintaining all the other parameters fixed. In particular, we are going to consider the following heat loads at the evaporator:

- 5 W, 15 W, 25.5 W for the grooved wick heat pipe
- 5 W, 15 W, 25.5 W, 40 W and 57.25 W for the Primitive wick heat pipe

The maximum heat inputs tested for both heat pipe configurations are equal to half the maximum heat input given by the capillary limit: 25.5 W for the grooved and 57.25 W for the Primitive. We are only running device-scale simulations up to half the maximum heat input as a safety factor, to account for more complex effects that can not be considered with this simple analytical model.

The first key performance parameter (KPI) that we are interested in evaluating is the overall thermal resistance of the device, defined as:

$$R_{tot} = \frac{\Delta T_f}{\dot{Q}_{in}} \quad (72)$$

where ΔT_f is the maximum temperature difference between evaporator and condenser. Given that $\dot{Q}_{in}$ is an input parameter, we just need to evaluate ΔT_f to obtain R_{tot} . In tables 19 and 20 are reported the results of the device scale simulations for the two different wicks at various heat inputs.

Grooved - $h = 250 \text{ W/m}^2\text{K}$				
$\dot{Q}_{in} \text{ [W]}$	$T_f^{\max} \text{ [K]}$	$T_f^{\min} \text{ [K]}$	$\Delta T_f \text{ [K]}$	$R_{tot} \text{ [K/W]}$
5	301.49	301.45	0.04	0.008
15	318.18	318.06	0.12	0.008
25.5	335.70	335.50	0.2	0.008

Table 19: Overall thermal resistance for the grooved wick.

First of all, from the results, we can see how for both the grooved and the Primitive wicks the overall thermal resistance R_{tot} is constant with the heat input. Another important result is that the overall thermal resistance of the Primitive heat pipe is greater than the one of the grooved one by $\sim 40\%$. This tells us that, for the same heat input, the grooved heat pipe thermally outperforms the Primitive one. This result is actually to be expected if we think about how the COMSOL model is set up: an effective thermal conductivity of the whole porous medium is calculated using analytical formulations where the only wick's parameter being used is the porosity. The effective thermal conductivity is estimated, basically, by doing a weighted average of the thermal conductivities of the liquid and the

Primitive - $h = 250 \text{ W/m}^2\text{K}$				
$\dot{Q}_{in} [W]$	$T_f^{\max} [K]$	$T_f^{\min} [K]$	$\Delta T_f [K]$	$R_{tot} [K/W]$
5	301.52	301.46	0.06	0.0115
15	318.26	318.09	0.017	0.0115
25.5	335.83	335.54	0.29	0.0115
40	360.10	359.64	0.46	0.0115
57.25	388.98	388.32	0.66	0.0115

Table 20: Overall thermal resistance for the Primitive wick.

solid phases using the porosity and its complementary as weights. Being that the solid (aluminum) has a higher thermal conductivity than the liquid (ammonia), lower porosities will translate to higher effective thermal conductivities, and since the effective thermal conductivity is directly correlated with the heat transport capabilities of the device, this will translate to lower $\Delta T_f^{\max}$ for the wick with higher porosities, and thus higher R_{tot} . To prove that a Primitive wick has equal thermal performances to the grooved one when porosities are equal, we can run the same analysis as before, this time using the same heat input, the same porosity and only different permeabilities (which, for what has been said, will not affect the temperature distribution). The results of this analysis are reported in table 21.

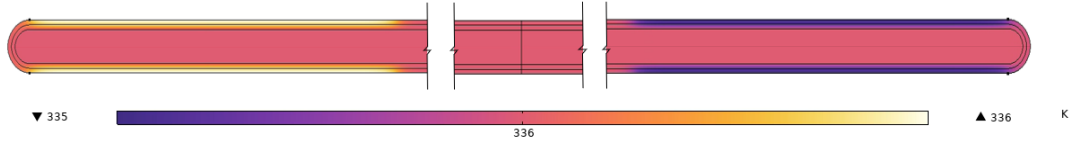
$\phi = 0.67$					
Wick type	$\dot{Q}_{in} [W]$	$T_f^{\max} [K]$	$T_f^{\min} [K]$	$\Delta T_f [K]$	$R_{tot} [K/W]$
Grooved	25.5	335.70	335.50	0.2	0.008
Primitive	25.5	335.70	335.50	0.2	0.008

Table 21: Overall thermal resistance for the grooved and Primitive wicks with equal porosity.

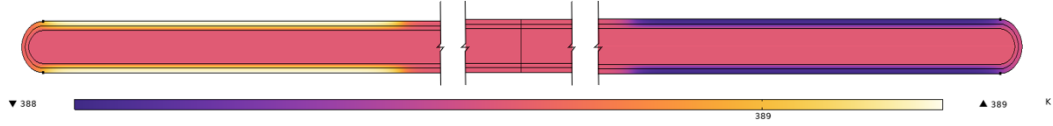
As we can see, R_{tot} is exactly the same for both wicks.

Having said that, a higher thermal resistance for the Primitive-wick heat pipe would still be acceptable, given that the capability of disposing more than twice the maximum heat load without incurring in dry-out offsets this negative aspect. Figure 89 shows the temperature field for both the solid casing and the wick (with averaged properties) for both the grooved (figure 89b) and the Primitive (figure 89b) wicks.

To check if the results make physical sense, we can verify the conservation of mass and energy in the device. Specifically, for the mass conservation we can check if the vapor mass flow rate coincides with the liquid flow rate in the wick in a generic section of the device (e.g. middle section); for the energy conservation, we can see if the heat being dissipated at the condenser equals the heat input at the evaporator. The results of this two checks are reported in table 22.



(a) Temperature field for the grooved wick.



(b) Temperature field for the Primitive wick.

Figure 89: Temperature field plots for both wick types at maximum heat input.

Mass conservation		
$\dot{m}_{vapor} [kg/s]$	$\dot{m}_{liquid} [kg/s]$	$\Delta \dot{m} [kg/s]$
$2.9 \cdot 10^{-12}$	$-2.9 \cdot 10^{-12}$	0
Energy conservation		
$\dot{Q}_{in} [W]$	$\dot{Q}_{out} [W]$	$\Delta \dot{Q} [W]$
57.25	-57.25	0

Table 22: Mass and energy conservation for Primitive wick heat pipe with $\dot{Q}_{in} = 57.25 W$.

We can also verify the no-slip boundary condition. From the plot in figure 90, we can see how the minimum velocity is $\sim 1.6e^{-7} m/s$, which is pretty close to zero, thus the no-slip BC is verified.

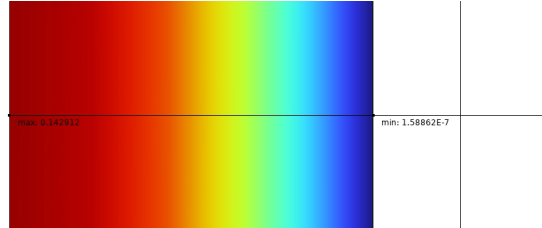


Figure 90: Velocity magnitude near the walls.

Now that we know that the simulations make physical sense, we finalize the analysis by plotting the velocity fields.

Figure 91 shows the velocity profiles for both the vapor and the liquid flows for the Primitive wick at 57.25 W power input.

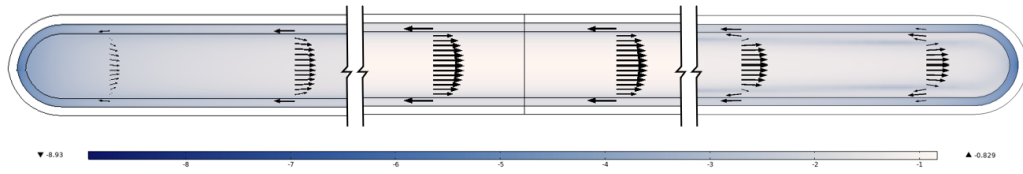


Figure 91: Velocity profiles for vapor and liquid flows (Primitive wick).

Figure 92 shows the 3D velocity magnitude field for the vapor flow for the same configuration.

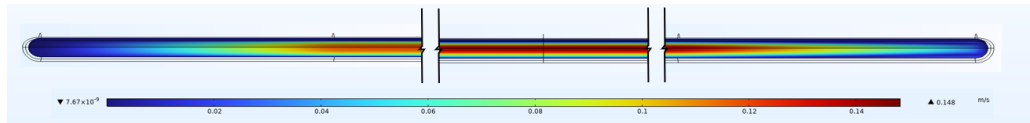


Figure 92: 3D velocity magnitude field for vapor flow (Primitive wick).

8 Conclusions

The main goal of this work was the development of a numerical workflow, based on a multi-scale modeling approach, for the estimation of the characteristic hydraulic parameters of 3D printed wick heat pipe for space thermal management applications. Three different triply periodic minimal surfaces (Diamond, Gyroid and Primitive) were considered for this study, given their promising topological features for heat transfer applications. The parameters obtained via the numerical workflow were then used to estimate the performances of the whole device, comparing them to the ones of a grooved heat pipe taken as a benchmark. The two parameters we were interested in evaluating were the hydraulic permeability of the lattice structure and its effective pore radius. To estimate permeability, we rigorously applied the homogenization theory framework and solved the resulting closure problem, which allowed us to obtain the permeability tensor for the specific unit cell being considered. The closure problem results were validated with both pore-scale simulations and by comparison with results found in literature. The relative error was below 5% for all unit-cell topologies and sizes, indicating excellent agreement between the homogenized and pore-scale models and supporting the validity of the upscaling approach. Even the literature cross-verification confirmed the accuracy of the results. For the estimation of the effective pore radius, an energy-conservation approach was used. The results for r_{eff} were then validated with 3D drainage simulations. As it was done for permeability, these results were also cross-validated using literature.

Finally, once the overall numerical workflow was validated as described, we used the hydraulic parameters obtained to evaluate the performances of the whole heat pipe. First, we evaluated a performance index, which characterizes the capillary performance of the wick: the results showed that the TPMS-based wicks present an increase in the PI, compared to a grooved wick heat pipe found in literature, of 4.3% for the Diamond, 19.3% for the Gyroid and 125% for the Primitive, all with a unit cell size of $775 \mu m$ (equal to the wick thickness) and an 80% porosity. Then, we run device scale simulations by implementing a heat pipe template model in COMSOL Multiphysics. In particular, we compared the overall thermal resistance of the grooved benchmark heat pipe with the one of the Primitive wick heat pipe for different heat inputs. These simulations showed that, for the same heat input, the grooved heat pipe has a lower thermal resistance than the 3D printed heat pipe. This is to be expected, given that the porosity of the grooved wick (67%) is smaller than the Primitive one (80%) and that porosity is the only parameter that influences the overall thermal resistance with the simplified model being implemented. Nevertheless, the Primitive wick can tolerate more than twice the power input at the evaporator than the grooved one, showing that 3D printed lattice structures can effectively be used for these kinds of applications.

This preliminary work can be expanded on many fronts. First of all, many other topologies

could be analyzed using this exact numerical workflow. Furthermore, the same upscaling procedure for the momentum equation could be extended to higher Reynolds numbers. Finally, the multiscale framework could be applied to derive homogenized transport equations not only for momentum but also for heat transfer, allowing thermal conductivity to be computed directly from the pore-scale geometry.

Acronyms

- AI** anisotropy index. xi, 53, 55
- AM** additive manufacturing. 16, 17, 19, 23, 24, 25
- ASME** American Society of Mechanical Engineers. 47
- BC** boundary condition. x, xi, 36, 45, 46, 58, 59, 69, 70, 71, 96, 97, 101
- BVP** boundary value problem. 30, 33, 43, 44, 50
- CFD** computational fluid dynamics. 22, 38, 47
- CHT** conjugate heat transfer. 96
- CT** computer tomography. 25
- DOF** degree of freedom. 59
- EBM** electron beam melting. 17
- GCI** Grid Convergence Index. 50, 61
- KPI** key performance parameter. 99
- LBB** Ladyzhenskaya-Babuska-Brezzi. 59
- ODR** off-diagonal ratio. xi, 53, 55
- PBF** power bed fusion. 17
- PDE** partial differential equation. 30, 33, 36, 42, 56
- PI** performance index. 86, 88, 89, 98, 103
- RE** Richardson extrapolation. 47, 50, 60
- SLM** selective laser melting. x, 17, 23, 24, 25, 82

TCS thermal control system. 3

TM thermal management. 1

TPMS triply periodic minimal surface. i, vii, ix, x, xii, 17, 20, 21, 22, 23, 24, 25, 26, 38, 40, 47, 50, 53, 60, 69, 73, 81, 82, 85, 86, 88, 89, 98, 103

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