EFFECT OF PORE SIZE DISTRIBUTION OF AGGREGATES ON THE THERMAL AND MECHANICAL BEHAVIOR OF LIGHTWEIGHT AGGREGATE CONCRETE

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Thesis submitted to the Office of Research and Graduate Studies in partial fulfillment of the requirements for the Degree of Master of Science in Engineering

Advisor:
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Santiago de Chile, January 2022
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ABSTRACT

Traditional concrete is the most widely used material in the construction worldwide. However, its high thermal conductivity makes it difficult for concrete envelopes to comply with thermal regulations of building energy codes. Incorporation of lightweight aggregates within concrete improves its thermal behavior but diminishes the mechanical performance. Most research about lightweight concrete analyze principally the mineralogy and fraction of components for the evaluation of its thermal conductivity and compressive strength. Nevertheless, these properties also depend on the pore size distribution (PoSD) contained in the aggregates, which could represent up to 80.0% of the concrete volume.

This thesis focuses on evaluating the effect of PoSD on the thermal and mechanical properties of lightweight aggregate concrete using a new thermal and mechanical model (LWAC-TMM) based on the finite element method. The thermal model uses the Fourier's law, while the mechanical model uses the Hooke's law and the Drucker-Prager yield surface. The model validation shows that it is able to estimate properly the thermal conductivity, Young's modulus, and compressive strength of composite porous materials. Regarding the influence of PoSD on thermal conductivity of LWAC, it was found that the effect is negligible, changing an 1.4% when the average pore size decreases from 161 to 25 μm for LWAC with 53.2% of porosity. However, for the same change in average pore size, the LWAC compressive strength increases up 30.8%. Therefore, the PoSD affects mechanical behavior more than thermal behavior in this range of porosity. Such difference is associated with the effect of tortuosity and pathways through which heat flow between pores. Future work should focus on smaller pore sizes, since they are related with a better mechanical performance, and the optimization of the PoSD and location to reduce thermal conductivity.

Keywords: lightweight aggregate concrete, pore size distribution, thermal conductivity, compressive strength, porous material model.
RESUMEN

El hormigón es el material más utilizado en la construcción a nivel mundial. Sin embargo, su alta conductividad térmica dificulta a las envolventes de hormigón cumplir con las normativas térmicas. La incorporación de agregados livianos al hormigón mejora su comportamiento térmico, pero un reduce su desempeño mecánico. La mayoría de las investigaciones de hormigones livianos consideran solo la materialidad y proporción de sus componentes en la evaluación de conductividad térmica y resistencia a compresión. No obstante, estas propiedades también dependen de la distribución de tamaño de poros contenida en los agregados, donde estos agregados representan hasta un 80% del volumen del hormigón.

Esta tesis se enfoca en evaluar el efecto de la distribución de tamaño de poros sobre las propiedades térmicas y mecánicas del hormigón con agregados livianos utilizando un nuevo modelo térmico y mecánico (LWAC-TMM) basado en el método de elementos finitos. El modelo térmico utiliza la ley de Fourier, mientras que el mecánico usa la ley de Hooke y la superficie de fluencia de Drucker-Prager. La validación muestra que el modelo estima adecuadamente la conductividad térmica, módulo de Young y resistencia a compresión de materiales porosos compuestos. Respecto a la influencia de la distribución de tamaño de poros sobre la conductividad térmica, el efecto es insignificante, cambiando 1.4% al disminuir el tamaño promedio de poros de 161 a 25 μm en hormigones con 53.2% de porosidad. Sin embargo, para el mismo cambio de tamaño promedio de poros la resistencia a compresión aumentó 30.8%. La distribución del tamaño de poros afecta en mayor medida al comportamiento mecánico que al térmico en este rango de porosidad. Dicha diferencia se explica por el efecto de tortuosidad y cantidad de caminos a través de los cuales fluye el calor entre los poros. El trabajo futuro debería evaluar menores tamaños de poros, asociados a un mejor desempeño mecánico, así como mejorar las propiedades térmicas a través de la optimización de distribuciones de tamaño y localización de poros.

Palabras claves: hormigón con agregados livianos, distribución de tamaño de poros, conductividad térmica, resistencia a compresión, modelo para material poroso
1. INTRODUCTION

1.1. Background information

The residential sector accounts for 22% of the total energy consumption in United States (U. S. Energy Information Administration, 2021). More than 60% of the energy consumed in buildings is used for heating and cooling indoor spaces, this energy consumption in buildings could be reduced up to 15% using lightweight concrete instead of normal weight concrete (Real et al., 2016).

Concrete is the most consumed material worldwide after water (Gagg, 2014). Although normal weight concrete shows good mechanical performance, it presents a high thermal conductivity compared to traditional thermal insulation materials (Remesar, Vera & López, 2017). Therefore, to improve its thermal performance is necessary to analyze the components of concrete: cement, water and aggregates; where the aggregates represents between 60 and 80 % of the concrete volume (Ninčević et al., 2019; Chan, 2013).

The research of lightweight aggregate concrete (LWAC) mostly focuses on studying the effect of the aggregate mineralogy, density, and porosity, but leaves aside microstructure aspects such as the pore size distribution (PoSD) (Asadi, Shafigh, Abu Hassan, & Mahyuddin, 2018). For a complete understanding of the thermal and mechanical behavior of a porous material is necessary to analyze the volumetric fraction of each phase of the composite material, and the geometry of the microstructure (Hasselman & Johnson, 1987; Phan-Thien & Pham, 2000; Tang, Zheng, Gao, & Zhou, 2019; Sumirat, Ando, & Shimamura, 2006; Topçu & Uygunoğlu, 2007).

Therefore, this research aimed to evaluate the effect of porosity and PoSD contained in the lightweight aggregate (LWA) on the LWAC’s thermal conductivity and on the compressive strength by a new numerical model using the finite element method (LWAC-TMM). The model considered the grading and volume fraction of LWAs, and the porosity and PoSD of the microstructure of LWAs.
Commercial Liaver® LWA were measured in this research, obtaining its PoSD and porosity, these LWAs were made from recycled soda-lime glass (Liaver, 2021). Then, based on the range of pore size and porosity of Liaver® LWA, three microstructures of LWAs with different PoSD were generated and simulated to evaluate the effect of PoSD on the thermal conductivity and compressive strength of lightweight aggregate concrete.

A classification of lightweight aggregates and concretes are shown in section 1.1.1, along with the main variables considered in the experiments with lightweight concrete. Simplifications about heat transfer mechanisms are considered according to the range of pore size treated (section 1.1.2). Finally, a literature review of experimental, analytical, and numerical advanced models of porous materials and concrete are shown in section 1.1.3.

1.1.1. Lightweight aggregates and concretes

LWA have a high fraction of air that lead to a lower density and a lower thermal conductivity than normal aggregates (Asadi et al., 2018; American Concrete Institute, 2014a). These aggregates are used in LWAC to reduce weight and to improve thermal performance. However, this lower density implies lower compressive strength that reduces the concrete’s mechanical performance (Remesar et al., 2017).

According to ASTM C330, LWA are classified in two categories: produced by a sintering process or based on a natural material. Also, to be classified as a lightweight aggregate, the maximum apparent density must be equal to 1120 and 880 kg/m³ for fine and coarse aggregates, respectively (ASTM, 2017). On the other hand, lightweight concretes are classified as structural (SLWC) if they have a minimum compressive strength at 28 days of 17 MPa, and a balance density between 1440 and 1840 kg/m³ (American Concrete Institute, 2014b). Usually concretes with low density are considered non-structural concretes (NSLWC), and they are used for insulation and lightweight components (Hedjazi, 2019). Due to the high air fraction contained in the aggregates, the
high LWA volume fraction on concrete, and the properties of cement paste, the concrete considered in this research is classified as NSLWC.

To improve the thermal and mechanical properties of lightweight aggregate concrete, the literature on experimental research is extensive considering a wide variety of LWA such as recycled perlite, polystyrene, expanded glass, clay or slate. Gandage et al. (2013) studied the effect of perlite incorporation, finding that a higher replacement proportion implied a lower thermal conductivity and density of the concrete.

Remesar et al. (2017) have evaluated the effect of expanded clay, shale, and polystyrene as aggregates, showing that the incorporation of these materials reduced thermal conductivity, but significantly reduced the compressive strength of concrete. Increasing the fraction of lightweight aggregates from 0 to 50% reduced the thermal conductivity from 1.44 to 0.75 W/mK, but the compressive strength decreased from 84.6 to 17.6 MPa. Similar results are shown by Ali, Maslehuddin, Shameem, & Barry (2018), who studied the incorporation of polyethylene beads as a replacement for thick limestone aggregates, reporting that total replacement with polyethylene beads produced the greatest reduction in compressive strength.

Wang & Meyer (2012) incorporated high-impact recycled polystyrene as aggregates, showing that compressive strength decreased by half when replacing 50% of normal aggregates by polystyrene; they also show that these aggregates made concrete more ductile, the energy dissipation capacity increased, and the thermal conductivity decreased by 44%.

Wu et al. (2015) have incorporated air into the concrete through cenospheres to decrease their density and thermal conductivity, showing that compressive strength increased by 3% and thermal conductivity decreased by 80% for 38% volume’s fraction of cenospheres, whereas the compressive strength and thermal conductivity decreased by 39% and 84% respectively, when cenospheres were greater than 48% of concrete’s volume. Yun, Jeong, Han, & Youm (2013) used shale, clay, slate, and glass microbubbles
to replace normal aggregates to analyze their effect on thermal conductivity. They found that glass microbubbles were the most effective aggregates for reducing the thermal conductivity. Most LWAC investigations evaluate the effect of LWA on concrete properties experimentally, and do not analyze the effect of the PoSD on the behavior of aggregate concrete.

1.1.2. Thermal behavior of porous materials

Heat transfer is governed by three transfer modes: convection, radiation and conduction (Incropera & DeWitt, 1999). Specifically, in porous materials the heat is transferred by a combination of mechanisms: solid wall conduction, and the conduction, convection, and radiation within the pores (Solórzano et al., 2009). In building materials, pore size does not exceed 3 mm, and specifically the lightweight aggregates evaluated in the present research have a maximum pore size of 0.5 mm. Thus the convection and radiation effects are negligible (Bhattacharjee & Krishnamoorthy, 2004). Similarly, Van De Walle (2019) considered that natural convection is insignificant for pores smaller than 4 mm. Moreover when pores are closed, such as those considered in this research, the convective effect is not significant (Arriagada, 2018). Solórzano et al. (2009) pointed out that radiation in cellular materials is negligible for porosities below 80%. Also Petersen (2015) exposed that radiative heat transfer is negligible in materials below a 94% of porosity. In the present research, the aggregates have an average porosity equal to 76%, so the thermal transfer by radiation is insignificant.

On the other hand, the heat transfer by conduction is a mixture of molecular vibrations and energy transport by free electrons (Bhattacharjee & Krishnamoorthy, 2004). Porous materials, such as lightweight aggregates, have lower thermal conductivities due to a high air volume fraction, distributed in pores. Air has lower thermal conductivity than solid materials, with a value close to 0.025 W/mK (She et al., 2018; Van de Walle, 2019).

The thermal conductivity of the air within the pores varies when the diameter is less than 10 μm by the Knudsen effect, which shows that the thermal conductivity of the gas
phase decreases when the pore diameter decreases. This effect is produced when the mean free path between gas particles is larger than the diameter of the pore, being the gas molecule more likely to collide with the wall than with another gas molecule, and the collision between gas particles produces more energy transfer than if it collides with the solid wall (Berge & Johansson, 2012). This phenomenon affects the thermal conductivity of the air inside the pore, as shown in the Figure 1-1, depending on the pore diameter. In the present research lightweight aggregates have a pore size above 10 μm diameter, in over 90% of the pores evaluated. According to Berge & Johansson (2012) over this pore size, the Knudsen effect is negligible, so the thermal conductivity above 10 μm is invariant.

Because heat transfer by convection and radiation are negligible, and the lower fraction of smaller pores, the Knudsen effect is neglected, the energy flows only by conduction in the solid phase of cement paste, solid phase of aggregates, and in the air contained in pores.

![Figure 1-1. Thermal conductivity of air according to pore size, by Knudsen effect (adapted from Berge & Johansson, 2012).](image)
1.1.3. Thermal and mechanical behavior models of composite materials

Previous research have proposed several numerical models to estimate the thermal conductivity (Lee, Yun, & Choi, 2015; She, Yiqiang, Yunsheng, & Jones, 2013; Van De Walle, Claes, & Janssen, 2018; and Chung, Elrahman, & Stephan, 2017), Young’s modulus (Tang et al., 2019; Youssef, Lavergne, Sab, Miled, & Neji, 2018), and compressive strength (Chung et al., 2017; Cui, Hao, & Shi, 2018; Jin, Yu, & Du, 2020) of porous materials and/or concrete. However, none of these models considers the effect of PoSD of aggregate LWAC, and most of them evaluate thermal or mechanical behavior separately.

Askari, Taheri, & Hejazi (2015) stated that analytical models work only for simplified cases, and in recent years the use of computational techniques has increased because materials can be modeled in greater detail. Also, they pointed out that experimental work, its logistics and demand for resources limits the practicality of experimental tests of composite materials. Regarding experimental investigation of porous materials, Lu, Lu, & Xiao (1999) exhibited analytical expressions for Young’s modulus estimation, but considering porosity as the unique variable. Morgan, Wood, & Bradt (1981) evaluated the effect of cell size of foamed materials on mechanical performance, exposing that flexural, tensile, and compressive strength increased by decreasing cell size and were proportional to the inverse square root of the cell size.

Remesar et al. (2017) pointed out that there is a gap in the knowledge concerning the effect of the type and volume of lightweight aggregates on the thermal and mechanical properties of lightweight concretes. Muñoz, Castillo & Torres (2018) exposed the necessity of numerical models to evaluate the effect of pore structure of solid materials, such as the lightweight porous aggregates evaluated in this research. Moreover, there are many advantages of numerical models over experimental trials, where sensitivity analyses are possible without compromising higher-cost and time-consuming resources in their
development (Banks, 1999). Finally, from the state-of-the-art and models for LWAC, it is not possible to obtain relationships between geometry and its mechanical behavior.

1.2. Knowledge gap

The effect of aggregates on the thermal and mechanical concrete performance in most researches is done through experimental tests, using aggregates with different materiality and density (Asadi et al., 2018). Most of the models for concrete and porous materials analyze only thermal or mechanical behavior, and advanced concrete models that consider both assume the aggregates as a continuous material grading (Chung et al., 2017; Chung et al., 2018) and they do not model the internal geometry of them, such as the PoSD. About geometric modeling, only the fraction of each material is not enough to describe the thermal or mechanical behavior of the composite, where it is necessary to consider the distribution of the air into the aggregates considering the PoSD (Phan-Thien & Pham, 2000; Tang, Zheng, Gao, & Zhou, 2019). Therefore, in literature there is a lack of knowledge about the effect of internal geometry of aggregate over the thermal and mechanical behavior of LWAC.

Regarding concrete investigations with lightweight aggregates, Moreno, Martinez, & López (2014) and Chandra & Berntsson (2002) have proposed analytical models for compressive strength, while Asadi et al. (2018) and ACI 213R (American Concrete Institute, 2014a) have proposed analytical model for the thermal conductivity estimation, based on the oven-dry density of lightweight concrete. Nonetheless, these models do not explicitly consider parameters such as porosity or PoSD of aggregates in thermal and mechanical estimations.

To analyze the effect of different aggregates, new experiments must be carried out, which are costly compared to more efficient methodologies such as numerical models. The literature shows a lack of numerical models for thermal and mechanical behavior of porous materials such as concrete with lightweight aggregates considering the internal
geometry of the aggregates. Therefore, this research addresses the following research opportunities:

- The lack of numerical models to estimate the thermal conductivity and compressive strength of LWAC considering the internal geometry of the aggregates.
- The lack of research studying the effect of the PoSD within the aggregates on the thermal and mechanical performance of LWAC.

This research will contribute to the lightweight aggregate concrete design to provide the amount of each aggregate type size in the concrete, based on its properties associated with the PoSD of the aggregates. Currently there are no advanced numerical methods that consider the distribution of pore size, it is only done by experimental tests that are expensive and time-consuming.

1.3. Hypothesis

This research tests the following hypothesis: the thermal conductivity and compressive strength of the LWAC are significantly influenced by the PoSD contained in its aggregates.

1.4. Objectives

The main objective of this research is to evaluate the effect of the PoSD contained in the aggregates on the thermal conductivity and compressive strength of LWAC.

The specific objectives are:

- To develop and validate a numerical model that estimates the thermal conductivity and compressive strength of LWAC, considering the PoSD contained in the aggregates.
- To generate the PoSD and aggregate grading to evaluate the effect of different PoSD on the thermal and mechanical properties.
• To estimate the thermal conductivity and compressive strength of LWAC for different PoSD.

1.5. Methodology

To evaluate the effect of PoSD on the thermal and mechanical behavior of LWAC, other parameters are fixed, such as: porosity, aggregate volume fraction, grading, and the thermal and mechanical properties of the phases. Porosity, grading and the properties of the aggregates are obtained from Liaver® lightweight aggregates characterization. Aggregate volume fraction of aggregates is set at 50 and 70% (Jin et al., 2020; Cui et al., 2018; Shahbeyk, Hosseini, & Yaghoobi, 2011; and Chung et al., 2017), while cement paste properties are based on the binder evaluated by Chung et al. (2018).

The estimation of the properties of LWAC were carried out by a 2D thermal and mechanical model (named LWAC-TMM) that consists of a two-stage process; the two-stage avoids having a high complex model, allowing to evaluate with the current computational tools. The first stage is focused on obtaining the equivalent properties of LWA, while the complete equivalent properties of LWAC are obtained in the second stage. The modeling was carried out using a package of three software: Microsoft Excel 365, Python 3.7 and Ansys® Mechanical (2020).

A similar process is used to randomly place pores within the aggregate, and the aggregates into the concrete. First, the specimen dimensions of aggregate or concrete are established, along with the fraction of each size of pore or aggregate. Excel allows to compute the quantity of each pore or aggregate size that must be placed inside the specimen. Second, the data is taken by a Python script that randomly positioned the pores inside the aggregate. A similar script is used to place the aggregate inside the concrete, the script is shown in Appendix A. The location of pores and aggregates is based on two key principles: objects do not overlap and do not get off the edges of the specimen. In the case of aggregate location in concrete, a spacing proportional to the aggregates size is used according to Wriggers & Moftah (2006). Third, from the Python script, a text file is
exported to pass the data to Ansys® Workbench to generate the geometry, using the script shown in Appendix B. Finally, the Steady-State Thermal and Static-Structural tools of Ansys® are used to perform the thermal and mechanical analysis of aggregates and concretes.

The validation of the LWAC-TMM is separated in thermal and mechanical. Experimental results of foamed concrete evaluated by She et al. (2013) are used to validate the thermal conductivity estimation, while the mechanical validation was based on normal weight and foamed concrete shown by Cui et al. (2018), Jin et al. (2020), and Youssef et al. (2018). The validation considers the fraction, the distribution, and the properties of the phases that compose the materials.

To test the hypothesis, the thermal conductivity and compressive strength of LWAC with 50 and 70% of aggregate volume fraction were evaluated, considering three PoSD distribution for each of them.

1.6. Thesis structure

Chapter 2 shows the development of the model LWAC-TMM that estimates the thermal conductivity and compressive strength of both aggregate and lightweight concrete using finite element method. Chapter 2 shows the validation of the model based on experimental data obtained from literature. Chapter 3 details the properties of materials and characterization of the internal geometry of Liaver® lightweight aggregates, such as the porosity and PoSD. Then, these parameters are used to describe the microstructure geometry of the LWAC. Finally, the thermal conductivity and compressive strength of the lightweight aggregate concretes are estimated.

1.7. Conclusions

Chapter 2 concludes that the geometry of lightweight aggregate concrete is highly complex. Therefore, a 2D model composed by a two-stage process was necessary to
estimate the thermal and mechanical properties of lightweight aggregate concrete, according with the current computer limitations of the author.

The validation of LWAC-TMM demonstrates that the model accurately estimates the thermal and mechanical properties of composite materials, obtaining coefficients of determination $R^2$ equal to 0.95, 0.93 and 0.99 for the thermal conductivity, Young’s modulus, and compressive strength estimation respectively, with respect to the experimental results. The developed model improves the estimation of thermal and mechanical properties compared with other models due to the incorporation of the internal geometry of aggregates. Besides, LWAC-TMM is a complement to the thermal and mechanical behavior analysis of LWAC, and a practical alternative to evaluate the effect of different lightweight aggregates on the concrete behavior. This could reduce cost and time of the investigation about thermal and mechanical behavior of LWAC.

The hypothesis is tested in Chapter 3 for LWAC with different LWA volume fraction and PoSD. The main conclusion is that the pore size presents a higher effect in the mechanical than thermal behavior of LWAC. In a LWAC with 53.2% of total porosity and 70% of LWA volume fraction, the compressive strength increases up to 30.8% when the average pore size decreases from 161 to 25 μm; at the same time, the thermal conductivity increases 1.4%. On the other hand, regarding the LWA, the decrease of the average pores size distribution from 263 to 25 μm generated an increase of 80.0% in the compressive strength of the aggregate with 76.0% of porosity, while the thermal conductivity increased by up to 3.3% for the same pore size change.

The increase in the compressive strength when the average of pore size decreases is explained due to the higher number of walls into the microstructure of the aggregates that support the stress, while the less variation on the thermal conductivity is explained by the counterweight between the tortuosity and number of pathways through which heat flows across the porous aggregates, both affected by the pore size. Regarding the mechanical performance of the aggregates, the failure plane was found in areas with less solid material
fraction concentration. Two main patterns were found in this failure plane: zones with the longest pore size concentration and zones with porous in a weak position, i.e., various pores placed in one direction, where interstitial porous walls are narrow. Therefore, pore size close to 25 μm must considered for the design and fabrication of LWA, or in the selection of LWA for LWAC dosage design, These pore sizes exhibit better mechanical performance without impairing thermal properties.

1.8. Limitations and future work

In the methodology there was a set of experimental data planned to be tested in the laboratory and used in the validation of the developed model. However, due to the sanitary measures of the health authority because of COVID, it was not possible to carry out such experiments. However, the model was validated by experimental data found in literature. A complementary validation could be performed in the future, based on LWAC experimental results.

Regarding the developed LWAC-TMM model, the future work should improve it by a more detailed internal geometry characterization using micro computed tomography (micro-CT scan) images directly to generate the finite element meshing, improving the accuracy in the evaluation of the properties of porous materials. On the other hand, the nonlinear mechanical behavior could be improved by incorporating the softening-hardening parameters of the materials.

Future work should consider smaller pore sizes, specially at nanometric scale, which should improve the mechanical behavior of porous aggregates, increasing the compressive strength. Future work should also focus on improving the thermal properties of LWAC varying the location and size of pores to control the tortuosity and the heat pathways.
2. A NOVEL NUMERICAL MODEL FOR THE ESTIMATION OF THE THERMAL AND MECHANICAL BEHAVIOR OF LIGHTWEIGHT AGGREGATE CONCRETE

2.1. Abstract

The building sector is responsible of 30% of end-energy consumption, whose majority is used for space conditioning. The thermal performance of building improves using lightweight aggregate concrete (LWAC) instead of normal-weight concrete, incorporating pores within the lightweight aggregates (LWA). However, the air into LWAC reduces the mechanical performance, thus, improving the thermal behavior of LWAC without sacrificing mechanical performance is challenging. The state-of-the-art evaluates the effect of aggregates with different mineralogy and volume fraction over the thermal and/or mechanical properties of concrete. Nevertheless, previous investigations leave aside the impact of the microstructure of aggregates, such as the pore size distribution (PoSD). Therefore, this research aims to evaluate the LWAC’s thermal and mechanical properties considering the porosity and PoSD of LWA by a new developed thermal and mechanical model (LWAC-TMM) based on the finite element method using Ansys®. The LWAC-TMM estimate the thermal conductivity, Young’s modulus, and compressive strength of porous materials with $R^2$ values of 0.95, 0.93 and 0.99, respectively. The model accurately estimates LWAC properties considering the LWA’s grading, LWA’s volume fraction, porosity, and air phase distribution. The LWAC-TMM is a new alternative for thermal and mechanical concrete evaluation allowing incorporate the microscale geometry and concrete’s component properties.

2.2. Introduction

The main challenge worldwide is to reduce the energy consumption and greenhouse gas emissions (Liu, Zheng & Zhang, 2018; Martínez-Molina, Tort-Ausina, Cho, & Vivancos, 2016), and the building sector plays a relevant role been responsible of 30% of
total energy consumption, and 28% of CO₂ emission during 2019 (Global Alliance for Buildings and Construction, 2020).

Between 60 and 80% of the total energy required by buildings corresponds to use of heating and cooling of spaces (ODYSSEE-MURE, 2015). Most of the energy consumption is caused to heat losses through walls and ceiling (Asadi et al., 2018), being the thermal properties of the building materials a relevant factor. Concrete is one of the main materials used in buildings (American Concrete Institute, 2018) but heavy-weight or normal weight concrete show high thermal conductivity in comparison with other building materials. Concrete is mainly composed by cement, water and aggregates (Mamlouk & Zaniewski, 2011), while aggregates are the largest fraction representing between 60 and 80% of the volume of concrete (Ninčević, Boumakis, Marcon & Wan-Wendner, 2019; Chan, 2013).

The advantage of concrete is its high mechanical compressive strength, with values usually used between 5 and 60 MPa (Instituto Nacional de Normalización, 2016), reaching values even above 150 MPa (Azmee & Shafiq, 2018), but normal weight concrete has high thermal conductivity values in the range of 1.4 to 2.3 W/mK (Remesar et al., 2017). Consequently, building envelopes made of concrete need to accomplish thermal insulation requirements by adding layers of thermal insulation and finishings. LWAC reduces or avoids the insulation needed by reducing energy losses due to its lower thermal conductivity with values close to 0.2 W/mK (Asadi et al., 2018). Nevertheless, reducing the thermal conductivity of concrete usually reduces its compressive strength (Remesar et al., 2017), which is an undesired effect.

The main parameters that describe their internal geometry of LWAC are:

- **Porosity**: air volume fraction of the total volume of a body, referring to the porosity of the aggregates or the complete concrete.
- **PoSD**: the relationship between pore sizes and the fraction of each of them.
• Aggregate volume fraction: fraction of aggregates with respect to the total volume of concrete.
• Aggregate grading: the aggregate particle size distribution inside the concrete.

Wu et al. (2015), Hasan, Saidi, & Afifuddin (2021), Wang & Meyer (2012), Gandage et al. (2013), Topçu & Uygunoğlu (2007), Yun, Jeong, Han, & Youm (2013), Arriagada (2018), Remesar et al. (2017) and Yu, Spiesz, & Brouwers (2015) have empirically analyzed the thermal and mechanical properties of concrete based on different LWA such as cenospheres, diatomaceous earth, recycled polystyrene, perlite, expanded glass, pumice, shale, clay and slate. Most of them consider the mineralogy, fraction, density, or the porosity of the aggregates as main variables, but they do not consider in detail the PoSD contained in the aggregates.

Regarding the numerical modeling of concrete, porous, or granular materials, several research studies evaluated their thermal and/or mechanical behavior through numerical modeling, these models present advantages regarding experimental tests. The experimental tests are more expensive and time-consuming (Van De Walle, 2019), and they must be carried out in a laboratory with controlled conditions that require equipment and materials, and usually waiting 28 days between the manufacture and testing for concrete samples (Supit, Rumbayan, & Ticoalu, 2017; Choi & Yuan, 2005; Li & Li, 2015).

Chung et al. (2017) and Chung et al. (2018) have evaluated the thermal and mechanical properties of LWAC but without considering the internal geometry of the aggregate, thus, the aggregates are modeled only as continuous materials. Most of the porosity of LWAC are into the LWA, and for a complete analysis of the porous material’s behavior, the distribution of phases have to be considered, such as the PoSD of the air inside the aggregates (Hasselman & Johnson, 1987; Phan-Thien & Pham, 2000; Tang, Zheng, Gao, & Zhou, 2019; Sumirat, Ando, & Shimamura, 2006; Topçu & Uygunoğlu, 2007).
The objective of the present research is to evaluate the effect of the PoSD contained in the aggregates on the thermal and mechanical behavior properties of LWAC at 28 days, this research presents a new thermal and mechanical numerical model for lightweight aggregate concrete based on finite elements method that allows to consider the volume fraction and grading of LWA, and the porosity of aggregates for geometrical characterization. The evaluation of the properties of LWAC is usually performed by experimental tests (Asadi et al., 2018; Yu et al., 2015), and there are few models for porous building materials (Van De Walle, 2019), and most of them are focused in external geometry of aggregate, and do not incorporate the PoSD on the LWAC evaluation. A resume of state-of-the-art models that estimate the thermal and mechanical behavior of both porous materials and concrete are described below.

2.2.1. Thermal models for porous and composite materials

Analytical models for thermal conductivity estimation for porous and composite materials have been summarized by Van De Walle (2019), Remesar et al. (2017), and She et al. (2018). The analytical models are shown in Table 2-1, where $\lambda$ is the thermal conductivity of composite material, $\phi$ is the volume fraction of the dispersed phase, $\lambda_1$ and $\lambda_2$ are the thermal conductivity of the continuous and dispersed phases, respectively. Asadi et al. (2018) and ACI 213R (American Concrete Institute, 2014a) proposed numerical models based on experimental results of lightweight concrete, which depended on $\rho$ which is the concrete oven-dry density.

The series, parallel, Hashin & Shtrakman, Bruggeman and Landauer (EMT) models are presented in Figure 2-1 for LWAC with different volume fractions of aggregates, these consider a cement paste matrix with a thermal conductivity $\lambda_1$ equal to 0.52 W/mK, a continuous phase is assumed, while the dispersed phase is represented by the aggregates with an thermal conductivity $\lambda_2$ of 0.10 W/mK (Chung et al., 2018). For porous materials, Van De Walle pointed out that the thermal conductivity should vary between Landauer (EMT) and upper Hashin & Shtrakman limits.
Table 2-1. Thermal analytical models for porous and composite materials.

<table>
<thead>
<tr>
<th>Model</th>
<th>Equation</th>
<th>Detail</th>
</tr>
</thead>
<tbody>
<tr>
<td>Series and parallel (She et al., 2018)</td>
<td>$\lambda_s = \frac{1}{\frac{\phi}{\lambda_2} + \frac{1 - \phi}{\lambda_1}}$</td>
<td>For materials in series and parallel distribution.</td>
</tr>
<tr>
<td></td>
<td>$\lambda_p = (1 - \phi)\lambda_1 + (\phi)\lambda_2$</td>
<td></td>
</tr>
<tr>
<td>Upper and lower H-S. (Hashin &amp; Shtrikman, 1962)</td>
<td>$\lambda_{HS\ upper} = \lambda_1 + \frac{3\lambda_1(\lambda_2 - \lambda_1)\phi}{3\lambda_1 + (\lambda_2 - \lambda_1)(1 - \phi)}$</td>
<td>For dilute concentrations of spheres in a continuous medium, based on homogeneous and isotropic materials.</td>
</tr>
<tr>
<td></td>
<td>$\lambda_{HS\ lower} = \lambda_2 + \frac{3\lambda_2(\lambda_1 - \lambda_2)(1 - \phi)}{3\lambda_2 + (\lambda_1 - \lambda_2)\phi}$</td>
<td></td>
</tr>
<tr>
<td>Bruggeman (Bruggeman, 1935; Van De Walle, 2019)</td>
<td>$\left(\frac{\lambda_2 - \lambda_{Brugg}}{\lambda_2 - \lambda_1}\right)\left(\frac{\lambda_1}{\lambda_{Brugg}}\right)^{\frac{1}{\phi}} = 1 - \phi$</td>
<td>For spherical inclusions dissolved in a solid matrix, according to Van De Walle (2019) this model matches with cellular materials.</td>
</tr>
<tr>
<td>Landauer 'effective medium theory' (EMT) (Landauer, 1952)</td>
<td>$\lambda_{EMT} = \frac{1}{4} \left[ \lambda_2(3\phi - 1) + \lambda_1(2 - 3\phi) + \sqrt{\left(\lambda_2(3\phi - 1) + \lambda_1(2 - 3\phi)\right)^2 + 8\lambda_2\lambda_1} \right]$</td>
<td>For pore structure with random distribution.</td>
</tr>
<tr>
<td>Asadi et al. (2018)</td>
<td>$\lambda = 0.0625e^{0.0015\rho}$</td>
<td>For lightweight concrete based on their dry density.</td>
</tr>
<tr>
<td>ACI 213R (American Concrete Institute, 2014a)</td>
<td>$\lambda = 0.072e^{0.00125\rho}$</td>
<td>For lightweight concrete based on their dry density.</td>
</tr>
</tbody>
</table>
Figure 2-1. Results of the estimation of thermal conductivity of LWAC by analytical models.

There are complex models that consider a cubic structure geometry or ellipsoid-shaped pores. Still none depend on the average pore size (Van De Walle, 2019), and most of them have a limited range of applicability due to adjustment factors that must be adjusted to match the model with the experimental results.

Regarding advanced numerical models, She et al. (2013) and She et al. (2018) proposed a 2D thermal model based on a resistor network analogy method to estimate the thermal conductivity of foamed concrete. However, they do not study the effect of PoSD for the same porosity and consider only one phase, which is no applicable to LWAC with several phases such as cement paste, the solid phase of aggregate and pores. Askari et al. (2015) and Lee et al. (2015) proposed models to estimate thermal conductivity of granular materials using finite and discrete element methods; nevertheless, these models consider a surface strength that is not applicable for porous cellular materials. Van De Walle (2019) and Van De Walle et al. (2018) proposed a 3D thermal model using finite element method for granular and cellular materials. Although their model considers the PoSD, these studies
did not investigate the effect of the pore size at equal porosity to evaluate the effect of PoSD.

A mesoscale model to estimate the thermal conductivity of concrete was proposed by Zhang, Min, Gu, Xi, & Xing (2015), their model is based on the volume fraction of the sand and coarse aggregates, with pores in an unsaturated state distributed through the cement mortar, but it does not consider the pores within the aggregates. Huang et al. (2018) developed a 2D thermal model using the finite element method considering the grading of the aggregates; they found out that the effective thermal conductivity of concrete varies logarithmically with the thermal conductivity of coarse aggregate. Finally, they concluded that the most practical and effective way to improve the thermal behavior of concrete is changing the thermal conductivity of the cement mortar or aggregates.

2.2.2. Mechanical models for porous and composite materials

Table 2-2 shows a summary of analytical compressive strength models for porous materials and LWAC. Zheng, Zheng & Luo (1992) featured an analytical model for brittle materials, where $f_c$ is the compressive strength of the porous material, $f_{c0}$ is the compressive strength of the continuous material without porosity, and $\phi$ is the porosity. This model is useful for materials with porosity less than 50%, and over this threshold the results are undefined, which is a significant limitation of the model.

Duckworth (1953) developed an analytical model using the $b_\sigma$ factor, it is an empirical constant that depends on experimental tests. Liu (1997) compared this model with experimental results of the compressive strength in porous ceramics with pore sizes between 0.093 and 0.42 mm, and porosities from 33% to 78%, showing a $R^2$ higher than 0.96. However, this model does not explicitly consider the PoSD in the porous material, and the internal effects of the PoSD are incorporated through $b_\sigma$; the model is not applicable for materials with more than one phase, such as concrete.
Regarding particular models for the LWAC compressive strength estimation, a two-phases model has been proposed by Chandra & Berntsson (2002). This model depends on LWA volume fraction, compressive strength of matrix and the aggregates (f_{LWA}). Bogas & Gomes (2013) have validated the expression for concretes but only for LWA volume fraction between 25 and 40%, showing that the model was representative for concrete when the aggregate strength is lower than the mortar strength. It should be noted that the matrix assumed in this model is made of mortar and not cement paste. However, mortar is considered to have a similar isotropic and homogeneous behavior.

Moreno et al. (2014) proposed an analytical model for LWAC, which depends on the compressive strength of the cement paste or mortar continuous matrix (f_m), the LWA volume fraction (V_{LWA}) and an aggregate weakness factor (\alpha) obtained from linear regression of experimental test results. Nevertheless, this model for LWAC does not explicitly consider dependence on the PoSD, although there is an implicit dependence through the factor \alpha. The use of this factor has some drawbacks, it needs a battery of experiments to determinate this value, and the model implicitly considers dependence on pore size as well as the effect of grading of aggregates, without being able to evaluate the PoSD effect directly.

<table>
<thead>
<tr>
<th>Model</th>
<th>Equation</th>
<th>Detail</th>
</tr>
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<tbody>
<tr>
<td>Zheng, Zheng &amp; Luo (1992)</td>
<td>( f_c = f_{c0}(1 - 2\phi)^{0.925}(1 - \phi^2)^{1/2} )</td>
<td>For porous materials with porosity less than 50%.</td>
</tr>
<tr>
<td>Duckworth (1953)</td>
<td>( f_c = f_{c0}e^{-b\sigma\phi} )</td>
<td>For porous materials for porosities between 30 and 78%.</td>
</tr>
<tr>
<td>Chandra &amp; Berntsson (2002)</td>
<td>( \log(f_c) = V_{LWA}\log(f_{LWA}) + (1 - V_{LWA})\log(f_m) )</td>
<td>For LWAC for LWA fraction between 25 to 40%.</td>
</tr>
<tr>
<td>Moreno, Martinez, &amp; López (2014)</td>
<td>( f_c = f_m10^{aV_{LWA}} )</td>
<td>For LWAC for LWA fraction between 20 to 66%.</td>
</tr>
</tbody>
</table>
The previous two analytical models for LWAC are shown in Figure 2-2 for the relationship between compressive strength and aggregate volume fraction. In the case of a compressive strength of a continuous matrix and aggregate of 64.53 MPa and 3.2 MPa, respectively (Chung et al., 2018). The model of Moreno et al. (2014) matches with model of Chandra & Berntsson (2002) for a weakness factor $\alpha$ equal to 1.3. The figure denotes that the model of Moreno et al. (2014) is adaptable through different values of weakness factor $\alpha$ for the same aggregate volume fraction and compressive strength of the continuous matrix, depending on the experimental tests mentioned above.

![Figure 2-2. Results of the estimation of compressive strength of LWAC by the models of Chandra & Berntsson (2002) and Moreno et al. (2014).](image)

Regarding advanced numerical models, Liu et al. (2017) evaluated experimentally and by finite element method the Young’s modulus and flexural strength of porous materials consisting of a gypsum matrix with expanded spherical polystyrene. They found out that Young’s modulus was reduced less than strength when porosity increased up to 31%. For titanium materials, Muñoz et al. (2018, 2015) developed a finite element model and they
evaluated experimentally the Young’s modulus and compressive strength; however their model considers only one phase, while the LWAC is a three phase composite material. Finally, they exposed that there is a lack of models to estimate the mechanical behavior depending on the structure of porous materials to improve the use of materials. Torres-Sanchez et al. (2017) evaluated experimentally Young’s modulus and compressive strength of porous titanium used in medical implants, testing materials with porosities up to 70%, they found that at the same porosity, larger pores size caused a lower compressive strength.

Regarding concrete modeling, a cause-and-effect relationship between geometric and physical properties cannot be established when the concrete is considered like a single homogeneous material (López, Carol & Aguado, 2008). Due to the strong relationship between the internal geometry of composite materials and their compressive strength, more complex models have been developed that consider aggregate geometry.

Kim & Abu Al-Rub (2011) showed 2D and 3D numerical models for concrete that evaluate Young’s modulus and tensile strength considering the grading of aggregates; nevertheless, these models do not consider the internal geometry of aggregates. Similarly, Youssef et al. (2018) proposed a model to estimate Young’s modulus of foamed concrete model estimation using fast Fourier transform algorithm. This model is for a continuous material with holes incorporated and does not consider the porous aggregates and the evaluation of compressive strength. On the other hand, Tang et al. (2019) proposed a 2D finite element model for Young’s modulus estimation of porous materials, for low values porosities up to 10%. Yu & Wu (2019) showed a 2D mesoscale model using the discrete element method for compressive strength estimation of recycled lump concrete. This model does not take into account porous materials and requires six parameters of materials that make complex its application. Jin et al. (2020) and Cui et al. (2018) developed finite element models to evaluate the compressive strength of normal weight concrete; they have validated their results with experimental data measured on concrete considering 45% of
aggregate volume fraction. The main drawback of these models is that they do not consider internal geometry of aggregates.

Finally, Chung et al. (2017, 2018) developed a model for LWAC, evaluating the thermal conductivity, compressive strength and Young’s modulus for different grading of aggregates and cement paste, however, their model considers the aggregates like a unique phase without pores, it does not allow to evaluate the effect of the PoSD of aggregates on the concrete’s properties. No models or investigations were found to evaluate the effect of pore size within aggregate on the thermal or mechanical behavior of LWAC. A novel numerical model that allows incorporating in detail the internal geometry of lightweight concrete aggregates is presented in this research.

2.3. Research methodology and materials

2.3.1. Lightweight aggregate concrete geometry and simplifications

The LWAC geometry characterization considers the porosity and PoSD placed within the aggregates and LWA volume fraction and grading of aggregates within the concrete (Yu et al., 2015). A representative illustration of LWAC is shown in Figure 2-3.

The geometry representation and properties of LWAC considers some simplifications such as: the cement paste matrix is a continuous and homogeneous material, the aggregates have spherical shape; the pores are placed inside the aggregates, they have also a spherical shape and they are separated without coalescence between them; and pores do not exceed the aggregates dimensions.
2.3.2. Overview of lightweight aggregates concrete thermal and mechanical model (LWAC-TMM) and validation

A thermal and mechanical 2D model is developed to estimate the thermal conductivity and compressive strength of LWAC. Because of the highly complex geometry of LWAC the model is composed of a two-stage process: first, each LWA is evaluated to obtain its properties that consider the same PoSD and porosity. The second stage is to generate the LWAC geometry and evaluate its properties, the inputs of this stage are the aggregate properties obtained in the first stage. Therefore, assessing the properties for the different kind of aggregates inside the concrete is required to estimate the properties of one LWAC.

The geometries of aggregates and full concrete are generated using Excel to obtain the size and quantity of pores or aggregates. This data is transferred to a script based on Python 3.7, to place the pores randomly within the aggregates and then the aggregates within the concrete. Finally, the output of Python is transferred to Ansys® Mechanical 2020-R1 to
generate the final geometry, the meshing, and finally to evaluate the thermal and mechanical properties of LWA and LWAC.

The thermal and mechanical validation of the LWAC-TMM is carried out separately, comparing modeling outcomes with analytical and experimental results. Thermal modeling validation is carried out using analytical and experimental results of foamed concrete. Regarding mechanical validation, first the linear behavior range is validated, evaluating Young's modulus compared with experimental tests of foamed concrete. Finally, a nonlinear validation of the compressive strength is carried out using analytical cases and experimental results of normal weight concrete.

2.3.3. Governing equations

The thermal and mechanical properties of aggregates and concrete are evaluated using the Steady-State Thermal and Static Structural tools of Ansys®. The governing equations of materials behavior are shown below.

2.3.3.1. Thermal behavior

Convection and radiation inside the pores are negligible due to the pore size does not exceed 3 mm (Bhattacharjee & Krishnamoorthy, 2004). Similarly, Van De Walle (2019) considers that natural convection is not significant for pores smaller than 4 mm. On the other hand, the pore sizes considered in this research are over 10 μm and the Knudsen effect does not affect the thermal behavior of air (Berge & Johansson, 2012). Therefore, the thermal flux in the model is only by conduction.

The thermal behavior was based on a linear model considering invariant properties of the material concerning temperature, using a steady-state and the Fourier's law shown in Equation (2.1) (Incropera & DeWitt, 1999; Liang & Wu, 2018), where \( q \) is the unit heat flow \([W/m^2] \), \( \lambda \) the thermal conductivity \([W/mK] \), and \( \nabla T \) is the temperature gradient \([K/m] \).
\[ q = -\lambda \nabla T \] (2.1)

Therefore, the LWAC-TMM requires the thermal conductivity of each phase that compose the material and a thermal gradient.

### 2.3.3.2. Mechanical behavior

According to the length scale of observation, the mechanical behavior of the concrete is simulated under different level approximations: (i) microscopic, where atomic or particle interaction of elements are considered; (ii) mesoscopic, which consider the mortar, the aggregates, and their interactions as different parts and properties; and (iii) macroscopic, where the concrete is considered as a homogeneous material with isotropic behavior.

The concrete with normal weight aggregates at the mesoscopic level is usually simulated considering a three-phase model that includes aggregates, mortar, and an interfacial transition zone (ITZ) (Jin, Yu, & Du, 2020; Pedersen, Simone, & Sluys, 2013). The normal weight concrete failure is usually propagated through the ITZ. Nevertheless, LWAC can be characterized as a two-phase model, where only the aggregates and a mortar matrix are considered, without ITZ consideration (Bogas & Gomes, 2013). This simplification can be hold because the LWAC increases the water absorption capacity of the porous aggregate, compacting and strengthening the ITZ behavior (Elsharief, Cohen, & Olek, 2005; Sarkar, Chandra, & Berntsson, 1992). Moreover, Topçu & Uygunoğlu (2007) stated that cement paste penetrates on the surface of the porous aggregate, thus the quality joint between the aggregate and the cement paste is higher that than in normal weight concretes. Both characteristics motivate the development of lightweight concretes and modeling them without the ITZ.

Several models simulate the different components of the concrete at the mesoscopic scale, such as models that consider the aggregates with linear-elastic behavior (Xiong, Wang, & Jivkov, 2020; Wittmann et al., 1984), or models considering the strength of
aggregate (Cui, Hao, & Shi, 2018; Jin, Yu, & Du, 2020). The mortar and aggregate are modeled using plastic behavior models such as Drucker-Prager (Klabník & Králik, 2017; Jankowiak & Lodygowski, 2005; Kmiecik & Kamiński, 2011), Menetrey-Willam (Hokeš, Ji, Hušek, & Král, 2016; Papanikolaou & Kappos, 2005), or Willam-Warnke (Labbane, Saha, & Ting, 1993).

The Drucker-Prager Concrete plasticity model (DPC) available in Ansys® R1 (2020) is considered to simulate the nonlinear behavior of the mortar and solid phase of aggregates. This model is a variation of the original Drucker-Prager criterion, which fit more adequately the asymmetric tensile/compressive strength of concrete considering a composed yield surface. Firstly, this plastic model considers that the strain tensor \( \varepsilon \) is divided into its elastic \( \varepsilon_e \) and plastic part \( \varepsilon_p \) (de Souza Neto, Peri, & Owen, 2008), as follows

\[
\varepsilon = \varepsilon_e + \varepsilon_p. \tag{2.2}
\]

Then, using the Hooke’s law, the elastic strain tensor \( \varepsilon_e \) is related with the Cauchy stress tensor \( \sigma \) by

\[
\sigma = D^e : \varepsilon_e = D^e : \left( \varepsilon - \varepsilon_p \right), \tag{2.3}
\]

where \( D^e \) is the fourth-order linear-elastic tensor. Moreover, the model considers two different yield surfaces (ANSYS Inc., 2020a), \( F^+ \) for the tensile and tensile-compressive regime and \( F^- \) for the compressive regime, which are defined as

\[
F^+(\sigma, \kappa) := \eta^+(\kappa)p + q - \sigma^+_y(\kappa), \quad \text{and} \tag{2.4}
\]

\[
F^-(\sigma, \kappa^-) := \eta^- p + q - \sigma^-_y(\kappa^-),
\]

where \( p = \frac{1}{3}I_1 \) is the hydrostatic stress to include the pressure-dependence behavior, with \( I_1 \) the first invariant of the stress tensor \( \sigma \) (i.e., \( I_1 = \text{trace}(\sigma) \)); \( q = \sqrt{3}J_2 \) is the von Mises equivalent stress, with \( J_2 \) the second invariant of the deviatoric stress tensor \( s \) (i.e., \( J_2 = \)
and $\eta^+(\kappa)$, $\eta^-(\kappa)$, $\sigma_y^+(\kappa)$, and $\sigma_y^-(\kappa)$ are tensile/compressive material parameters, which are function of the hardening strain vector $\kappa = [\kappa^+, \kappa^-]^T$, (with the exception of $\eta^-$ parameter), with $\kappa^\pm$ are the tensile/compressive hardening variables, respectively. Generally, the $\eta^\pm$ and $\sigma_y^\pm$ parameters are fitted according to the desired Mohr-Coulomb approximation or the tensile/compressive strength of concrete. In this case, the parameters $\eta^+(\kappa)$ and $\sigma_y^+(\kappa)$ are chosen to fit the uniaxial tensile $f_t'$ and the uniaxial compressive strength $f_c'$ of concrete, whereas the parameters $\eta^-$ and $\sigma_y^-(\kappa^-)$ are chosen to fit the uniaxial $f_t'$ and biaxial compressive strength $f_b'$ of concrete. Then, all these parameters, are expressed as follows:

\[
\eta^+(\kappa) = \frac{3[\alpha^-(\kappa^-) - \alpha^+(\kappa^+)]}{\alpha^-(\kappa^-) + \alpha^+(\kappa^+)} \quad \sigma_y^+(\kappa) = \frac{2\alpha^-(\kappa^-)\alpha^+(\kappa^+)}{\alpha^-(\kappa^-) + \alpha^+(\kappa^+)} \tag{2.5}
\]
\[
\eta^- = \frac{3(f_b' - f_c')}{2f_b' - f_c'}, \quad \sigma_y^- = \frac{f_b'f_c'}{2f_b' - f_c'} \Omega^-(\kappa^-) \tag{2.6}
\]

where $\alpha^+(\kappa^+) = f_t'\Omega^+(\kappa^+)$ and $\alpha^-(\kappa^-) = f_c'\Omega^-(\kappa^-)$ are functions associated with the normalized tensile/compressive $\Omega^\pm(\kappa^\pm)$ function, respectively. The normalized functions $\Omega^\pm(\kappa^\pm)$ can be hardening/softening relations such as exponential, linear-decay, elasto-plastic, and can also include the fracture energy. Particularly, in the elasto-plastic case, i.e., $\Omega^\pm(\kappa^\pm) = 1$, the $\eta^\pm$ and $\sigma_y^\pm$ parameters are constants and given by

\[
\eta^+ = \frac{3(f_c' - f_t')}{f_c' + f_t'}, \quad \sigma_y^+ = \frac{2f_c'f_t'}{f_c' + f_t'} \tag{2.7}
\]
\[
\eta^- = \frac{3(f_b' - f_c')}{2f_b' - f_c'}, \quad \sigma_y^- = \frac{f_b'f_c'}{2f_b' - f_c'} \tag{2.8}
\]

Moreover, the model considers two flow potentials surfaces, $G^+$ for the tensile and tensile-compressive regime and $G^-$ for the compressive regime, which are defined as

\[
G^+(\sigma, \kappa) := \delta^+\eta^+(\kappa)p + q \quad \text{and} \quad G^-(\sigma, \kappa) := \delta^-\eta^-(\kappa)p + q \tag{2.9}
\]
\[ G^-(\sigma) := \delta^- \eta^- p + q, \]

with \(\delta^\pm \in [0,1]\) are the tensile/compressive dilatancy factor, respectively. Then, the yield surface is a composed function, the non-associated flow rule for the plastic strain tensor is given by the Koiter’s rule as follows

\[
\dot{\varepsilon}_p := \sum_{\kappa=1}^{2} \gamma^{\kappa}_R \frac{\partial G^\kappa}{\partial \sigma}, \quad \text{with} \quad \frac{\partial G^+}{\partial \sigma} = \frac{\delta^+ \eta^+(\kappa)}{3} I + \frac{3}{2q} s, \quad \text{and} \quad \frac{\partial G^-}{\partial \sigma} = \frac{\delta^- \eta^-}{3} I + \frac{3}{2q} s,
\]

where \(N\) denotes the active yield surface, \(\gamma^{\kappa}_R\) is the active plastic operator rate, and \(I\) is the second order identify tensor (i.e., \((I)_{ij} = \delta_{ij}\), with \(\delta_{ij}\) Kronecker function). Note that the flow rule is associate when \(\delta^\pm = 1\). The evolution law for the tensile/compressive hardening variables \(\kappa^\pm\) are stated as

\[
\kappa^\pm := \sum_{\kappa=1}^{2} \gamma^{\kappa}_R \frac{\partial G^{\kappa}}{\alpha^\pm(\kappa^\pm)}.
\]

Finally, the loading-unloading Karush-Kuhn-Tucker rules and the consistency condition are considered for the \(N\)-th active yield surface \(F^N\) and expressed by

\[
gamma^{\kappa}_R \geq 0, \quad F^N(\sigma, \kappa) \leq 0, \quad \text{and} \quad \gamma^{\kappa}_R F^N(\sigma, \kappa) = 0.
\]

The mechanical complete model requires seven material parameters, \(E, \nu, f_t', f_c', f_b', \delta^\pm\), and the normalized tensile/compressive \(\Omega^\pm(\kappa^\pm)\) functions, where \(E\) and \(\nu\) are the Young’s modulus and Poisson’s ratio, respectively. Since this research is interested to simulate the response of concrete at the maximum compressive strength, therefore it only requires the perfect elasto-plastic behavior model, neglecting the softening behavior at post-peak. Moreover, the associative flow rule is assumed, and only the \(E, \nu, f_t', f_c'\) and \(f_b'\) material parameters are required.
2.3.4. Materials for thermal and mechanical validation

Different materials are considered for the analytical and validation of thermal and mechanical properties estimation by the developed LWAC-TMM. The experimental data considered has been evaluated at 28 days. For thermal validation, properties and geometry of experimental test results of foamed concrete were considered, with a thermal conductivity equal to 0.5 W/mK for the solid phase of the foamed concrete, and 0.025 W/mK for the air (She et al., 2013). The analytical validation of thermal behavior of porous materials uses the same thermal conductivities for their phases.

Regarding the mechanical model, experimental test results of foamed concrete were considered to validate the Young’s modulus estimation, using a solid phase with a Young modulus of 24 GPa and Poisson’s ratio of 0.2 (Youssef et al., 2018). For validation of compressive strength estimation, normal weight concrete was used with the properties shown in Table 2-3; these comparative experimental results of normal weight concrete are based on the experimental data shown by Cui et al. (2018) and Jin et al. (2020). They have developed advanced numerical models to estimate the compressive behavior of normal weight concrete and used these experimental data to validate their models. An analytical validation is carried out for compressive strength, considering a first material with $E$, $v$, $f'_c$, $f'_t$, and $f'_b$ equal to 40.0 GPa, 0.2, 80.0 MPa, 6.0 MPa, and 93.6 MPa, and for a second material 24.0 GPa, 0.2, 20.0 MPa, 2.0 MPa and 23.4 MPa, respectively.

Table 2-3. Properties of normal weight concrete components for validation.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Material</th>
<th>Young’s Modulus (GPa)</th>
<th>Poisson’s ratio</th>
<th>Uniaxial compressive strength (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cui et al.</td>
<td>Mortar</td>
<td>25</td>
<td>0.18</td>
<td>35</td>
</tr>
<tr>
<td>(2018)</td>
<td>Aggregate</td>
<td>70</td>
<td>0.14</td>
<td>90</td>
</tr>
<tr>
<td>Jin et al.</td>
<td>Mortar</td>
<td>24</td>
<td>0.2</td>
<td>20</td>
</tr>
<tr>
<td>(2020)</td>
<td>Aggregate</td>
<td>40</td>
<td>0.2</td>
<td>80</td>
</tr>
<tr>
<td></td>
<td>ITZ</td>
<td>18</td>
<td>0.22</td>
<td>15</td>
</tr>
</tbody>
</table>
2.4. Model description, validation, and results

2.4.1. Lightweight aggregate concrete thermal and mechanical model

2.4.1.1. Stages of the model

Due to the complex geometry associated with the LWAC, a 2D geometry was considered, and the process of modeling had to be separated into two stages, which are shown in Figure 2-4. In the stage 1, the equivalent properties of the aggregates are evaluated. Then, these properties of aggregates are introduced into the concrete model plus the properties of cement paste in stage 2, evaluating the thermal and mechanical properties of LWAC.

Regarding geometry generation to simplify the modeling, the pores are considered as spherical (She et al., 2013; She et al., 2018; Youssef et al., 2018). Similarly, the aggregates incorporated in concrete are considered as spheres too (Wittmann, Roelfstra, & Sadouki, 1984; Xiong, Wang, & Jivkov, 2020; Pedersen, Simone, & Sluys, 2013; Cui, Hao, & Shi, 2018; Jin, Yu, & Du, 2020; Chung et al., 2017; Chung et al., 2018).

In the stage 1, the PoSD and porosity within the aggregate geometry are considered, and the thermal and mechanical properties of aggregates are estimated. These evaluations are required for each kind of aggregate that has the same PoSD and porosity. The results of stage 1 are the thermal conductivity, Young’s modulus, and compressive strength of aggregates. In stage 2, the geometrical parameters required are the aggregate volume fraction and grading of aggregates. Here, the aggregates’ properties obtained from stage 1 are used.
Figure 2-4. Geometry of LWAC and stages of 2D LWAC-TMM. (a) 2D representation of LWAC, (e) stage 1, LWA properties evaluation, and (f) stage 2, LWAC properties evaluation.

Depending on the evaluated model, one, two or three phases (materials) are considered as explained below:

1. One phase is considered in a continuous porous material like LWA, where the continuous phase could be glass for example (Liaver, 2021). As shown in Figure 2-4 in stage 1, the mechanical aggregate evaluation, the air inside the pores does not contribute to mechanical behavior, neglecting its effect, considering a one phase model.

2. Two phases are required for the thermal LWA model: air and solid phase of aggregate, considering the thermal properties of each of them. Also, in thermal and mechanical concrete model, cement paste is the continuous phase, while the aggregates are presented as dispersed, thus two phases are considered (as shown in Figure 2-4 in stage 2 for concrete evaluation with aggregate equivalent properties case).
3. Three phases composed by a continuous matrix, aggregates and ITZ are presented only in the validation section, for a normal weight concrete model exposed by Jin et al. (2020).

The geometry is generated through Excel, Python 3.7 and Ansys®, and finally, the properties evaluation is done in Ansys®. The workflow of the model is shown in Figure 2-5.

![Workflow diagram]

Figure 2-5. Workflow of geometry generation and properties evaluation of LWA and LWAC.
The following explains in more detail the geometry generation of the developed model, aggregate and of the complete concrete.

2.4.1.2. Geometry generation and meshing

For stage 1, the inputs of Excel are specimen dimension, porosity, and PoSD; the outputs of Excel are the quantity and size of pores to be placed. The pore data is transferred to Python script that randomly places the pore in the aggregate. The flowchart of this script is shown in Figure 2-6, while the script is found in Appendix A.

Regarding stage 2, the random aggregate location is similar to the process of pore location described above, considering the LWA volume fraction and grading of aggregates, and the dimensions of concrete specimen. However, a minimum distance criterion among aggregates has been considered, due to the thickness of the matrix covering the aggregates depends on the LWA volume fraction and size of aggregates. Wriggers & Moftah (2006) established a minimum spacing distance among aggregates of \( \gamma d \), where \( \gamma \) was a distribution factor depending on LWA volume fraction, and \( d \) is the particle diameter being positioned. A lower value of \( \gamma \) implies less difficulty to place aggregates, but macroscopically the concrete becomes less uniform, then the greatest value of \( \gamma \) was sought. This location process has been reported by literature known as take-and-place method and used for the generation of concretes with randomly distributed aggregates (Bazant et al., 1991; Wriggers & Moftah, 2006).
Figure 2-6. Process of random pore location in aggregates by a Python script.

An example of a geometry generation of foamed concrete using the Python script is shown in Figure 2-7(b), based on the PoSD shown in Figure 2-7(a). This geometry will be used for thermal validation section based on the data of She et al. (2013).
Figure 2-7. Porous material geometry of foamed concrete. (a) Pore size distribution (adapted from She et al. (2013)). (b) Pore geometry generated.

The random geometric location of pores (or aggregates within the concrete) done by Python script generates a text file containing information of the pores size and their location. Then, this data file is transferred to SpaceClaim in Ansys® Mechanical, it is a drawing tool that works with Python scripts. A second script was developed to generate the aggregates geometry in SpaceClaim. The geometry generation script used for this process is shown in Appendix B. This geometry is the input of the Static Structural and Steady-State Thermal tools in Ansys®, for thermal and mechanical behavior analysis, respectively.

The meshing for the finite element method considered tetrahedral element of 10 nodes. This type of elements was better suited to the complex geometry observed. Continuing with the previous example of location of pores, Figure 2-8 shows the geometry of a foamed concrete and the meshing.
Figure 2-8. Geometry and meshing of foamed concrete for validation section. (circles with different colors are pores, the random colors are assigned by the software by default, but all them are the same material) (source: Ansys® Mechanical).

This research proposes that the mesh refinement is given by the relationship between size of the finite element and the size of the specimen [specimen length/element size] or SE ratio, using values between 60 and 300. Higher values cause higher computing time for software execution, and the value used depends specifically on the geometry generated. A computer with an AMD Opteron(tm) Processor 6172 with 2.1GHz, 16 GB of RAM memory and 12 virtual processors was used to generate the mesh and the finite element evaluation.

Below are the evaluations that allow to obtain the thermal and mechanical properties, as well as the boundary conditions of the specimen for each case simulation to be performed.

2.4.1.3. Thermal conductivity evaluation

The boundary conditions are two different prescribed temperatures on opposite sides, $T_1$ and $T_2$ ($T_1 > T_2$). The rest of the faces remained adiabatic (Figure 2-9). The average
heat flux \((q_{av})\) was used to calculate the effective thermal conductivity of the composite material, \(\lambda_{ef} \text{ [Wm}^{-1}\text{K}^{-1}]\), as Equation (2.13) shows, where \(L\) is the specimen length [m].

\[
\lambda_{ef} = q_{av} \frac{L}{T_1 - T_2}
\]  

(2.13)

Figure 2-9. Boundary conditions of composite material for thermal analysis.

2.4.1.4. Mechanical properties evaluation

There are several studies that report the values of the uniaxial compressive strength \(f'_c\) of each component of concrete (Arriagada, 2018; Muñoz et al., 2018; Remesar et al., 2017; Cui, Hao, & Shi, 2018; Jin et al., 2020; Xiong et al., 2020). The uniaxial tensile strength \(f'_t\) is evaluated such as 0.1\(f'_c\) for cement paste and 0.075\(f'_c\) for the aggregates (Li & Li, 2015; Xiong et al., 2020; Jin et al., 2020). Conversely, it is experimentally observed that the value of the biaxial compressive strength \(f'_b\) of the aggregate and cement paste is about 1.16-1.17 \(f'_c\) (Dong, Wu, Zhou, & Huang, 2016; Kedziora & Anwaar 2019).

Boundary conditions are applied on opposite faces as shown in Figure 2-10. Side offsets are restricted at the left edge and the horizontal and vertical displacements are restricted in the upper left corner, whereas a prescribed offset is applied at the right edge. Also, plain stress is assumed, and there is no confinement on the transverse faces to the
direction of the load (Jin et al., 2020; Zhou & Lu, 2018; Häfner, Eckardt, Luther, & Könke, 2006; Yu & Wu, 2019).

In the modeling of compressive strength estimation, a prescribed deformation is attributed achieving its maximum compressive strength. The outputs of the mechanical model are the force reaction \( F_R \) [N] in the direction of the applied displacement, getting Young’s modulus \( E \) [Pa] and the stress of compressive strength \( f'_c \) [Pa] according to equation (2.14), where \( A \) is the cross-sectional area, \( \delta \) [m] the prescribed offset. The numerical model developed in this research considered that the materials do not have micro-fissures that could change the mechanical properties of the phase with the load application.

\[
f_c = \frac{F_R}{A}, \quad E = \frac{f_c}{\delta/L}
\]

Figure 2-10. Boundary conditions of composite material for mechanical analysis.

2.4.2. Validation and results

Most of the previous experimental investigations about LWAC do not show all the data needed to validate the thermal and mechanical model, such as the PoSD, aggregate grading or the properties of the phases. Because of that, the validation of the model developed was carried out by searching investigations with different materials that show
the geometry and material properties to estimate the thermal conductivity, Young’s modulus and compressive strength by the LWAC-TMM. Therefore, foamed concrete was used to validate the model regarding the linear properties: thermal conductivity and Young’s modulus, while normal weight concrete was considered to validate estimations of compressive strength prediction. Also, analytical comparisons have been used to complement the model validation.

2.4.2.1. Validation of the thermal modeling

Analytical and experimental cases are considered in the thermal validation considering materials in different geometric distributions. First, two materials distributed in series and parallel were evaluated to validate the model based on analytical solutions. Secondly the model was validated against experimental data of foamed concrete of She et al. (2013).

a. Thermal validation based on analytical cases

A validation based on analytical using material with series and parallel distribution is done, using the geometries shown in Figure 2-11, assuming two thermal conductivities, $\lambda_1$ and $\lambda_2$, equal to 0.025 W/mK and 0.5 W/mK, respectively. Figure 2-12 shows a comparison between analytical and LWAC-TMM results of the parallel and series cases. These results show a very good agreement with differences below 2.9% between analytical and simulated solutions.
Figure 2-11. Geometry of series and parallel analytical cases and boundary conditions for thermal analytical validation.

Figure 2-12. Comparison of thermal conductivity results from analytical and LWAC-TMM estimation.

b. Thermal validation based on experimental results

The second validation step was performed using the experimental results of foamed concrete with porosities between 10.5 to 68.4% evaluated by She et al. (2013). Lognormal
fit representation regarding experimental geometry evaluation of the PoSDs of the foamed concrete are shown in Figure 2-13 for the different porosities. The geometries for each kind of foamed concrete generated by the LWAC-TMM are shown in Figure 2-14. The specimens’ geometry is not at the same scale in Figure 2-14 due to the greater complexity of finite element meshing when porosity increases. Thermal conductivities equal to 0.025 and 0.5 W/mK are used for air and the solid phase (She et al., 2013).

![Figure 2-13. Pore size distribution of foamed concrete for different porosities (adapted from She et al. (2013)).](image)

Figure 2-15 shows the independence of the results regarding the finite element meshing refinement for the highest porosity specimen of 68.4%. Different mesh sizes were tested, exposed as the SE ratio respect to thermal conductivity; a higher ratio value implies a smaller element size. Depending on the mesh size, the thermal conductivity is underestimated between 17 and 25%, while it was underestimated by 34% by numerical model of She et al. (2013) numerical model. Moreover, it is observed that mesh size does not affect the estimated thermal conductivity for SE ratios above 200. Based on these results, the thermal conductivity estimation of porous materials was performed for a SE ratio of 200.
Figure 2-14. Generated geometry of foamed concrete geometry based on the experiments of She et al. (2013). Porosities: a) 10.5%, b) 21.0%, c) 32.5%, d) 47.3%, e) 57.9%, and f) 68.4%.

Figure 2-16 shows that the predicted thermal conductivities agree well with the experimental data of She et al. (2013) for all foamed concrete samples with different porosities, thus a coefficient of determination $R^2$ equal to 0.95 was obtained. The differences could arise because the PoSD evaluated is a simplified representation of the actual foamed concrete's internal geometry, and possible differences in the measurement of the thermal conductivity of the porous material.
Figure 2-15. Relationship between finite element size ratio and thermal conductivity results for foamed concrete with 68.4% of porosity.

Figure 2-16. Comparison of experimental (She et al., 2013) and estimated results by LWAC-TMM of thermal conductivity of foamed concrete. For porosities between 10.5 and 68.4%.
2.4.2.2. Validation of the mechanical modeling

Concrete mechanical behavior models have been presented over the years as a major challenge due to its internal complex geometry (Forti et al., 2020; Kim & Abu Al-Rub, 2011). In the design of concrete structural element the main parameter evaluated is the compressive strength, being the tensile strength neglected for bending and axial strength calculations according to ACI-318 (American Concrete Institute, 2014b). Hence, this research focused on obtaining the concrete compressive strength of LWAC. However, Young’s modulus of aggregates is required to evaluate the compressive strength of concrete. Therefore, two validations based on experimental tests are considered: a) a linear behavior mechanical validation for porous materials evaluating Young’s modulus and b) a nonlinear plastic behavior mechanical validation for concrete, which also evaluates the compressive strength. The plasticity of concrete was modelled according to the Drucker-Prager criterion.

a. Linear mechanical validation for Young’s modulus estimation

Yousseff et al. (2018) conducted several experiments on foamed concrete, evaluating the bulk, shear, and Young’s modulus. The research of interest in this kind of concrete is due to its low density, low thermal conductivity, and high fire resistance.

Young’s modulus of the solid phase (Em) of foamed concrete is 24 GPa, and Poisson’s ratio is 0.2. Young’s modulus, and PoSD for different porosities from 29.0 to 67.0% were obtained experimentally by Youssef et al. (2018). The same PoSD was observed for all porous materials with a maximum size of 2210 μm (Figure 2-17).
Figure 2-17. Pore size distribution of foamed concrete (Adapted from Youssef et al. (2018)).

Based on the PoSD shown in Figure 2-17, the geometries of five samples were generated and shown in Figure 2-18. Figure 2-19 shows the meshing convergence for the foamed concrete with the highest porosity (67.0%). It can be seen that the LWAC-TMM estimates Young’s modulus with difference from experimental results below 1.0%, using a SE ratio equal to 300. Youssef et al. (2018) also developed a numerical model showing a similar difference to the LWAC-TMM. Therefore, the mesh generation for Young’s modulus estimation considers a SE ratio of 200 to reduce computing time, which shows an acceptable difference of 3.5% between numerical and experimental values in the case of 67.0% of porosity.
Figure 2-18. Foamed concrete’s geometries foamed concrete based on the experiments of Youssef et al. (2018), for porosities: a) 29.0, b) 45.0, c) 55.0, (d) 61.0, and e) 67.0%.

Young’s modulus (E) of the porous materials obtained by the LWAC-TMM, normalized by the Young’s modulus of the solid phase (Em) were compared with the experimental results of Youssef et al. (2018) in Figure 2-20. LWAC-TMM shows a coefficient of determination $R^2$ equal to 0.93 about Young's modulus estimation. The LWAC-TMM showed a good agreement between estimated and experimental data for porosities above 45%. However, the model significantly underpredicts E/Em at the lowest evaluated porosity of 29%. This result might be due to the solid phase of foamed concrete was modeled as one-phase material, while it is composed of cement paste and normal-weight fine aggregate (i.e. sand). At 29% of porosity, foamed concrete is more rigid because of the higher Young’s modulus of sand (95.5 GPa) that matrix, where the sand represent 25% of the total concrete volume (Youssef et al., 2018). Therefore, sand plays
a crucial role in Young’s modulus, but the LWAC-TMM does not consider this effect of sand because of one-phase assumption modeling.

Figure 2-19. Relationship between finite element size ratio and Young’s modulus results for a foamed concrete with 67.0% of porosity.

Figure 2-20. Comparison of experimental (Youssef et al., 2018) and estimated results by LWAC-TMM of normalized Young’s modulus of foamed concrete. For porosities between 29.0 and 67.0%.
b. Nonlinear validation for uniaxial compressive strength estimation

The evaluation of the uniaxial compressive strength of concrete requires the incorporation of the Drucker-Prager nonlinear concrete criterion, considering the following five parameters: $E$, $v$, $f_c'$, $f_t'$, and $f_b'$. As mentioned above, $f_t'$ is $0.1f_c'$ and $0.075f_c'$ for matrix and aggregates, respectively, and $f_b'$ as $1.17f_c'$. The validation of compressive strength is composed by analytical and experimental cases.

i. Nonlinear mechanical validation based on analytical cases

Regarding the analytical validation, two materials in series and parallel distribution were evaluated, these are shown in Figure 2-21. The analytical result for materials placed in series assume that the compressive strength is dominated by the material with the lowest $f_c'$, which is equal to 20 MPa. In the parallel case, the composite compressive strength is the result of an equitable contribution between both materials, obtaining a $f_c'$ equal to 50 MPa. The compressive strength estimations of the series and parallel configurations by the LWAC-TMM and the analytical solutions are compared in Figure 2-22. The differences between simulated and analytical solutions are below 1.0%, showing that LWAC-TMM can properly deal with this basic cases.

![Figure 2-21. Geometry of analytical cases in series and parallel for compressive strength validation.](image)


Figure 2-22. Comparison of experimental, analytical and estimated results by the model LWAC-TMM for compressive strength.

**ii. Nonlinear mechanical validation based on experimental cases**

The validation of the compressive strength estimation of the LWAC-TMM against experimental results is based on normal weight concrete using the geometries and results shown by Cui et al. (2018) and Jin et al. (2020). The properties of the phases that compose the concrete were presented in Table 2-3. Cui et al. (2018) developed a model for the estimation of compressive strength of concrete considering mortar, aggregates, and pores randomly distributed. The aggregate volume fraction was 45%; the aggregate sizes were 3-5 mm, 5-8 mm, and 8-10 mm, and their volume fractions were 16, 17 and 12% respectively; it is also considered 0.1% pore volume with size of 1 mm. Based on these properties and characteristics, the corresponding concrete geometry was generated (Figure 2-23(a)).

Secondly, the geometry and properties exposed by Jin et al. (2020) were considered. The concrete’s volume has 45% of aggregates, with two sizes of aggregates: 8 and 16 mm. The ITZ is included in the model with a thickness of 1 mm according to Jin et al. (2020).
Figure 2-23(b) shows the geometry generated while the properties assigned to each phase were exposed in Table 2-3.

Figure 2-23. Geometry of models of normal weight concrete for the nonlinear mechanical validation. (a) 2-phase concrete (mortar and aggregates) (based on the experimental results of Cui et al. (2018)); and (b) 3-phase concrete
Regarding the validation based on experimental results of Cui et al. (2018), the stress-strain behavior obtained is depicted in Figure 2-24(a) for different mesh sizes. The estimated compressive strength is 36.2 MPa, with an error of 4.9% compared to the experimental result (34.5 MPa). Figure 2-25(a) shows the stress field, it is distributed across all the specimen showing stress concentration in the cement paste-aggregate joint, associated with the redistribution of forces inside the concrete components. Figure 2-25(b) shows the permanent equivalent plastic deformation, observing that the maximum deformation is located along the cement paste section, this result is explained due to the lower compressive strength of lower cement paste equal to 35 MPa while the aggregates have a compressive strength equal to 90 MPa.

The stress-strain curve of the LWAC-TMM based in Jin et al. (2020) is illustrated in Figure 2-24(b), obtaining a compressive strength of 18.6 MPa for the finest meshing; whereas, the experimental compressive strength is 18.5 MPa, difference of 0.5%. The stress field is shown in Figure 2-25(c) and the permanent equivalent plastic deformation in Figure 2-25(d). It is worthy to notice that the higher stress is concentrated mostly in the ITZ interphase, associated to the force distribution among the phases, similarly the highest values of permanent plastic deformation are across the ITZ sections, associated to its lower compressive strength regarding the rest of components. Therefore, the compressive strength values estimated by the LWAC-TMM have small differences regarding experimental values shown by Cui et al. (2018) and Jin et al. (2020), differences were 4.9% and 0.5% respectively, showing good agreement for compressive strength.

In Figure 2-24 relevant differences between estimated and experimental Young’s modulus values in concrete evaluated are observed. This is explained because the research of Cui et al. (2018) and Jin et al. (2020) have proposed the Young’s modulus values of the phases by an inverse method, adjusting the modulus of the phases used in their models to
match with the complete behavior of concrete evaluated in the experimental results, so the Young’s modulus used is not precisely the real value of materials. However, it did not affect the ultimate compressive strength behavior of the tested concretes, presenting low errors with respect to the experimental results.

Figure 2-24. Estimation of the mechanical behavior of concrete for different sizes of finite elements. (a) Based on concrete evaluate by Cui et al. (2018); and (b) Based on concrete evaluate by Jin et al. (2020).
Figure 2-25. Results of mechanical behavior of concrete. (a) Equivalent stress of concrete evaluated by Cui et al. (2018), (b) equivalent plastic strain field of concrete evaluated by Cui et al. (2018), (c) equivalent stress of concrete evaluated by Jin et al. (2020), and (d) equivalent plastic strain field of concrete evaluated by Jin et al. (2020) (source: Ansys® Mechanical).

The compressive strength’s results evaluated by the LWAC-TMM for analytical and experimental cases shows that the mechanical part of the developed model can predict the compressive strength accurately, with a coefficient of determination $R^2$ equal to 0.99 for the results shown in Figure 2-22, and a maximum difference between estimated and experimental results less than 4.9%.
2.5. Conclusions

This paper aimed to develop a numerical model to estimate the thermal and mechanical behavior of LWAC, considering the effect of the PoSD of the aggregate explicitly. Based on the author’s best knowledge, no simplified analytical or advanced numerical models have considered the effect of PoSD on the thermal and mechanical behavior of LWAC previously, which could significantly influence its thermal and mechanical properties. The development of complex models can be an alternative to consider these characteristics (Van De Walle, 2019; Askari et al., 2015; Jin et al., 2020; Cui et al., 2018). The main conclusions obtained are as follows.

- It is proposed a novel model LWAC-TMM that estimates thermal conductivity and compressive strength of LWAC. The LWAC-TMM can incorporate the grading, volume of aggregate, PoSD, porosity of pores in aggregates and the properties of LWAC’s phases. In addition, the model’s geometry can be adapted, being able to incorporate voids and ITZ, depending on the representative geometry of the concrete to be modeled.

- The LWAC-TMM was validated against analytical solutions and experimental results of porous and composite materials. The thermal section of the LWAC-TMM shows that the PoSD can be considered in detail for the thermal conductivity estimation. The difference between estimated and analytical/experimental thermal conductivities is below 17.3%, and coefficient of determination $R^2$ equal to 0.95 for porosities evaluated between 10.5 and 68.4% is obtained in comparison with experimental results. Similarly in the mechanical behavior analysis with materials with a complex geometry, the validation shows a $R^2$ equal to 0.93 for Young’s modulus estimation, and 0.99 for mechanical compressive strength estimation, obtaining a difference of 4.9% with respect to experimental results of compressive strength. It shows that the LWAC-TMM can obtain reliable results of the effect of pore size on the conductivity and compressive strength of LWAC.
• The main challenge were the computational limitations, the 2D model had to be subdivided into two steps due to complex geometry associated to the LWAC. However, the coefficients of determination for porous materials in the validation section show that the model nevertheless estimates reliable results for thermal and mechanical behavior of porous materials.

The future work also should be focused on evaluating the properties of LWAC considering aggregates with equal porosity and different PoSD through the LWAC-TMM. Since if only the PoSD changes, concretes with the same quantities of materials but different distributions can be analyzed, to broaden knowledge about the pore’s distribution of the materials in LWAC. The LWAC-TMM has the advantage over classical experimental test by keeping all geometrical parameters the same and varying only PoSD to evaluating its effect directly.
3. EFFECT OF PORE SIZE DISTRIBUTION ON THE THERMAL AND MECHANICAL PROPERTIES OF LIGHTWEIGHT AGGREGATES CONCRETE THROUGH NUMERICAL MODELING

3.1. Abstract

Lightweight concrete has significant advantages over traditional concrete such as lower density, lower thermal conductivity, along with the possibility of using recycled materials as aggregates. Previous research of lightweight aggregate concrete (LWAC) has studied the effect of material and porosity on its thermal and mechanical performance, disregarding the microstructure of the porous aggregates, given by the pore size distribution (PoSD). This paper aims to evaluate the effect of PoSD on the thermal conductivity and compressive strength of LWAC. Three types of proposed aggregates with different PoSD were developed and simulated, also two types of LWAC with different PoSD and with equal porosity, volume fraction and grading of lightweight aggregate (LWA), and materials properties were generated. The properties estimation was done using a finite element model. The concrete behavior results showed that by decreasing the average pore size from 161 to 25 μm, the compressive strength of concrete increased up to 30.8% and the thermal conductivity varied 1.4% for concrete with a LWA volume fraction of 70%. Regarding the properties of the LWAs, the results showed that by decreasing the average pore size from 263 to 25 μm, the compressive strength and thermal conductivity of aggregates increased up to 80.0% and 3.3%, respectively. The increase in compressive strength is explained by the higher number of solid partitions within aggregates having a smaller pore size, while the low thermal conductivity variation is associated to the balance between the tortuosity and the number of heat flows paths, both increasing with smaller pores. In conclusion, the mechanical behavior is more affected than the thermal behavior by the size of the pores, and an average pore size less than 25 μm is recommended. Future research should seek to a widen pore size range studied, mainly at the nanoscale.
3.2. Introduction

Concrete is the most used man-made material worldwide (Adesina, 2020), and the construction of residential buildings is one of its main consumers (American Concrete Institute, 2018; Ninčević et al., 2019). In the European Union, buildings use about 40% of the total primary energy consumption, while up to 66% is consumed for space heating (Cao, Dai, & Liu, 2016). The lightweight concrete shows a lower density and higher insulation compared with normal weight concrete (Chung et al., 2017), improving the thermal performance of building envelopes and decreasing the space heating energy consumption.

LWAC is composed by porous aggregates embedded in a continuous cement paste matrix. The aggregates are composed by a the solid phase and air pores, like a cellular structure (Yu et al., 2015). Several investigation have evaluated thermal or mechanical performance of concrete using different lightweight aggregates (LWA) such as cenospheres, diatomaceous earth, recycled polystyrene, perlite, expanded glass, pumice, shale, clay or slate (Wu, Wang, Monteiro & Zhang, 2015; Hasan, Saidi, & Affifuddin, 2021; Wang & Meyer, 2012; Gandage et al., 2013; Yun et al., 2013; Arriagada, 2018; Topçu & Uygunoğlu, 2007). The improvement of thermal properties by lightweight aggregates undermines the mechanical properties (Remesar et al., 2017). Most of the literature considered the material and fraction of aggregates as the main factors that affect the concrete properties. However, literature review disregards the internal microstructure of aggregates that is relevant for a better understanding of the thermal and mechanical behavior of porous materials such as LWAC, as described below.

The thermal behavior of the LWAC depends on the internal structure of the LWA (Topçu & Uygunoğlu, 2007) that is characterized by the PoSD. However, the effect of the PoSD is not well understood, showing different and opposite results over the thermal behavior of different materials and structures (Van De Walle, 2019). Considering the mechanical modeling, the porosity does not fully describe by itself the behavior properties
of porous materials. Therefore, consideration of the internal geometry is required (Tang et al., 2019) because the strength of lightweight concrete is significantly affected by the microstructure (Nguyen, Bui, Ngo, & Nguyen, 2017; Moreno et al., 2014). The effect of PoSD over normal weight concrete have been studied by Zhao, Xiao, Huang, & Zhang (2014), they show a high variability of compressive strength experimental results for concrete with similar porosities but different PoSD. The classic models between porosity and compressive strength are not applicable to their results because these models do not consider the pore structure, they proposed a model to estimate the compressive strength depending on the experimental cement paste parameters and mean pore diameter, thus the strength varies inversely with the mean pore size.

The analysis of porous materials can be carried out using analytical models, but they are valid for simple geometries considering ideal conditions and assumptions (Van De Walle, 2019). However, advanced numerical models allow to evaluate more realistic geometries (Muñoz et al., 2015). There are complex models that consider the microstructure of porous materials in thermal evaluation (Van De Walle & Janssen, 2018; She et al., 2013) and mechanic evaluation (Torres-Sanchez et al., 2017; Wittmann et al., 1984), although these studies does not consider the geometry of LWAC and evaluate materials with only one phase. Additionally there are normal weight concrete models considering grading and volume fraction of aggregates (Jin et al., 2020; Cui et al., 2018), however they do not apply for a LWAC geometry with porous aggregates. Finally, Chung et al. (2017, 2018) have studied the thermal and mechanical behavior of LWAC, considering the aggregate as a phase embedded in a matrix, nevertheless they consider the aggregates like a continuous phase, thus they do not evaluate the internal geometry of aggregates.

Therefore, the objective of the present research is to analyze the effect of PoSD contained in the aggregates on thermal conductivity and mechanical compressive strength of LWAC. The investigation is carried out using a 2D lightweight aggregate thermal and mechanical model (LWAC-TMM) based on the finite element method. The evaluation of
different PoSD distributions for the same total porosity of LWAC is performed. It considers an aggregate porosity of 76%, an aggregate grading based on the Andreasen & Andersen distribution, and a LWA volume fraction of 50 and 70%. The geometric characterization of the LWA was carried out by the micro computed tomography technique (micro-CT scan). Porous Liaver® aggregates from Germany were evaluated, which are made of recycled glass (Liaver, 2021). LWACs with equal fractions of materials and different microstructures are generated, thus different thermal and mechanical behaviors properties are expected. This research will support the future work to improve the thermal and/or mechanical performance of LWAC based on the modeling the mix design stage concrete.

3.3. Research methodology and materials

The thermal and mechanical evaluation is done through the numerical model LWAC-TMM that considers the porosity and PoSD of pores within the aggregate, the grading and volume fraction of aggregates within the concrete. The range of pore size based on Liaver® aggregates evaluates the PoSD and porosities for aggregates with diameter between 0.1 to 4 mm. Then LWAC with three PoSD with an average pore size of 25, 111 and 161 μm are proposed.

3.3.1. Numerical estimation by LWAC-TMM

The geometrical parameters needed for the 2D numerical model are the porosity, PoSD, LWA volume fraction and grading of LWAC. Due to the complexity of the internal geometry of LWAC, the model works in two-stage process: firstly, the equivalent properties of porous aggregates are evaluated, grouping them by equal porosity and PoSD. Then, the second stage evaluates the properties of the complete LWAC, this stage considers the equivalent properties of the aggregates obtained from the first stage, plus the cement paste matrix properties. Both stages have a similar framework using three software packages: Microsoft Excel 365, Python 3.7 and Ansys® release 2020-R1.
Firstly, regarding the porous aggregates’ evaluation, the porosity and PoSD are processed in Excel; then, the output of Excel are used by a Python script to randomly places the pores within the aggregate; and finally, the aggregate’s geometry is generated, and their equivalent thermal and mechanical properties are estimated in Ansys®. Once the equivalent properties of aggregates are obtained, the full concrete properties evaluation uses the same methodology, replacing the porosity and PoSD by the grading and LWA volume fraction respectively.

The element type used in the finite element method is a tetrahedral of 10 nodes due to its better adaptation to complex geometries such as those considered in this research. The validation of LWAC-TMM was done by comparing estimated results with analytical and experimental results.

3.3.2. Lightweight aggregate characterization

Expanded glass aggregates produced by Liaver® were used in this research because previous studies (Remesar et al., 2017; Chung et al., 2017, 2018; Yu et al., 2015) showed the potential on these aggregates to improve the thermal and mechanical performance of LWAC. These expanded glass aggregates are made of recycled soda-lime glass. The PoSD and porosity of aggregates are evaluated. The thermal and mechanical properties of the solid phase of aggregates were obtained from an inverse process using the aggregate properties and the geometry of the largest category of expanded glass aggregate. The estimation of the properties was done using the model outlined in the previous section. Finally, based on the range of range pore size evaluated from expanded glass aggregates, PoSDs with an average diameter between 25 and 263 μm were selected, with a porosity of 76%.

3.3.2.1. Porosity and pore size distribution of Liaver® aggregates

The sizes of LWA analyzed were between 0.1 and 4 mm. The micro-CT scan, using a 3D X-ray microscope SkyScan1272 desktop and Bruker manufacturer manuals, MCT-
059 (Bruker, 2014) and MCT-011 (Bruker, 2012a) were used to evaluate the porosity and PoSD of these aggregates with a resolution up to 1.8 μm. This non-invasive method has been used previously for materials analysis by Arriagada (2018), Hafsa et al. (2014), Remesar et al. (2017), and Videla, Lin, & Miller (2007). The micro-CT scan output is a collection of images showing black and white voxels regarding to the solid and non-solid material sections. Postprocessing the images was done in CT-Analyser software (CTAn) of Bruker (2012b) that consists of selecting: a collection of images, the aggregate to analyze (Volume of Interest, VOI), and the thresholding colors of the image to select the corresponding material to be analyzed. Then, a noise cleaning process was performed, and finally, the PoSD and porosity of each aggregate is obtained. The steps to perform image cleanup and PoSD evaluation are described in Appendix C. Table 3-1 shows the size, porosities, and the average pore size for each aggregate. The average porosity of all categories of aggregates is 76%.

Table 3-1. Geometry characterization of expanded glass aggregates.

<table>
<thead>
<tr>
<th>Aggregate category</th>
<th>Range size (*) [mm]</th>
<th>Average size [mm]</th>
<th>Porosity [%]</th>
<th>Average pore size [μm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.10-0.30</td>
<td>0.20</td>
<td>71.80</td>
<td>59.40</td>
</tr>
<tr>
<td>B</td>
<td>0.25-0.50</td>
<td>0.38</td>
<td>76.90</td>
<td>96.00</td>
</tr>
<tr>
<td>C</td>
<td>0.50-1.00</td>
<td>0.75</td>
<td>75.30</td>
<td>100.00</td>
</tr>
<tr>
<td>D</td>
<td>1.00-2.00</td>
<td>1.50</td>
<td>78.60</td>
<td>136.70</td>
</tr>
<tr>
<td>E</td>
<td>2.00-4.00</td>
<td>3.00</td>
<td>79.40</td>
<td>166.10</td>
</tr>
</tbody>
</table>

(*) Based on Liaver (2021)

The increase of the aggregate size implies a greater range of pores size, with the largest pore reaching a size close to 470 μm in the aggregate E. The cumulative PoSD for each aggregate is presented in Figure 3-1. In the smaller aggregate, there are more abrupt jumps on the distribution curve, while the curve of the aggregate category E is the smoothest. The difference in jumps is explained by the aspect ratio (aggregate size/average pore size) because in larger aggregates there are greater number of pores, allowing a more varied...
distribution of them. On the other hand, in smaller aggregates the effect is the opposite, decreasing the variation of pores sizes.

Figure 3-2 shows the relation between aggregate size and average pore size. In the smallest aggregate, type A, with medium size equal to 0.20 mm, the size of the average pore size is about 4 times less than the size of the aggregate, whereas on the largest aggregate, type E, with medium size of 3 mm, the average pore size is around 18 times smaller than the size of the aggregate.

Figure 3-1. Cumulative pore size distribution of Liaver® aggregates.
Figure 3-2. Aspect ratio between aggregate size and average pore size.

Regarding the aggregate geometry generation in the model, the coalescence effect between pores is neglected. Arriagada (2018) pointed out that the pores within LWA are mostly closed, associated to the production of pore sizes below 500-700 μm. This is the case of pores evaluated in expanded glass aggregates as shown in Figure 3-1. Additionally, pores near the surface of the specimen are assumed to be closed because they are embedded with cement paste of the concrete (Bumanis, Bajare, & Korjakins, 2013; Yu et al., 2015). The assumption of closed pores was corroborated by visual analysis of aggregates through micro-CT scan. Figure 3-3 shows a 2D image of a Liaver® aggregate. Image analysis of micro-CT scan allows to study the 3D aggregate from a collection of 2D images taken at different sample heights. Despite that there are pores coalescence in an image, in the adjoining images these pores are presented as closed again, and the coalescence observed is minimal.
Figure 3-3. Image of Liaver® aggregates, size 1.1 mm. (a) solid walls (b) air pores. (source: CT-Analyser Bruker®)

3.3.2.2. Thermal and mechanical properties of Liaver® aggregates

The thermal and mechanical properties of Liaver® aggregates were provided by the manufacturer and previous literature, which are shown in Table 3-2.

Table 3-2. Thermal and mechanical properties of Liaver® aggregates.

<table>
<thead>
<tr>
<th>Property</th>
<th>Category</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal conductivity [W/mK] (*)</td>
<td></td>
<td>-</td>
<td>0.08</td>
<td>0.75</td>
<td>0.73</td>
<td>0.07</td>
</tr>
<tr>
<td>Young’s modulus [GPa] (*)</td>
<td></td>
<td>-</td>
<td>0.83</td>
<td>0.80</td>
<td>0.79</td>
<td>0.76</td>
</tr>
<tr>
<td>Compressive strength [MPa]</td>
<td></td>
<td>3.50</td>
<td>2.90</td>
<td>2.60</td>
<td>2.40</td>
<td>2.20</td>
</tr>
</tbody>
</table>

(*) (Chung et al., 2017; Chung et al., 2018)
The chemical composition of aggregates was reported by the manufacturer (Table 3-3). These aggregates are acid resistant, non-combustible and thermally stable to frost and up to 750 °C (Liaver, 2021).

Table 3-3. Chemical composition of soda-lime glass.

<table>
<thead>
<tr>
<th>Component</th>
<th>mass/mass %</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO₂</td>
<td>72</td>
</tr>
<tr>
<td>Na₂O</td>
<td>13</td>
</tr>
<tr>
<td>CaO</td>
<td>8</td>
</tr>
<tr>
<td>MgO</td>
<td>3</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>2</td>
</tr>
<tr>
<td>K₂O</td>
<td>1</td>
</tr>
</tbody>
</table>

Source: Liaver (2021)

Nevertheless, the intrinsic properties of the crystalline phase with the composition shown in Table 3-3 are not representative of the solid phase materials of aggregates because the thermal and mechanical properties does not depend solely on mineralogical composition, but they also depend on the crystallinity degree, associated to the treatments to which the materials have been undergone (Bansal & Doremus, 1986; Nguyen, Beaucour, Ortola, & Noumowé, 2014). The porous aggregates were synthesized through a high-temperature process between 750 to 900°C, in a rotary kiln (Liaver, 2021).

3.3.3. Materials

A cement paste with a water-binder ratio of 0.34, and additions of fly ash of 131 kg/m³ has been used as the matrix for the LWAC (Chung et al., 2018; Cui et al. 2018). The thermal conductivity, Young’s modulus, and compressive strength of the solid phase of the aggregate of glass were obtained by an inverse method, similar to a previous research (Jin et al., 2020) using the model described in section 3.3.1. The properties and geometry of the Liaver® category E aggregate shown above were used, and the properties of the
solid phase were obtained by setting them to match with the equivalent properties of the aggregate given in Table 3-2. The aggregate category E was used because it has the largest variety of pore size and most of its properties are available from the manufacturer. The PoSD of aggregate E used is shown in Figure 3-1, with 79.4% of porosity.

The estimation of the properties of the solid phase is based on the specimen shown in Figure 3-4. Regarding the thermal model evaluation, the finite element mesh considers material within the pores that represent air (Figure 3-4 (a)) but it is not incorporated in the mechanical analysis (Figure 3-4 (b)) because the air do not contribute to mechanical behavior of the porous material. Finally, the properties of the phases of LWAC are shown in Table 3-4.

Figure 3-4. Finite element model of aggregate category E, Liaver®. (a) thermal model. (b) mechanical model. (source: SpaceClaim Ansys® Mechanical).
Table 3-4. Thermal and mechanical properties of lightweight aggregate concrete components.

<table>
<thead>
<tr>
<th>Property</th>
<th>Cement paste (*)</th>
<th>Solid phase of LWA</th>
<th>Air</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal conductivity [W/mK]</td>
<td>0.52</td>
<td>0.72</td>
<td>0.025 (***</td>
</tr>
<tr>
<td>Young’s modulus [GPa]</td>
<td>32.14</td>
<td>34.00</td>
<td>-</td>
</tr>
<tr>
<td>Poisson’s ratio [-]</td>
<td>0.180</td>
<td>0.25 (**)</td>
<td>-</td>
</tr>
<tr>
<td>Compressive strength [MPa]</td>
<td>64.53</td>
<td>550.00</td>
<td>-</td>
</tr>
<tr>
<td>Density [kg/m³]</td>
<td>1253.00</td>
<td>2500.00 (**)</td>
<td></td>
</tr>
</tbody>
</table>

(*) Based on Chung et al. (2018) and Cui et al. (2018)

(***) based on Bansal & Doremus (1986)

(**) based on She et al. (2018) and Van De Walle (2019)

3.3.4. Cases of study: pore size distributions in lightweight aggregate concrete

Three PoSD are developed and assigned into the aggregates; the ranges of pore sizes were based on those evaluated from the Liaver® aggregates. Then, concrete geometries with dispersed aggregates are developed considering LWA volume fractions of 50 and 70%.

3.3.4.1. Aggregate geometry

Three normal shape distributions are generated based on the pore size range of Liaver® aggregate. Normal distribution is set to simplify the choice of average and variation of pore size. In this research, the average for the finest PoSD was proposed as the pore diameter reaches 20% of the accumulated porosity of the smallest Liaver® aggregate category A, which is equal to 25 μm. On the other hand, the average for the coarsest PoSD was considered as the 20% of accumulated porosity for the largest aggregate category E,
which is 263 μm, these values are shown in Figure 3-1. A third PoSD is considered with an average equal to the weighted average of the two previous selections, which results in 144 μm. A porosity of 76% was fixed for the three distributions, which represents the average porosity of Liaver® aggregates. The normal distribution considered a standard deviation of 66.7% of the average that allows enough variety of pore size to obtain the high target porosity. Finally, the three PoSD are shown in Figure 3-5.

![Figure 3-5. Pore size distributions obtained in the proposed lightweight aggregates, with 76% porosity (μ = average, σ = standard deviation).](image)

### 3.3.4.2. Concrete geometry

Regarding the design of normal and lightweight concretes, the modified Andreasen & Andersen model has been used for the grading of aggregates within the concrete (Yu, Spiesz, & Brouwers, 2014):

\[
P(D) = \frac{D^q - D_{\text{min}}^q}{D_{\text{max}}^q - D_{\text{min}}^q} \quad (3.1)
\]
where \( P(D) \) is the fraction of accumulated particles; \( D \) is the diameter of the particle; \( D_{\text{min}} \) and \( D_{\text{max}} \) are the minimum and maximum particle size, respectively; \( q \) is the distribution module, with a fixed value of \( q = 0.37 \), it allows the highest aggregate volume fraction of dispersed spherical particles (Fennis, 2011; Brouwers, 2006).

The grading of the aggregates obtained is shown in Figure 3-6 with \( D_{\text{max}} = 4 \) mm and \( D_{\text{min}} = 0.1 \) mm. However, a minimum particle size up to 0.5 mm is assumed due to the computational limitations associated with the high complexity of the geometry and meshing on the finite element model (Chung et al., 2017). The grading of aggregates were characterized in three size ranges: 0.5 - 1 mm, 1.5 - 2 mm, and 3 mm, obtaining fractions of aggregates equal to 27, 31, and 42% of volume, respectively.

Two different LWA volume fractions were considered, equal to 50 and 70%. Similar values have been found in previous studies (Jin et al., 2020; Cui et al., 2018; Shahbeyk, Hosseini, & Yaghoobi, 2011; Chung et al., 2017).

![Figure 3-6. Aggregate grading based on Andreasen & Andersen modified model.](image)
3.3.5. Pore size distribution of lightweight aggregate concrete

The three PoSDs of LWA described in 3.3.4.1 are assigned to the different aggregate size ranges to generate three PoSDs in the LWAC. The cases are shown in Table 3-5, characterizing each PoSD by its average pore size. The total PoSD of LWACs is independent of the aggregate volume fraction because the q factor is constant.

Regarding the first combination case C1, the smaller PoSD have been assigned to all the aggregates, obtaining an average pore size of concrete equal to 25 μm. For combination C2, only the aggregates with diameter of 0.5-1.0 mm have a PoSD with average 25 μm, while the rest has assigned the PoSD averaged on 144 μm, getting an average pore size of concrete equal to 111 μm. Finally, the last combination C3 considers a different PoSD for each aggregate size range, with an average pore size of concrete equal to 161 μm. These combinations allow to generate LWAC with different PoSD, while all of them present the same dosage of materials because the porosity, LWA volume fraction, and grading of the aggregates remains constant. This PoSD allocation allows to directly evaluate the effect of the pore size on the thermal and mechanical concrete behavior. The PoSDs for the full concrete are set out in Figure 3-7. The resulting concretes with 50 and 70% of LWA volume fraction, obtain 38 and 53.2% of porosity, respectively.

Table 3-5. Cases of pore size distribution assigned to aggregates.

<table>
<thead>
<tr>
<th>Case</th>
<th>Aggregate size [mm]</th>
<th>Average PoSD</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.5-1</td>
<td>1.5 – 2</td>
</tr>
<tr>
<td>C1</td>
<td>25 μm</td>
<td>25 μm</td>
</tr>
<tr>
<td>C2</td>
<td>25 μm</td>
<td>144 μm</td>
</tr>
<tr>
<td>C3</td>
<td>25 μm</td>
<td>144 μm</td>
</tr>
</tbody>
</table>

The pores are placed within the aggregates, while the cement paste matrix phase joining the aggregates was considered homogeneous and isotropic (Jin et al., 2020; Chung et al., 2017; Chung et al., 2018; Y. Yu & Wu, 2019).
Figure 3-7. Pore size distributions of the proposed lightweight aggregate concretes.

### 3.4. Results and discussion

The results are separated into two sections. Firstly, the internal microstructure of the LWA and the geometry of LWAC are shown. Secondly, the thermal and mechanical properties estimation of the LWA for the different PoSD, and LWAC properties are evaluated, the LWAC evaluation considers the equivalent properties of aggregates. Both, the geometry generation, and the property estimation were carried out using the LWAC-TMM model.

#### 3.4.1. Geometry results

##### 3.4.1.1. Geometry of lightweight aggregates

The numerical model detailed in 3.3.1 uses as input the PoSD described in 3.3.4.1, this allow to obtain the internal geometry of the three types of aggregates shown in Figure 3-8, all of them with porosity equal to 76%.
3.4.1.2. Geometry of lightweight aggregate concretes

In the second stage evaluation, for the geometry of LWAC, the models consider the aggregates as a continuous phase using the equivalent properties of the porous aggregates, the evaluation of these properties will be exposed in the next section. Regarding the geometry of LWAC, a minimal spacing $\gamma d$ between aggregates was used, where $\gamma$ is a distance factor called distribution factor depending on aggregate volume fraction, and $d$ is the diameter of the particle being placed (Wriggers & Moftah, 2006), where different distribution factors $\gamma$ for concretes with aggregate fraction 50 and 70% were obtained. The geometry was also based on the modified Andreasen & Andersen packing curve, with a packing factor of $q = 0.37$. The LWAC geometries are shown in Figure 3-9, these show that concrete with LWA volume fraction of 50% has a greater spacing between the aggregates, given by a $\gamma$ factor of 0.3, while for concrete of 70% the aggregates tend to come together because there was a higher proportion of aggregates using $\gamma$ equal to 0.04.
Figure 3-9. Lightweight aggregate concrete geometries. a) LWA volume fraction of 50% with $\gamma = 0.3$ and b) LWA fraction of 70% with $\gamma = 0.04$. (source: SpaceClaim Ansys® Mechanical)

3.4.2. Thermal and mechanical properties estimation

3.4.2.1. Equivalent properties of lightweight aggregates

a. Estimation of thermal properties of lightweight aggregates

The geometries of the aggregates shown in 3.4.1.1 are evaluated using the phases properties exposed in Table 3-4, the finite element meshing for the geometry of each case of PoSD are shown in Appendix D. The results of thermal conductivity show a reduced impact of the pore size (Table 3-6). The average thermal conductivity of the three aggregates was 0.100 W/mK, with a coefficient of variation equal to 2.3%.

Table 3-6. Estimated thermal conductivity of lightweight aggregates.

<table>
<thead>
<tr>
<th>Average pore size [μm]</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.102</td>
<td>0.098</td>
</tr>
<tr>
<td>144</td>
<td></td>
<td></td>
</tr>
<tr>
<td>263</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The thermal conductivity varies 3.3% when the average pore size decreases from 263 to 25 μm. This low variation is explained by two opposite geometric effects that affect thermal behavior in different ways: firstly, decreasing the pore size increases the tortuosity (Caravella, Hara, Obuchi, & Uchisawa, 2012), increasing the heat resistance, and therefore generating a decrease in equivalent thermal conductivity (Kou et al., 2009; B. Yu & Cheng, 2002). On the other hand, decreasing the pores sizes increases the number of paths among the pores through which the heat flows, generating an increase in the equivalent thermal conductivity of the aggregate (Babaei, McGaughey, & Wilmer, 2016). Therefore, the balance between both effects means that the heat flow through the aggregate does not present considerable variations when the pore size changes, presenting a low variation result. This low thermal conductivity variation is also observed by She et al. (2018), who showed that the impact of the PoSD is negligible. However, the 3.3% increase in thermal conductivity when the average pore size decreased from 263 to 25 μm is explained by the greater effect of increased number of pathways through which heat flows in contrast to the increase in tortuosity, producing a low reduction on heat resistance when the pore size decreases.

The thermal conductivity of aggregates obtained by the LWAC-TMM are compared with thermal analytical models of composite materials: series and parallel models (She et al., 2018), H-S (Hashin & Shtrikman, 1962), EMT (Landauer, 1952) and Bruggeman model (Bruggeman, 1935) are shown in Figure 3-10. The thermal results of the LWA with the different PoSD are closer to the Bruggeman model, with an average difference of 16.2% considering a porosity equal to 76%. In addition, the values estimated agree well with results of Van De Walle (2019), exposing that the thermal conductivity of porous cellular materials are contained between the models of Landauer (EMT) and the upper Hashin & Shtrikman (H-S) limit the range of its thermal conductivity.

For instance, the internal thermal behavior of the aggregate with a PoSD averaged on 263 μm is shown in Figure 3-11. It is observed that the heat fluxes mostly through the
solid phase of glass, which has a thermal resistance 29 times lower than the air contained in the pores, concentrating the greatest heat fluxes in the glass areas narrowed by the pores.

Figure 3-10. Comparison of thermal conductivity results of lightweight aggregates by LWAC-TMM and analytical models.

Figure 3-11. Result of heat flux of aggregate with a pore size distribution average on 263 μm. (source: Ansys® Mechanical)
b. Estimation of mechanical properties of lightweight aggregates

The estimated mechanical properties of LWA are shown in Table 3-7. The Young’s modulus and compressive strength increased in 17.3 and 80.0% respectively, when the average pore size decreased from 263 to 25 μm. This mechanical behavior of porous aggregates with different pore size is consistent with data reported in literature (Table 3-2), where smaller aggregates with smaller pore size have higher compressive strength and Young’s modulus values.

Table 3-7. Estimated mechanical properties of lightweight aggregates.

<table>
<thead>
<tr>
<th>Average pore size [μm]</th>
<th>25</th>
<th>144</th>
<th>263</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus [GPa]</td>
<td>1.18</td>
<td>1.13</td>
<td>1.01</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.17</td>
<td>0.19</td>
<td>0.20</td>
</tr>
<tr>
<td>Compressive strength [MPa]</td>
<td>4.48</td>
<td>3.44</td>
<td>2.49</td>
</tr>
</tbody>
</table>

Regarding the microstructure of aggregates and their mechanical behavior, the stress is distributed through the solid phase. According to Leguillon & Piat (2008), the failure propagation in porous materials presents a bottlenecks effect in the circular pores, and the failure propagation among porous depends on the thickness of solid separation between the pores. Morgan et al. (1981) have experimentally obtained that the strength of porous materials has a proportional relationship with the inverse square root of the pore size. However, various pore sizes were used in the microstructure of LWAs in the present research, so this relationship was not exactly observed. Nevertheless, the result shows that the compressive strength decreases for larger pore sizes, being consistent with the relationship proposed by Morgan et al. They also stated that the strength of porous materials is produced by accumulated damage by a failure plane propagation sequentially on adjacent walls, increasing the crack through the porous material. The smaller pores size has more interstitial walls between pores to a better distribution of compressive stress.
Figure 3-12 shows the equivalent plastic strain results using an amplification factor for deformations of 3.7 in the aggregate geometry with a PoSD averaged on 263 μm. The failure surface is influenced by the pore size, the random location of the pores, and the thickness of the walls. Failure planes are observed inside the microstructure of the aggregates, similarly to those presented by Morgan et al. (1981); the failure is propagated through the weakest areas with less fraction of solid material, and where the higher stresses are concentrated. Liu (2010) has modeled materials with high porosity such as a strut and node system, exposing that the failure tends to be on the struts, which in this case are the walls of pores, and the failure is generated when the maximum stress within these struts reaches the maximum permissible strength of the material conforming the walls.

Figure 3-12. Result of equivalent plastic strain of aggregate with average of pore size distribution of 263 μm, using an amplification factor of 3.7. (a) LWA, (b) larger pores concentration failure, and (c) pores in a weak location. (source: Ansys® Mechanical)
Two geometric characteristics were observed and are related to a possible structural failure: areas of the material with a higher concentration of larger pores (Figure 3-12 (b)); and areas with pores in a certain unfavorable location, along with thin walls of solid material, as shown by the line in the red box in Figure 3-12 (c), which become the area into a weak section of the material.

3.4.2.2. **Lightweight aggregate concrete**

The assignation of PoSD in the aggregates within the LWAC model was done by setting properties of each PoSD to the respective aggregates, based on the results of thermal and mechanical behavior exposed in Table 3-6 and Table 3-7. These assignations generate the LWAC in the cases C1, C2 and C3 for the different PoSD of full concrete shown in 3.3.5. The thermal conductivity and compressive strength of the LWAC are evaluated and shown above. The finite element meshing for the LWAC with 50 and 70% of LWA volume fraction are shown in Appendix D.

**a. Estimation of thermal properties of lightweight aggregate concretes**

The thermal conductivities of LWAC are shown in Figure 3-13 for the pore combinations C1, C2 and C3, which have average pore size of 25, 111 and 161 μm, respectively. LWAC with an aggregate volume fraction of 50 and 70% were evaluated, obtaining an average of thermal conductivity of 0.259 and 0.182 W/mK, and coefficients of variation of 0.5% and 0.9% for each LWA volume fraction, respectively. The thermal conductivity of LWAC increased by about 0.9% and 1.4% when the average pore size decreased from 161 to 25 μm for the LWAC with 50 and 70% of LWA volume fraction, respectively. This low effect of the pore size in thermal conductivity of LWAC is explained by the low difference of thermal conductivities between LWA categories. Nevertheless, the increase of thermal conductivity is the effect that by decreasing the pore size, the decreases of the thermal resistance by higher number of paths through which heat flows is greater than the effect of increasing the thermal resistance by increasing the tortuosity.
Figure 3-13. Estimation of thermal conductivity of LWAC for different average pore size distribution.

The heat flux and temperature distribution through the LWAC are similar for the three cases C1, C2 and C3 due to the low variation of the thermal conductivity of the LWAs, and the geometry location of aggregates are the same for all combination. The C2 case is shown in Figure 3-14, while the rest of the cases are in Appendix D. Due to the difference of thermal conductivity between cement paste matrix and aggregates, the heat flows mostly through the cement paste. The average of thermal conductivities of aggregates is 0.100 W/mK, while the thermal conductivity of cement paste is 0.524 W/mK.
Figure 3-14. Results of thermal behavior of LWAC for pore size distribution C2. (a) Temperature field of LWAC with LWA volume fraction of 50%, (b) heat flux for LWA fraction of 50%; (c) temperature field for LWA fraction of 70%, and (d) heat flux for LWA fraction of 70% (source: Ansys® Mechanical).

The low variation of thermal conductivities of LWAC cases are directly related to the thermal behavior of aggregates, which internally shows a balance between the tortuosity and the number of paths through the heat flows. The larger pores imply fewer number of pathways where heat flows, reducing the cross-section of materials with lower thermal resistance, causing a increases in thermal resistance. On the other hand, the larger pores are also associated to a reduced tortuosity and path length, increasing the thermal
resistance. If the location of the pores could be controlled in detail, i.e., by avoiding the pores aligned in the direction of the thermal gradient, the tortuosity should increase, and the effective thermal conductivity of the aggregates decreases.

Figure 3-15 shows a comparison between the results obtained by LWAC-TMM and analytical models. The literature model that better approximate the thermal conductivity was EMT, with a difference in 0.6 and 3.2% for the cases of LWA volume fraction of 50 and 70%, respectively. The EMT model proposes an equation for material composed by mixing dispersed in the continuous phase. The EMT model aims to improve the thermal estimation of composite materials with a high fraction of the dispersed phase (Landauer, 1952). It is relevant to consider that the EMT model can accurately estimate the thermal behavior because the aggregates dispersed have similar thermal conductivity, nevertheless if the phases have a greater difference in thermal conductivity, the EMT could lose accuracy in the estimation of the value of this property.

Figure 3-15. Comparison of thermal conductivity results of LWAC by LWAC-TMM and analytical models.
Thermal numerical models from literature based on experimental results of LWAC are used to compare it with the results obtained by LWAC-TMM. Asadi et al. (2018) and American Concrete Institute committee 213 R-03 (2014a) proposed two relationships given by $0.0625e^{0.0015\rho}$ and $0.072e^{0.0125\rho}$, respectively, where $\rho$ is oven-dry density of concrete, the results are shown in Table 3-8. The model of Asadi et al. shows differences of -3.1 and 13.0% for 50 and 70% of LWA volume fractions, respectively. On the other hand, the model of ACI committee 213 R-03 shows differences of -11.4% and 6.9%, respectively. The differences between the results are explained by the different relationships assumed in the models that consider aggregates with different mineralogy, microstructure, grain size, cement content and pore structures (American Concrete Institute, 2014a).

Table 3-8. Comparison of thermal conductivities with Asadi et al. (2018) and American Concrete Institute (2014a) models.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>50%</td>
<td>927</td>
<td>0.259</td>
<td>0.251</td>
<td>0.229</td>
</tr>
<tr>
<td>70%</td>
<td>796</td>
<td>0.182</td>
<td>0.206</td>
<td>0.195</td>
</tr>
</tbody>
</table>

Therefore the PoSD does not seem to be a relevant factor in the thermal behavior of porous materials such as LWAC, and the EMT and Asadi et al. models seem to estimate accurately the thermal conductivity of LWAC based on few parameters, respect to values obtained with LWAC-TMM.

**b. Estimation of mechanical properties of lightweight aggregate concretes**

If the average pore size of full LWAC decreased from 161 to 25 $\mu$m, the compressive strength increased by 14.4 and 30.8% for LWA volume fraction of 50 and 70%, respectively, as shown in Figure 3-16. LWAC with 70% of volume fraction is mostly...
affected by the properties of aggregates, being more sensitive to the size of pores contained in the aggregates.

Figure 3-16. Estimation of compression strength of LWAC with LWA volume fraction equal to 50 and 70%, by LWAC-TMM.

The stress is mostly concentrated in the cement paste because its Young’s modulus is 29 times higher than that of the aggregates. For case C2 of concrete with 50 and 70% of LWA volume fraction the equivalent stress and equivalent plastic strain are exposed in Figure 3-17. The stress strain results for LWAC case C2 are shown in Figure 3-18. The C1 and C3 cases are in Appendix D.

The major strain was concentrated in the aggregates, due to the lower Young’s modulus, and the failure surface is mainly propagated through the aggregates, this is observed in the equivalent plastic strain (Figure 3-17 (b) and (d)). This behavior agrees with literature regarding the aggregates showing lower compressive strength than cement paste, thus failure is propagated through the aggregates (Zivkovic & Øverli, 2019) limiting the compressive strength of LWAC (Moreno et al., 2014). Yu et al. (2015) highlighted that a crack caused by compression over lightweight concrete expands along the
aggregates. Therefore, the effect of LWA on the mechanical behavior of concrete is significant.

Figure 3-17. Results of mechanical behavior of LWAC for pore size distribution C2. (a) Equivalent stress of LWAC with LWA volume fraction of 50%, (b) equivalent plastic strain field for LWA fraction of 50%, (c) equivalent stress for LWA fraction of 70%, (d) equivalent plastic strain field for LWA fraction of 70% (source: Ansys® Mechanical).
Figure 3-18. Result of stress-strain relationship of LWA for pore size distribution C2. (a) LWAC with LWA volume fraction of 50%, and (b) LWAC with LWA fraction of 70%.

Moreno et al. (2014) proposed a model to estimate the compressive strength of lightweight concrete based on three parameters: fresh density, relative volume of aggregates and mortar strength. However, this model applies to densities over 1100 kg/m$^3$ and a fraction of aggregates up to 50%. They also proposed a model for compressive strength by the expression $f_c = f_m 10^{\alpha V_{LWA}}$, based on the compressive strength of the matrix ($f_m$), LWA volume fraction ($V_{LWA}$) and an experimental weakness factor ($\alpha$). Chandra & Berntsson (2002) have proposed a biphasic model for LWAC given by $\log(f_c) = V_{LWA} \cdot \log(f_{LWA}) + (1 - V_{LWA}) \cdot \log(f_m)$, where $f_{LWA}$ is the compressive strength of aggregates. This last model has been validated by Bogas & Gomes (2013) for concretes with volume of LWA between 25 and 40%, showing that it is useful for concrete when the strength of the aggregate is lower than that of mortar.

The models of Moreno et al. (2014) and Chandra & Berntsson (2002) have been used to compare with the results obtained using LWAC-TMM. For a compressive strength of the cement paste matrix of 64.53 MPa, and an average compressive strength of aggregates equal to 3.47 MPa, a graph of the relationships between compressive strength and LWA
volume fraction are shown in Figure 3-19. The model of Moreno et al. matches well with the model of Chandra & Berntsson using a $\alpha$ equal to 1.27. This shows that both models have a similar behavior to estimate the compressive strength of LWAC with respect to the volume of aggregates.

Regarding the model of Chandra & Berntsson, for concrete with 50 and 70% of LWA volume fraction, the compressive strengths obtained were 14.96 and 8.34 MPa. These values overestimated the results obtained with the method of the present article in 29.3 and 43.3%, respectively. Otherwise, the model of Moreno et al. (2014) fit to the result for 50 and 70% of LWA fraction for an $\alpha$ value equal to 1.49, as shown in Figure 3-19. The estimation of compressive strength by LWAC-TMM and Moreno et al. models show differences less than 1.4%.

![Figure 3-19. Comparison of compressive strength results of LWAC by LWAC-TMM and the models of Chandra & Berntsson (2002) and Moreno et al. (2014).](image)

Although the $\alpha$ value of the model of Moreno et al. has been adjusted with only two values, it showed a good approximation for both LWA volume fractions. The model of
Chandra & Berntsson, (2002) did not show a good fit, which may be because this model is valid for LWA volume fraction up to 40% (Bogas & Gomes, 2013). Hence, the compressive strength of LWAC does not depend only of the aggregate fractions, it also varies with the geometry of the composite material and the model of Moreno et al. (2014) allows to fit this geometrical effect through the $\alpha$ factor. However, the model of Moreno et al. does not incorporate the effects of grading, porosity and PoSD separately, since the $\alpha$ factor is obtained from experimental results, therefore is the main limitation of their model.

Finally, the LWAC-TMM estimates the thermal conductivity and compressive strength of LWAC incorporating as input two main parameters that characterize the phase distribution: PoSD and grading. The PoSD does no show considerable effect over the thermal behavior of LWA or LWAC but has a high impact on their compressive strength.

3.5. Conclusions

This article aims to study the effect of different PoSDs on the thermal and mechanical behavior of LWAC. A finite element model developed in Ansys® was used to evaluate this effect directly. Some geometric parameters that are difficult to control accurately even in the laboratory conditions, such as: total porosity of concrete, thermal and mechanical properties of materials, location and grading of aggregates, were fixed, for the two cases evaluated (LWA volume fraction of 50 and 70%). The control of the geometric parameters allows to evaluate the PoSD impact on the concrete behavior directly through the model. The main conclusions reached are set out below.

Regarding the thermal behavior, the thermal conductivity did not change considerably as a function of pore size due to opposite effects of tortuosity and the heat flow pathways developed. The results show that the thermal conductivity in aggregates increases 3.3% when the average pore size decreased from 263 to 25 μm. Moreover, the thermal conductivity of the LWAC increases 1.4% or less changing the average pore size from 161 to 25 μm. However, compressive strength of the aggregate was affected strongly,
increasing 80.0% by changing the average pore size from 263 to 25 μm. While the compressive strength of LWAC increased 14.4 and 30.8% when average pore size of concrete decreased from 161 to 25 μm, for LWA fraction of 50% and 70%, respectively.

About the analysis of the pore size of Liaver® aggregates, the average pore size increased slower than the aggregate size: for each 1 μm that the diameter of the aggregate grows, the average of pore size grows 0.035 μm. This is advantageous according to the results of this paper, because even if larger aggregates are incorporated, pore size will grow to a lesser extent than the aggregate, this lower growth is accompanied by a better mechanical performance, increasing compressive strength.

LWAs with smaller pore size are recommended. They show higher compressive strength with a marginal variation of the thermal conductivity, smaller pores are found in smaller LWA. These have two advantages for LWAC: a better mechanical performance related to its smaller pore size, and on the other hand, a more homogeneous distribution of water delivery to continue the concrete curing process, when LWA are used as internal curing agents (Paul, 2010).

The main limitation of the study was the generation of geometry in the model, due to the high complexity of the microstructure of LWAC, the study considers a 2D model of two-stage to be able to incorporate the full concrete geometry. Future work should focus on evaluating the effect of the LWAC microstructure on a smaller scale, possible to obtain by Scanning Electron Microscope (SEM) images, or mercury intrusion porosimetry. Furthermore, the future research should consider the spatial distribution of pores in the aggregate to improve the aggregate thermal and mechanical behavior.
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A. Python script for the pore location in aggregate (and aggregates in concrete).

Example for concrete with 70% of LWA volume fraction

```python
import numpy as np
import matplotlib.pyplot as plt
plt.close('all')
from time import time

# INPUT

d = 14  # specimen edge length in mm
name = "Concrete_q_0.37"  # file name
initial_t = time()  # time calculator

DNP= [5.00E-01, 95 , 1.00E+00, 24 , 1.50E+00, 12 , 2.00E+00, 7 , 3.00E+00, 8 ]
gamma=0.04  # Wriggers & Moftah (2006)

DP1=[]  # Circle diameter array
NP1=[]  # circle type quantity array
for i in np.arange(int(len(DNP)/2)):
    DP1.append(DNP[2*i])
    NP1.append(DNP[2*i+1])
A_agrr=edge**2
A_pores_1=0

for j in np.arange(int(len(DNP)/2)):
    A_pores_1+=np.pi*(DP1[j]/2)**2*NP1[j]

# Aggregate fraction:"+str(round(A_pores_1/A_agrr*100,1))"%

def rand_xy(center, edge, r_pore):  # random location
e_agg=gamma*2*r_pore  # in aggregate use 0.0002 [mm]
delta_edge=e_agg+r_pore
x = delta_edge + np.random.uniform(0,1)*(edge-2*delta_edge)
y = delta_edge + np.random.uniform(0,1)*(edge-2*delta_edge)
return center[0]+x , center[1]+ y
```
def LP(center, edge, DNP):  # circles location
    DP = []  # circles diameter
    NP = []  # circles quantity
    for i in np.arange(int(len(DNP) / 2.)):
        DP.append(DNP[2 * i])
        NP.append(DNP[2 * i + 1])
    DP = DP[::-1]
    NP = NP[::-1]

    porous_rad = []  # list that adds the radius of each aggregate repeatedly
    for i in range(len(NP)):
        for j in range(NP[i]):
            porous_rad.append(DP[i] / 2)

    xyr_pores = np.zeros((1, 3))

    for r_pore in porous_rad:
        need_check = True
        while need_check:
            x, y = rand_xy(center, edge, r_pore)
            no_touch = True
            for i in xyr_pores:
                dist = np.sqrt((i[0] - x) ** 2 + (i[1] - y) ** 2)
                e_agg = gamma * min(2 * i[2], 2 * r_pore)  # in aggregate use 0.0002 [mm]
                if dist < i[2] + r_pore + e_agg:  # sume of each radius
                    no_touch = False
                    if no_touch:
                        pore = np.array([x, y, r_pore])
                        xyr_pores = np.append(xyr_pores, [pore], axis=0)
                        need_check = False
                        print(str(len(xyr_pores)) + " of " + str(sum(NP1)))
    return xyr_pores[1:,]

center = [0, 0]
a = LP(center, edge, DNP)
# figure print script
segment_number = 60
angle = np.linspace(0, 2*np.pi, segment_number+1)
x = np.array([0, edge, edge, 0, 0])
y = np.array([0, 0, edge, edge, 0])
plt.plot(x, y, color="red", markersize=1)

for pore in np.arange(len(vect_x)):
    rad_pore = a[pore, 2]
    angle = np.linspace(0, 2*np.pi, segment_number+1)
    x = rad_pore * np.cos(angle) + vect_x[pore]
    y = rad_pore * np.sin(angle) + vect_y[pore]
    plt.plot(x, y, color="blue", markersize=1)

title_print = name + "_" + str(edge) + "mm_" + str(round(A_pores_1/A_aggr*100,1)) + "%_gamma_" + str(gamma) + "_" + str(sum(NP1)) + "_units"
plt.grid()
plt.title(title_print)
plt.xlabel("X")
plt.ylabel("Y")
plt.gca().set_aspect('equal')
plt.show()

final_t = time()
print("time:" + str(final_t - initial_t) + " seg.")
f = open(title_print + ".txt", "w+")
f.write("[
"
for i in range(len(a)):
    f.write(str(a[i][0]) + ", " + str(a[i][1]) + ", " + str(a[i][2]) + ", \n, [
f.close()
B. Python script for geometry generation of LWAC and LWA in SpaceClaim tool of Ansys ® Mechanical release 2020-R1

```python
# Python Script, API Version = V18

# array with location [x-y] and radius [r] of the circle in mm [x,y,r]
xyr=[[x1, y1, r1], [x2, y2, r2], ...]  # add the location of the circles before run

edge=14  # specimen edge length in mm
z2=edge/20.

for i in xyr:
    # Sketch Circle
    plane = Plane.PlaneZX
    result = ViewHelper.SetSketchPlane(plane)
    origin = Point2D.Create(MM(i[0]), MM(i[1]))
    result = SketchCircle.Create(origin, MM(i[2]))
    # EndBlock

    # Solidify Sketch
    mode = InteractionMode.Solid
    result = ViewHelper.SetViewMode(mode, Info1)
    # EndBlock

    # Extrude 1 Face
    selection = Facel
    options = ExtrudeFaceOptions()
    options.ExtrudeType = ExtrudeType.Add
    result = ExtrudeFaces.Execute(selection, MM(z2), options, Info2)
    # EndBlock

    for i in xyr:
        # Sketch Circle
        plane = Plane.PlaneZX
        result = ViewHelper.SetSketchPlane(plane)
        origin = Point2D.Create(MM(i[0]+2*edge), MM(i[1]))
        result = SketchCircle.Create(origin, MM(i[2]))
        # EndBlock

    # Sketch Rectangle
    plane = Plane.PlaneZX
    result = ViewHelper.SetSketchPlane(plane)
    point1 = Point2D.Create(MM(2*edge), MM(0))
    point2 = Point2D.Create(MM(3*edge), MM(0))
    point3 = Point2D.Create(MM(3*edge), MM(edge))
```
result = SketchRectangle.Create(point1, point2, point3)
# EndBlock

# Solidify Sketch
mode = InteractionMode.Solid
result = ViewHelper.SetViewMode(mode, None)
# EndBlock

# Extrude 1 Face
Selection = Selection.Create(GetRootPart().Bodies[len(xyr)].Faces[len(xyr)])
options = ExtrudeFaceOptions()
options.ExtrudeType = ExtrudeType.Add
result = ExtrudeFaces.Execute(selection, MM(z2), options)
# EndBlock

# Delete Selection
selection = Selection.Create(GetRootPart().Bodies[len(xyr)])
result = Delete.Execute(selection)
# EndBlock

# Translate Along Z Handle
selection = Selection.Create(GetRootPart().Bodies[len(xyr)])
direction = Direction.DirZ
options = MoveOptions()
result = Move.Translate(selection, direction, MM(-2*edge), options)
# EndBlock
C. Methodology of micro-CT scan image processing by CTAn software

**Step 1:** Upload micro-CT scan images in .bmp format to CTAn.

**Step 2:** Go the *regions of interest* option. Select manually the region of interest (ROI) in the various images where the aggregate is presented, a collection of images generates the volume of interest (VOI). Save the VOI.

**Step 3:** Go to *custom processing* option. Specify the *thresholding*, it generates a binary image to differentiate the material to analyze. Within the Plug-In *thresholding*, selected *global* and the range 1 to 255.

**Step 4:** Select the Plug-In *morphological operations*, and the *erosion*, the *3D space* option, and select 1-unit radius, removing the more external pixel from the ROI.

**Step 5:** Add *bitwise operation* and incorporate *image= copy region of interest*.

**Step 6:** Add *reload* and choose *region of interest*.

**Step 7:** Add *bitwise operations* and incorporate *region of interest= region of interest sub image*.

**Step 8:** Add *reload*. Select *image*.

**Step 9:** Add *thresholding*, select *global*, in the range 1 to 255.

**Step 10:** Add *despeckle*, and select:
where the value of voxels depends directly on the noise presented by the image and the size of particles that are observed to be not a real part of the sample.

**Step 11:** Add bitwise operations. Select image=image or region of interest.

**Step 12:** Add reload and select region of interest.

**Step 13:** Add thresholding, choose global, and select the range 0 to 1. With this new range the not solid material is selected, i.e., the pores of the aggregate are selected to evaluate the size distribution.

**Step 14:** Add 3D analysis. Activate additional values and select only structure thickness. After this step, the analysis of pore selection will be carried out, obtaining total porosity and pore size distribution.
D. Finite element meshing and thermal and mechanical results of LWA and LWAC by LWAC-TMM

i. Finite Element Meshing for LWA

Figure D-1. Finite element meshing for LWA with average pore size equal to 25 μm. (a) Complete specimen of 0.2 mm, and (b) zoom of the specimen meshing (source: Ansys® Mechanical).

Figure D-2. Finite element meshing for LWA with average pore size equal to 144 μm. (a) Complete specimen of 1.1 mm, (b) and zoom of the specimen meshing (source: Ansys® Mechanical).
Figure D-3. Finite element meshing for LWA with average pore size equal to 263 μm. (a) Complete specimen of 2.2 mm, (b) and zoom of the specimen meshing (source: Ansys® Mechanical).

ii. Finite Element Meshing for LWAC

Figure D-4. Finite element meshing for LWAC with 50% of LWA volume fraction. (a) Complete specimen of 14 mm, (b) and zoom of the specimen meshing (source: Ansys® Mechanical).
Figure D-5. Finite element meshing for LWAC with 70% of LWA volume fraction. (a) Complete specimen of 14 mm, (b) and zoom of the specimen meshing (source: Ansys® Mechanical).
iii. Results of thermal behavior of LWACs

![Figure D-6](source: Ansys® Mechanical)

(a) Temperature field of LWAC with LWA volume fraction of 50%, (b) heat flux for LWA fraction of 50%; (c) temperature field for LWA fraction of 70%, and (d) heat flux for LWA fraction of 70% (source: Ansys® Mechanical).
Figure D-7. Results of thermal behavior of LWAC for pore size distribution C3. (a) Temperature field of LWAC with LWA volume fraction of 50%, (b) heat flux for LWA fraction of 50%; (c) temperature field for LWA fraction of 70%, and (d) heat flux for LWA fraction of 70% (source: Ansys® Mechanical).
iv. Results of mechanical behavior of LWACs

Figure D-8. Results of mechanical behavior of LWAC for pore size distribution C1. (a) Equivalent stress of LWAC with LWA volume fraction of 50%, (b) equivalent plastic strain field for LWA fraction of 50%, (c) equivalent stress for LWA fraction of 70%, (d) equivalent plastic strain field for LWA fraction of 70% (source: Ansys® Mechanical).
Figure D-9. Results of mechanical behavior of LWAC for pore size distribution C3. (a) Equivalent stress of LWAC with LWA volume fraction of 50%, (b) equivalent plastic strain field for LWA fraction of 50%, (c) equivalent stress for LWA fraction of 70%, (d) equivalent plastic strain field for LWA fraction of 70% (source: Ansys® Mechanical).
Figure D-10. Result of stress-strain relationship of LWA for pore size distribution C1. (a) LWAC with LWA volume fraction of 50%, and (b) LWAC with LWA fraction of 70%.

Figure D-11. Result of stress-strain relationship of LWA for pore size distribution C3. (a) LWAC with LWA volume fraction of 50%, and (b) LWAC with LWA fraction of 70%.