ORIGINAL ARTICLE

The Effect of Porosity and Contact Angle on the Fluid Capillary Rise for Bone Scaffold Wettability and Absorption

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ABSTRACT

Introduction: Wettability and fluid absorption are two important bone scaffold characteristics that determine proper cell attachment and flow of nutrition and oxygen. To imitate the human bone structure, the current study was carried to investigate the effect of the porosity of bone scaffold and contact angle of the fluid by evaluating the height of capillary rise. **Methods:** The structure was simplified based on the circle and square pattern and evaluated using Computational Fluid Dynamic (CFD). Porosity and contact angle were varied from 50% to 80%, while the contact angle ranged from 0 degrees to 60 degrees. The result was evaluated further using statistical analysis. **Results:** The CFD result was in agreement with Jurin's law (9% error). The height of capillary rise was found to be excellent for the square pattern, while the circle was found to work across all the investigated parameters better. The porosity was correlated with the height of capillary rise (r = -0.549). The strongest correlation happened to contact angle (r = -0.781). **Conclusion:** The study concludes that water absorption and wettability can be altered and improved based on porosity. Meanwhile, the height of capillary rise depends strongly on the contact angle.

Keywords: Bone scaffold, Capillary Rise, Pore pattern, Porosity, Contact angle

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INTRODUCTION

Recently the study of bone scaffolds is receiving much attention as the scope of the study is related to regeneration of bone tissue researches (1, 2). Bone scaffold contains organic and non-organic substances with complex and organized microstructure frameworks. Besides, the bone scaffold is designed to allow and stimulate the attachment of cells responsible for bone regeneration on its surfaces. Several factors need to be considered in designing bone scaffolds, such as biocompatibility, biodegradability, and mechanical properties (3). Wettability and fluid absorption are two essential characteristics of the bone scaffold related to the bone scaffold's biocompatibility. Wettability is affected by the surface properties of the material. The characteristic can be classified as either hydrophilic or hydrophobic and is influenced by factors such as the surface tension of the liquid, contact angle of the solid surface, and porosity level of the bone scaffold (4). On the other hand, absorption is related to the ability of the structure to absorb liquid and keep it inside.

Porosity with the proper pore size and interconnections between microstructure forms a suitable environment to attract cell migration, facilitate the flow of nutrients, and supply oxygen (5-7). Besides, its mechanical properties allow bone scaffolds to withstand the applied working load (8-10). Excellent bone growth requires suitable porosity while promoting advantages to the cell. Several studies showed that suitable pore size and interconnections between bone microstructure improve regeneration performance. Danilevicius et al. reported a higher efficiency of cell ingrowth on the 3D scaffold up to 86% of structure porosity (5). Even in the study, there were a few porosities tested from 82% to 90%, only certain porosity significant to encourage cell growth. Besides the mentioned advantages, increasing the structure porosity affect the compression strength which jeopardized the mechanical strength of the bone scaffold structure (11).

Porosity and pore size plays an essential role in cell migration and attachment. On average porosity of the bone scaffold range between 50% to 90% and the pore size range between the smallest of 150um to the larger 1200 um (11). The study done by Ciara M. Murphy et al showed higher pore size of 325 μm successfully increase the number of cell attachments compared to lower pore size which then lead to encouraging bone scaffold growth (12). This situation happens because the bigger pore size allows a higher number of cells to migrate far away and infiltrate the bone scaffold. Based on these previous studies, the current research continues to understand the effects of porosity which is by modifying the scaffold structure and pore size. At the same time relate those aspects to the fluid capillary performance to provide better insights about wettability and fluid absorption of the bone scaffold.

The enhancement in the wettability and absorption provides advantages to cell attachment, cell proliferation, and cell-scaffold interactions (7, 13, 14). Therefore, this study was carried out to investigate the effect of the porosity bone scaffold and contact angle of the fluid by evaluating the height of capillary rise. Two-dimensional models were used by simplifying the porous structure based on smooth and sharp curves besides varying its size to alter structure porosity.

MATERIALS AND METHODS

The study was divided into three sections; i) Computational Fluid Dynamic (CFD) validation of capillary rise, ii) effect of bone scaffold porosity and contact angle of the fluid on the height of capillary rise, and iii) statistical analysis of the investigation parameters. All the applied methods were used to elucidate the study interest comprehensively. The work was different from the previous work as most of the previous studies work with CFD focus on the permeability of the scaffold which is the ability of the liquid to pass through the structure from inlet to outlet (15-17). For instance, Davar Alie (2019) and Hasan Basri et al. (2017) simulate the flow within a porous scaffold by setting the CFD with several velocities at the inlet and zero pressure at the outlet (17, 18). Meanwhile, the wettability causes the fluid to flow within the structure due to the surface tension and contact angle between fluid and solid surface as a boundary condition. This condition can be achieved at a microfluidic level.

Validation of Computational Fluid Dynamic

The CFD was validated using a two-dimensional (2D) model of capillary rise in a small tube vessel according to Jurin's law (19). The theory explains the force balance between the weight of the rising fluid and its surface tension as the rise occurs due to capillary action.

Capillary rise Equation

Jurin's law or the theory of capillary rise mentions that the height of capillary rise in a tube is inversely proportional to the tube's internal diameter or pore size (19, 20). The height of capillary rise depends on the surface tension of the fluid. When a fluid touches the wall and gets wet on the surface, it climbs upward against gravity (20). In the scope of this study, the fluid rises vertically and stops at the maximum height. The maximum height can be calculated as the magnitude of the force from the surface tension component equal to the weight of the raised fluid, or in simple words, force equilibrium is achieved. The situation can be represented by Equation 1.

$$\text{Height of capillary rise, } h = \frac{4\gamma\cos\theta}{\rho g d} \qquad \text{Equation 1}$$

Where γ is the surface tension of the fluid in contact with the bone scaffold surface, θ is the fluid contact angle, ρ is the density of the fluid, g is gravity acceleration, and d is the diameter of the tube used in the study.

CFD model and description

CFD validation was carried out using the COMSOL Multiphysics software package (COMSOL Inc., Sweden). The fluid was modelled as a 2D model using an internal model builder provided by the software, as illustrated in Figure 1(a). The fluid domain was modelled into two parts, fluid reservoir and tube vessel. These parts then form a union using the initial interface boundary condition. Water properties were assigned to the fluid reservoir part, and air properties were assigned to the tube vessel to represent the pore at the initial condition as in Table I. The fluid domain with two material properties was set up to initiate surface tension of the fluid interface and Two-Phase flow. Water was chosen as the fluid medium as reported by Jeremy C.M. Teo et al. to investigate the permeability of the cancellous bone (16).

Table I : Material properties of water

Item	Detail
Surface tension (N/m)	72.1
Density (kg/m3)	1000
Viscosity (Pa.s)	8.90×10^{4}
Contact angle (degree) [14]	25

The model was built with a 1 mm x 3 mm size for the water reservoir part and 30 mm x 1 mm for the tube vessel part. Inlet is then assigned on the vertical side of the water reservoir model, as shown in Fig. 1(a). The normal flow direction with zero pressure was set to the inlet. Zero pressure was then assigned at the outlet, and a no-slip wetted wall with a 25-degree contact angle was assigned to the model. Through the setting, water flowed purely by the surface tension of the fluid without presenting any external forces. The magnitude of the contact angle is then applied directly to the solution of the matrix during the solving process. Hexa mesh element types with a maximum and minimum size of 0.08 and 0.006 mm were used to discretize the fluid domain.

The model was discretized using linear element order to consider the stable characteristic of the surface tension according to phase field. Step time of 4.0 x 10-4 s and the total time of 0.3 s were applied to run this computational

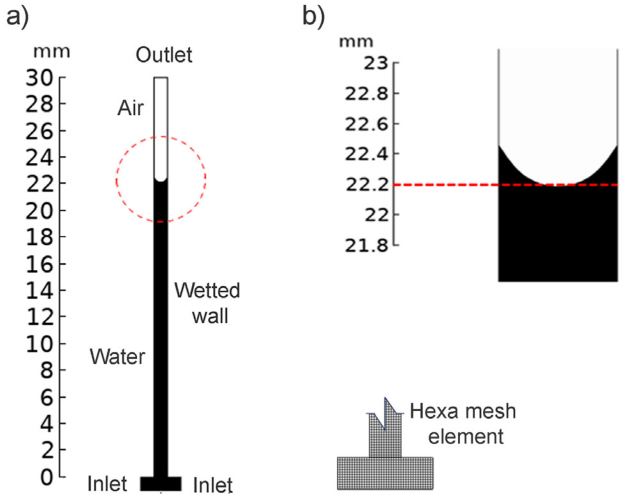

Figure 1: Computational fluid dynamic setting for the capillary flow study of the bone scaffold (A) Boundary condition of the CFD for tube vessel and meshing element, and (B) Height of capillary rise at it achieved the equilibrium between surface tension and weight of the water.

study. The solution was managed based on laminar flow, and the surface tension between the water-air interface was managed by including the surface tension in the momentum equation and its gradient effect. Data collection was done by taking the height of the lower point of the liquid-water interface as in Fig. 1(b).

Effect of porosity and contact angle on the capillary rise of the bone scaffold

The simplified bone scaffold was built as 2D with two different patterns, as in Fig. 2. These two patterns represent the smooth and sharp curve of the human bone, which later these patterns were evaluated for their effect on the height of capillary rise using statistical analysis.

The contact angle that ranged lower than 90 degrees is considered in this section to include hydrophilic characteristic which allows water to wet and climb on

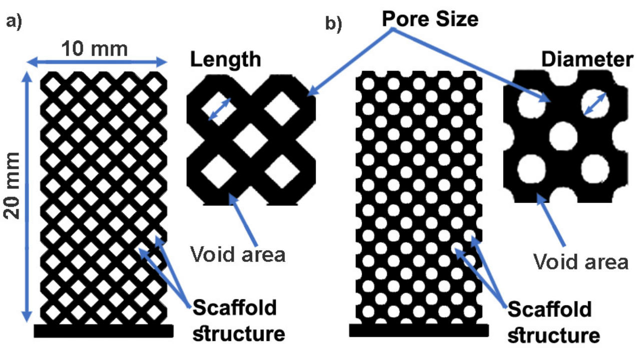

Figure 2: Size of specimen and pore pattern of the bone scaffold where the blade region represents the void area that will fill by fluid of the capillary rise (A) square pattern, and (B) circle pattern.

the wall. Therefore to investigate the contact angle effect, 0 degrees, 25 degrees, and 60 degrees were selected to represent highly hydrophilic, normal hydrophilic, and lower hydrophilic, respectively.

The simplified bone scaffold was modelled with the dimension of 10 mm x 20 mm. The fluid reservoir is still included in the CFD study as a validation section to allow fluid to be absorbed freely by the sample model and rise to a specified height to fulfil Equation 1. The porosity was altered by increasing and decreasing the pore size by changing the length of the square and the circle's diameter of the scaffold structure from 0.6 mm to 1.13 mm (refer to Figure 2). Eventually forming the structure porosity of 50 %, 60 %,70 % and 80 %. As the study focused on the 2D model, the porosity was calculated based on the ratio of the void area and total area (Equation 2). To consider three important parameter related factors (simplified bone scaffold pattern, porosity and contact angle), a total of 24 simulations were carried out, and the result was then plotted in two separate 3D graphs.

The equation below was altered from the 3D model, which in the 3D model, the volume is considered in the calculation. However, in this study, the model's thickness is assumed to be consistent and can be ignored.

$$\text{Porosity}, \varnothing = \frac{\text{Void area}, V_v}{\text{Total area}, V_T} \qquad \text{Equation 2}$$

Statistical test

Statistical analysis was carried out for data post-processing to examine further all the parameters involved. Two types of the test, (i) Pearson correlation test and (ii) T-test, were selected using IBM SPSS Statistics 23 (IBM Corp, USA) at 0.05 significance level. In addition, the correlation for the porosity of bone scaffold and fluid's contact angle toward the height of capillary rise in simplified bone scaffold was tested for all 24 CFD data.

RESULTS

Validation

It is found that the height of the capillary rise is in agreement with Jurin's law, as provided in Table II and Fig. 1(b). The percentage of error between Jurin's law and CFD is less than 10% and acceptable for further analysis. The acceptable decision was made based on the previous study related to the capillary flow done by Argьelles-Vivas et. al., which was 20% on average in their study. The result was two times higher than the current result, which shows its acceptable level (21). It is expected that the disparity in the present study happens due to element order, and its one of the study limitations since the applied element order was the most compatible element to cope with the complicated bone scaffold models. Due to this issue, the first-order

Table II: Height of capillary rise

Method of study	Height of capillary rise
Jurin's law [12]	24.4 mm
Current CFD study	22.2 mm
Percentage of error	9 %

Lagrange hexa element with the fine element size setting was preferred.

The simulation study captured that the capillary flow rises faster at the beginning, but once the water reaches the higher position, it then climbs slowly before it stops as the magnitude of the surface tension was equal to the weight of the fluid.

Parameters study on the scaffold structure

Fig. 3 shows the 3D graph of two simplified bone scaffold patterns. The data was collected by the average height of the highest and lowest point of the capillary, as illustrated on the bone scaffold model. In general, this model applied a similar understanding based on the model from the validation section. In this section, the difference is that a single water column was divided into tiny micro-pore according to the porosity. The equilibrium was achieved as the weight of the water-filled micro-pore equal to the surface tension of the water touched the pore structure. Based on that understanding, the height of capillary rise for the circle pattern overall was higher about 3 % across the model than the square pattern.

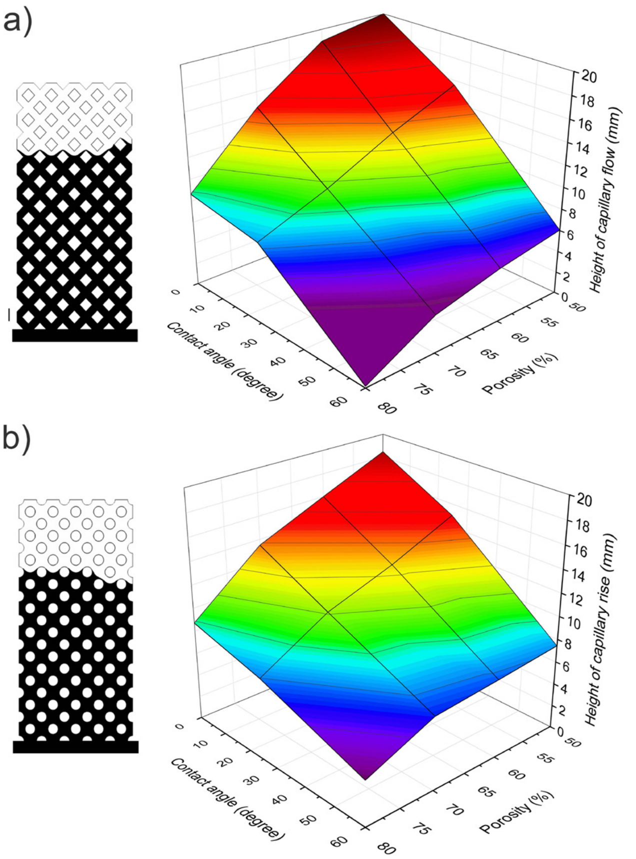

Figure 3: Three-dimensional data of the height of capillary rise. (A) The effect of the bone scaffold porosity and contact angle of the fluid for a square pattern of the simplified bone scaffold, and (B) the effect of the porosity and contact angle for the circle pattern of the simplified bone scaffold.

Statistical analysis

Statistical analysis for 24 CFD validations was carried out to see the correlation of the parameters to the study interest. It is found that the porosity correlates to rise with the coefficient ($r = -0.549$ $p < 0.05$ %). The strongest correlation was between contact angle and capillary rise height ($r = -0.781$, $p < 0.05$). Both of the parameters inversely impacted the absorption and wettability of the bone scaffold. Meaning a lower value of porosity and contact angle will increase the capability to raise the fluid.

DISCUSSION

The square pattern of the scaffold structure shows the most excellent capillary capability as it can reach 20mm for 50 % porosity of 0-degree contact angle. It was driven by the smallest and consistent pore size of 424 µm between other investigated porosity. This gap is representing the distance between scaffold walls of the void area as the size of the scaffold structure was altered from 0.6 mm to 1.13 mm (Refer Fig 2). The square pattern shows the lowest capillary capability for the 80 % porosity of 60-degree contact angle. Fluid hard to climb on the wetted wall because of the pore size of 784 µm which was double than mentioned before at 424 µm. The circle pattern even though perform less than square because of overall pore size was 5 % bigger ranged from 448 µm to 815 µm while the square pattern went from 424 µm to 784 µm, but it was found to be consistent, which capable of raising the fluid for all the study parameters. Eventually, pore size plays an essential aspect in the height of the capillary rise as it affects how fluid attaches and climbs on the wetted wall.

The capillary capability may reduce if the fluid change from water to the simulated body fluid as the surface tension of the body fluid is lower than water. The surface tension of the blood for example is 55 N/m which is 20 per cent lower than water at 72.1 N/m, thus the capability of the fluid will reduce 20 per cent lower.

The height of capillary rise from this CFD study is in agreement with the study done by Daniel S. Oh et al. (14). In their study, the same scaffolds with dimensions of 20 mm x 10 mm and porosity ranged from 79 % to 86 % were used. The study mentioned that the height of capillary rise was 15 mm for human allograft and 20 mm for micro-channel and nano-pores scaffold, which was also captured in this study using the 2D model. Besides, Daniel S. Oh [14] also supported the obtained result for the pore size aspect. With a similar width of 10 mm, the height of the capillary rise obtained is 15 mm for the specimen with 350 µm pore size and 10 mm for 750 µm pore size, which concluded. Smaller pore size shows the higher capillary rise, while larger pore size shows the lower capability of the capillary rise.

As mentioned in the methodology section, the scaffold pattern, either square or circle, is one of study interest and tested based on a T-test. Independent T-test was carried out at a 95 % confidence level. The mean value and standard deviation for square are Ms = 10.54 sd = 4.49, and the mean value and standard deviation of the circle pattern are Mc = 10.42 sd = 6.06. The obtained result was not statistically significant difference at degree of freedom of 22 (tt = -0.061, dr = 0.952, $p < 0.05$). It is found that the smooth and sharp corners, respectively represented by square and circle, do not contribute much to the height of the fluid rise capability. This insignificant difference happens because both of the patterns are designed to have a similar aspect ratio of its side length for square and major and minor axis for circle.

CONCLUSION

The investigation of simplified bone structure with a variety of parameters studied was successfully carried out. The study concludes that water absorption and wettability can be altered and improved based on porosity and contact angle. The porosity is associated with pore size; changing the pore size will adjust the bone scaffold porosity. Meanwhile, the height of capillary rise, which influences the wettability, depends strongly on the contact angle. The scaffold pattern, either square or circle representing a smooth and sharp corner, does not contribute to the study interest, especially for the geometry with a similar aspect ratio.

REFERENCES

1. Samavedi S, Whittington AR, Goldstein AS. Calcium phosphate ceramics in bone tissue engineering: a review of properties and their influence on cell behavior. Acta biomaterialia. 2013;9(9):8037-45.
2. Li X, Wang L, Fan Y, Feng Q, Cui FZ, Watari F. Nanostructured scaffolds for bone tissue engineering. Journal of Biomedical Materials Research Part A. 2013;101(8):2424-35.
3. Ghassemi T, Shahroodi A, Ebrahimzadeh MH, Mousavian A, Movaffagh J, Moradi A. Current concepts in scaffolding for bone tissue engineering. Archives of bone and joint surgery. 2018;6(2):90.
4. Menzies KL, Jones L. The impact of contact angle on the biocompatibility of biomaterials. Optometry and Vision Science. 2010;87(6):387-99.
5. Danilevicius P, Georgiadi L, Pateman CJ, Claeyssens F, Chatzinikolaidou M, Farsari M. The effect of porosity on cell ingrowth into accurately defined, laser-made, polylactide-based 3D scaffolds. Applied Surface Science. 2015;336:2-10.
6. Lien S-M, Ko L-Y, Huang T-J. Effect of pore size on ECM secretion and cell growth in gelatin scaffold for articular cartilage tissue engineering. Acta biomaterialia. 2009;5(2):670-9.
7. O'Brien FJ, Harley BA, Waller MA, Yannas IV, Gibson LJ, Prendergast PJ. The effect of pore size on permeability and cell attachment in collagen scaffolds for tissue engineering. Technol Health Care. 2007;15(1):3-17.
8. Limmahakhun S, Oloyede A, Sitthiseripratip K, Xiao Y, Yan C. 3D-printed cellular structures for bone biomimetic implants. Additive Manufacturing. 2017;15:93-101.
9. Chen Y, Frith JE, Dehghan-Manshadi A, Attar H, Kent D, Soro NDM, et al. Mechanical properties and biocompatibility of porous titanium scaffolds for bone tissue engineering. Journal of the mechanical behavior of biomedical materials. 2017;75:169-74.
10. Baptista R, Guedes M. Morphological and mechanical characterization of 3D printed PLA scaffolds with controlled porosity for trabecular bone tissue replacement. Materials Science and Engineering: C. 2021;118:111528.
11. Prasadh S, Wong RCW. Unraveling the mechanical strength of biomaterials used as a bone scaffold in oral and maxillofacial defects. Oral Science International. 2018;15(2):48-55.
12. Murphy CM, O'Brien FJ. Understanding the effect of mean pore size on cell activity in collagen-glycosaminoglycan scaffolds. Cell Adh Migr. 2010;4(3):377-81.
13. Goddard JM, Hotchkiss J. Polymer surface modification for the attachment of bioactive compounds. Progress in polymer science. 2007;32(7):698-725.
14. Oh DS, Kim YH, Ganbat D, Han M-H, Lim P, Back J-H, et al. Bone marrow absorption and retention properties of engineered scaffolds with micro-channels and nano-pores for tissue engineering: a proof of concept. Ceramics International. 2013;39(7):8401-10.
15. Ali D, Ozalp M, Blanquer SB, Onel S. Permeability and fluid flow-induced wall shear stress in bone scaffolds with TPMS and lattice architectures: A CFD analysis. European Journal of Mechanics-B/Fluids. 2020;79:376-85.
16. Teo JC, Teoh SH. Permeability study of vertebral cancellous bone using micro-computational fluid dynamics. Computer Methods in Biomechanics and Biomedical Engineering. 2012;15(4):417-23.
17. Basri H, Nasution JD, Syahrom A, Sulong MA, Saad APM, Prakoso AT, et al. The effect of flow rate characteristic on biodegradation of bone scaffold. Malaysian Journal of Fundamental and Applied Sciences. 2017;13:546-52.
18. Ali D. Effect of scaffold architecture on cell seeding efficiency: A discrete phase model CFD analysis. Computers in biology and medicine. 2019;109:62-

9.
19. Liu S, Li S, Liu J. Jurin's law revisited: Exact meniscus shape and column height. The European Physical Journal E. 2018;41(3):1-7.
20. Barozzi GS, Angeli D. A note on capillary rise in tubes. Energy Procedia. 2014;45:548-57.
21. Argьelles-Vivas F, Babadagli T. Gas (air)–heavy oil displacement in capillary media at high temperatures: A CFD approach to model microfluidics experiments. Chemical Engineering Science. 2016;140:299-308.