CHARACTERIZATION OF FLUID DYNAMIC PROPERTIES OF SCHWARZ'S PRIMITIVE CELLULAR MATERIALS

Che-Cheng Chang, Shewei Zhou, Yuhang Chen and Qing Li

School of Aerospace, Mechanical and Mechatronic Engineering, J07, University of Sydney, NSW 2006, Australia.

Introduction

Recent studies on design optimization of cellular composites have identified Schwarz's primitive surface (Schwarz-P) is a potential microstructure [1, 2]. Schwarz-P structure can provide maximised mechanical properties in terms of solid, fluid, heat and electromagnetic problems [3]. Particularly, it is of great interest in the design of scaffold architecture where the multi-objective optimization is required to resolve property confliction.

Schwarz-P surface is a mathematically fully-defined minimal surface. It can be organized periodically along three Cartesian coordinates, dividing the space into two equal and identical volumes and each representing the solid phase and the fluid phase of a scaffold. Such volumetric division can be modified by adding a constant term, which in turn tailors the porosity of the scaffold.

This paper aims to characterize mass flow properties, wall shear stress (WSS), and the energy dissipation rate in relation to the variable scaffold porosity. Current research in scaffold microstructure design and simulation has been widely adopting brick elements to take advantage of its versatility in homogenization and optimization algorithm [2, 4]. Homogenization is commonly applied in post-processing to normalize the computational outputs [2, 4, 5]. However, the accuracy of such models inevitably suffers as a result of the zig-zag surface geometry at relatively low resolution. This paper will attempt to overcome this problem by means of smooth surface modelling with non-brick elements.

Methods

In this paper, the modified Schwarz-P surface is defined by the following equation:

$$\cos(x) + \cos(y) + \cos(z) + k = 0, -1 < k < 1 \quad (1)$$

The Schwarz-P models were generated and exported in triangulated STL format.

The computational fluid dynamics (CFD) simulation process was performed on the representative volumes on a commercial CFD platform (ANSYS ICEM CFD, Fluent). The triangulated models were meshed using tetrahedron elements. The flow was governed by the periodic boundary conditions and was then solved for a given constant pressure drop (1Pa/m) in the x-direction; all y/z inlets and outlets were defined as symmetry.

The raw solution data were used to compute the homogenized properties. In the tissue engineering case scenario, the advection term was assumed negligible given that the Reynolds number is relatively small, the constitutive equation for the fluid governed by Stokes flow can be written as:

$$\sigma = -p + \varepsilon^2 \mu \partial u_k \quad (2)$$

where $\varepsilon = L_1/L_0$; subscripts 0 and 1 denote global and local scales, respectively. The weak form of expanded homogenization is expressed in asymptotic expansion as follows:

$$\int_V \partial^{1T} \mu D \partial^1 u^0 dV = \int_V \partial^{0T} p^0 dV \quad (3)$$

The energy dissipation rate is computed according to the following formula:

$$E = u^T [K] u \quad (4)$$

The diffusivity matrix K is obtained from integration:

$$K = \mu \int_\Omega B^T D B \cdot d\Omega \quad (5)$$

where $[B] = \partial^1 = \partial N_j \partial X_i$, j is the number of nodes per element; and i is the degree of freedom (x,y,z). [B] represents the derivative of the shape functions N_i, which depend on the elemental nodal coordinates. In an unstructured mesh (e.g. in tetrahedron elements), the diffusivity matrices differ from element to element.

Results and Discussion

The porosity of the Schwarz-P construct as a function of k can be approximated using the following formula:

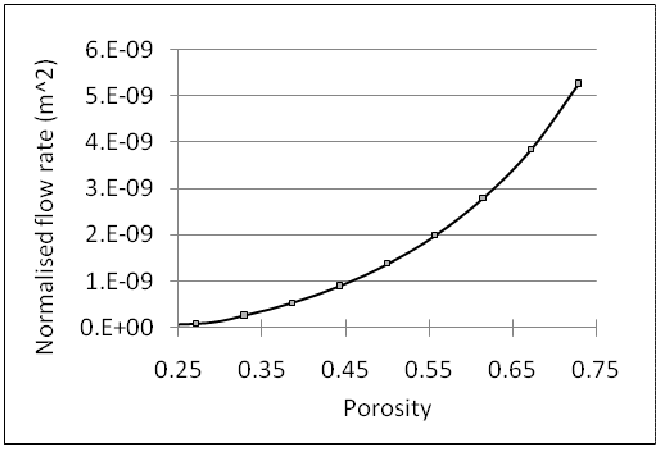

Fig. 1 Mass flow rate at various porosity

$$\text{porosity} = 0.286 \times \text{k} + 0.5, -1 < k < 1 \quad (6)$$

The porosity is virtually a linear function of the constant *k*. The constraint for k is often required to maintain the continuity of both fluid and solid phases.

Fig. 1 shows a non-linear relationship between mass flow rate and porosity. A power law formula can be derived from curve-fitting as:

$$\dot{m} = a \times (porosity - 0.213)^{2.28} \quad (7)$$

The sole coefficient a is a function of viscosity, density, pressure drop, and geometric parameters. The exact value of a is irrelevant to the constitutive equation for incompressible flow. The constant inside the bracket is an x-offset at which point the flow domain becomes discontinuous ($k = -1$). Darcy's Law is applied to obtain a normalised flow rate:

$$\kappa = \dot{m}\frac{\mu}{\rho A}\frac{\Delta x}{\Delta P} = (2.33e-8)(por - 0.213)^{2.28} \quad (8)$$

where μ is the fluid viscosity; ρ is the fluid density; ΔP is the pressure drop across the representative volume of element (RVE); A and $\triangle x$ are the cross-sectional area and the length of the RVE, respectively.

The WSS as shown in Fig. 2 suggests a relatively steady and linear increase in the maximum WSS across most of the porosity range; the steep decrease in WSS at low porosity is attributed to the rapidly reducing flow rate as the pores become isolated. In contrast, the minimum WSS follows a non-linear increasing pattern with a larger gradient compared to the maximum values. Note that the trend reverses at both ends of porosity scale.

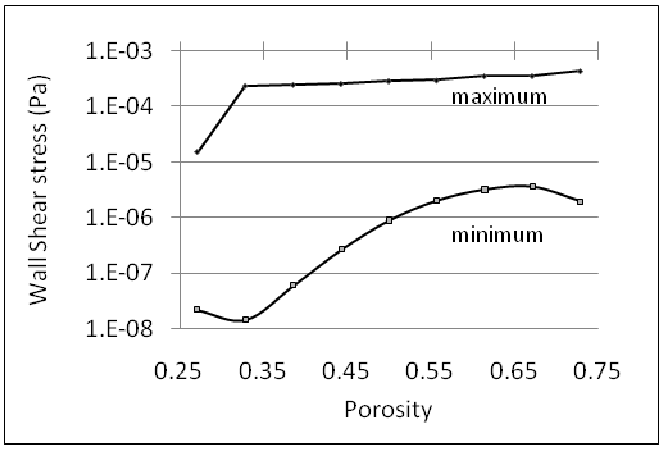

Fig. 2 Wall shear stress at various porosity

The homogenized energy dissipation rate shown in Fig 3 follows a trend similar to that of the mass flow rate, with a power value fairly close to that found in equation (7). The use of simple power law sufficiently relates different variables to the porosity. For the given flow and boundary conditions, high porosity is correlated to high flow rate, leading to a high energy dissipation rate. The coefficient in front of the porosity term also depends on the modelling parameters and the intrinsic fluid properties as given in equation (8).

The integration of energy can be expressed directly as functions of elemental nodal coordinates (x,y,z). Unlike the homogenization process of brick elements, translation to natural coordinates is not required.

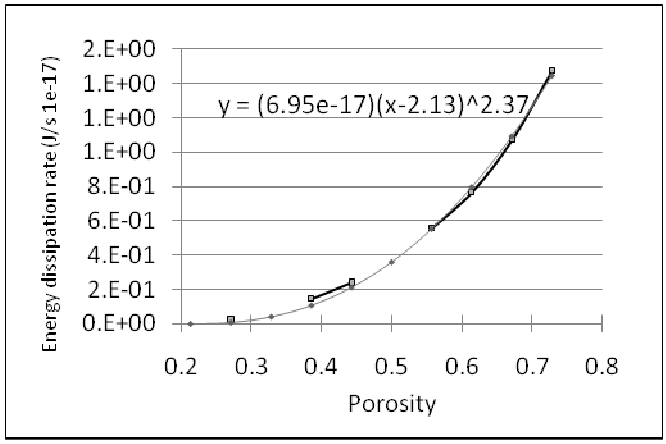

Fig. 3 Homogenized energy dissipation rate by curve fitting

Conclusion

The "smooth" Schwarz-P structures were tested and characterized through the CFD simulation and homogenization process by asymptotic expansion. The study demonstrates the viability of tetrahedron mesh in the creation of geometrically accurate CFD models and applicability of the homogenization process. The increase in fluid flow rate and energy dissipation rate can be represented by simple power law in terms of porosity. The maximum and minimum wall shear stresses are positively related to porosity with exceptions at extreme cases.

References

1. Zhou SW, Li Q (2008) A variational level set method for the topology optimization of steady-state Navier-Stokes flow. Journal of Computational Physics, 227:10178–10195.
2. Chen YH, Zhou SW, Cadman J, Li Q (2010) Design of cellular porous biomaterials for wall shear stress criterion, Biotechnology & Bioengineering 107(4):737-746.
3. Torquato S, Hyun S, Donev A, 2002. Multifunctional composites: optimizing microstructures for simultaneous transport of heat and electricity. Phys. Rev. Lett. 89, 266601–1–4.
4. Chen YH, Zhou SW, Li Q (2009) Computational design for multifunctional microstructural composites. International Journal of Modern Physics B, 23:1345–1351.
5. Guest JK, Prevost JH. 2006b. Optimizing multifunctional materials: Design of microstructures for maximized stiffness and fluid permeability. International Journal of Solids and Structures 43(22-23):7028-7047.