AN *IN SILICO* STUDY OF TRANSPORT PHENOMENA IN 3D POROUS SCAFFOLDS USING LATTICE BOLTZMANN SIMULATIONS

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Introduction

Transport phenomena through the scaffold have a marked impact in tissue engineering (TE) processes [Schiavi, 2012]. In this work we present a virtual test bench where realistic 3D models of porous TE scaffolds are reconstructed from micro-CT images and the transport phenomena are simulated applying the Lattice Boltzmann Method (LBM). Here, the virtual tool is applied to evaluate the *in silico* permeability (k_C) of three scaffolds for bone tissue regeneration and validated with experimental permeability (k_E) measurements.

Methods

Scaffolds were fabricated by using the freeze-drying technique and contain bioactive glasses (BG), and a polymeric blend (PS) made of chitosan and gelatin. Foams with three different BG/PS fractions (0/100 (S1), 40/60 (S2) and 70/30 (S3)) were prepared [Gentile, 2012]. The permeability was evaluated experimentally and computationally. The experimental set up was recently proposed [Schiavi, 2012]. As for the in silico model, a square region of interest (ROI) was selected from micro-CT images (pixel size: 8.7 μm) and the 3D model was reconstructed. For each scaffold, porosity (*n*) was evaluated by counting the number of "void" voxels and dividing by the total number of voxels. The open-source LBM software Palabos was used to solve the single phase flow within scaffold models. Models were padded with walls (i.e. no net flow at side walls). A constant pressure gradient between the inlet and outlet sections (i.e. Reynolds number Re <<1) and the bounce-back boundary rule at the solid walls of scaffold models were imposed. The standard BGK collision operator was applied and a 3D lattice with 19 velocities (D3Q19) was used.

Results & Discussion

Table 1 shows that the porosities and the permeability values evaluated both experimentally and *in silico* exhibit the same decreasing trend as the BG percentage into the scaffold increases. Moreover, the *in silico* values are always higher than the experimental ones. This discrepancy is mainly due to two reasons. First, the reconstructed scaffold volumes are two orders of magnitude smaller than the experimentally investigated samples. In this study, the sample size influence (i.e. boundary effects) was investigated (data not shown) and results confirmed that a computational model size between six to twelve times the average pore size is needed to reduce the dispersion of permeability data, but maybe this size is insufficient to represent the experimental samples. Secondly, an inadequate resolution of the micro-CT images was used to reconstruct the 3D models: the investigated scaffolds are characterized by narrow throats that, if not solved with adequate lattice points, lead to an overestimation of the permeability. On the contrary, the k_E values account for those small structures that could not be discriminated whit a resolution of 8.7 μm.

Sample	n [-]	k_C [m^2]	k_E [m^2]
S1	81	$9.5 \cdot 10^{-11}$	$(2.05 \pm 0.85) \cdot 10^{-11}$
S2	70	$1.77 \cdot 10^{-11}$	$(4.6 \pm 1.45) \cdot 10^{-12}$
S3	68	$9.8 \cdot 10^{-12}$	$(2.28 \pm 0.62) \cdot 10^{-12}$

Table 1. Computational (k_C) and experimental (k_E) permeability values.

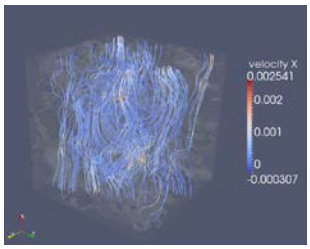

Fig. 1: Streamlines through S1 are color-coded with the values component of the velocity vector (x direction).

References

Schiavi *et al.* Meas. Sci. Technol. 23 105702, 2012.
Gentile *et al.* J Biomed Mater Res A 2012:100A:2654-2667.