A 3D Simulation Model for Porous Polymer Network Formation

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In this paper the 3D simulation model of typical porous polymer is presented. Porosity growth was caused by numerical handling of a spatial pores network. Although the algorithm has a good accuracy it is noticed that the final average pore sizes for simulated polymer networks are larger than the desired pore size.

Keywords: polymer network, porosity, tissue engineering

In terms of technology, creation and development of porous structure in polymer scaffolds are difficult tasks. Today one of the most effective techniques in tissue engineering has proven to be the polymer scaffolds construction followed by seeding of progenitor cells. The subsequent 3D culture and implantation of these biocompatible, biodegradable scaffolds has found widespread experimental and limited clinical use. The design of such scaffolds permits culture of these tissues in structures with porosity, surface area, and surface characteristics optimized for each tissue type cultured [1]. Fine control of these architectural characteristics at micrometric level influences the scaffold mechanical behavior. In fact, at macroscopic level, the polymeric structures response used and particularly the relaxation produced in time should not be neglected even if both stress and temperature conditions remain unchanged [2, 3].

Tissue engineering scaffolds benefit from a porous structure, whether being used to seed cells *in vitro* prior to implantation or as conductive structures *in vivo*. Typical desirable porosities for tissue engineering scaffolds are around 90%, with pore sizes in the range of 100–200 microns [4].

Theoretical part

Porous Polymer Network Formation

In a classical pore-network modeling framework, a porous medium is described by a network of wide pore spaces. The porous medium morphology is incorporated in the network structure using pore distribution, throat size distribution and their connectivity [5]. On the other hand the inverse problem consists in building a topologically equivalent skeleton to describe the network for a real porous medium. In this sense the generation of random pore-network structure is calibrated with known physical properties of the equivalent porous material.

The polymer network shows as a 3D logical array (100 x 100 x 100), where TRUE represents the presence of polymer, and FALSE no polymer. To generate a porous network, spherical holes (diameter of 1, 3, 5, or 9) were sequentially removed from a solid (all true) polymer array. The location of each hole was randomly selected, and all points described by the sphere were set to zero. This process continued until the desired porosity (50 - 90%) was achieved. Polymer spheres were permitted to overlap to allow for pore size distribution and interconnection. Periodic boundary conditions were used for the formation of the polymer networks. All indices within 2 units from the edge of the polymer were set to true, in order to create "walled" boundary conditions in the random walk simulations. Each network was saved with and without a 3 unit gap between the wall and polymer. One polymer network was generated for each pore size and porosity.

According to our model, in figure 1 we show a formal representation of the 3D logical matrix. Each cube in the picture stands for 1 bit of memory that will hold the TRUE/ FALSE value. For example a spherical pore, with a 3 unit diameter, is a sphere-shaped spatial distribution of 7 bits set to zero.

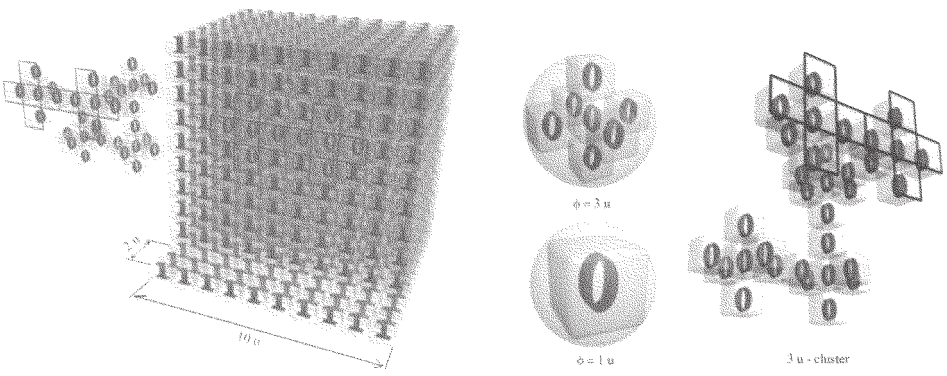

Fig.1. (10 x 10 x 10) segment of the main matrix (left) with a porous network of spherical holes (zeros) with a 3 unit diameter (right)

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In figure 2 we present a logical porous network (3 unit diameter interconnected pores) in a region of the matrix and the detail of a vertical cross section. Each one of these lines will represent an input to our algorithm.

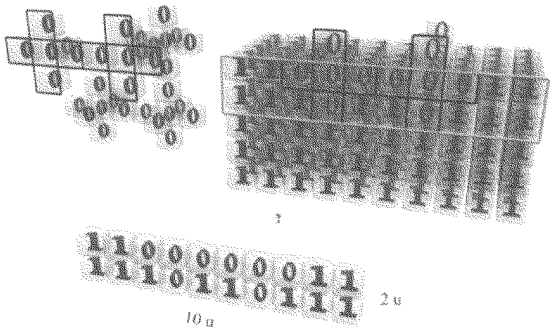

Fig.2 Logical vision of porous network and the detail of a vertical cross section

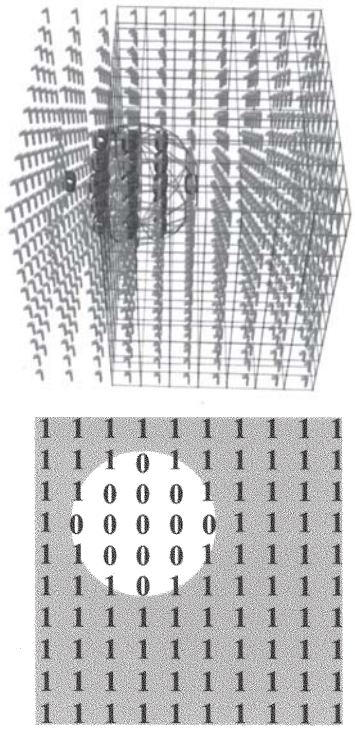

Fig.3. The 3D binary matrix (on the left) and a cross section (on the right)

A simple array scanning technique was used to obtain statistics on pore size distribution consisting in searching for the 1 (TRUE) values and outputting a sequential index of their locations that is used to find the gap size between each polymer. The 3D structure of the matrix is used to find an orientation bias by applying the algorithm along the three Cartesian axes.

The representation of a polymer by a 10 x 10 x 10 logical matrix of TRUE values with a sigle pore (a sphere of zeros – FALSE - with 5 unit diameter) and a cross section (parallel with the paper's plane) giving a 2D logical matrix.

Results and discussion

Several polymeric cubic structures, with a fixed number of randomly distributed spheres, were constructed by the method described above. Each configuration is considered to be macroscopically homogeneous but microscopically heterogeneous. Obviously, the physical and chemical properties are assumed to be constant in the polymer network.

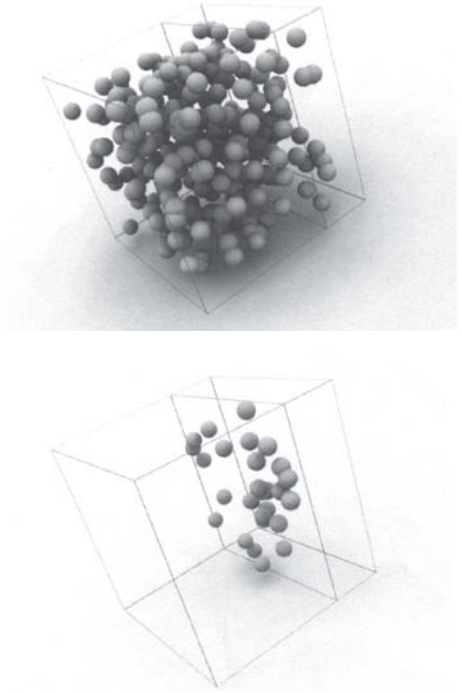

Fig.4. The porous network inside a 100 x 100 x 100 cube (left) and a cross section (right)

The figure 4 depicts randomly distributed spheres in a cube with a 100 unit side. The spheres overlap forming pores with a dimension superior to their initial size (5 unit diameter). We also show the spheres touching that section plane in the right-hand side picture. In order to analyze the simulated 3D structure we slice it to obtain 2D matrices and use their lines as input in our algorithm.

Even though in figure 5 we have circles of different sizes, all the generated pores are greater than the minimum pore size because of the overlapping of spheres with distances between the centers inferior to their diameter. The circles that appear smaller are in fact sections of the pore at a certain distance from the pore center.

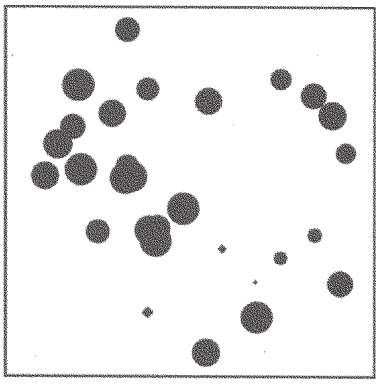

Fig.5. Cross section of the polymer showing the pores (black) and the polymer walls (white)

According to a qualitative observation, the unconnected pore space appeared to consist of only small cavities within individual struts. Such interconnectivity would be valuable in medicine domain, for perfusion and cell migration throughout a scaffold. The mechanism of determining interconnectivity through 3D reconstruction of pore-space and subsequent region growing performed robustly in the analysis of the simulate samples.

Mathematical models and simulations can be used in conjunction with experiments as a means of evaluating competing mechanistic hypotheses [6-10]. The analysis of the described polymer shows that the average pore sizes

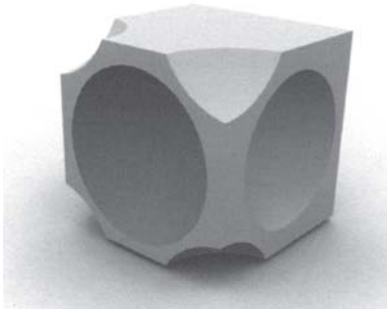

Fig.6 Detail of the polymer in the region where two pores are interconnected.

for all polymer networks are larger than the desired pore size. Due to the pore generation technique, no pore sizes smaller than the reference pore are possible so the networks simulated were considered useful representations of materials with known pore sizes.

The porosity of a porous medium describes the fraction of void space in the material. Technically, the porosity is defined as the ratio of void-space volume and the total or bulk volume of material, including the solid and void components.

Conclusions

A pore-network 3D model is developed to study the polymer porosity. In general, the porosity has a direct relationship to surface area. Still, the correlation procedure can be difficult to compute in a spatial complex sample.

The model suggests that the final average pore sizes for all simulated polymer networks are larger than the desired pore size.

The initial conditions that were established were to closely approximate the conditions that are found for typical porous real structures. From simulations, site occupancy was not significantly different than that of no real polymer network. Moreover, the pores system and the porosity are in good agreement with the known experimental results [11].

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