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METHODOLOGY FOR NUMERICAL SIMULATION OF THE DEGRADATION PROCESS OF 3D PRINTED BIOPOLYMERIC SCAFFOLDS

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Abstract *3D printed biopolymeric scaffolds are porous implants manufactured by additive manufacturing of biomaterials, with hierarchical structure, which enable the tissue regeneration process [1]. The durability of these implants mainly depends on the physical properties of the material used. In this work, a predictive model of the degradation process of the biopolymeric scaffold is presented, using open source tools. It consists of a numerical simulation to compute the dynamic degradation of the scaffold manufactured by additive manufacturing. The model consists of a chamber with an inlet and outlet ducts [2,3] where the fluid goes through a cylindrical scaffold. Once the geometric model is done, a mesh of both fluid and solid domains is generated [4]. Afterwards, it simulates the fluid flow with transient Navier Stokes to obtain the velocity field using a Finite Element software [5]. Once the velocity is calculated, it allows the determination of the shear stress field over the surface. Then, a threshold shear stress value is defined to remove the elements that exceed this limit value. The removed elements are assigned to the fluid domain by means of the advanced management tools of FreeFem++ [6], in 3D. The threshold value decreases at the time that the scaffold is being degraded. This tool allows the prediction of the durability and suitability of the scaffold before the experimental degradation test, previous to in vitro or in vivo test.*

1 INTRODUCTION

First of all, G.Erkizia et al. [1] made a computational model that simulates the degradation process of the scaffolds. The geometry is discretized in small cubes named voxels. The model simulates the scaffold degradation by means of the Montecarlo method, accounting the curvature of the structure's fiber surfaces. By geometry, it is known what voxel is fiber or liquid and based on this you know the probability that said voxel will be degraded. In other words, for each voxel of the initial geometry, it is calculated the number of neighbour voxels that are liquid or solid. If all of them are solid, the probability of degradation will be zero. Indeed, it is also taken into account the neighbour voxels with different probability of degradation depending of the number of normalized liquid neighbours, which takes into account if the liquid neighbour has an adjacent face or edge.

For example, for a liquid neighbour with an adjacent face, the weight would be 0.069, while in the case of an adjacent edge, the weight would be 0.049. With these data, they created a probability function depending on the normalized number of liquid neighbours. The Montecarlo method generates an aleatory number between 0 and 1 for each voxel, then the normalized number of liquid voxels is calculated (following the aforementioned approach) and if the aleatory value exceeds the probability of degradation, the voxel degrades and, consequently, it converts into a liquid. This is how it simulates the degradation process over time.

This method allows the simulation of the degradation of the material but it is exclusively based on the degree of exposure of the material to the fluid, without considering parameters associated with the dynamic flow of the corporal fluids.

Another aspect related to the topic is the fluid effect on the degradation process of the scaffolds. In this term, the authors Hasan Basri et al. [7] start from three models of scaffolds of different porosities and the same size of pore. For each one, it is applied an inlet flow with different velocities that there are similar to those generated in the bone marrow. The scaffolds stay in the camera for 24, 48 and 72 hours.

For simulations, it is needed, in the first place, the reconstruction of the 3d geometry of the scaffold. Micro computerized tomography is used, and it consists of obtaining images of the transversal sections of the scaffold at different heights. Then, these images are combined by using a u-CT package, and generates, then, the model. This model is exported in .stl format to use it in the simulation software.

The model is imported in the COMSOL software and it performs the flow simulations to obtain the corresponding shear stresses.

2 MATERIALS AND METHODOLOGY

2.1 Materials

Bio-fluid within scaffold microstructures transports nutrients and metabolites for osteocytes and forms a crucial component to maintain newly-regenerated tissue alive. Joints present a particular case for the scaffolds because of the characteristics of the synovial fluid, which speeds up the degradation process due to the enzymes present in it.

For this reason, it is of capital importance the choice of the materials in the scaffold to complete the healing process of the tissue. Indeed, it is important that the materials of the scaffold are biocompatible with the patient, otherwise the scaffold will be rejected from the body. For the simulation tests, Polylactic-acid (PLA) scaffolds will be considered, due to its wide acceptation in the medical community.

On the other hand, the synovial fluid is non-newtonian, so that implies a more complexity in the formulation and resolution of the Navier-Stokes equations. Indeed, most of the experimental tests use Newtonian fluids that behave similar to the biological ones. One of these fluids could be the PBS solution, widely used in the in-vitro tests, so it will be considered for the simulations.

2.2 Methodology

2.2.1 Preprocessing

The scaffold geometry is based on a real model used for experimental tests. Our model is a cylindrical scaffold, which is 10 mm depth, with 10 mm diameter and with a 0.5 mm pore size. The geometry was modelled using the open source SALOME software.

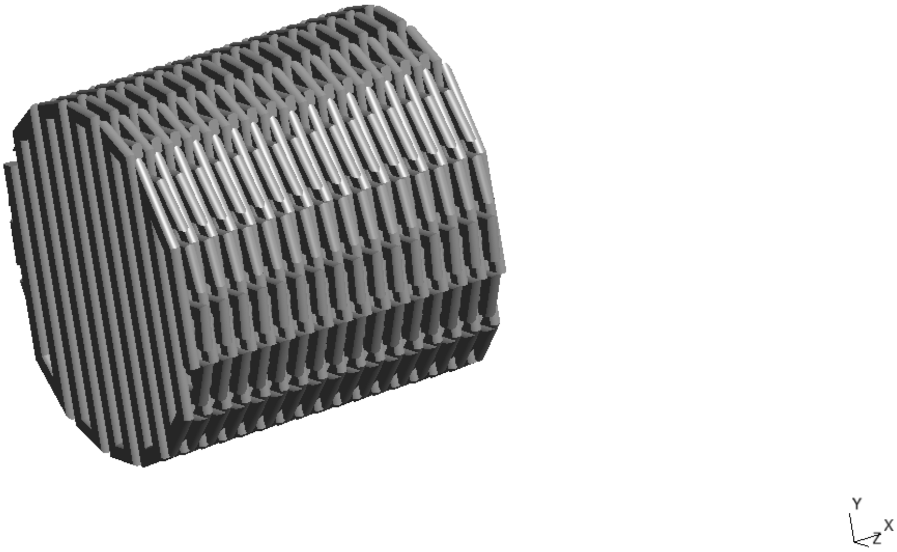

Figure 1. Geometrical model of the scaffold

The model will be placed inside a bioreactor in which the inlet and outlet boundary conditions will be imposed. The bioreactor model basically consists of three parts: the inlet channel where the fluid enter with a predefined velocity; the chamber, where the scaffold is placed, and the outlet channel.

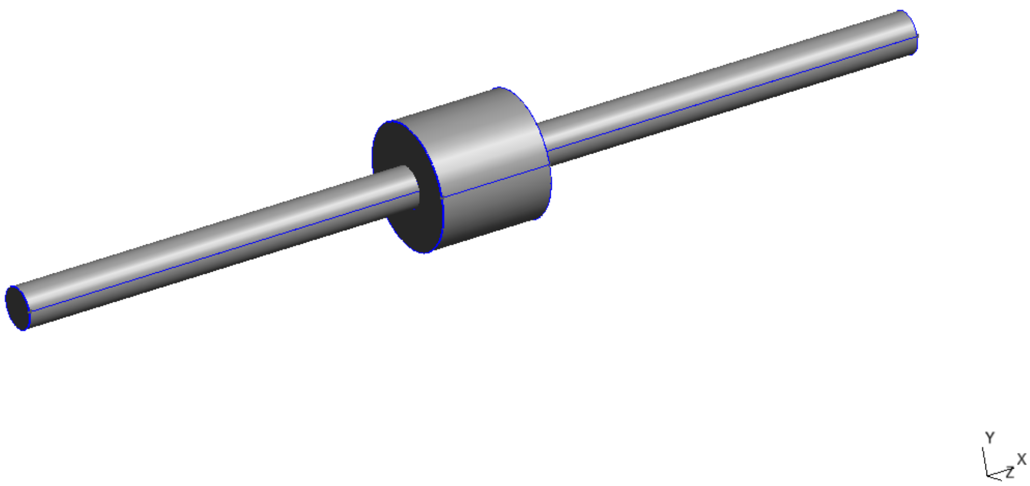

Figure 2. Geometrical model of the chamber

Once defined the study domains, the mesh size will be defined for each boundary. For the scaffold, it will be applied a mesh size of 0.1 mm. However, for the chamber it will be applied a size of 0.5 mm, to not exceed the computation time. Once the boundary are defined, we create the tethraedral mesh.

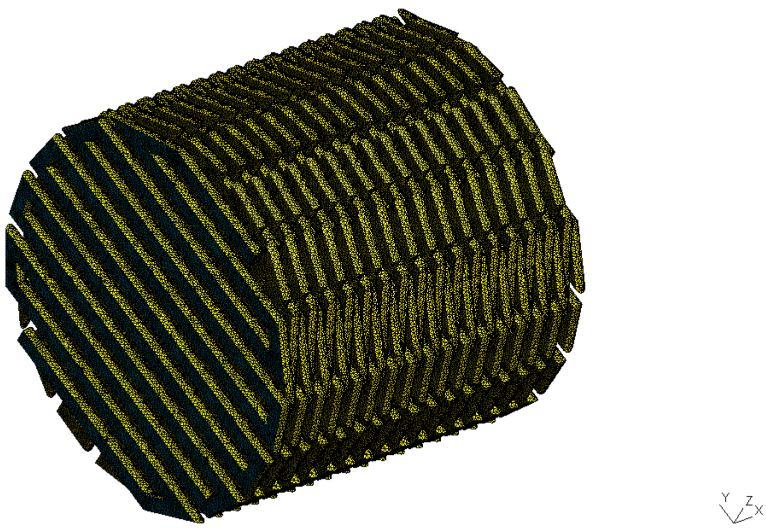

Figure 3. Mesh of the scaffold

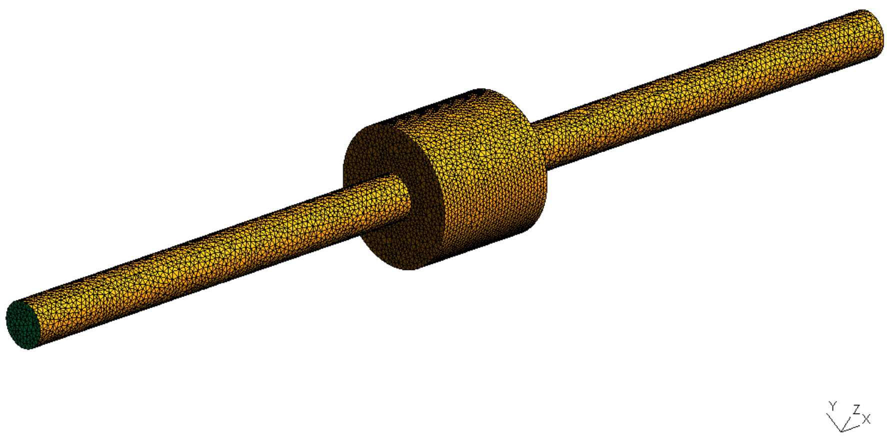

Figure 4. Mesh of the chamber

2.2.2 Degradation algorithm

Previous to the definition of the degradation, it is required a computation of the velocity variables to determine the velocity field of the fluid domain. As the degradation process is continuous over time, it has been decided to use transient Navier Stokes equations. In this work, a Projection method of the Navier Stokes called **Chorin Rannacher** was used. This scheme is characterised by using P1 finite element functions both for velocity and pressure and its lower computational cost compared with other methods.

Once the velocity is calculated, we can obtain the shear rate and, hence, the shear stress. As it is said, the scaffolds are subjected to degradation process due to the fluid flow through the walls. The degradation process does not imply a pure mechanical degradation, but also a loose of its chemical properties. Among many factors, one of the most important in the degradation is the shear stress. When the value of the shear stress exceeds a threshold, previously defined, the degradation occurs. For a Newtonian Fluid, the shear stress is a function of the viscosity and the shear rate:

$$\tau = \sqrt{\left[\mu\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right]^2+\left[\mu\left(\frac{\partial v}{\partial z}+\frac{\partial w}{\partial y}\right)\right]^2+\left[\mu\left(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x}\right)\right]^2}$$

By using advanced tools of FreeFem++, we can remove those elements where the shear stress is higher than the threshold. The removed elements will be added to the fluid mesh. This process will be repeated until there are no elements left in the scaffold mesh.

Below we can see a scheme that overviews the explanation above.

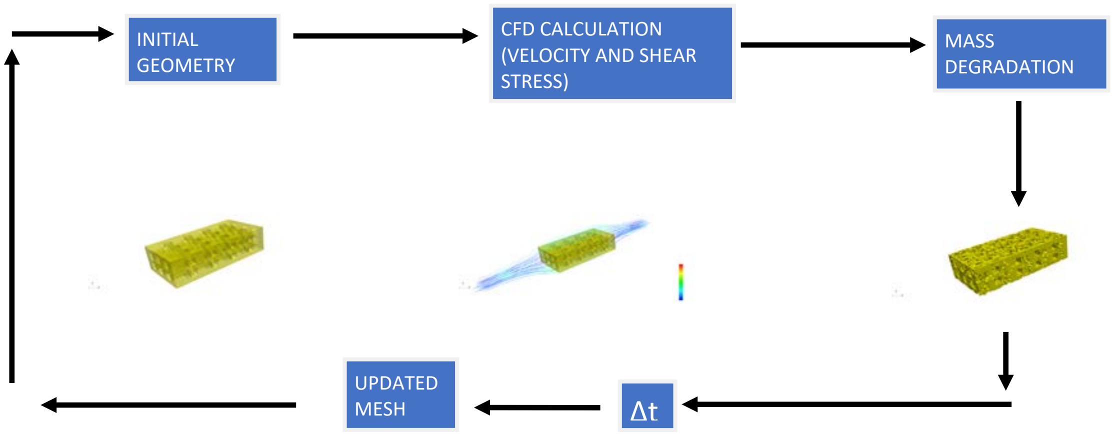

Figure 5. Diagram of the simulation algorithm

3 RESULTS

A brief summary of the velocity and the degradation results is presented below. Figure 6 show the velocity streamlines through the scaffold.

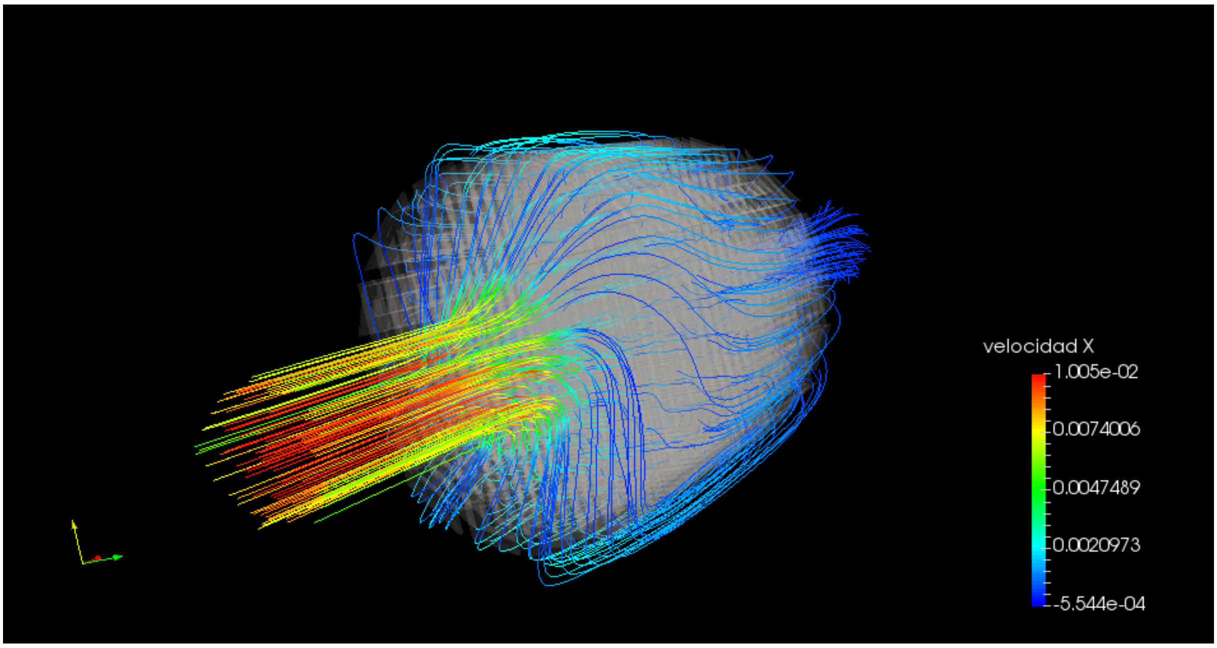

Figure 6. Velocity streamlines for t=4

The next figures show the mass loss of the scaffold through time:

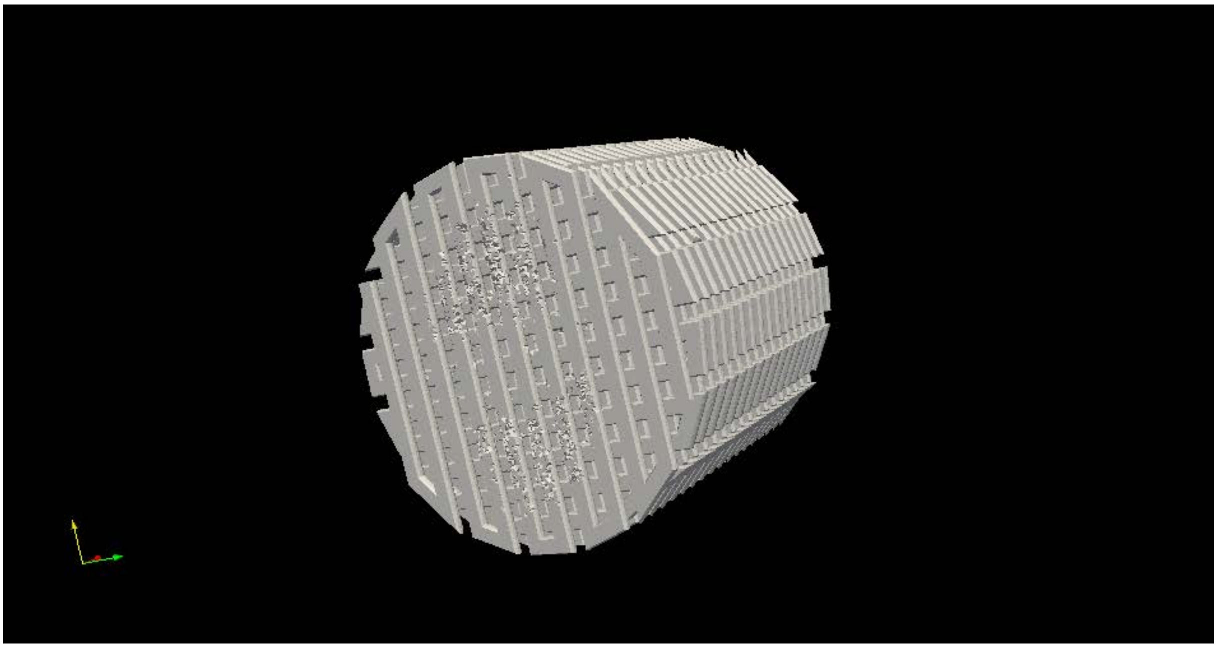

Figure 7. Degradation evolution t=0.005

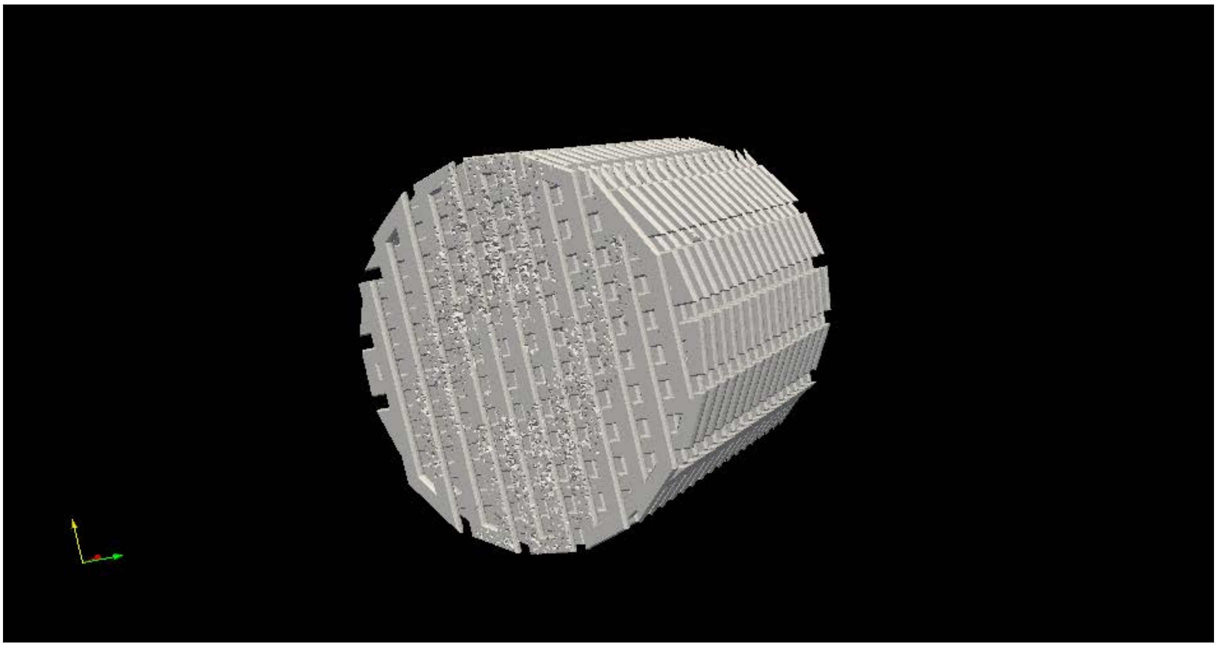

Figure 8. Degradation evolution t=0.02

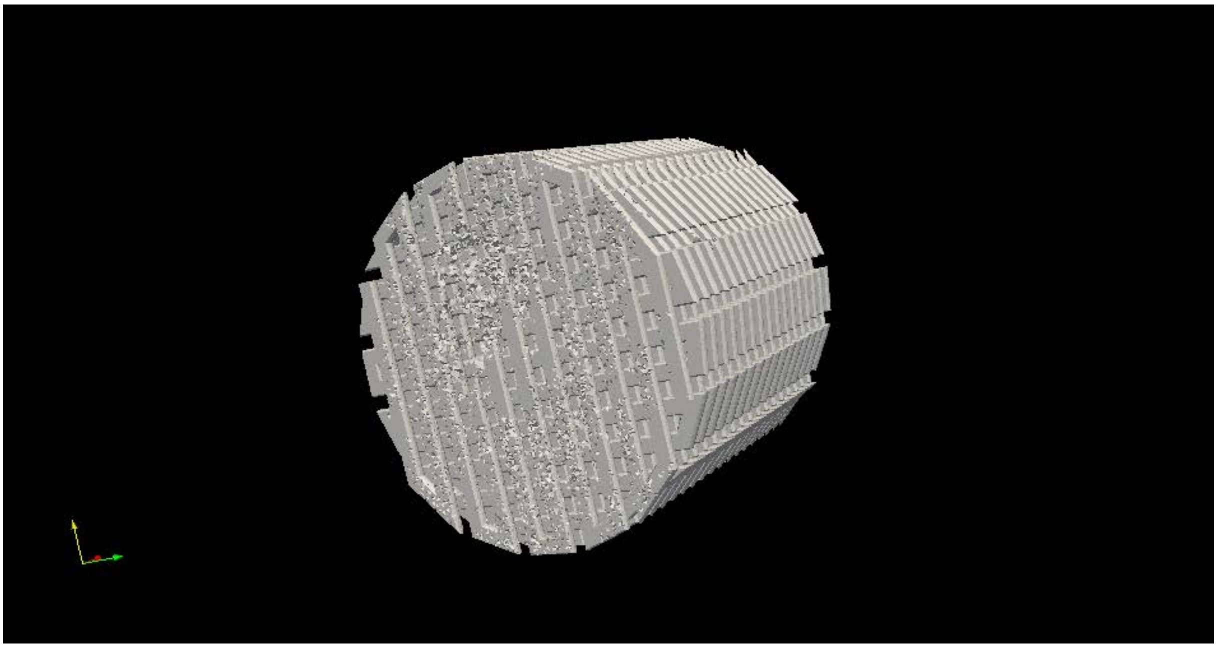

Figure 9. Degradation evolution t=0.037

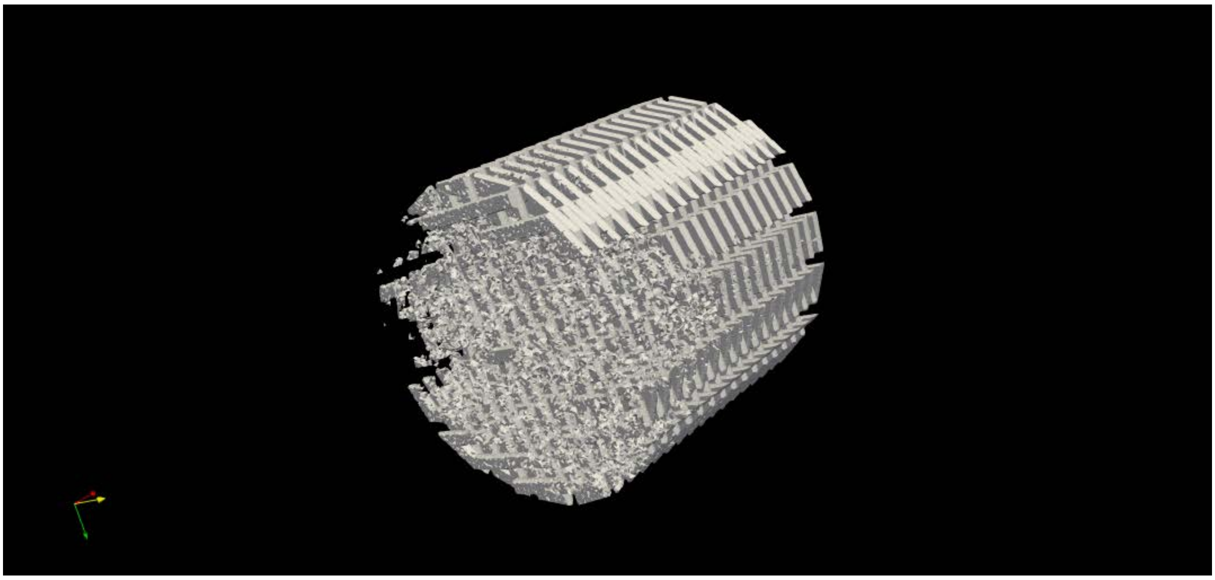

Figure 10. Degradation evolution t=0.05

4 CONCLUSIONS

This work proposes a methodology that allows to predict the degradation time of 3d printed biopolymeric scaffolds by using finite element method. So far, simulations have been carried out on both simplified and “real” models. We have seen that the degradation is predominant in the face oriented to the inlet, but it is also produced in the internal and lateral walls. We have seen when the velocity increases, the degradation rate is higher. That is because the shear rate is greater.

On the other hand, this simulation requires high computational resources due to the number of nodes of the mesh, specially in the scaffold walls.

5 ACKNOWLEDGMENTS.

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