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ACEX022

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Simulation of variation of intraocular pressure

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Abstract

The human cornea has five layers. The epithelium is a thin layer of tissue multicellular fast-growing and easily-regenerated cells in a period of seven days, it is external, it occupies approximately 10% corneal thickness and it is composed of about six layers of cells. The stroma constitutes about 90% of the total thickness of the cornea and it consists of Approximately 200 layers parallel and its fibers are arranged in a manner orthogonal to the fibers of the layers adjacent. The Bowmans's layer lies between the epithelium and the stroma. It is tough layer, very fine and very resistant to trauma, pressure and infection. The move of the corneal leaves the surface of the Bowmans's layer with its uniform curvature due to moving between the sub-layers of the stroma, whose movement are facilitated by mixing of aqueous humor and metabolic secretions. The cornea receives nutrients via forced convection from the tear fluid at the outside and the aqueous humor at the inside. The accumulation of metabolic secretions in the epithelium cause stinging and blurred vision and the metabolic secretions accumulation of between the sub-layers of the stroma hinder the movement between its sub-layers and weaken the mechanism of forced convection. Then, gradually, the mass transport will be carried out by diffusion. Deficiency of the forced convection reduces of the movement of the metabolic secretions, causing its dehydration, by decanting, and the consequent increase of its viscosity.

Because of the difficulty to convince a professional to measure intraocular pressure under certain conditions, to prove the transient intraocular pressure, we developed a simulator that is presented in this work demonstrates the transient pressure and help to understand the risk of life of patients underwent surgery laser trabeculoplasty, to reduce intraocular pressure.

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ACEX035

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Blood Flow in Cylindrical Stenosed Channel – Numerical Approach

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Abstract

Arthrosclerosis means literally "arteries hardening". However, arthrosclerosis it is a generic term that is related with three patterns of vascular diseases, which have the hardening and loss of elasticity of the arteries walls as a common factor [1]. The dominant pattern is atherosclerosis, characterized by the formation of atheroma, which is comprised by fibrous plaques that generally exhibit a centre rich in lipids.

In the present work, the flow of blood in a cylindrical channel, containing an atheroma at the walls, has been numerically studied using the finite-element software package POLYFLOW®. In the simulations, blood was considered an incompressible homogenous fluid and the flow regime was the laminar regime. The rheology of the mentioned fluid was described by distinct constitutive equations [2] - constant viscosity, power-law model and Carreau model. The local behaviour of properties such as pressure, interstitial velocities, shear rate and shear stress was explored in the present investigation. The local behaviour of these properties can help to understand the formation and detachment of thrombi.

[1] S.L. Robbins, R.S. Cotran, V. Kumar and T. Collins, Fundamentos de Robbins – Patologia estrutural e funcional, 6ª ed. (Editora Guanabara Koogan, Rio de Janeiro, 2000).

[2] B.M. Johnston, P.R. Johnston, S. Corney, D. Kilpatrick, J Biomech, 37, 709 (2004).

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ACEX080

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Molecular dynamics study of oligomer-membrane complexes with biomedical relevance

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Abstract

The use of liposomes as drug delivery systems (DDS) is well know. However, for this kind of application the stability of liposomes (shelf stability and in blood stream) is an issue. One way to address this problem is the development of polymer-liposome complexes for providing improved stability as well as better selectivity characteristics.

This work reports the modeling and simulation studies, by molecular dynamics (MD), on polymer-membrane complexes with biomedical interest. For computational resources reasons, a bilayer membrane was used to mimic the liposome surface, whereas the targeted polymers, which have been recently synthesized in our laboratory, were replaced by representative oligomers. The MD simulations were performed by using the united-atoms 53a6 GROMOS force-field, with the GROMACS 4.5.2 package in a Linux cluster consisting of eight computer nodes, two Intel Xeon™ 2.4GHz CPUs (Gulftown) each, and Infiniband intercommunication. Different oligomers with different chain lengths were tested, and their interactions with the bilayer surface analyzed. Some heating ramps were also simulated to understand how the oligomer-membrane complex reacts under different environment temperatures.