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A review of models in bioengineering developed by the group led by Miloš Kojić in the period 2006-2016

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Abstract

A brief summary of results in the period 2006-2016 of the group led by Milos Kojic is given in this report. Three fields are included: general bioengineering problems, models for transport in capillary systems and tissue, and modeling of underground water flow. This research has been published in books, journal papers and conference proceedings. The research has been supported by various grants, national (Ministry of Education, Science and Technological Development of Serbia) and international, and industry. The computational models have been implemented into our software PAK.

Keywords: FE models in bioengineering, tissue, muscles, transport in capillaries and tissue multiscale, underground water flow, FE package PAK

1. Introduction

Our group started with the development of computational FE models and our software package PAK back in 1975 (founder and main author M. Kojic). Over decades, significant progress was continuously made, so that the original structural linear and further nonlinear FE modeling problems have been enriched by other fields such as heat transfer, fluid flow, solid-fluid interaction, damage mechanics, multiphysics, multiscale, and biomechanics and transport within capillary systems and tumors. This work has been initiated at the Computer Center of the Serbian car factory “Zastava” in the City of Kragujevac, followed by work at the Faculty of Mechanical Engineering of the University of Kragujevac, Center for Scientific Research of the Serbian Academy of Science and Arts and the University of Kragujevac, Bioengineering R&D Center for Bioengineering in Kragujevac, and the Faculty of Science of the University of Kragujevac.

We here summarize the main results in the last 10 years of the group led by M. Kojic. Results of the other groups led by professors who originally worked under the leadership of M. Kojic are reported separately in this volume. Some representative results in several bioengineering topics are given first, followed by transport models within capillary systems and tissue (developed in the period 2009-2016), and with models of underground water flow where the group was partly involved. Concluding remarks are given in the last section. List of publications (journal papers and one book) in this period is given in the References.

2. Computational models in bioengineering

Our group was involved in the development of computational models and software for various problems in bioengineering since 1995. These models include tissue mechanics, muscle mechanics, cartilage mechanics, bones, cells, transport of ligands within extracellular space, models of biological membranes, blood flow and thrombosis. The results in the period 1995-2008 are summarized in the book (Kojic et al. 2008). From 2009 to 2016 there were two major directions of research of the M. Kojic group: (a) development of models for motion of deformable and rigid bodies in fluid flow, with solid-fluid interaction and solid-solid interaction; and (b) methods and software for modeling mass transport (convective and diffusive) of particles and molecules within capillaries and tissue. Here we selected two typical examples for the group (a), while the topic (b) will be addressed in Section 3.

2.1 The model of biological membrane covered with surfactant

Alveolated structure deep in the lung is composed of membranes in the form of alveolae and connective tissue as fibers and rings (Wilson 1982; Bachofen and Schurch 2001; Bachofen et al. 1979). Exchange of oxygen occurs due to contact of air and membranes and that exchange depends on the airflow within alveolae. The flow is conditioned by motion of alveola membranes. During breathing, the overall lung structure is subjected to cyclic motion and deformation. The supporting structure of the lung is the connective tissue which contains muscle and other connective tissue cells, and displays hysteretic characteristics when the force-deformation relationship is considered. The alveolar membranes deform during breathing and their surface change has a cyclic character. Membranes are covered by surfactant which generates surface stresses, with hysteretic character. Hysteresis of the fibers and membranes have the opposite character and their superposition results in the hysteretic motion of the lung walls - which produces air mixing deep in the lung. This mixing is crucial for normal lung functioning. In our study (Kojic et al. 2011) we investigated the mechanical behavior of an alveolar duct and used our model of biological membrane covered by surfactant (Kojic et al. 2006).

In Fig. 1, the concept of stress integration which includes nonlinear constitutive curves for biological tissue of membrane and hysteretic characteristics of alveolar ring and surfactant are shown. The numerical results for the spherical membrane and alveolar duct illustrate hysteretic responses under cyclic loading.

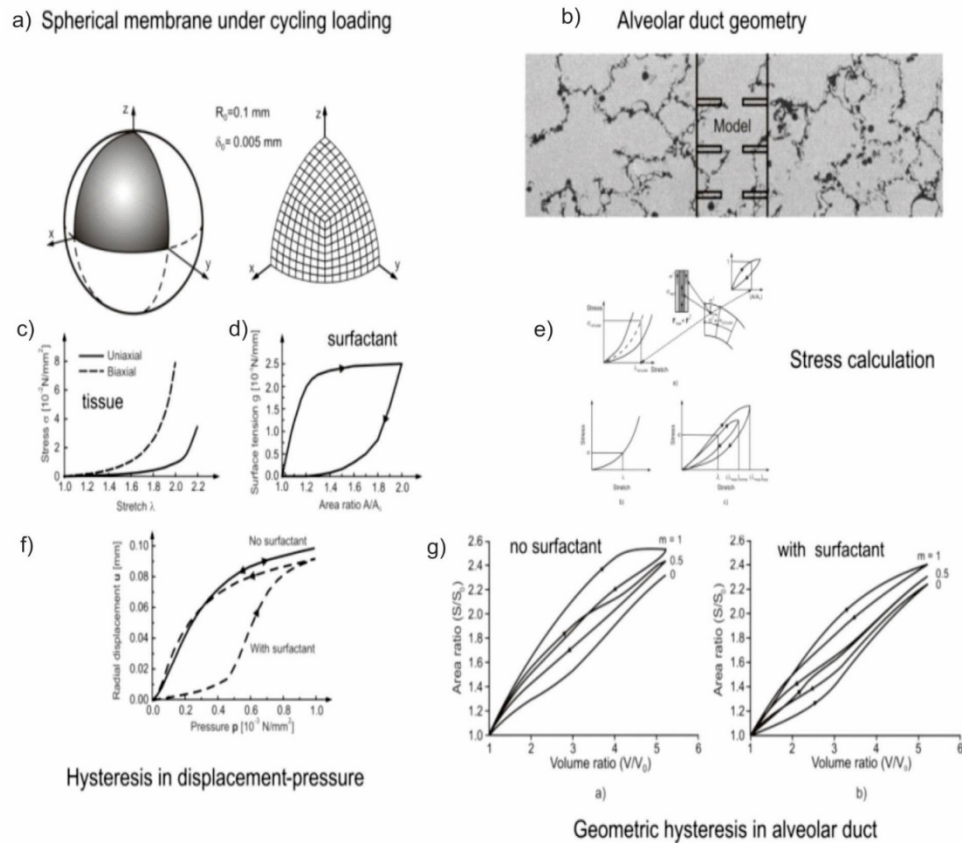

Fig. 1. The model of biological membrane according Kojic et al. (2006) and of alveolar duct according to Kojic et al. (2011). a) Geometry and FE model of the spherical membrane. b) Geometry of the duct. c) Uniaxial and biaxial constitutive curves for membrane tissue. d) Hysteretic characteristic of surfactant. e) Stress integration which includes membrane tissue, alveolar ring and surfactant. f) Radial displacement-pressure relationship for the spherical membrane. g) Geometric hysteresis expressed as the ratio of the duct surface to duct volume for the alveolar duct

2.2 Cancerous cell passing through capillary narrowing

This example illustrates our developments in the field of modeling solid-fluid and solid-solid interaction. We investigated various concepts of modeling motion of deformable and rigid bodies within fluid, which is of particular importance to various problems in cardiovascular systems. We have found that the most robust and reliable is the concept of direct coupling, where solid surface and fluid have common nodes, with common (equal) velocities within time step, and with the common solid-fluid system of equations which is formed and solved simultaneously over time steps and iterations. When this solution is obtained for velocities and pressures (for fluid and solid if mixed formulation is used) for a time step, the body is displaced, and remeshing of the fluid domain is performed, Fig. 2 (Isailovic 2012). The detailed analysis of this methodology is presented in Isailovic (2012) and Isailovic et al. (2014).

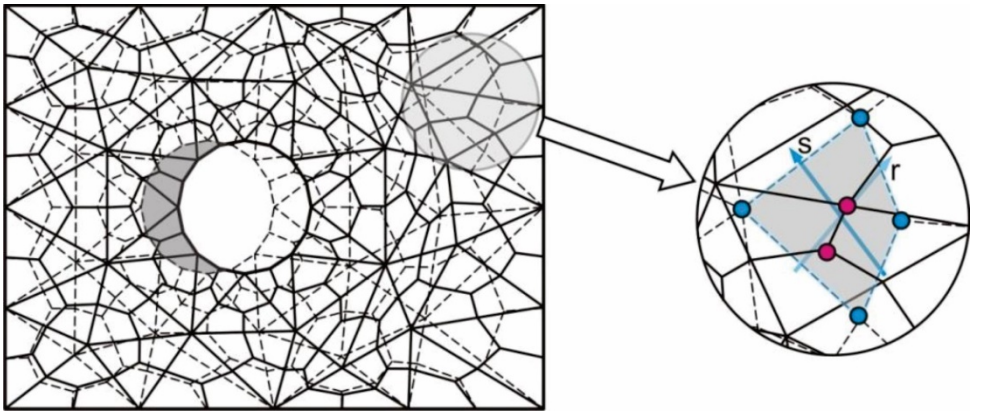

Fig. 2. Schematics of the remeshing procedure. After the solution for the current time-step is obtained, the solid is displaced, a new fluid mesh is generated (with common solid and fluid nodes at the solid surface), and solutions from the old mesh are mapped to the new mesh [80]

Among other applications, we present here the results given in Kojic N. et al. (2015) where conditions must be fulfilled for circulating tumor cell (CTC) to pass a capillary narrowing. In Fig. 3a,b the concept of solving interaction between deformable bodies using 1D fictitious elements is schematically shown. This is one of the simple methods in computational mechanics summarized in Kojic (2013). Regarding deformation of the solid, a mixed formulation introduced in Kojic (2015) is implemented.

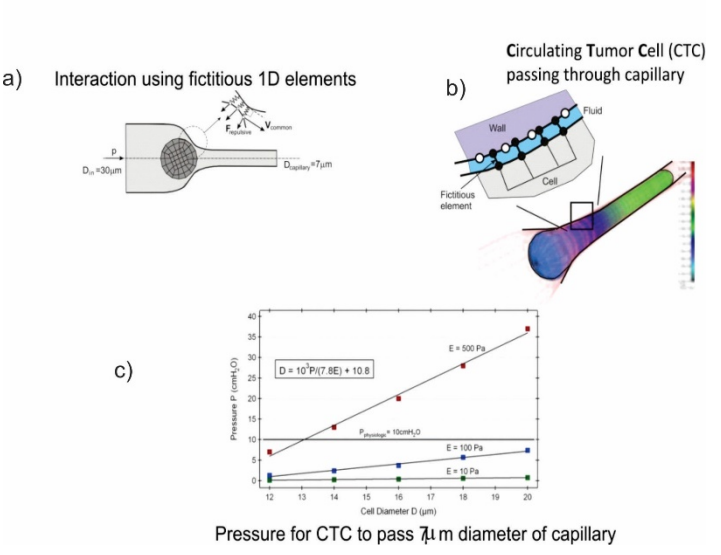

Fig. 3. Model of circulating tumor cell (CTC) passing capillary narrowing according to Kojic (2015). a) and b) Use of fictitious 1D elements to model interaction between cell and wall. c) Relation between blood pressure and cell diameter to pass 7 micrometer capillary diameter, for several cell stiffnesses (elastic modulus E)

Results in Fig. 3c show that the relationship between cell diameter, blood pressure and elasticity modulus can be established for a CTC to pass circular capillary narrowing. In Fig. 4

we show two cells within capillary together with velocity field, to demonstrate the applicability of our models to very challenging computational problems.

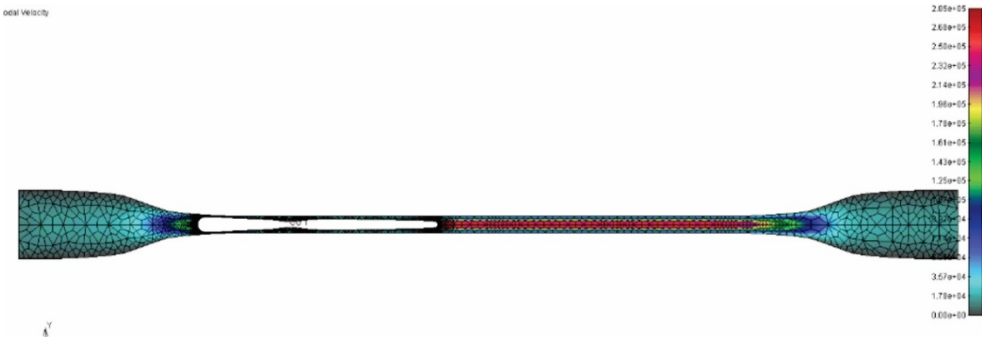

Fig. 4. Two cells as a CTC cluster passing through capillary. Cells are subjected to very large deformation (direct coupling, interaction algorithm and mixed formulation are implemented to demonstrate robustness of our methodology and applicability to very challenging problems of computational mechanics)

3. Models for mass transport within capillaries and tissue

From 2009, our group was engaged to develop models for convective and diffusive mass transport within small blood vessels and tissue, with the emphasis on tumor problems. In the previous section, we have briefly presented convection due to blood flow. Here, we summarize the main results for the transport which is mainly governed by diffusion.

3.1 Hierarchical multiscale model for diffusion

This model is basically established in Ziemys et al. (2011) by investigating molecular transport within nanodevices (NDS) originally invented by Professor Mauro Ferrari. The hierarchical model relies on the concept that the constrained diffusion within small channels, as in nanochannels of the NDS, can be adequately modeled by evaluating interaction between transported particles and molecules and wall surface; this is achieved by using molecular dynamics (MD). Scaling functions are introduced and used to determine diffusion coefficient in terms of distance from the wall surface and concentration. The model was further generalized to diffusion within porous media with complex microstructure (Kojic et al. 2014). The basic concept of the hierarchical multiscale model is shown in Fig. 5.

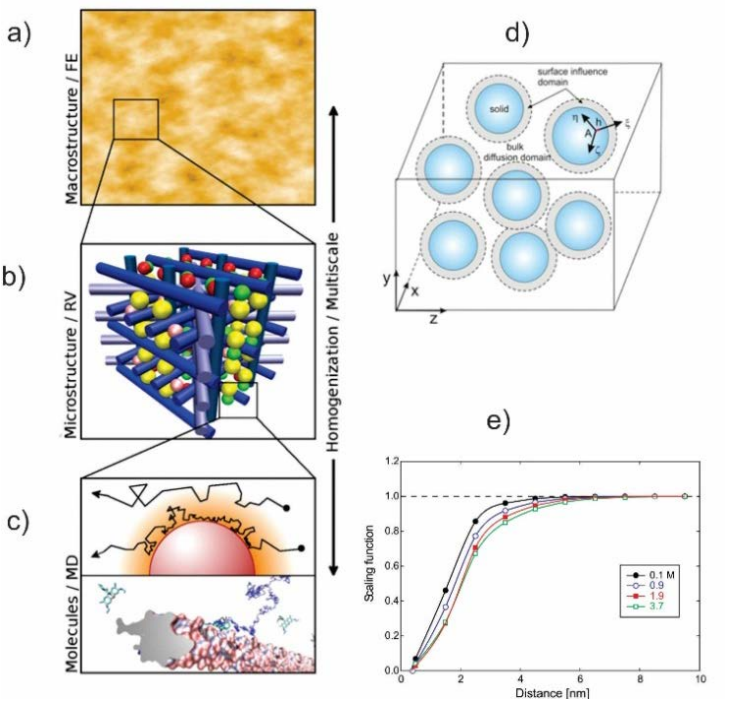

Fig. 5. Hierarchical multiscale model. a) A reference volume (RV) of the porous continuum is selected. b) General microstructural geometry. c) Molecular dynamics (MD) is used to determine dependence of diffusion coefficient on the distance from solid microstructural surface. d) Domain of restrained diffusion due to interaction of solute particles and surfaces, and domain of free (bulk) diffusion. e) Scaling functions as the ratios of the effective and bulk diffusion coefficient

Using the scaling functions we can determine the field of the effective diffusion coefficient in the pore space and employ that field for the FE model during evaluation of diffusion matrices of elements and nodal fluxes. The scaling functions are shown in Fig. 5e. We have implemented this model to compute diffusion through an agarose solution, Fig. 6.

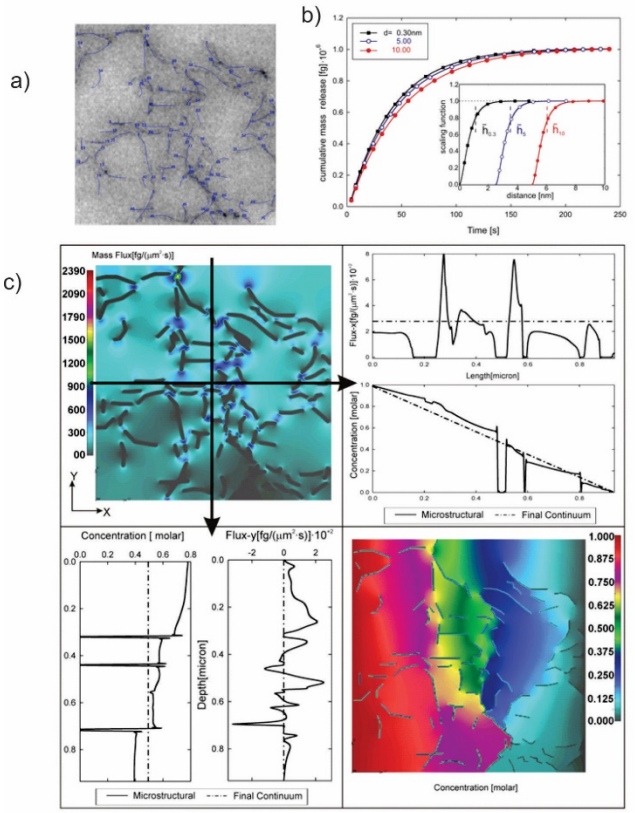

Fig. 6. Diffusion within an agarose polymeric solution according to Ziemys et al. (2011)**.** a) Internal microstructure obtained by imaging. b) Mass release curves for three particle diameters 0.3, 5 and 10 nm, corresponding to rhodamine 6G and two general nanoparticles. c) Field of mass flux distribution in *x*-direction (left upper panel), concentration and flux distributions along *x* and *y* directions, and concentration field (right lower panel)

We have introduced pipe elements for transport within large vessels (Kojic et al. 2014) and fictitious elements to connect pipe elements with continuum (Kojic et al. 2015). These developments established the basis for modeling large systems, such as entire tumor or organ. The data can be used from imaging recordings, as shown in Fig. 7.

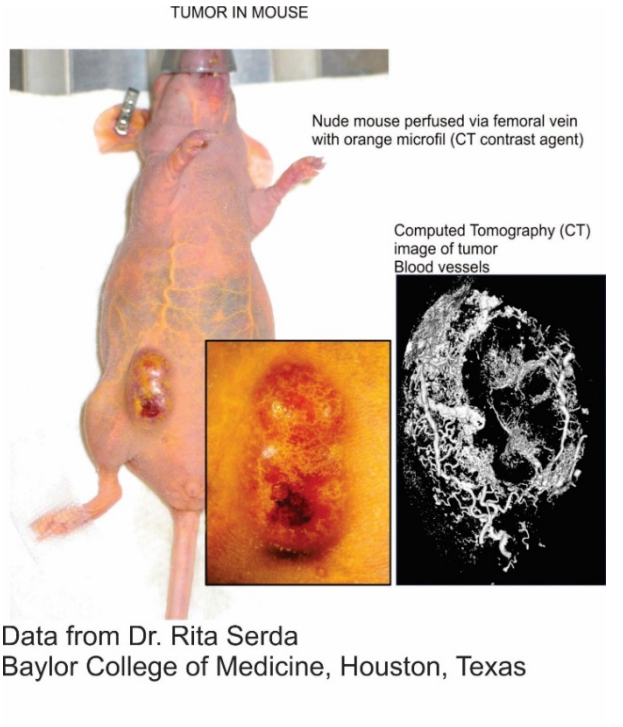

Fig. 7. Experimental investigations with use of imaging for recording blood vessel network in a tumor. Data from Dr. Rita Serda, Baylor College of Medicine, Houston, Texas, USA (private communication)

Application of our methodology and software PAK (Kojic et al. 2010) to modelling transport in tumor is shown in Fig. 8 where concentration distribution within the tumor is displayed.

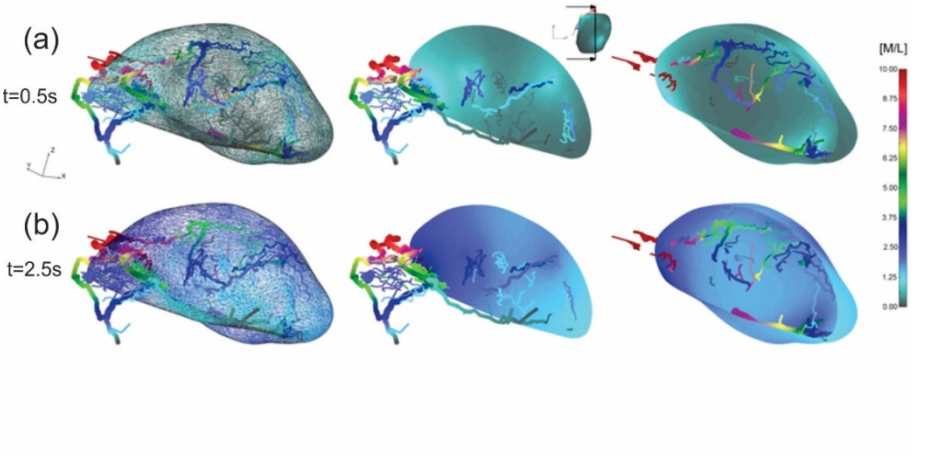

Fig. 8. Concentration distribution within tumor according to Kojic et al. (2015). Concentration within capillaries in plane and in front of plane, in plane and capillaries looking through the plane. (a) time t=0.5s. (b) time t=2.5s

4. Model of underground water flow

Our group has been involved over several years in the development of methodology and software for modeling underground water flow. This research has been performed together with the Institute "Jaroslav Černi", Belgrade. A very sophisticated user-friendly interface software Lizza (Fig. 9a) was developed. Also, a number of publications appeared from this work.

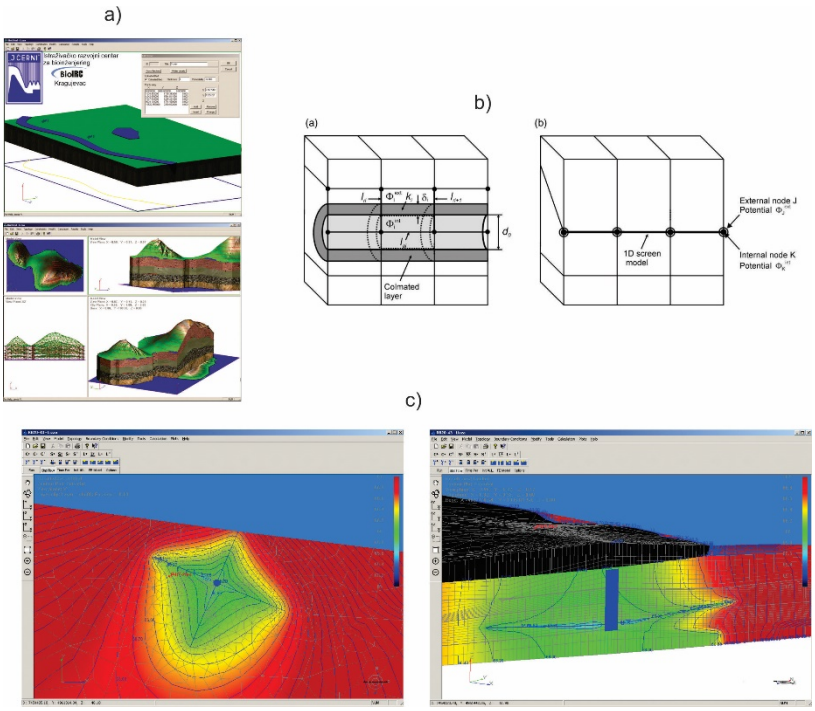

Fig. 9. Modeling underground water flow. a) Illustration of the menu of the interface software Lizza. b) One-dimensional FE of wall screen connected to the continuum (Dimkic et al. 2013). c) Field of potential in models of Belgrade Water Supply System obtained by application of the Lizza and PAK software

Here we show in Fig. 9b the concept of modeling well screens by 1D elements, which are connected to the 3D space (discretized by isoparametric FEs) by fictitious-dimensionless finite elements (Dimkic et al. 2013); these fictitious elements take into account permeability of colmatted soil layers close to the screens. This concept is very important in practical applications since it does not require a fine mesh near the screens – the screens are represented by 1D elements imbedded to the 3D mesh and directly connected to the 3D element nodes. The applications of this methodology and packages Lizza and PAK (Kojic et al. 2010) to the Belgrade Water Supply System is shown in Fig. 9c.

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Извод

Преглед модела у области биоинжењеринга развијених од стране истраживачке групе професора Милоша Којића у периоду 2006-2016

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Резиме

У овом раду се представља преглед резултата групе предвођене од стране Милоша Којића у периоду 2006-2016. Наведене су три области: општи проблеми биоинжењеринга, модели транспорта у капиларним системима и ткиву, и моделирање струјања подземних вода. Овај истраживачки рад је публикован у књигама, радовима у часописима и у зборницима са конференција. Истраживања су подржана кроз пројекте, националне (Министарство просвете, науке и технолошког развоја Србије) и интернационалне, и од индустрије. Компјутерски модели су уграђени у наш софтвер ПАК.

Кључне речи: ФЕ модели у биоинжењерингу, ткива, мишићи, транспорт у капиларним системима и ткиву, струјање подземних вода, ФЕ пакет ПАК

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