NUMERICAL MODELING OF CONVECTIVE AND DIFFUSIVE MASS TRANSPORT IN BIOLOGICAL MEDIA

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Abstract. Mass transport represents the fundamental processes within living organisms. It is of enormous importance to have computational methods to model transport within biological media. In principle, two types of mass transport can be distinguished: convective and diffusive. Further, these two types can occur simultaneously. Biological conditions are far more complex than those usually met in nature or engineering so that computational modeling is still a big challenge. The complexity comes not only due to different time and length scales, spanning from picoseconds to days and from nano – to macro-scales, but also due to bio-chemical interactions between the transported matter (biofluid, cells, molecules, particles and drugs) and the surroundings as vessel walls or tissue microstructure. Classical methodology of modeling based on standard formulations for solids and fluids and their interactions must be extended to include biological phenomena. For example, blood flow in small vessels must include motion of cells, or, in diffusive transport - interaction between transported molecules and solid phase within the porous medium must be taken into account.

In the R&D Center for Bioengineering in Kragujevac and the Methodist Hospital Research Institute in Houston, our primary focus has been in last few years on development of methods and software for modeling of transport of cells and particles within small vessels and on diffusion of molecules and particles within complex biological media. Also, we have participated in an FP7 EU grant (University of Kragujevac) for developing models for atherosclerosis. Here, we summarize the main results, which include our original concepts in computational methodology and a number of solutions that are of interest for medical applications. The original comutational software relies on our solvers PAK developed over 40 year period, and modern interfaces for connecting computational medels with imaging records, as well as graphical pre-and post-processors.

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