



HAL
open science

A numerical framework for the simulation of molecular diffusion in the micro-vascular system

Vincent Doyeux, Yohan Davit, Sylvie Lorthois

► **To cite this version:**

Vincent Doyeux, Yohan Davit, Sylvie Lorthois. A numerical framework for the simulation of molecular diffusion in the micro-vascular system. 22nd Congress of the European Society of Biomechanics, Jul 2016, Lyon, France. pp.0. hal-03660264

HAL Id: hal-03660264

<https://hal.science/hal-03660264>

Submitted on 5 May 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Open Archive TOULOUSE Archive Ouverte (OATAO)

OATAO is an open access repository that collects the work of Toulouse researchers and makes it freely available over the web where possible.

This is an author-deposited version published in : <http://oatao.univ-toulouse.fr/>
Eprints ID : 16562

To cite this version : Doyeux, Vincent and Davit, Yohan and Lorthois, Sylvie *A numerical framework for the simulation of molecular diffusion in the micro-vascular system*. In: 22nd Congress of the European Society of Biomechanics, 10 July 2016 - 13 July 2016 (Lyon, France).

Any correspondence concerning this service should be sent to the repository administrator: staff-oatao@listes-diff.inp-toulouse.fr

A NUMERICAL FRAMEWORK FOR THE SIMULATION OF MOLECULAR DIFFUSION IN THE MICRO-VASCULAR SYSTEM

Vincent Doyeux (1), Yohan Davit (1), Sylvie Lorthois (1)

1. CNRS, IMFT (Institut de Mécanique des Fluides de Toulouse),
Allée Camille Soula, F-31400 Toulouse, France

Introduction

Cerebral microcirculation is linked to a large number of applications: angiogenesis and neo-angiogenesis, long term remodeling in ageing and/or disease (hypertension, metabolic syndrome, neurological disease such as Alzheimer's), patho-physiology (cerebro-vascular disease -stroke-, brain tumors), and functional neuroimaging. In this context, direct numerical simulation of molecule transfer (e.g. tracers, nutrients) in the brain microcirculatory system where diffusion and transport processes are fully coupled between the vessels and tissue is of a great interest. Although direct simulations of the whole cerebral microcirculation is computationally cumbersome, we will show that they can be carried out on a smaller scale (about 50 to 10000 vessels).

Simulations of mass transfer at this intermediate scale enable a fine comparison with experiments. Indeed, experiments of tracer or oxygen diffusion are available at that scale and make a direct comparison possible with matching geometries. Such simulations can thus be used to validate models, as for example the coupling model for diffusion between vessels and tissue (often expressed as boundary conditions) or extract parameters of a given model (e.g. diffusion coefficients).

Some works have been done to model the mass transfer from capillaries to tissue taking into account the coupled interaction on very simple geometries [1,2]. Other works used more complex networks, where the vessels were segmented and the cross-sectional variations of concentration were either neglected [3] or fitted from other simulations [4].

Methods

We introduce a numerical framework able to solve the fully coupled problem: tissue-diffusion and vessels-advection/diffusion. The equations are solved by finite element method, using the library Feel++ [5]. Several boundary conditions are tested to model the coupled interaction between vessels and tissue. The simulation method uses a two-domains approach to differentiate tissue and vessels domains. Two methods have been derived to construct the geometries of these domains:

1) two different sub-domains are automatically defined and meshed by scripting the mesh generator Gmsh

2) the vascular and tissue are pure fictitious domains: in that case a cubic mesh is generated and a distance function to the segmented network is computed efficiently through the use of fast algorithms.

The later method can incorporate a mesh refinement process in order to better match some regions of interest.

Results

The simulation using both methods will be compared on simple test cases as in [1]. Results of tracer diffusion on anatomical geometries (figures 1) will be presented and compared to experimental results.

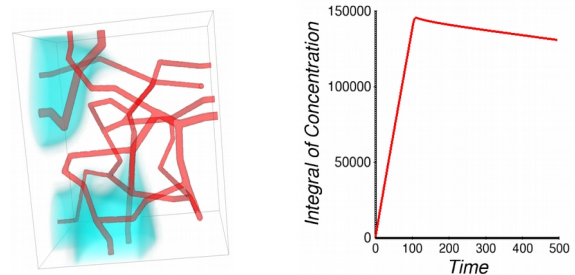


Figure 1

Figure 1: (left) Concentration of tracer (in blue) diffusing into a cerebral capillary network where the vessels (in red) are taken into account through a fictitious domain approach. (right) Integral of concentration over time following a transient injection. After time $T=100$, where injection stops, the wash-out is observed.

Discussion

The advantages and drawbacks of this numerical approach will be discussed from several points of view, including: performances, error estimations, algorithm complexity. Moreover the boundary conditions at the vessel/tissue interface will also be examined.

References

1. Lorthois et al, Journal of Theor. Bio. 353:157-169, 2014.
2. Krogh, J. Physiol. 52:409, 1919.
3. Beard et al, Annals of Biom. Eng. 29:837-843, 2001.
4. Tsoukias et al, Journal of Theo. Bio. 248:657-674, 2007.
5. Prud'homme et al, ESAIM: Proc. 38:429-455, 2012.

Acknowledgements

This work was supported by ERC BrainMicroFlow GA615102.