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Review of the doctoral thesis manuscript entitled "Microstructurally oriented model of ionic transport in porous medium"

presented by

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to obtain academic degree of

doctor in Applied Mechanics

from the

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A targeted application of the proposed approach consists in deciphering the complex coupled interstitial fluid phenomena governing living tissue behaviour. In particular, cortical bone is identified as a valuable avenue of research and numerical illustrative results are presented toward this direction.

The chapter #2 contains the key ingredient of the multiscale strategy developed through this work. Indeed, the accuracy of the effective model obtained through any periodic homogenization method strongly depends of the modelling choices made at the microscopic scale. These microscopic ingredients are presented in this chapter. First, the fully saturated porous medium is seen as a periodic two-scale structure assuming scale separation.

The idea here is to consider the movement of (i) an electrolyte made of multivalent ions (seen as point charges) in an incompressible Newtonian solvent (ii) within an elastic piezo-electric porous structure presenting a surface charge on the pores. As a result, the fluid description combines the Poisson-Boltzmann non-linear equation to describe the electric double-layer phenomena occurring at the pore scale, the Stokes equation for an incompressible fluid (including the Coulombic effect), and the Nernst-Planck equation for ions transport. In parallel, the elasto-piezoelectricity description of the solid phase is proposed. Finally, convenient solid-fluid interface and periodicity conditions are introduced. Since being the core part of the multiphysical description of the problem, the main assumptions and their implications might have been a little bit more extensively discussed at this stage with respect to the targeted physical applications. Notwithstanding this remark, the microscale description is rich enough to capture possible coupling at the macroscale through the upscaling procedure presented in the following chapter.

Chapter 3, for its part, presents the methodological heart of the thesis. Here, the unfolding method is introduced and its application to the microscopic description of the previous chapter is detailed. If the desire to be didactic comes through on reading, some points still especially at the microscale, an explicit comparison of the typical pore size r to the Debye-length and the order of magnitude of the zeta potential could be very helpful to support the discussion of the Fig. 4.1. Indeed, this Figure seems to indicate that there is no bulk phase in the middle of the pore, and thus very strong electro-hydraulic couplings that may limit the accuracy of the Debye-Hückel assumption.

Concerning the results of Fig. 4.2, the legend should also include D12 & D21 cases, and explain the last graph. Furthermore, what is the significance of a negative diffusion coefficient here?

Finally, the macroscopic illustrations are presented. Notwithstanding the fact that they could have been more deeply discussed, the feasibility of the numerical treatment of the approach has been shown in this chapter.

The final chapter presents an application to the peculiar case of the osteonal structures of bone. To be able to perform convenient calculations, an iterative algorithm to identify the material parameters is proposed. Then, two macroscopic coupled simulations of the behaviour of a single osteon under compression are presented, corresponding to an impervious or semi-permeable property for the inner surface of the osteon. The physiological meaning of this set of boundary conditions could be clarified. Thus, in its present form, this numerical illustration is more a toy approach that proves the interest of the developed tools. It now requires to be more efficiently correlated to existing works or experiments to support the concepts. In particular, the macroscopic values that are obtained here present very limited variations and are sometimes physically unrealistic due to surprising order of magnitudes of the evaluated quantities (see for instance the values of the effective displacement).

That is why, the prospects proposed in the concluding final chapter are necessary and valuable. However, before investigating the proposed avenue of research in the wake of the osteon's study of chapter #5 by considering wet bone including osteocytic cells or including wave propagation, a first applicative stage could be to properly investigate less tricky

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Posudek disertační práce

Uchazeč Jana Camprová Turjanicová

Název disertační práce Mikrostrukturálně orientovaný model transportu iontů v porézním prostředí

Studijní program

Školitel Prof. Dr. Ing. Eduard Rohan, DSc.

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Aktuálnost tématu disertační práce

komentář: In silico modeling of various biomechanical processes is an ever growing field gaining popularity even among physicians. Surgeons for example may take advantage of such a modeling approach in preparation of a patient specific treatment and surgery planning. To understand physical and chemical mechanisms driving bone remodeling processes plays an important role in the prediction of bone/implant performance. In light of this, the selected topic is at the forefront of present research trends and the presented work deserves attention.

☒ vynikající	☐ nadprůměrný	☐ průměrný	☐ podprůměrný	☐ slabý

Splnění cílů disertační práce

komentář: The goals of the thesis were introduced in the introductory chapter, properly addressed throughout the thesis, and fully achieved as indicated by the presented results. What I miss, and I understand it is difficult to provide, is the presence of a physical experiment the implemented computational work could be supported with. This an important step forward which should complement the list of future objectives presented in the last chapter. The author may wish to briefly address this issue during the thesis defense.

☐ vynikající	☒ nadprůměrný	☐ průměrný	☐ podprůměrný	☐ slabý

Metody a postupy řešení

komentář: The thesis examines a complex task of a coupled ionic transport throughout a deformable porous medium. To address microstructural details while maintaining computational feasibility the proposed solution strategy grounds on a two-scale computational homogenization. The formulation falls into the category of asymptotic homogenization and adopts the unfolding method to separate the two scales. The formulation begins with an elastic matrix and is further extended to consider a weakly piezoelectric porous medium. The strong formulation including all necessary constitutive equations and boundary conditions is presented in detail in Chapter 2. The essential steps of upscaling is then described in Chapter 3 for both types of problems. I was not able to check all the equations by they seem, in most parts, sound. Implementation into a SfePy software is outlined in Chapter 4 together with the presentation of the results of several illustrative examples. The proposed methodology is then exploited in the identification of non-directly measurable material parameters. Although general in potential applications, the approach is demonstrated on one particular set of material data for the sake of illustration. The data derived assuming a virtual laboratory test are finally adopted in the macroscopic simulation of the

Formální úprava disertační práce a její jazyková úroveň

komentář: The thesis is written in good English with minor grammatical errors. The graphical representation of the results could be improved. In most parts, the legends, labels, or scales are too small and difficult to read. However, neither this nor the grammer does not reduce the overall high quality of the thesis.

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Připomínky

1. Please explain the linearization step, Section 3.2.2, in more details. I suppose, the only source of nonlinearity is the potential Ψf. But how the issue of EDL is treated via the proposed linearization is not clear to me.

2. Given the comment regarding the dimensionless analysis, would it be possible to re-derive Eq. (3.3.4_1)? I do not understand, where the term g¯ (g bar), in my opinion just replacing the term g', comes from.

2. The proposed identification method is deterministic. Given the variability in material properties, would it make sense to address this issue in the stochastic manner, for example in the framework of Bayesian inference? I understand, this would require a formulation of a certain surrogate model on macroscale, which could be problematic. On the contrary, this approach opens the door to the identification of an experimental error, which is typically not of the main interest. I would appreciate your opinion on this.

Závěrečné zhodnocení disertace

Na základě předloženého posouzení vědeckého významu, dosažených výsledků, organizace, stylu a teoretické správnosti práce lze práci hodnotit kladně. Jelikož vyhovuje všem požadavkům doktorské práce, doporučuji ji k další obhajobě. V případě úspěšné obhajoby doporučuji udělit Ing. Ludvíku Kolpaskému titul Ph.D.

Doporučuji po úspěšné obhajobě disertační práce udělení titulu Ph.D.	***ano*** ☒	***ne*** ☐

Datum: ....

Podpis oponenta: ....