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# Numerical modeling of diffusion within composite media

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**Abstract.** *Within biological systems, which contain complex and composite media, diffusion may depend not only on internal geometry, but also on the chemical interactions between solid phase and transported particles. New hierarchical multiscale microstructural model for diffusion within complex media is presented. Hierarchical modeling approach is then employed to construct a continuum diffusion model based on a novel numerical homogenization procedure, using which we evaluate constitutive material parameters.*

**Keywords:** diffusion; hierarchical modelling; microstructural and continuum model; numerical homogenization.

## 1 INTRODUCTION

In complex biological media diffusion transport is affected by molecular interactions with the surface, and predictions following Fick's law may become inaccurate. MD modeling and experiments have shown that diffusion of molecules in nanochannels is affected by proximity to a solid surface [1]. Therefore, modeling of these transport regimes needs novel approaches that could bring molecular scale information into complex macroscale models. An ideal scenario is to properly transfer MD information to macroscopic models. Hierarchical (multiscale) modeling approach [2], [3], which couples MD and Finite Element Method (FEM), offers this possibility. We will then introduce a multiscale hierarchical model for diffusion at the microstructural level. Further, we formulate a 'continuum' model which employs the results obtained by the microstructural model for diffusion within the RV. The continuum model is based on constitutive parameters, which include equivalent 'bulk' diffusion coefficients and equivalent distances from an imaginary surface. Constitutive parameters depend only on the structural geometry and the material properties of the diffusing constituents.

## 2 METHODS

### 2.1 MD simulations and scaling functions for diffusion coefficient

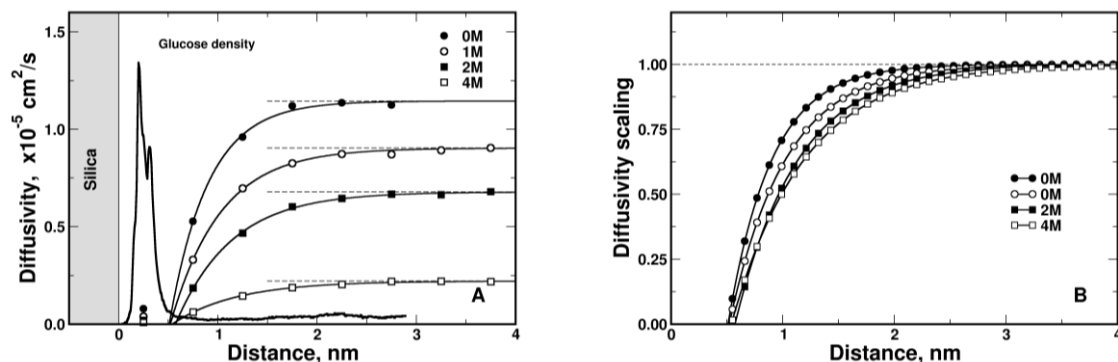


Figure 1: Calculated glucose diffusivity (A) and scaling functions of the proximity to the silica surface for several concentrations (B); according to [1].

MD simulations for calculating diffusion coefficient in nanochannels were carried out within [1],[2]. Diffusion coefficients were then calculated by using the mean square displacement  $\langle r^2 \rangle$ . The diffusivity along the surface normal ( $z$ -direction) was evaluated, from the surface up to the middle of the nanochannel. The diffusivity results include dependence on distance from the wall and glucose concentrations (Figure 1A).

The MD calculated diffusivity is normalized with respect to the “bulk” value  $D_{bulk}$  corresponding to diffusivity far from the surface, where influence of the surface is negligible. Calculated scaling function is shown in Figure 1B.

## 2.2 Finite element model

We here consider unsteady diffusion where the diffusion coefficient depends on both concentration and spatial position of a point within the model. FE solution procedures for nonlinear diffusion problems have been well established and successfully used in various applications (e.g. [4],[5],[6]). The basic mass balance equation, which also includes Fick’s law in equation, is transformed into the incremental-iterative system of linear balance equations for a finite element [6]:

$$\left( \frac{1}{\Delta t} \mathbf{M} + {}^{n+1} \mathbf{K}^{(i-1)} \right) \Delta \mathbf{C}^{(i)} = {}^{n+1} \mathbf{Q}^{S(i-1)} + {}^{n+1} \mathbf{Q}^{V(i)} - {}^{n+1} \mathbf{K}^{(i-1)} {}^{n+1} \mathbf{C}^{(i-1)} - \frac{1}{\Delta t} \mathbf{M} {}^{n+1} \mathbf{C}^{(i-1)} - {}^n \mathbf{C} \quad (1)$$

In our FEM model we have incorporated concentration and interface effects. Implementation of the incorporated expression is illustrated in Figure 2. Note that linear interpolation between scaling curves is used.

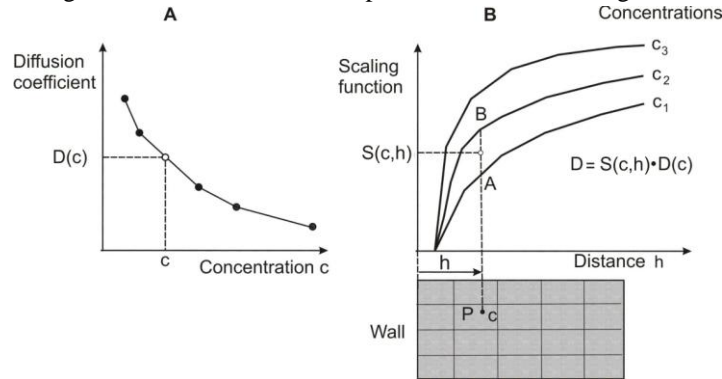


Figure 2: Determination of diffusion coefficient at a spatial point P using dependence on concentration and surface effects. a) The “bulk” value is determined from the curve  $D(c)$ ; b) the scaling function is evaluated from family of curves. Linear interpolation curves  $S(c,h)$  is adopted; according to [7].

## 2.3 Generalization of the hierarchical model to porous media

The main idea here is to determine equivalent diffusion parameters of a homogenous porous medium which capture the internal structure of a composite medium in a way that diffusion properties are preserved. To achieve this, we first take a reference volume around a material point (in a form of a cube) around that point, Figure 3a, and discretize it into finite elements (Figure 3b).

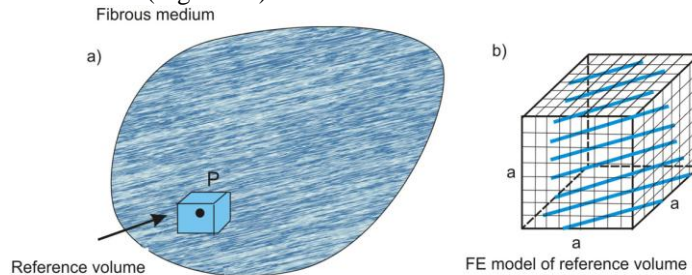


Figure 3: Concept of extension of hierarchical model to porous medium with fibers. a) Fibrous medium with reference volume at a material point P; b) Reference volume discretized into finite elements; according to [3],[8].

## 2.4 Numerical homogenization procedure and continuum model

We introduce a novel numerical homogenization procedure to determine the appropriate diffusion properties of a continuum model with a given microstructure. The basic condition governing this procedure is the equivalence of mass fluxes (through any surface in the diffusion domain) for the microstructural and continuum model, at any time during diffusion process.

Next, we calculate diffusion through the reference volume using equivalent quantities of a porous homogenous medium within the RV. The porosity  $n$  is evaluated from the internal structure of the RV. For each diffusion direction  $i$  (i.e. x,y,z), the steps are as follows: First we calculate mass release using initial diffusion using given  $D_{bulk} \cdot c$ . Then, perform changes on the value  $D_0$  until the mass release curve is close enough to the true curve, when the value is  $\bar{D}_0$ . After that, using  $\bar{D}_0$  calculate initial mass release curve taking into account equivalent values of the transformation matrix  $\bar{\mathbf{T}}$  and equivalent distance from the solid surface  $\bar{h}_0$ . Finally, search for the distance  $\bar{h}_i$  when difference between the calculated and true mass release curves is within a selected error tolerance. In the above calculations of the equivalent transformation matrix and initial equivalent distance  $\bar{h}_0$  a weighted procedure, which takes into account volumes belonging to FE nodes, is implemented [3],[8].

## 3 RESULTS

### 3.1 Dependence of equivalent parameters on concentration range and concentration gradient

For given solvent and diffusing particles we show that material parameters of the continuum model (equivalent diffusion coefficients and equivalent distances from surface) only depend on the geometry of the microstructure and its material characteristics [3]. To demonstrate this statement, we take a reference volume (RV) with solid silica nanofibers with fibers diameters of 10nm, angle of fiber direction is 75 degrees and porosity equal to 80%. For this model we change the boundary conditions to achieve various mass release curves.

### 3.2 Effect of total fiber's area in RV on values of equivalent parameters

In order to check influence of total fibers' surface area we used three different configurations of internal microstructure, consisting of fibers which direction is orthogonal to direction of diffusion. All examples are approximately with 80% porosity. Input parameter for each example, together with calculated values of total surface areas and total volume of solid phase in system, are given in table 6.

Table 1: Equivalent diffusion coefficient and equivalent distance from the surface results for three examples with different fiber's area, and same porosity.

Example	$\bar{D}_0^{eff}$	$\bar{D}_1^{eff}$	Surface Area [ $\mu m^2$ ]	$H_{eff}$
1	4.33908e+7	2.78251e+6	0.010050	1.6768E-3
2	4.33800e+7	2.77214e+6	0.007634	1.9002E-3
3	4.34844e+7	2.87622e+6	0.005026	2.2727E-3

According to results for  $\bar{D}_0^{eff}$  from table 1 it can be concluded that equivalent diffusion coefficient of free diffusion depends on porosity (results for  $\bar{D}_0^{eff}$  are approximately the same for all three examples). Result for equivalent distance from the surface  $H_{eff}$  show that  $H_{eff}$  depends on total surface area in the system ( $H_{eff}$  decreases with increasing of total surface area).

## 4 CONCLUSIONS

Our approach, consisting of a microstructural model and numerical homogenization procedure is general and robust, and offers new possibilities in modeling diffusion through complex materials, including molecular transport in biological systems (e.g. intercellular spaces and tissues).

The presented methodology can serve as a tunable platform for constructing intricate multiscale hierarchical diffusion models with additional complexity and effects, such as multiple molecule types (e.g. different proteins/ligands), multiple surfaces (e.g. various cell types with different receptors), and various media (e.g.

different solvents). These multiscale models provide a basis for a deeper, more accurate representation of fundamental transport processes occurring throughout nature.

Numerical homogenization procedure presented in this work is analogous to homogenization procedures previously presented in linear and nonlinear solid mechanics, heat transfer and diffusion, where different types of RV were used (e.g. [9],[10],[11]). Previous homogenization procedures have limitations due to the special assumptions made regarding microstructure (e.g. periodicity) as well as relying on various asymptotic expansions of analytic forms. Our method is not only general, but also includes concentration-dependent parameters within a wide range of concentrations over which diffusion occurs.

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