An Analytical Model of Diffusion in a Sphere with Semi-Permeable Boundary

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***Abstract*—Modeling biological systems is of high interest in molecular communications. Exact analytical models of biological environments, e.g. cells or blood vessels offer several advantages in analysis and design of molecular communication channels. For the diffusion of particles in cells or their transport through a chain of cells functional transformations are a promising modeling approach. This contribution considers the modeling of particle diffusion in a sphere with impedance boundary conditions, serving e.g. as a simple model for diffusion in cells bounded by a semi-permeable membrane.**

I. Problem Description

The design and analysis of biological channels for the transmission of information by particles is of high interest in molecular communications (MC). At the moment only a few testbeds are available (e.g. [1]) and their design is very complex. Biological experiments mostly are slow and the accuracy of experiments is restricted. Helpful tools for the design of experiments and therefore for MC channels are simulation models of biological systems. Therewith the impulse response of a channel can be derived, before a complex experiment or measurement has to be set up. Beside numerical methods or Monte-Carlo simulations also an analytical model can be derived by the application of functional transformations to an initial-boundary value problem [2], [3].

In this contribution an initial-boundary value problem for the particle diffusion in a sphere is considered. The sphere is bounded by a membrane with an adjustable permeability. A simulation model follows by the application of functional transformations and the boundary conditions are incorporated by a feedback loop. The derived model serves as a simple cell model for the modeling of inter/intra-cell and cell-to-environment communication. It can be extended in further works to: Traveling calcium waves through a cell cascade (see [4]); Cells pumping protons into a substrate according to the presented testbed in [1].

In this abstract, the exact calculations are only roughly outlined. The simulation results show the coherence of the derived analytical model.

II. Physical Description

The diffusion of particles in a spherical volume $V = \{\boldsymbol{x} : [r, \theta, \varphi] \,|0 \leq r \leq R, -\pi \leq \varphi \leq \pi, 0 \leq \theta \leq \pi\}$ is described by a set of partial differential equations for the particle concentration $p(\boldsymbol{x}, t)$ in $\mathrm{mol\,m^{-3}}$ and flux $\boldsymbol{i}(\boldsymbol{x}, t) = [i_r \, i_\theta \, i_\varphi]^{\mathrm{T}}$ in $\mathrm{mol\,m^{-2}\,s^{-1}}$

$$\boldsymbol{i}(\boldsymbol{x}, t) + \frac{1}{D} \cdot \mathbf{grad}\, p(\boldsymbol{x}, t) = 0, \tag{1}$$

$$\frac{\partial}{\partial t} p(\boldsymbol{x}, t) + \mathbf{div}\, \boldsymbol{i}(\boldsymbol{x}, t) = f_{\mathrm{e}}(\boldsymbol{x}, t). \tag{2}$$

The function f_{e} is an excitation function containing all source signals. A constant diffusion coefficient D specifies the propagation of particles within the sphere.

The boundary of the sphere at $r = R$ is semi-permeable, which leads to boundary conditions of the third kind

$$i_r(\boldsymbol{x}, t) = \gamma \cdot p(\boldsymbol{x}, t), \qquad r = R. \tag{3}$$

The real-valued parameter γ controls the rate at which particles can leave the sphere. At time $t = 0$ there are no particles in the sphere, so that $p(\boldsymbol{x}, 0) = 0$.

For the derivation of a simulation model the PDE's (1), (2) are reformulated in a unifying vector form according to [3]

$$\left[\frac{\partial}{\partial t}\boldsymbol{C} - \boldsymbol{L}\right] \boldsymbol{y}(\boldsymbol{x}, t) = \mathbf{0}, \qquad \boldsymbol{L} = \boldsymbol{A} + \nabla \boldsymbol{I}, \tag{4}$$

with the spatial differential operator $\boldsymbol{L}$ and the matrices

$$\boldsymbol{A} = \begin{bmatrix} 0 & -\boldsymbol{I} \\ 0 & \mathbf{0} \end{bmatrix}, \; \boldsymbol{C} = \begin{bmatrix} 0 & \mathbf{0} \\ 1 & \mathbf{0} \end{bmatrix}, \; \nabla = \begin{bmatrix} -\mathbf{grad} & \mathbf{0} \\ 0 & -\mathbf{div} \end{bmatrix}. \tag{5}$$

The vector of variables $\boldsymbol{y}$ contains all physical quantities

$$\boldsymbol{y}(\boldsymbol{x}, t) = \begin{bmatrix} p(\boldsymbol{x}, t) & \boldsymbol{i}(\boldsymbol{x}, t)^{\mathrm{T}} \end{bmatrix}^{\mathrm{T}}. \tag{6}$$

III. Functional Transformations

The solution $\boldsymbol{y}$ of the initial-boundary value problem in (4) is expanded into a set of bi-orthogonal eigenfunctions [2], [3] and is formulated in terms of a state-space description. The boundary conditions in (3) are realized by a feedback loop. The eigenvalues s_μ of the system are derived for boundary conditions with $\gamma = 0$, then they are shifted by a feedback matrix to fulfill the boundary conditions with $\gamma > 0$ [5].

A. Eigenfunctions and Eigenvalues

The eigenfunctions for the concentration p are derived by the solution of an eigenvalue problem dedicated to (4) as described in [3] and follow as

$$K_p(\boldsymbol{x}, \mu) = j_n(k_{n,\nu} \cdot r) \cdot Y_n^m(\theta, \varphi). \tag{7}$$

The function j_n denotes the spherical Bessel function of order n and $k_{n,\nu}$ are the real-valued zeros of $j_n'(k_{n,\nu} \cdot R) = 0$. The

function Y_n^m is the spherical harmonic function of order n and degree m. The three indexes $n = 0 \dots N$, $\nu = 0 \dots M$, $m = -n \dots n$ are combined into the index $\mu = [n, \nu, m]$ numbering the eigenfunctions $K(\boldsymbol{x}, \mu)$ and eigenvalues s_μ.

The eigenvalues s_μ of the system with boundary conditions for $\gamma = 0$ are derived within the solution of the eigenvalue problem for K_p. All eigenvalues indexed by μ can be arranged into a state matrix $\boldsymbol{\mathcal{A}}$ with the s_μ-values on its main diagonal

$$s_\mu = -Dk_{n,\nu}^2, \qquad \rightarrow \qquad \boldsymbol{\mathcal{A}} = \operatorname{diag}(\dots, s_\mu, \dots). \tag{8}$$

The influence of the boundary conditions for $\gamma > 0$ on the eigenvalues is concentrated into a feedback matrix acting on the matrix $\boldsymbol{\mathcal{A}}$ [5]

$$\boldsymbol{\mathcal{A}}_\mathrm{c} = \boldsymbol{\mathcal{A}} - \gamma \cdot \boldsymbol{\mathcal{B}}\boldsymbol{\mathcal{K}}. \tag{9}$$

The amount of the variable permeability γ from (3) determines the eigenvalues of the matrix $\boldsymbol{\mathcal{A}}_\mathrm{c}$.

IV. Simulation Model

By the application of the transformation steps described in [3], [5] the solution of the vector PDE in (4) is formulated in terms of a state-space description in the discrete time domain. The multidimensional state equation follows as

$$\bar{\boldsymbol{y}}[k] = e^{(\boldsymbol{\mathcal{A}} - \gamma \cdot \boldsymbol{\mathcal{B}}\boldsymbol{\mathcal{K}})T} \bar{\boldsymbol{y}}[k-1] + \bar{\boldsymbol{f}}_\mathrm{e}[k], \tag{10}$$

with T as the discrete sampling time and $t = kT$. The vector $\bar{\boldsymbol{y}}$ is the vector of system states in the transform domain and $\bar{\boldsymbol{f}}$ is the transform domain representation of the excitation functions. The output equation for the concentration $p(\boldsymbol{x}, t)$ in the sphere is given by

$$p[\boldsymbol{x}, k] = \boldsymbol{c}^\mathrm{T}(\boldsymbol{x}) \bar{\boldsymbol{y}}[k], \quad \boldsymbol{c}^\mathrm{T}(\boldsymbol{x}) = [\dots, K_p(\boldsymbol{x}, \mu), \dots]. \tag{11}$$

V. Simulation

The simulations show the validity of the derived simulation model. The geometry of the sphere is described by the normalized radius $R = 1$. The normalized diffusion coefficient is $D = 1 \cdot 10^{-2}$. The excitation signal $f_\mathrm{e}(\boldsymbol{x}, t)$ is a sequence of two particle injections at $t = 0.25\mathrm{s}, 3\mathrm{s}$. The injections are modeled by a spatial raised cosine function in the center $r_0 = 0$ of the sphere. As the source is located in the center, only modes of order $n = 0$ are excited, and therefore $N = 0$, $M = 30$ is used for simulation. The simulations are performed with the model in (10) and are compared with the results of the particle based AcCoRD simulator [6].

The simulation results for the normalized concentration $p(\boldsymbol{x}, t)$ are shown in Fig. 1 for different observation positions and permeability γ. The upper plot in Fig. 1 shows the particle concentration near the boundary at $r_1 = 0.9 \cdot R$. For a value of $\gamma = 0$ the boundary of the sphere is completely reflective as can be seen in the black curve. Choosing $\gamma > 0$ the sphere boundary becomes permeable so that all particles can leak for $t \rightarrow \infty$ (blue, red curves). The plot in the bottom of Fig. 1 shows the same scenario for a different observation point $r_1 = 0.4 \cdot R$. The same effects can be observed, but, conclusively, they are not as pronounced as on the boundary.

Both simulations show, that the derived model (10), (11) perfectly agrees with the results of the particle simulator. While

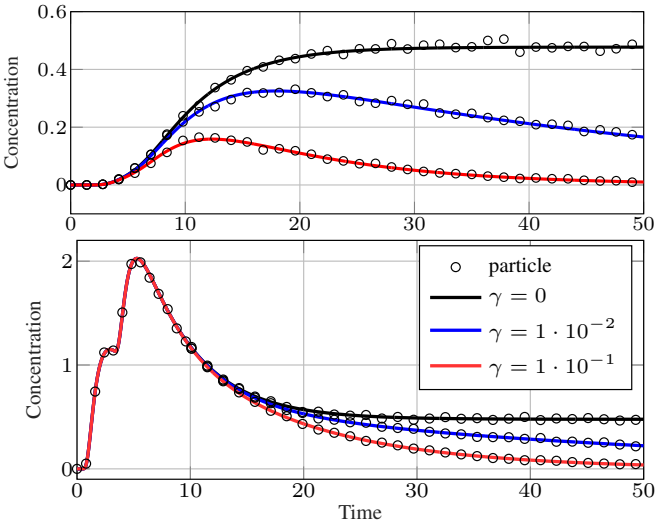

Fig. 1. Normalized concentration $p(\boldsymbol{x}, t)$ at $\boldsymbol{x} = [r_1, \pi/3, \pi/4]$, with $r_1 = 0.9$ (top) and $r_1 = 0.4$ (bottom) over time for different values of $\gamma = 0, 1 \cdot 10^{-2}, 1 \cdot 10^{-1}$, simulated with the simulation model (10), (11) (black, blue, red) and with a particle simulator [6].

the AcCoRD simulator needed approx. $15\mathrm{min}$ to simulate one scenario, the proposed model needed $15\mathrm{s}$, respectively $0.2\mathrm{s}$ for the pure time iterations. Furthermore, the model preserves the closed form of the solution and allows a system theoretic analysis of the process and the influence of the permeability. It is also able to handle e.g. time- and space dependent permeability at the boundary.

VI. Conclusions

This abstract outlined the derivation of an analytical model for particle diffusion in a sphere with a semi-permeable boundary. The incorporation of the boundary conditions by a feedback loop makes the permeability γ an adjustable parameter in the discrete time simulation algorithm.

The derived model serves as a starting point for further works: intra- and inter cell communication, propagation of calcium waves trough a cell-cascade, transmitter/receiver design.

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