Channel Modeling for Time-Varying Dispersive Closed-Loop MC Systems with Pulsatile Flow

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***Abstract*—Molecular communication (MC) is a communication paradigm in which information is conveyed through the controlled release and propagation of molecules. Especially in in-body application environments, the channel topology is closed-loop, and particle propagation is determined by the joint influence of diffusion and pulsatile flow induced by the heartbeat. However, most existing analytical models for dispersive closed-loop MC channels assume a constant flow velocity, whereas flows in biological environments are in many cases pulsatile. Therefore, in this paper, we present a time-varying one-dimensional (1D) channel model for closed-loop MC systems under pulsatile flow, operating in the dispersive regime. An analytical expression for the channel impulse response (CIR) is derived, resulting in a wrapped Normal distribution with time-variant mean and variance. The proposed model is validated by comparison to three-dimensional (3D) particle-based simulation (PBS) results.**

I. Introduction

Molecular communication (MC) enables information transfer in biological environments, and targets various biomedical and healthcare applications. In vascular and circulatory systems, transport takes place in highly branched closed-loop channels and is governed by diffusion and flow [1]. The closed-loop nature of such channels motivates the development of models that account for the periodicity of transport. However, most existing models assume constant flow velocity [2], [3], although physiological flows can exhibit pulsatile behavior due to the periodic pumping of the heart.

Recent advances in transport modeling have shown that, in the dispersive regime [4], diffusion and pulsatile flow with a Womersley velocity profile [5] can be approximated by a one-dimensional (1D) advection–diffusion equation with time-varying flow velocity [6], similar to the Aris-Taylor approximation for time-invariant scenarios. To this end, this work addresses the modeling of dispersive closed-loop MC channels under pulsatile flow.

The main contributions of this work are as follows. First, we extend an existing closed-loop MC channel model to account for pulsatile flow by introducing a time-varying flow velocity expression. Second, we derive an analytical expression for the channel impulse response (CIR) with time-variant mean and variance. Finally, we validate the proposed analytical 1D model through three-dimensional (3D) particle-based simulations (PBSs) of the underlying transport processes.

II. Channel Model

This section adopts the reduced 1D transport model for pulsatile flow proposed in [6] and derives an analytical expression for the corresponding CIR in a closed-loop MC system.

Particle transport in a cylindrical MC channel is governed by advection and diffusion in three dimensions. For sufficiently long and slender channels, transverse diffusion is much faster than axial transport, leading to an approximately uniform particle distribution over the cross section. Under these conditions, the underlying transport processes can be approximated by an equivalent 1D description along the axial direction [4]. The resulting 1D axial transport is described by the following advection-diffusion equation [6, Eq. (41)]

$$\partial_t p(x,t) + u(t)\partial_x p(x,t) = D_{\mathrm{1D}}(t)\partial_{xx} p(x,t), \qquad (1)$$

where ∂_x and ∂_t denote the first derivatives with respect to space and time, respectively, and ∂_{xx} denotes the second derivative with respect to space. Moreover, $p(x,t)$, $u(t)$, and $D_{\mathrm{1D}}(t)$ are the particle concentration, the cross-sectionally averaged, time-variant axial flow velocity, and the corresponding time-variant effective diffusion coefficient. As we consider a closed-loop system of total length L, (1) will be solved for periodic boundary conditions and an impulsive release of particles at $t = 0$, see [1, Sec. III-C].

The axial flow velocity $u(t)$ in (1) is time-varying and periodic, and can be modelled by a finite Fourier series as follows [6, Eq. (48)],

$$u(t) = \bar{u}\left(1 + \sum_{n=1}^{N} M_n \cos(n\omega t + \phi_n)\right), \qquad (2)$$

where $\bar{u}$ denotes the temporal mean velocity over one pulsation period, $\omega = 2\pi f$ is the fundamental angular frequency, f is the pulsation frequency, M_n are dimensionless amplitude coefficients, ϕ_n are phase shifts, and N is the number of harmonics used to approximate the pulsatile velocity waveform. An example waveform is shown in Fig. 1. The representation in (2) allows flexible modeling of physiologically realistic pulsatile waveforms and is consistent with the 3D velocity model in [6, Eq. (31)] used in PBSs.

Similar to the derivation of the effective diffusion coefficient for time-invariant systems [4], the time-varying effective diffusion coefficient in (1) is determined by the pulsatile velocity in (2). A key dimensionless parameter characterizing pulsatile flows is the Womersley number, $\mathrm{Wo} = R\sqrt{\omega/\nu}$, which measures how fast the flow velocity changes in time compared to how fast viscosity can adjust the velocity profile across the channel cross section [5]. Here, R denotes the channel radius, and ν the kinematic viscosity.

For the parameter ranges considered in this paper, the Womersley number Wo is within the range for which the diffusion coefficient approximation derived in [6, Eq. (43)] can be directly applied, i.e., $D_{\mathrm{1D}}(t) = D + \frac{\bar{u}^2 R^2}{48D}\left(\frac{u(t)}{\bar{u}}\right)^2$, where D is the corresponding 3D molecular diffusion coefficient of the signaling particles.

To obtain $p(x,t)$ from (1), we apply a sequence of variable transformations. First, a moving spatial coordinate is introduced as $\xi = x - \Xi(t)$, where $\Xi(t) = \int_0^t u(s)\,\mathrm{d}s$, and follows the instantaneous mean flow velocity. Using the chain rule, (1) reduces to

$$\partial_t p(\xi,t) = D_{\mathrm{1D}}(t)\partial_{\xi\xi} p(\xi,t). \qquad (3)$$

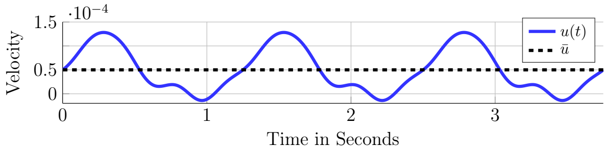

Fig. 1. **Time-varying axial flow velocity** $u(t)$ under pulsatile flow conditions in (2).

Next, a rescaled time variable is defined as $\tau(t) = \int_0^t D_{1\mathrm{D}}(s)\,\mathrm{d}s$, which absorbs the time dependence of the diffusion coefficient. Under this transformation, (3) turns into a diffusion equation with constant coefficients

$$\partial_\tau h(\xi,\tau) = \partial_{\xi\xi} h(\xi,\tau), \tag{4}$$

where $h(\xi,\tau) = p(\xi, t(\tau))$.

Solving (4) for periodic boundary conditions and an impulsive release of particles at $t = 0$, and then returning to the original variables by inverting the coordinate transformations, the particle concentration $p(x,t)$, which defines the CIR, in a dispersive closed-loop MC system with diffusion and time-variant flow ends up in a wrapped normal distribution as follows

$$p(x,t) = \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2(t)}} \exp\left(-\frac{[x-\Xi(t)+kL]^2}{2\sigma^2(t)}\right), \tag{5}$$

with time-variant mean $\Xi(t) = \int_0^t u(s)\,\mathrm{d}s$ and variance $\sigma^2(t) = 2\int_0^t D_{1\mathrm{D}}(s)\,\mathrm{d}s$. We note that the expressions for $\Xi(t)$ and $\sigma^2(t)$ can be obtained in closed form, but are omitted here for brevity due to the space limitations.

III. Simulation Results

In the following, the analytical model in (5) is validated by comparison to the results from 3D PBS. The PBS is implemented for a straight cylinder with reflecting boundaries at the channel walls and the closed-loop characteristic is realized by imposing periodic boundary conditions. Moreover, we compare the model in (5) to the time-invariant solution proposed in [1]. We consider a receiver of length Δx_{det}, located at $x = x_{\mathrm{det}}$. Therefore, the particle concentration inside the receiver follows as

$$p_{\mathrm{det}}(t) = \int_{x_{\mathrm{det}}-\Delta x_{\mathrm{det}}/2}^{x_{\mathrm{det}}+\Delta x_{\mathrm{det}}/2} p(x,t)\,\mathrm{d}x. \tag{6}$$

The parameters were chosen according to [1], [4] such that the system operates in the dispersive regime. Unless stated otherwise, the parameters are fixed to $D = 5\cdot 10^{-9}\,\mathrm{m}^2\,\mathrm{s}^{-1}$, $R = 0.1\,\mathrm{mm}$, $L = 1\,\mathrm{mm}$, and $\Delta x_{\mathrm{det}} = 0.1\,\mathrm{mm}$.

We employ the pulsatile velocity waveform $u(t)$ shown in Fig. 1, generated from (2) using $f = 0.8\,\mathrm{Hz}$ and $N = 4$ harmonics with amplitudes $M_1 = 1.26$, $M_2 = 0.27$, $M_3 = 0.18$, and $M_4 = 0.09$, and phases $\phi_1 = -1.4$, $\phi_2 = -2.6$, $\phi_3 = 1.0$, and $\phi_4 = 2.8$. Unless stated otherwise, the temporal mean velocity is $\bar{u} = 0.5\cdot 10^{-4}\mathrm{m\,s}^{-1}$. For the results in which $\bar{u}$ is varied, the same pulsatile waveform is used, and only the value of $\bar{u}$ is changed. For better comparability, all results are normalized by the equilibrium value $p_\infty = \Delta x_{\mathrm{det}}/L$, obtained from $\lim_{t\to\infty} p(x,t) = 1/L$.

Figure 2 shows the results from the proposed model in (5) (blue), from PBS (circle markers), and from the time-invariant

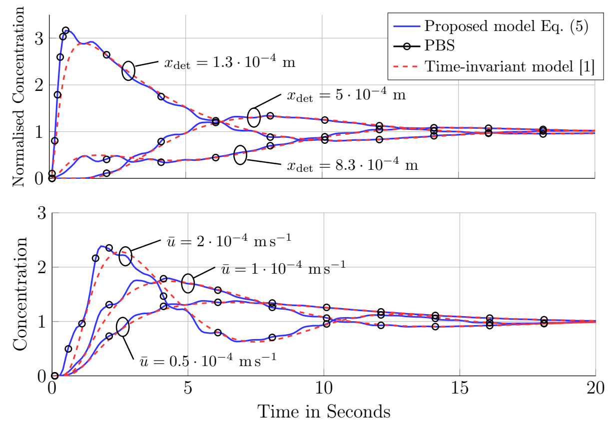

Fig. 2. **Received Signals** for varying receiver distance x_{det} (top) and mean flow velocity $\bar{u}$ (bottom).

model in [1] (red), for different receiver positions x_{det} with fixed mean flow velocity $\bar{u} = 0.5\cdot 10^{-4}\mathrm{m\,s}^{-1}$ (top) and for different mean flow velocities $\bar{u}$ for a fixed receiver position $x_{\mathrm{det}} = 0.3\,\mathrm{mm}$ (bottom). First, we can observe that the proposed model is in excellent agreement with the results from PBS in all considered scenarios. Moreover, we can observe that the time-invariant model from [1] is not able to capture the pulsations, while it is still capable of approximating the overall shape of the received signal. However, it can also be observed that the influence of the pulsatile background flow becomes less pronounced for increasing receiver distance, decreasing mean flow velocities, and over time. This behavior is expected, as for all these variations, the influence of the advective transport gets less important compared to diffusion yielding more dispersive system dynamics [4].

IV. Conclusion

In this work, we proposed a channel model for time-varying closed-loop MC systems under pulsatile flow. An analytical expression for the CIR was derived, yielding a wrapped Normal distribution form with time-variant mean and variance. The model extends our previous closed-loop channel model [1] by incorporating pulsatile flow and was validated through comparison with 3D PBSs. The results build the basis for our future work, including the in-depth investigation of the influence of pulsatile flow on the received signal.

References

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