Molecular Transport in Microfluidic Channels for Flow-induced Molecular Communication

A. Ozan Bicen   Ian F. Akyildiz
Broadband Wireless Networking Laboratory (BWN)
School of Electrical and Computer Engineering
Georgia Institute of Technology, Atlanta, Georgia 30332
Email: {bozan, ian}@ece.gatech.edu

***Abstract*—Fluid flow inside microfluidic channels can alleviate excessive dispersion and delay in diffusion-based molecular communication and lead to the emergence of Flow-induced Molecular Communication (FMC). To develop communication techniques for FMC, analysis of molecular transport by flow, i.e., convection, inside microfluidic channels is essential. In this paper, molecular transport, i.e., concentration propagation, is studied for FMC in rectangular microfluidic channels. First, solution of flow velocity inside rectangular microfluidic channels is presented. Then, impulse response and transfer function are determined for a point source based on the flow velocity, diffusion constant, channel cross-section, and length parameters. Frequency and phase responses for concentration propagation in rectangular microfluidic channels with different cross-section and length parameters are revealed via numerical results.**

I. Introduction

Molecular communication enables nano-scale networking in fluidic environments. Concentration of molecules is used to encode and transmit information in molecular communications. Diffusion is considered as mass transport phenomenon for concentration propagation from transmitter to receiver in molecular communication [2]. However, transmitted concentration is exposed to excessive attenuation and delay when diffusion is employed for mass transport.

Flow-based molecular transport, i.e., convection, provides opportunity to overcome shortcomings of the diffusion-based communications. In addition, via microfluidic channel between transmitter and receiver, concentration propagation can be directed. In this work, we address concentration propagation inside microfluidic channels with flowing fluid inside, which leads to Flow-induced Molecular Communications (FMC). A bacteria population can be used as a point source to encode and transmit, as well as receiving information based on molecular concentration in microfluidic channels [3]. In particular, utilization of flow alleviates attenuation and delay by enhancing concentration propagation and directing concentration propagation in microfluidic channels. Comparison of convection and diffusion is presented in Fig. 1 (a) and (b), respectively. The propagation delay and the attenuation are mitigated via convection in Fig. 1 (a) compared to Fig. 1 (b). Nanomedicine and microbiology can be some of the important application areas of FMC. To realize FMC, a rigorous analysis of concentration propagation inside microfluidic channels from FMC perspective is required to enable design of communication techniques. Effect of microfluidic channel parameters, i.e., cross-section and length, as well as flow velocity on concentration propagation from transmitter to receiver must be investigated.

Molecular communications attracted many researchers from different fields. Diffusion-based molecular communication model is proposed in [2], and noise sources are identified in [4] and [5], as well as capacity analysis in [6]. There have been works on analysis of microfluidic channels for chemical signal separation and mixing [7], [8], [9], [10], [11], [12], [13]. Furthermore, droplet-based communications for nanonetworking in microfluidic devices is proposed in [14]. Overall, existing models for diffusion-based molecular communication are not suitable for FMC, since they do not address effect of flow. On the other hand, existing models for concentration propagation in microfluidic channels lack communication perspective. Therefore, employment of flow for molecular communication requires new concentration propagation analysis that address flow and peculiarities of microfluidic channels for efficient design of communication techniques in FMC.

In this paper, first, velocity of flow in rectangular microfluidic channels is determined. Then, analysis of concentration propagation in FMC is performed which provides a framework to determine impulse response and transfer function of concentration propagation in rectangular microfluidic channels based on flow velocity and microfluidic channel parameters, i.e., cross-section and length. Furthermore, obtained analytic formulations are elaborated via numerical results for various cross-section and length parameters.

The remainder of this paper is organized as follows. In Section II, flow velocity solution for rectangular microfluidic channels is presented. Analysis of concentration propagation via convection in rectangular microfluidic channels is presented in Section III. Numerical results are presented in Section IV. Finally, in Section V, we conclude the paper.

II. Fluid Flow in Microfluidic Channels

In this section, the hydrodynamic behavior of the fluid flow inside microfluidic channels is presented. In microfluidic channels, fluid flows are taken as incompressible, i.e., constant density ρ [15]. The flow velocity $\mathbf{u}$ is related to pressure drop $\mathbf{p}$ via Navier-Stokes equation under the constant density ρ, constant viscosity μ, and conservation of mass $(\nabla \cdot \mathbf{u} = 0)$

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(a) (b)

Fig. 1. Illustration of the exposed dispersion at τ_1 and τ_2 instants via convection (a) and diffusion (b) for a concentration signal placed in the channel at τ_0 instant.

assumptions as

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = -\nabla\mathbf{p} + \mu\nabla^2\mathbf{u} \tag{1}$$

For a unidirectional flow through an infinite channel, the Navier-Stokes equation can be simplified due to $(\mathbf{u}\cdot\nabla)\mathbf{u} = 0$. Fluid flow inside microfluidic channels under this condition is termed as laminar, and by addition of each lamina, complete flow is formed. To analyze microfluidic channels efficiently, laminar flow should be preserved from disruptions. In the following subsections, the fluid flow velocity in rectangular microfluidic channels is formulated, and the solution for flow velocity is presented using the linear relationship between pressure drop and flow rate.

A. Poiseuille Flow

To model flow in microfluidic channels, Poiseuille flow is used [15], [16]. The Poiseuille flow is generated by pressure difference, and it is unidirectional and in steady-state [16]. The microfluidic channel is straight and parallel to x axis. Between the inlet and the outlet of the microfluidic channel, the pressure drop Δp is constant. Under these assumptions, Navier-Stokes equation (1) is reduced to

$$\partial_x p(x) = \mu(\partial_y^2 + \partial_z^2)u_x(y,z) \tag{2}$$

where μ is the viscosity of the fluid, and $u_x(y,z)$ is the fluid velocity field. Since there is no pressure drop in y and z directions, velocity field in these directions are 0. Both sides of the (2) are equal to a constant, hence, pressure along the channel is a linear function of position x as

$$p(x) = p(x_0) - \frac{\Delta p}{l}(x - x_0) \tag{3}$$

where l is the length of the channel. We obtain

$$(\partial_y^2 + \partial_z^2)u_x(y,z) = -\frac{\Delta p}{\mu l} \tag{4}$$

by replacing (3) into (2). The Poiseuille flow exhibits a parabolic velocity field, and the flow velocity reaches its peak value at the center of the channel, and it decays to 0 at the boundaries. In rectangular channels, flow velocity u_x for Poiseuille flow can be determined via solution of (4) as [16]

$$\begin{aligned} u_x(y,z) =& \frac{4h^2\Delta p}{\pi^3\mu l} \\ &\cdot \sum_{n=1,3,5,\cdots}^{\infty} \frac{1}{n^3}\left[1 - \frac{\cosh(\frac{n\pi y}{h})}{\cosh(\frac{n\pi w}{2h})}\right]\sin(n\pi z/h) \end{aligned} \tag{5}$$

where h and w are the height and width of the microfluidic channel, respectively.

B. Flow Rate

Volumetric flow rate Q can be found via integration over cross-section area S of the rectangular microfluidic channel as

$$Q \triangleq \int_S u_x(y,z)\mathrm{d}y\mathrm{d}z \tag{6}$$

By integrating the velocity contributions (5) of each lamina, volumetric flow rate inside rectangular microfluidic channel is found as

$$\begin{aligned} Q &= \int_0^w \int_0^h u_x(y,z)\mathrm{d}y\mathrm{d}z \\ &= \frac{8h^3 w}{\pi^4 \mu l}\sum_{n=1,3,5,\cdots}^{\infty}\left[\frac{1}{n^4} - \frac{2h}{\pi w n^5}\tanh(\frac{n\pi w}{2h})\right]\Delta p \end{aligned} \tag{7}$$

For high aspect-ratio rectangular channels, i.e., $w \gg h$, Q in (7) can be further approximated using $\tanh(\infty) = 1$ as [16]

$$Q \approx \frac{h^3 w}{12\mu l}\left(1 - 0.630\frac{h}{w}\right)\Delta p \tag{8}$$

The linear relationship between the flow rate and the pressure drop along the microfluidic channel is shown for the Pouseuille flow. This linear relation between flow rate and pressure drop is called Pouseuille-Hagen law and will be used to define hydraulic conductance and determine flow velocity.

C. Flow Velocity

Using the presented average flow rate in rectangular microfluidic channels, lumped parameter modeling is used to formulate flow velocity. Due to linear relation between pressure drop and flow rate, the flow rate in the channel is linked to the pressure drop along the channel via Hagen-Poiseuille law as

$$Q = G\Delta p \tag{9}$$

where G is the hydraulic conductance of the rectangular microfluidic channel. For rectangular channels with high aspect-ratio, i.e., $h/w \to 0$, the hydraulic conductance is given by

$$G_n = h_n^3 w_n/(12\mu l_n) \tag{10}$$

The Pouiseulle flow definition, i.e., steady and laminar flow, holds in added two finite length rectangular channels with different cross-sections, due to low Re numbers in microfluidics [7], [16]. The fluid flow velocity u is obtained by dividing fluid flow rate with cross-section area of the rectangular microfluidic channel A as

$$u = \frac{1}{A}Q \tag{11}$$

Next, concentration propagation analysis is performed for FMC in rectangular microfluidic channels.

III. Concentration Propagation Analysis

In this section, impulse and frequency response for concentration propagation through rectangular microfluidic channels is determined to enable analysis of FMC.

A. Impulse Response

The propagation of concentration ϕ inside rectangular microfluidic channels is modeled using the convection-diffusion equation, which is defined as

$$\frac{\partial \phi}{\partial t} = -u\nabla\phi + D\nabla^2\phi \tag{12}$$

where D is the diffusion constant. Variation of concentration in time ($\partial\phi/\partial t$) is related to convection ($u\nabla\phi$) and diffusion ($D\nabla^2\phi$) by convection-diffusion equation. Overall, concentration propagation can be expressed as a linear combination of propagation inside rectangular microfluidic channels having different cross-section.

Concentration propagation in microfluidic channels is analyzed using one-dimensional solution of convection-diffusion, which is sufficient to capture the convection-driven transport of molecules [7]–[11].

The injected finite amount of mass M at instant t_0 into the flow by a point source located at x_0 is given by

$$\phi(x_0, t_0) = \frac{M}{A}\delta(x - x_0, t - t_0) \tag{13}$$

where A is the cross-section area of the rectangular microfluidic channel. For $M/A = 1$, impulse response is obtained as [16]

$$h(l,\tau) = \frac{1}{\sqrt{4\pi D\tau}}\exp\big(-\frac{(l-u\tau)^2}{4D\tau}\big) \tag{14}$$

where $l = x - x_0$, and $\tau = t - t_0$.

Pe number is the determiner for dominance of role of flow over diffusion for concentration propagation, which is defined as

$$\mathrm{Pe} = ul/D \tag{15}$$

As Pe increases, concentration propagation is dominated by convection, and diffusion becomes negligible. Next, we obtain transfer function of concentration propagation inside rectangular microfluidic channels.

B. Transfer Function

The transfer function of the concentration propagation for a point source, i.e., frequency response for an impulse input concentration in frequency domain as $\Phi(0, f) = 1$, can be found via solving (12) in frequency domain. Fourier transform of (12) is

$$j2\pi f\Phi(l,f) = -u\frac{\partial\Phi(l,f)}{\partial l} + D\frac{\partial^2\Phi(l,f)}{\partial l^2} \tag{16}$$

The transfer function is obtained using boundary conditions $\Phi(0, f) = 1$ and $\Phi(\infty, f) = 0$ as

$$H(l,\omega) = e^{(u(1-\sqrt{1+\frac{j4\omega D}{u^2}})\frac{l}{2D})} \tag{17}$$

where the ordinary frequency f is converted to angular frequency ω using identity

$$\omega = 2\pi f. \tag{18}$$

To have a converging series expansion, assuming

$$|j4\omega D/u^2| < 1, \tag{19}$$

the term in square root can be approximated as

$$\sqrt{1 + j4\omega D/u^2} \approx 1 + j2\omega D/u^2 + 2\omega^2D^2/u^4 \tag{20}$$

Finally, we approximate the transfer function as

$$H(l,\omega) \approx e^{-(\frac{\omega^2 D}{u^3} + j\frac{\omega}{u})l} \tag{21}$$

where we assume

$$4\omega D < u^2 \tag{22}$$

during derivation to have a converging series expansion for the transfer function.

IV. Numerical Results

In this section, we investigate frequency and phase response of FMC in rectangular microfluidic channels. Viscosity μ of the fluid is set to $10^{-3}\mathrm{Pa}\cdot\mathrm{s}$. Diffusion constant D is set to $10\cdot 10^{-10}\mathrm{m}^2/\mathrm{s}$. Frequency and phase responses are studied for two different channel lengths, i.e., l of 10 and $100\mathrm{mm}$ in Fig. 2 and 3, respectively. Pressure drop Δp along the channel is set to $500\mathrm{Pa}$. Channel height is taken as $h = 5$ and $10\mu\mathrm{m}$, and width is taken as $w = 25$ and $50\mu\mathrm{m}$.

A. Attenuation

In Fig. 2 (a), Fig. 2 (c), Fig. 3 (a), and Fig. 3 (c), it is shown that concentration propagation inside rectangular microfluidic channel is exposed to significant attenuation with increasing frequency, i.e., concentration level decays rapidly with the increasing frequency. Therefore, usable frequencies for communication are limited in FMC. However, attenuation of the concentration depends on the cross-section parameters as well as frequency and distance. For the same width w, increasing the height of the channel yields significant reduction in the attenuation. Concentration level reduces below one half, i.e., $3\mathrm{dB}$ cut-off frequency, as angular frequency is further increased beyond $1\mathrm{rad/sec}$, and concentration level is below one third at $\omega = 2\mathrm{rad/sec}$ for a channel with $w = 25\mu\mathrm{m}, h = 10\mu\mathrm{m}$ in Fig. 2 (c). Compared to $w = 25\mu\mathrm{m}, h = 5\mu\mathrm{m}$ case in Fig. 2 (a), when the height of the channel is doubled, i.e., $w = 25\mu\mathrm{m}, h = 10\mu\mathrm{m}$ in Fig. 2 (c), achievable frequencies are significantly increased, i.e., cut-off frequency is doubled. Furthermore, when distance l is increased to $100\mathrm{mm}$ in Fig. 3 (a) and (c), achievable frequencies are significantly reduced for all different cross-section. However, increased height in rectangular channels, i.e., $h = 10\mu\mathrm{m}$ in Fig. 3 (b), have a higher range of usable frequencies compared to $h = 5\mu\mathrm{m}$ case in Fig. 3 (a).

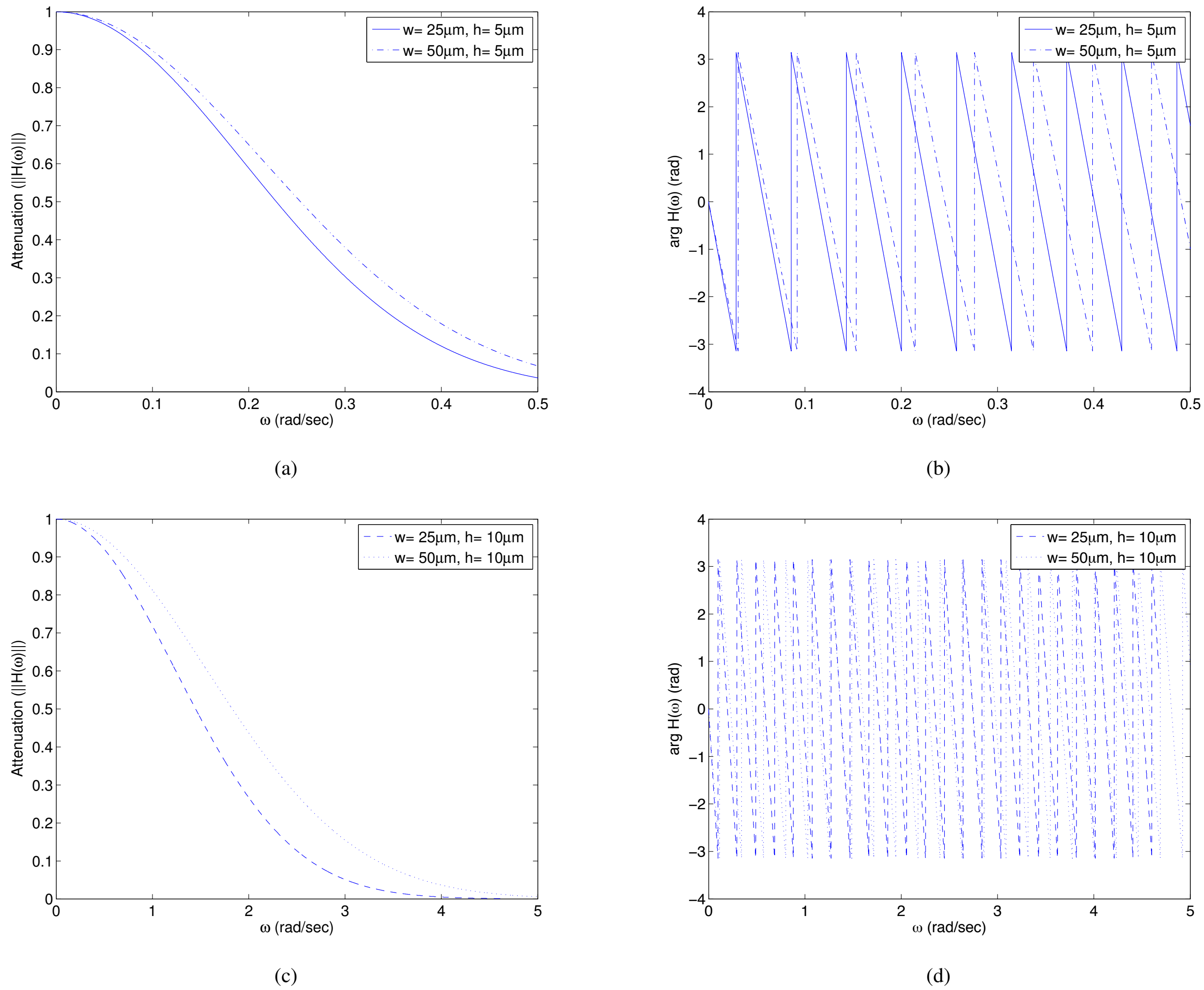

Fig. 2. For a rectangular channel of length $10\mu\mathrm{m}$, attenuation and phase response with respect to various cross-section parameters.

B. Bandwidth

Bandwidth of the rectangular microfluidic channels depends on both on cross-section parameters and distance. Bandwidth increases proportional to square of the reduction factor for the distance, i.e., when distance is reduced to $10\mu\mathrm{m}$ in Fig. 2 (a) and (c) from $100\mu\mathrm{m}$ in Fig. 3 (a) and (c). For the same area, higher height rectangular channels provide higher bandwidth compared to smaller height rectangular channels, i.e., a rectangular channel with $w = 25\mu\mathrm{m}, h = 10\mu m$ in Fig. 2 (c) and Fig. 3 (c) has a higher bandwidth than a channel with $w = 50\mu\mathrm{m}, h = 5\mu\mathrm{m}$ in Fig. 2 (a) and Fig. 3 (a) for a channel length of $10\mathrm{mm}$ and $100\mathrm{mm}$, respectively.

C. Phase

Phase of concentration changes periodically based on frequency. Rate of phase change decreases for higher bandwidth having channels, i.e., lesser bandwidth channels experience rapid phase fluctuations based on frequency. Phase of concentration in rectangular channel with $w = 25\mu\mathrm{m}, h = 5\mu\mathrm{m}$ in Fig. 2 (b) and Fig. 3 (b) changes two times faster than phase of concentration in channel with $w = 50\mu\mathrm{m}, h = 10\mu m$ in Fig. 2 (d) and Fig. 3 (d) for $l = 10$ and $100\mathrm{mm}$, respectively.

V. Conclusions

In this paper, molecular transport in microfluidic channels is investigated for Flow-induced Molecular Communications (FMC). The objective of this work is the analysis of concentration propagation inside rectangular microfluidic channels. To this end, flow velocity inside rectangular microfluidic channels is modeled first. Then, using developed flow velocity model, impulse response and transfer function is derived for FMC in rectangular microfluidic channels. Furthermore, attenuation of concentration, bandwidth of the FMC channel, and phase of concentration are reveled via numerical studies. Provided analysis of concentration propagation can be utilized to develop communication techniques for FMC.

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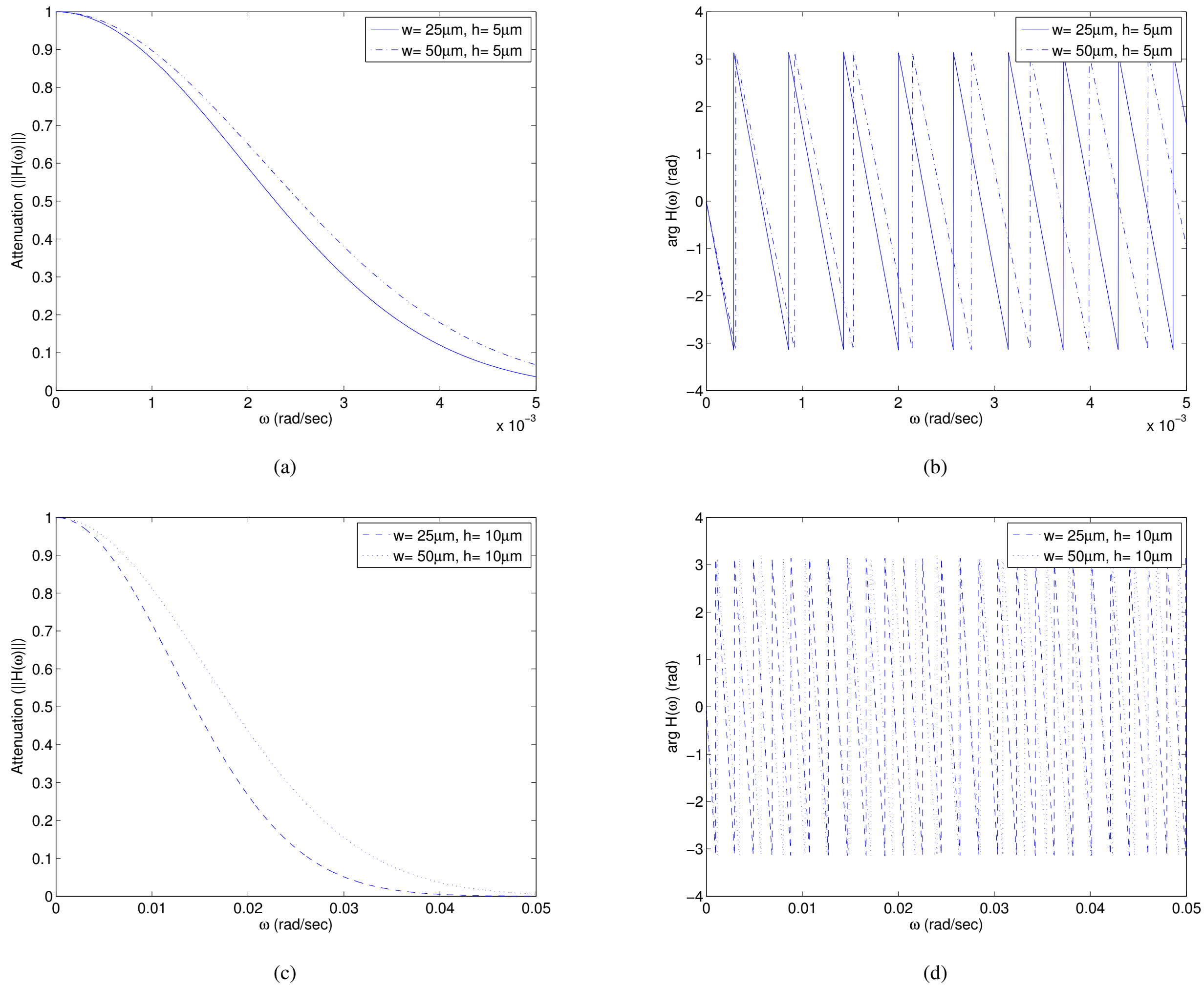

Fig. 3. For a rectangular channel of length 100μm, attenuation and phase response with respect to various cross-section parameters.

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