Mathematical model for propagating waves

The behavior of the propagating chemical waves can be predicted with the following mathematical model. From first principles, the propagating signal is represented by a space and time dependent concentration of a dilute solute $c(x,y,z,t)$ flowing through the channel with velocity $v(y,z)$. This concentration is periodic $c(x,y,z,t)=c(x,y,z,t+\tau)$, and it obeys a complex four dimensional convection diffusion PDE[9]. However if the channel height h and width w are small relatively to its length L, we can considerably simplify the problem if one considers the behavior of the average concentration $C(x,t)$ across its cross section under the influence of its average velocity V

$$C(x,t)=\frac{1}{w\cdot h}\cdot\int_0^w\int_0^h c(x,y,z,t)\cdot dy\cdot dz\,,$$

$$V=\frac{1}{w\cdot h}\cdot\int_0^w\int_0^h v(y,z)\cdot dy\cdot dz \tag{1}$$

$C(x,t)$ is also periodic $C(x,t)=C(x,t+\tau)$, and it approximately obeys the simplified, lumped one-dimensional convection-diffusion equation

$$D\cdot\frac{\partial^2 C}{\partial x^2}-V\cdot\frac{\partial C}{\partial x}=\frac{\partial C}{\partial t} \tag{2}$$

where D is the effective diffusion constant adjusted for Taylor-dispersion[1]. In Fourier space we can represent the average signal as $C(j\omega,x)$; hence the time derivative term in Eq. (2) is readily replaced with the complex term $j\omega\cdot C$.

$$D\cdot\frac{d^2C}{dx^2}-V\cdot\frac{dC}{dx}=j\omega\cdot C \tag{3}$$

with suitable boundary conditions $C(j\omega,0)=C_{in}(j\omega)$ and $C(j\omega,\infty)=0$, one can Solve this ODE to obtain the transfer function (T.F.) $T(j\omega,x)$ for the microfluidic channel. Solution of this ODE have the form

$$C(j\omega,x)=e^{\beta\cdot x}=e^{-\frac{x}{L_D}}\cdot e^{-j\gamma(\omega)\cdot x} \tag{4}$$

where $e^{-\frac{x}{L_D}}$ is the ampitude decay part with characteristic decay length L_D and $e^{-j\gamma(\omega)\cdot x}$ is the phase shift part. Substituting $C(j\omega,x)$ into the ODE, we can easily find that

$$\beta=-j\cdot\gamma(\omega)-\frac{1}{L_D}=\frac{V\pm\sqrt{V^2+4j\omega D}}{2D}=\frac{V}{2D}\cdot[1\pm(1+\frac{4j\omega D}{V^2})^{1/2}] \tag{5}$$

For decaying solutions, the minus sign before the square root part should be chosen and the transfer function for the microfluidic channel is hence

$$\begin{aligned}T(j\omega,x)&=C_{out}(j\omega,x)/C_{in}(j\omega)=C(j\omega,x)/C(j\omega,0)\\&=\exp[(V-\sqrt{V^2+4j\omega D})\cdot x/2D]\end{aligned} \tag{6}$$

where x is the distance measured from the channel inlet.

While at first the behavior of the complex exponential in Eq. (4) is difficult to ascertain, it becomes very clear when we plot the magnitude $\|T(j\omega, x)\|$ versus frequency as shown in the Bode plot of Fig 1.

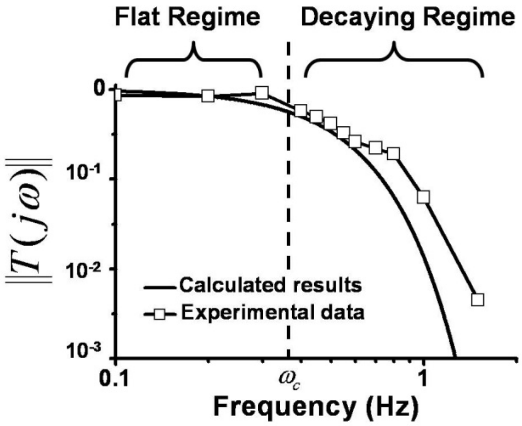

Fig. 1 Observed and calculated transfer function magnitude versus excitation frequency at 19.2 mm downstream from a PDMS channel inlet. The cross section of the channel was 25×16 μm^2 and the flow velocity was 1 cm/s. The spot size was 25×25 μm^2.

At low excitation frequencies the pulse distortion and amplitude decay are minimal yielding a near flat T.F. regime, but beyond a cut off frequency ω_c the amplitude attenuation is very large. By expanding Eq. (5) into a simple second order Taylor series, we can get the approximate cut off frequency. Let $\left|\frac{4j\omega D}{V^2}\right| << 1 = 0$, and with $(1+x)^{1/2} \approx 1 + \frac{x}{2} - \frac{x^2}{8} + \cdots$ we have

$$\begin{aligned} \beta &\approx (\frac{V}{2D}) \cdot \{1 - [1 + \frac{1}{2} \cdot (\frac{4j\omega D}{V^2}) - \frac{1}{8} \cdot (\frac{4j\omega D}{V^2})^2 + \cdots]\} \\ &\approx (\frac{V}{2D}) \cdot [-\frac{1}{2} \cdot (\frac{4j\omega D}{V^2}) - \frac{16}{8} \cdot (\frac{\omega^2 \cdot D^2}{V^2}) + \cdots] \\ &= -j \cdot (\frac{\omega}{V}) - (\frac{\omega^2 D}{V^3}) \end{aligned} \tag{7}$$

From Eq. (5) and Eq. (7), then

$$\frac{1}{L_D} = \frac{\omega^2 D}{V^3} \tag{8}$$

Therefore for a channel of fixed length L the amplitude will decay substantially for $\omega \geq \omega_c$, where

$$\omega_c \approx \left[\frac{V^3}{D \cdot L}\right]^{1/2} \tag{9}$$

and D is the corresponding dispersion adjusted diffusion constant which depends on velocity and capillary cross section dimensions.

At low frequencies and for short channels the amplitude decay is negligible, and Eq. (4) simply reduces to

$$T(j\omega, x) \approx \exp[-\gamma(\omega)\cdot x] = \exp[-j(\omega \cdot x / V)] = \exp(-j\theta) \tag{10}$$

Where

$$\theta = \frac{\omega \cdot x}{V} = \omega \cdot T = \frac{2\pi \cdot x}{\lambda} \tag{11}$$

is a characteristic phase delay angle proportional to the signal transit time $T = x/V$ and input frequency ω, and λ is the characteristic wavelength. Short channels in the flat regime therefore act as elementary delay line elements with phase angle linearly proportional to their length. On the other hand, long channels behave as low-pass filter elements that time average (and mix) the incoming pulses reducing the overall amplitude. In addition, since the propagating signal is periodic, it can also be expressed as a Fourier series. Very long channels strongly attenuate all of the high frequency series components basically leaving only the average and the first (fundamental) term of the series. This low-pass filter action explains why the observed output signal in Fig. 3 converges to a simple sinusoidal wave at the fundamental frequency.