Numerical Study on the Mass Transfer in a Two-Dimensional Channel with the Transversely Oscillating Wall*

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Abstract
Numerical study on the mass transfer in a two-dimensional channel with the transversely oscillating wall was carried out as the basic study to understand the mass transfer of the infused drug into the blood flow. It is clear that the actual oscillation of the blood vessel in vivo includes the many frequency components with a wide range. So, the numerical calculations were carried out varying the wall oscillation frequency widely and we considered the role of the Strouhal number mainly. The calculation results are summarized as follows. (1) In a low Strouhal number region, the wall oscillation has an effect to enhance the mass diffusion. However, further increase in the Strouhal number brings the restraint effect of the mass diffusion and brings the increase in the mass concentration at the wall. (2) The increase in the Schmidt number has an effect to clarify the restraint effect of the mass diffusion in a high Strouhal number region.

Key words: Mass Transfer, Bio-fluid Mechanics, Moving Boundary Problem, Boundary Layer, Computational Fluid Dynamics, Internal Flow

1. Introduction
The infused drug into the blood flow through the blood vessel forms a thin concentration boundary layer along the blood vessel, where the concentration of the drug is higher than that in the bulk flow. It is easily expected that the structure of this concentration boundary layer plays an important role in the cardiovascular regulatory process or the drug delivery. For example, the concentration distribution of the bioactive agent is expected to affect the endothelial cells and regulate the biological process(1). So, the concentration boundary layer of the drug in the blood flow has attracted the interest of many researchers and many theoretical and experimental studies have been carried out(2)-(4).

On the other hand, the oscillation of the blood vessel is an important problem to be considered for the case of the blood flow through the blood vessel(5),(6). It is clear that the contraction and relaxation of the heart creates the complicated oscillation of the blood vessel(5),(6) and we can easily expect that this complicated oscillation of the blood vessel has a strong influence on the concentration boundary layer of the drug. However, the influence of the wall oscillation on the concentration boundary layer of the drug has been hardly studied yet and remains unclear.

In the present study, a numerical study on the mass transfer in a two-dimensional channel with the transversely oscillating wall was carried out. As the present study is the first step to clarify the influence of the oscillating wall on the mass transfer of the drug in the blood flow, the numerical calculations were carried out under the conditions of the
simple geometry and simple oscillation conditions. Of course, these conditions are not equivalent to the biological conditions in vivo. However, it is easily expected that the numerical results of the present study will have an important meaning to understand the influence of the oscillating wall on the mass transfer of the drug in vivo.

Clearly, the actual oscillation of the blood vessel in vivo is highly complex and includes the many frequency components with a wide range \( f \). So, the dependency of the wall oscillation frequency on the concentration boundary layer will become an important problem. For this reason, the numerical calculations were carried out varying the wall oscillation frequency widely and we considered the role of the wall oscillation frequency mainly.

2. Methods

The schematic model of a two-dimensional channel bounded by a fixed wall and an oscillating wall is shown in Fig.1. As mentioned above, the simplified model was used to clarify the basic characteristics of the mass transfer in the blood flow. In the present study, the function \( F(t, x) \) indicating the transverse oscillation of the lower wall is expressed as

\[
F(t, x) = -KH_0 \cos(2\pi t/T_0) \exp[-\alpha(x - \beta)^2], \tag{1}
\]

where, \( t \) is time, \( T_0 \) is the period of wall oscillation, \( H_0 \) is the channel width far away from the oscillation region, and \( K \) is the non-dimensional amplitude of the wall oscillation. The coordinate component \( x \) is parallel to the bulk flow and coincides with the lower wall in the case of \( F(t, x) = 0 \). Additionally, \( \alpha \) and \( \beta \) are constants that denotes the geometry of the wall oscillation mode. In the present study, the values of \( \alpha \) and \( \beta \) were set at 1.5 and \( 0.4 H_0 \) respectively.

The flow is assumed to be incompressible and laminar. In addition, the fluid is assumed to be a Newtonian fluid. Therefore, the basic equations for the two-dimensional flow are written as

\[
\rho \left( \frac{\partial \omega}{\partial t} + \frac{\partial \Psi}{\partial y} \frac{\partial \omega}{\partial x} - \frac{\partial \Psi}{\partial x} \frac{\partial \omega}{\partial y} \right) = \mu \nabla^2 \omega, \tag{2}
\]

\[
-\omega = \nabla^2 \Psi, \tag{3}
\]

where \( \omega \) is the vorticity, \( \Psi \) is the stream function, \( \rho \) is the density, \( \mu \) is the viscosity coefficient, and \( \nabla^2 \) is the two-dimensional Laplacian. In addition, \( y \) is the coordinate component perpendicular to the \( x \) axis. On the other hand, the basic equation for the non-dimensional concentration of the drug (mass of the drug per unit mass of the blood) \( C \) can be written as

\[
\frac{\partial C}{\partial t} + \frac{\partial \Psi}{\partial y} \frac{\partial C}{\partial x} - \frac{\partial \Psi}{\partial x} \frac{\partial C}{\partial y} = D_0 \nabla^2 C, \tag{4}
\]

where \( D_0 \) is the diffusion coefficient.

Fig.1 Schematic model of a two-dimensional channel with the oscillating wall
In the present study, the geometry of the flow domain changes with time. So, we introduce the coordinate transformation method\(^{(7),(8)}\) to simplify the numerical calculations. The coordinate transformation clearly complicates the basic equations, but the moving boundary problem is converted into a fixed boundary problem. Therefore, we concluded that the coordinate transformation can facilitate the numerical calculations. The coordinate transformation from the \((x-y-t)\) system to the \((\xi-\eta-\tau)\) system can be written as

\[
\begin{align*}
\xi &= x, \\
\eta &= H_0(y - F)/(H_0 - F), \\
\tau &= t.
\end{align*}
\] (5)

Note that the flow domain becomes rectangular with the coordinate transformation.

Next, we show the boundary conditions of the flow fields. A fully developed steady-velocity profile in a two-dimensional channel is given as the inlet boundary conditions for the vorticity and stream function. At the outlet, the boundary conditions for the vorticity and stream function are given by the free flow-out condition\(^{(7)}\). The upper wall of the channel has the boundary condition of \(\Psi = \text{constant}\) for the stream function and has the Woods condition for the vorticity. The lower wall of the channel has the following boundary conditions for the stream function. That is,

\[
\begin{align*}
(\partial \Psi / \partial y)_{r=F} &= 0, \\
(\partial \Psi / \partial x)_{r=F} &= -\partial F / \partial t.
\end{align*}
\] (6)

For the vorticity, the lower wall of the channel also has the Woods condition. Of course, the modification of this condition is required because of the transverse oscillation of the lower wall\(^{(7)}\). Subsequently, we show the boundary conditions of the concentration fields of the drug. The boundary conditions at the lower wall are given by

\[
\begin{align*}
-(\rho D_0 \partial C / \partial y)_{r=F} &= j_C \quad (0 \leq x / H_0 \leq 1), \\
(\partial C / \partial y)_{r=F} &= 0 \quad (1 < x / H_0).
\end{align*}
\] (7)

These equations mean that the drug is infused at a constant rate \(j_C\) per unit area within the region of \(0 \leq x / H_0 \leq 1\) and the zero mass flux condition is applied to the region of \(1 < x / H_0\). As for the boundary condition of the upper wall, the zero mass flux condition is applied everywhere. That is,

\[-(\partial C / \partial y)_{r=H_0} = 0.\] (8)

Moreover, the inlet concentration of the drug is set at zero and the free flow-out condition is used as the outlet boundary condition.

Due to the present coordinate transformation mentioned above, the geometry of the flow domain was converted into a rectangular flow. So, we adopted the finite difference scheme to obtain the numerical results. The fully implicit scheme was used to improve the stability of the numerical analysis. Moreover, the central difference scheme was adopted for the discretization of the convection term. In the present study, the numerical calculations were carried out within the range of \(0 \leq x / H_0 \leq 10.0\). The total number of grid points was \(400 \times 160\), and we recognized within the present study that this mesh division was sufficient to reveal the detailed flow pattern and concentration fields of the drug correctly from the comparison of the calculated results with different grid points. Moreover, we found that the numerical calculation over the many pulsation cycles was required to obtain the periodic solution for the case of the low diffusion coefficient. In the present study, the numerical calculation was carried out over the thirty cycles to obtain the
periodic solution.

3. Calculation Results

The present numerical results are characterized by five non-dimensional parameters mainly, i.e. Reynolds number $Re$, Strouhal number $St$, Schmidt number $Sc$, non-dimensional amplitude of wall oscillation $K$ and non-dimensional infusion rate of drug $q$. The Reynolds number, Strouhal number and Schmidt number are defined by

$$Re = \frac{\rho u_0 H_0}{\mu}, \quad St = \frac{H_0}{(u_0 T_0)}, \quad Sc = \frac{\mu}{(\rho D_0)},$$

where $u_0$ is the section-averaged axial velocity at the inlet. Moreover, the non-dimensional infusion rate of drug $q$ is defined by

$$q = \frac{J_c H_0}{(\rho D_0)}.$$

In the present study, the values of $K$ and $q$ were set at 0.2 and 50.0 respectively. It should be noted that the value of $q$ corresponds to the typical parameter in the blood flow\(^2\).

Figure 2 shows the instantaneous contours of the non-dimensional drug concentrations for $Re = 500.0$, $St = 0.02$ and $Sc = 1000.0$. The values of the Reynolds number and Schmidt number correspond to the typical blood flow parameters in the artery\(^2\). As our main interest lies in the contours near the oscillating region, this figure shows the contours within the range of $2 \leq x/H_0 \leq 7$, $y/H_0 \leq 0.4$. Moreover, it should be noted that the scale along the $y$ axis is enlarged in order to assist the understanding. From the panel at $t/T_0 = 0/6$ of this figure, we can find that the thin boundary layer forms along the dip of the lower wall and separates in the downstream side of the dip. Of course, the distribution of the drug concentration changes with time due to the wall oscillation. That is, the panels at $t/T_0 = 2/6$, $t/T_0 = 3/6$ and $t/T_0 = 4/6$ show that the separation occurs near the top of the lower wall and the separated portion moves to the downstream side with the progress of time. From these results, we can understand the complicated nature of the drug concentration near the oscillating wall. Figure 3 shows the instantaneous contours of the non-dimensional drug concentrations for $Re = 500.0$, $St = 0.10$ and $Sc = 1000.0$. From the comparison of Fig.3 and Fig.2, we can find that the increase in the Strouhal number has an effect to restrain the occurrence of the flow separation. That is, we cannot find the separated flow region in the downstream side of the oscillating region for the case of Fig.3. Of course, we can find the symptom of the flow separation from the panels at $t/T_0 = 4/6$ and $t/T_0 = 5/6$ of this figure. However, this symptom does not grow up with the progress of time. These results mean the important role of the Strouhal number.

To clarify the influence of the Strouhal number, we consider the distributions of the non-dimensional drug concentration at $x/H_0 = 10.0$. The calculation results are shown in Figs.4-7. In these figures, the vertical axis gives the value of $y/H_0$ and the horizontal axis gives the value of the non-dimensional drug concentration. Additionally, the calculated distributions of the non-dimensional drug concentration under the condition of $K = 0$ (flat wall) are shown in Fig.8 for reference. Figure 4 shows the results for $Re = 500.0$ and $Sc = 1000.0$. This figure shows that the increase in the Strouhal number has an effect to restrain the change of the drug concentration with time and increase the drug concentration on the wall. That is, the drug concentrations on the wall for $St = 0.10$ are close to the values for $K = 0$ (flat wall) compared with the case of $St = 0.02$ (see Fig.4 and Fig.8). These results are in agreement with the results shown in Figs.2 and 3 qualitatively. Figure 5 shows the results for $Re = 250.0$ and $Sc = 1000.0$. The results of this figure agree with the results of Fig.4 qualitatively, but these figures show that the decrease in the Reynolds number has an effect to weaken the influence of the Strouhal
Fig. 2 Instantaneous contours of the drug concentration
(Re = 500.0, St = 0.02, Sc = 1000.0)

Fig. 3 Instantaneous contours of the drug concentration
(Re = 500.0, St = 0.10, Sc = 1000.0)
Fig. 4 Distribution of the drug concentration at $x/H_0 = 10.0$

$Re = 500.0$, $Sc = 1000.0$

Fig. 5 Distribution of the drug concentration at $x/H_0 = 10.0$

$Re = 250.0$, $Sc = 1000.0$

Fig. 6 Distribution of the drug concentration at $x/H_0 = 10.0$

$Re = 500.0$, $Sc = 100.0$

Fig. 7 Distribution of the drug concentration at $x/H_0 = 10.0$

$Re = 250.0$, $Sc = 100.0$
number. Figure 6 shows the results for $Re = 500.0$ and $Sc = 100.0$. It is well known that realistic Schmidt number of the blood flow is order of $10^3$. So, we can find that the calculation condition of this figure is not realistic. We should note that the purpose of this figure is to consider the influence of the Schmidt number. From the comparison of Fig.6 and Fig.4, we can find that the increase in the Strouhal number does not have an effect to restrain the change of the drug concentration with time and does not increase the drug concentration on the wall for the case of $Sc = 100.0$. That is, the drug concentrations on the wall for $St = 0.02$ are close to the values for $K = 0$ (flat wall) compared with the case of $St = 0.10$ (see Fig.6 and Fig.8). These results mean that the increase in the Schmidt number enhances the restraint effect of the mass diffusion in a high Strouhal number region. In addition, we can understand the important role of the Schmidt number easily. Figure 7 shows the results for $Re = 250.0$ and $Sc = 100.0$. We can find that the results of this figure agree with the results of Fig.6 qualitatively.

From a practical viewpoint, the drug concentration on the wall has an important meaning$^{(1), (2)}$. So, we show the calculated distributions of the drug concentration on the wall. The calculated results are shown in Figs.9-12 and $C_{wall}$ is defined by

$$C_{wall} = (C)_{y=0}.$$  

(11)

Additionally, the calculated distributions of $C_{wall}$ under the condition of $K = 0$ (flat wall) are shown in Fig.13 for reference. Figure 9 shows the results for $Re = 500.0$ and $Sc = 1000.0$. This figure means that the increasing Strouhal number can restrain the change of $C_{wall}$ with time, being in agreement with the results mentioned above. Moreover, we can find that the wall oscillation generates the notable change of $C_{wall}$ within the relative narrow region (see Fig.9 and Fig.13). The results for $Re = 250.0$ and $Sc = 1000.0$ are shown in Fig.10. We can find that the decrease in the Reynolds number does not have a strong effect on the distributions of $C_{wall}$. Figure 11 shows the results for $Re = 500.0$ and $Sc = 100.0$. Comparison of Fig.11 and Fig.9 reveals that the decreasing Schmidt number does not change the influence of the Strouhal number qualitatively. In addition, we can find the almost same results for the case of $Re = 250.0$ (see Fig.12 and Fig.10).

Subsequently, we show the calculation results of the time averaged drug concentration on the wall $\overline{C}_{wall}$ in order to reveal the influence of the Strouhal number and Schmidt number clearly. Figure 14 shows the results of $\overline{C}_{wall}$ at $x/H_0 = 10.0$. The left panel of this figure is the results for $Sc = 1000.0$. This panel shows that the increase in the Strouhal number has an effect to decrease the value of $\overline{C}_{wall}$ in a low Strouhal number region. However, further increase in the Strouhal number brings a increase in the value of
These results mean that the increase in the Strouhal number has an effect to restrain the diffusion of the drug and to increase the drug concentration on the wall. The right panel is the results for $Sc = 100.0$. This panel means that the increase in the Schmidt number has an effect to clarify the restraint effect of the mass diffusion in a high Strouhal number region. These results are worthy of attention.

![Fig.9 Distribution of the drug concentration on the wall (y = F)](image)

$Re = 500.0, Sc = 1000.0$

![Fig.10 Distribution of the drug concentration on the wall (y = F)](image)

$Re = 250.0, Sc = 1000.0$

![Fig.11 Distribution of the drug concentration on the wall (y = F)](image)

$Re = 500.0, Sc = 100.0$

![Fig.12 Distribution of the drug concentration on the wall (y = F)](image)

$Re = 250.0, Sc = 100.0$

![Fig.13 Distribution of the drug concentration on the wall under the condition of $K = 0$ (flat wall)](image)

$Re = 250.0, Sc = 100.0$
4. Discussion

The transverse oscillation of the wall produces the alternating fluid motion perpendicular to the bulk flow. And the increase in the Strouhal number increases the velocity of the alternating flow perpendicular to the bulk flow. So, it is expected easily that the increase in the Strouhal number has an effect to enhance the drug diffusion in the blood flow. However, the present study showed that the increase in the Strouhal number has an effect to restrain the drug diffusion and to increase the drug concentration on the wall for the case of a high Strouhal number region. This result will be one of the most important results in the present study, but this result gives a strange impression seemingly. For this reason, we consider the physical mechanism of this result subsequently.

In connection with this problem, we take up the synthetic jet. The restraint of the flow separation has an important meaning in various fields such as the design of the aircraft. So, the theoretical and experimental studies on the devices to restrain the flow separation have been carried out for a long time. Among these devices, the synthetic jet has been shown to be a useful tool for the separation control. The synthetic jet consists of the orifice driven by the acoustic source in a cavity. And the alternating flow perpendicular to the bulk flow is generated by the oscillating membrane within a cavity. In this case, it is clear that the vortex rings are formed between the discharged fluid and the surrounding fluid. This vortex rings transport the high momentum fluid of the bulk flow to the wall. So, we can easily expect that this transport can re-energize the boundary layer under a certain condition when the boundary layer begins to weaken and approach separation. After all, the boundary layer energization will lead to the restraint of the flow separation. From these considerations, we can understand the physical mechanism of the synthetic jet easily.

Here, let us compare the present model (see Fig.1) with the synthetic jet. It is clear that both systems share the alternating flow perpendicular to the bulk flow. For this reason, we can easily expect that the present model has a similar property to the synthetic jet under a certain condition. The reason that the present model has an effect to restrain the separation of the drug concentration can be explained qualitatively from this consideration. Well, for the case of the synthetic jet, the frequency of the alternating jet has an important meaning, too. So, the frequency dependence of the pressure loss or the flow separation has attracted the interest of many researchers and it has been suggested that the flow control mechanism can be divided into two types according to the value of the jet frequency. Of course, we cannot compare the present results with the results of the synthetic jet due to the difference of flow geometry. In future, we should continue the study of the frequency dependence by considering the analogy of the present model with the
synthetic jet. Moreover, the role of the Schmidt number will be the important subject in future. In the present study, we showed that the Schmidt number has a strong effect on the distributions of the drug concentration. However, the influence of the Schmidt number in a channel with the transversely oscillating wall has been hardly studied yet and there is much left to be studied hereafter. More detailed study should be performed in future.

5. Conclusions

As a model of the drug diffusion in the blood flow, we studied the mass transfer in a two-dimensional channel numerically. It is well known that the blood vessel shows the complicated motion in vivo. So, the transverse oscillation of the wall was included in the present numerical calculations and our main attention was paid to the influence of the wall oscillation to the distributions of the drug concentration. The most important results of the present study is that the increase in the Strouhal number has an effect to restrain the separation of the drug concentration in a high Strouhal number region. Moreover, the present study showed that the Schmidt number has a strong effect to the distributions of the drug concentration. It is easily expected that these results have an important meaning from the engineering viewpoint or the biomedical viewpoint. So, more detailed study should be performed in future. In addition, the medical meaning of these results will be the important subjects in future study.

Acknowledgements

The authors want to thank Dr. Hiroaki Hasegawa (Associate Professor of Akita University) for his excellent advices on the present study.

References