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Modeling for Fluid Mixing in Passive Micromixers Using the Vortex Index

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The present paper addresses the effects of molecular diffusion and the vorticity of microchannel flows on mixing in passive micromixers, which are essential components of a microfluidic chip. A model that can predict the mixing performance of passive micromixers is developed based on the physical characteristics of mixing such as the Peclet number and the vortex index that is newly defined in this paper. In order to investigate the flow physics in the passive mixers, we performed numerical simulations for a wide range of Peclet numbers and Reynolds numbers. The model is found to be able to accurately predict the mixing performance of passive mixers without solving the coupled, complex diffusion and momentum equations.

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I. INTRODUCTION

Recently microfluidics has been paid attention for the development of automated miniaturized analytical devices in (bio)analytical chemistry. Microfluidics deals with microscale, physical phenomena of fluid and particle flows in microchannels that connect various functional sites on a miniaturized analytical device. Analysis of bio-samples in a miniaturized device requires transport of various forms of the bio-samples in appropriate fluids from a functional site to another through microchannels on the device [1]. As a result, the device is often called a microfluidic chip. In addition, when the multiple functionalities required for a complete procedure of the analysis are integrated onto a single microfluidic chip, it is called Lab-on-a-Chip or micro Total Analysis System (μTAS) [2–4]. Typical functionalities contained on a microfluidic chip include sampling, purification, separation, mixing, reaction, concentration amplification, detection, etc. Lithography adapted from semiconductor production is commonly used to fabricate microfluidic chips [5]. Analysis using a microfluidic chip has many advantages against conventional biochemical analysis. It can automate the analysis processes, reduce consumption of precious bio-samples such as DNA, RNA, proteins, cells, bacteria, viruses or blood, reduce contamination of the bio-samples by minimizing human interaction, and reduce the analysis time [6].

Among the various functionalities, rapid mixing is crucial because biological analyses, like enzyme reactions, protein folding, and cell activation, require a rapid reaction process that can be controlled by the mixing of reactants. Unfortunately, mixing at a microscale mainly depends on molecular diffusion, resulting in an extremely slow process and long microchannel for complete mixing. This is because almost all microchannel flows are laminar, and the Reynolds number is so low that turbulent mixing can hardly be achieved.

Many micromixers have been developed in order to enhance and control mixing in a microchannel [7]. The micromixers can be categorized into two types: passive mixers and active mixers. An active mixer uses external energy sources to perturb a laminar flow. The perturbation methods include oscillation of a flow-driving source like pressure field [8,9] or electric field [10,11], acoustic wave generation [12–14], magnetic field variation [15], and so on. In general, active mixers stir up fluids better than passive mixers, but they require complicated fabrication techniques and sophisticated operation procedures [7].

A passive mixer uses special geometries embedded in a microchannel like grooves, rivets or posts, as shown in Fig. 1, to increase the vorticity and, subsequently, to cause a chaotic advection [16–22]. Chaotic advection improves mixing by enhancing the transversal motion of a fluid in a microchannel. The other type of passive mixers is a lamination mixer, which decreases the diffusion

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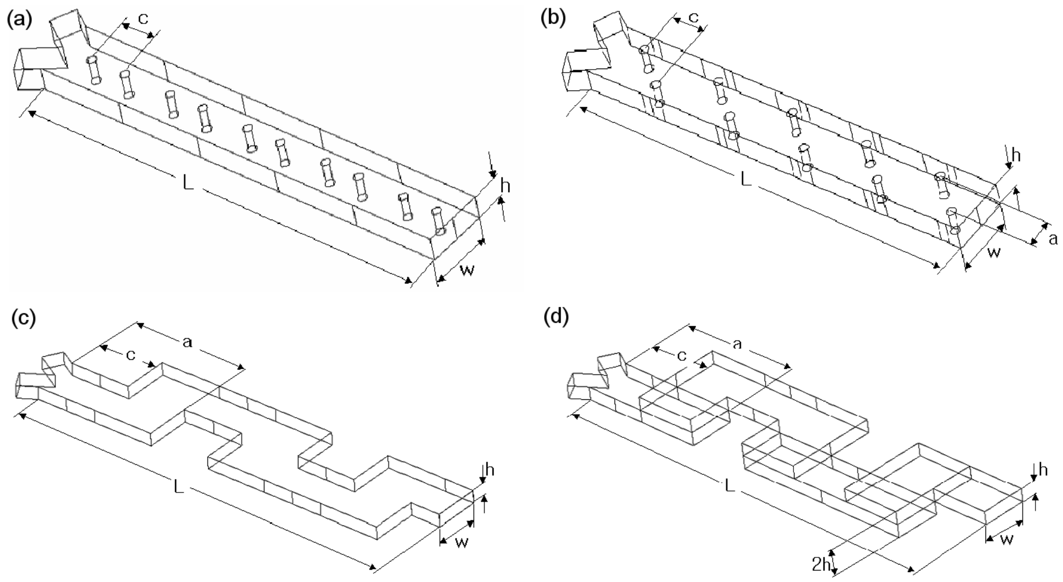

Fig. 1. Various flow geometries for passive mixers. (a) Central post mixer: L = 2375 μm, w = 300 μm, h = 100 μm, c = 200 μm, and post diameter = 20 μm. (b) Zigzag post mixer: L = 2375 μm, w = 300 μm, h = 100 μm, a = 150 μm, c = 200 μm, and post diameter = 20 μm. (c) Square wave mixer: L = 2800 μm, w = 300 μm, h = 100 μm, a = 800 μm, and c = 400 μm. (d) Serpentine mixer: L = 2600 μm, w = 300 μm, h = 100 μm, a = 800 μm, and c = 40 μm.

length and increases the contact area of fluids by splitting incoming streams into multiple substreams and then laminating them into one stream again [23–27]. Passive mixers are frequently adapted in the development of integrated microfluidic chips due to the simple concept.

Predicting mixing in a microchannel requires solving the coupled diffusion and momentum equations, which leads to complex numerical calculations. However, it is expected that one can effectively predict and evaluate mixing in passive mixers by simply considering the mass diffusivity of the mixed fluids and the vorticity of the flow without solving the coupled equations. This is because passive mixers, especially chaotic mixers, have been designed to utilize the vorticity generated in laminar flows. Maeng *et al.* developed a model to predict mixing in microchannels by using the so-called vortex index [28]. The vortex index was defined for 2-D planar mixers and represents only one-dimensional effects of vorticity on mixing for a fixed inlet flow condition. Thus, modification of the vortex index is required to utilize it for predicting the mixing performance of general 3-D mixers or for different inlet flow conditions.

The present paper proposes a simple model to predict the degree of mixing in passive mixers operated over a practical, wide range of Reynolds number from 0.1 to 1000. The model relates effects of both diffusion and chaotic advection to the mixing. In order to determine the vorticity and the mixing in various passive mixers, we performed numerical analyses by using a commercial software, CFD-ACE. The mixing index and the vortex index are newly defined to accurately quantify mixing and vorticity in commonly used passive mixers.

II. DEFINITIONS OF THE CHARACTERISTIC QUANTITIES FOR MIXING

Important physical mechanisms involved in microscale mixing are diffusion and chaotic advection. Diffusion can be characterized by the Peclet number that depends on the diffusivity of a species and the residence time of the species in the channel. Chaotic advection depends on the flow geometry, and the strength of the chaotic motion can be expressed by the vorticity. If mixing is to be predicted, the effects of both diffusion and chaotic advection should be considered. The first step is to quantify mixing and then relate it to the vorticity and the Peclet number of a microchannel flow.

1. Mixing Index

Let us consider a mixing of two identical fluids inserted into a Y-shaped microchannel as shown in Fig. 2 (a). However, the upper fluid is assumed to contain a species like protein or DNA, and the dimensionless concentration is set to unity. The concentration of the other is assumed to be zero. To perform a numerical analysis on a microchannel flow, we divide the microchannel into infinitesimal volumes by generating grids as shown in Fig. 2 (b).

A mixing index (M) to quantify mixing in the microchannel can be defined as follows:

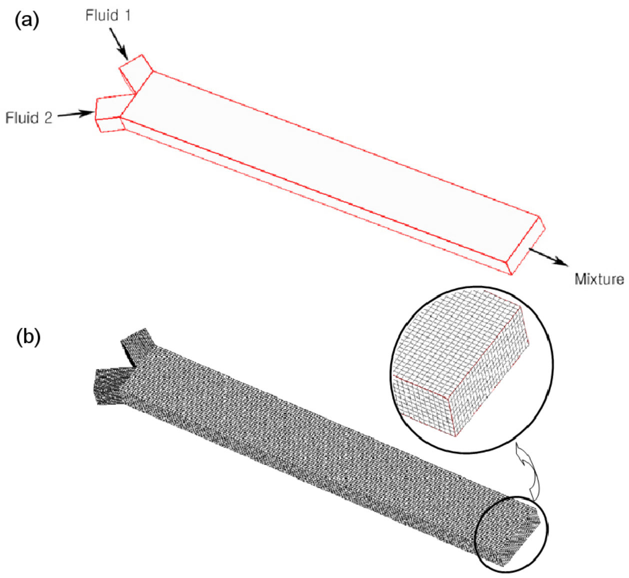

Fig. 2. Y-shaped microchannel and generated grid. (a) Y-shaped microchannel (b) Microchannel divided into infinitesimal volumes by generating a grid

$$M = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(C_i - C_{in})^2} \tag{1}$$

where C_i is the local, dimensionless concentration at a node of a given cross section of the channel. C_{in} is the dimensionless, average concentration at the inlet, which is the junction of the Y-shape channel, and N is the number of nodes at the cross section. The mixing index is equal to 0 when the two fluids are mixed completely and 0.5 at the inlet.

2. Vortex Index and Peclet Number

In order to consider the effects of chaotic advection on mixing, one should quantify the proper vorticity of the flow that induces chaotic motions and that subsequently contributes to mixing. However, it is not the local vorticity of the flow but the vorticity history that determines the degree of mixing at a cross section of the channel because the degree of mixing at a position depends on the upstream history of the flow. Thus, a vortex index representing the vorticity history of a flow can be defined as follows:

$$\Omega = \sqrt{\Omega_x^2 + \Omega_z^2} \quad for \quad 2-D \quad mixers, \tag{2}$$

$$\Omega = \sqrt{\Omega_x^2 + \Omega_y^2 + \Omega_z^2} \quad for \quad 3-D \quad mixers, \tag{3}$$

where

$$\Omega_x = \frac{\int_v |\omega_x| dV}{Q}, \ \Omega_y = \frac{\int_v |\omega_y| dV}{Q}, \ \Omega_z = \frac{\int_v |\omega_z| dV}{Q} \tag{4}$$

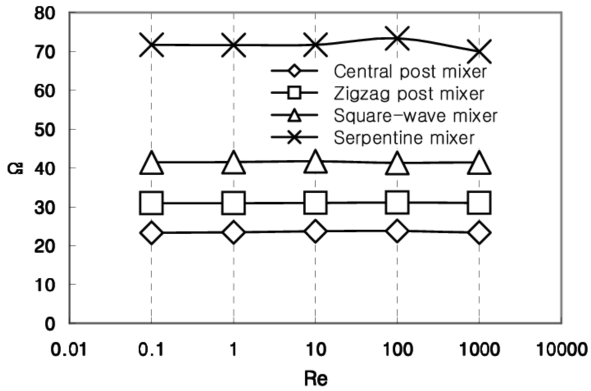

Fig. 3. Vortex index variations with Reynolds numbers.

with Q being the flowrate in the channel. The integration interval is from the inlet to the cross section of interest. The vortex index is defined separately for 2-D mixers (*e.g.*, a post mixer with posts and a square-wave mixer) and 3-D mixers (*e.g.*, a serpentine mixer) because the spanwise vorticity (ω_y) does not contribute to mixing at all for 2-D mixers. A vorticity normalization with Q is required to reflect variations of the inlet flow conditions, like the flow velocity or the flowrate, from one case to another. Thus, the normalization makes the vortex index depend on the flow geometry only and be independent of Reynolds number for a given geometry, as shown in Fig. 3.

The effects of diffusion on mixing can be represented by the Peclet number:

$$Pe = \frac{UL}{D}, \tag{5}$$

where U is the inlet velocity, L is the hydraulic diameter of the channel, and D is diffusivity. Physically, the Peclet number implies the ratio of the longitudinal convection to the lateral diffusion times. Fig. 4 shows the effects of Peclet number on mixing in a simple Y-shaped channel for different Peclet numbers. A Smaller Peclet number results in a more rapid and more uniform mixing, as expected.

III. RELATIONS OF THE MIXING INDEX, VORTEX INDEX, AND PECLET NUMBER

Numerical analyses are performed for four representative geometries of passive mixers as shown in Fig. 1, to develop a model that relates the mixing index to the vortex index and Peclet number. The inlet velocity for each channel varies from 1 mm/s to 5 mm/s, but is assumed to be uniform. Incoming fluids are assumed to be a dilute water solution of bio particles with a diffusivity of 1.7×10^{-9} m^2/s, and the pure water. The numerical results for each mixer are shown in Figs. 5 and 6 for a

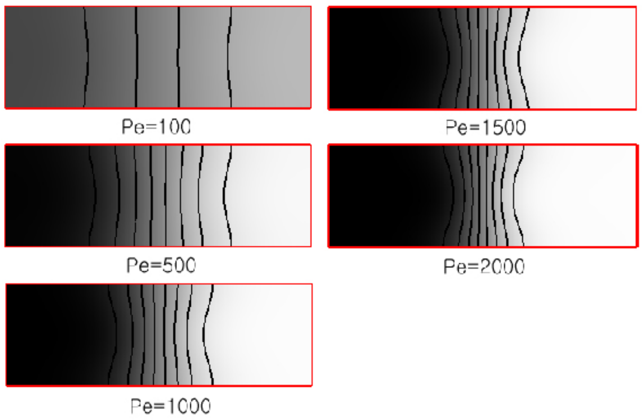

Fig. 4. Effects of Peclet number on mixing in a simple Y-shaped channel. The gray scale represents the concentration (0 ∼ 1) that is measured at the outlet.

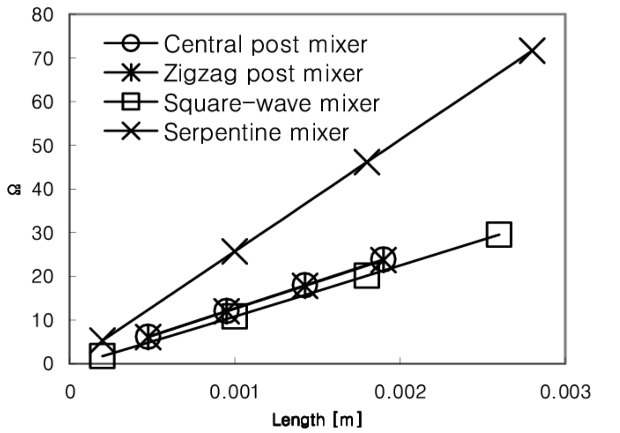

Fig. 5. Vortex index variations along the channel length. The length is defined along the streamline at the center of each channel for the square-wave and the serpentine mixers.

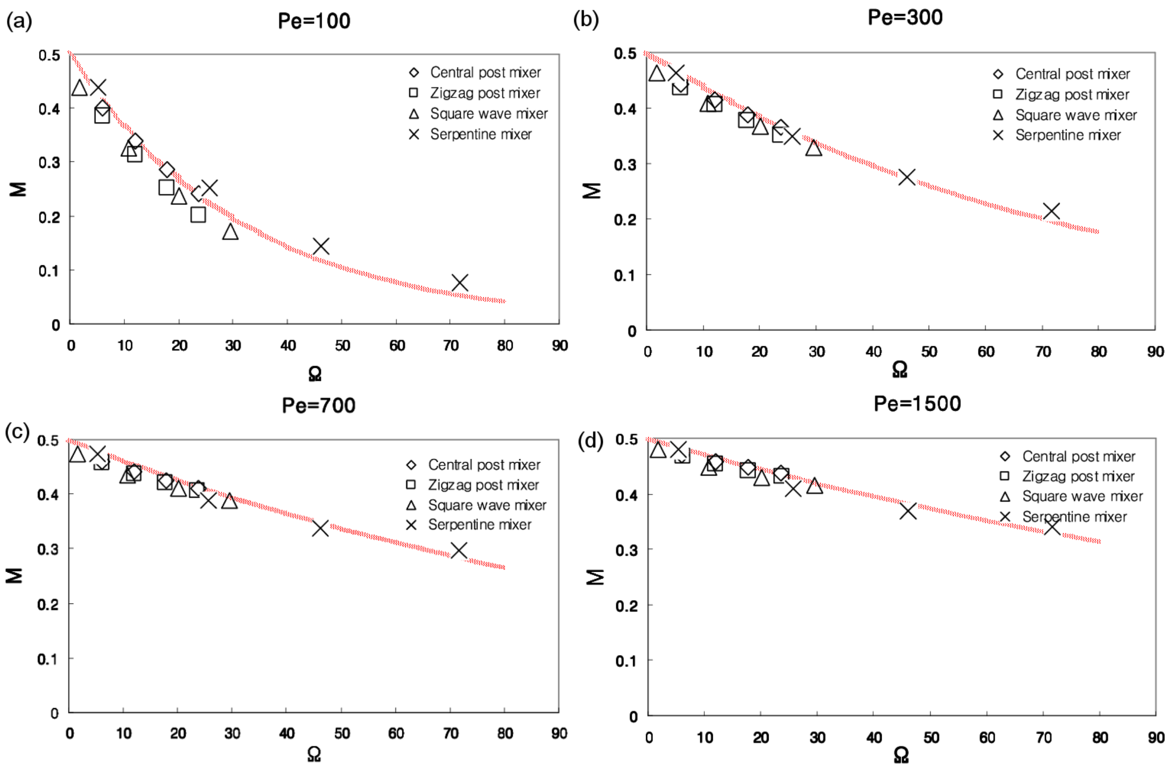

Fig. 6. Mixing index variations with the vortex index for different Peclet numbers.

wide range of Peclet numbers. The vortex index is the largest for the serpentine mixer at the same longitudinal length from the inlet as shown in Fig. 5 (a), indicating that the serpentine mixer induces chaotic motions most violently. The vortex index of the serpentine mixer is 2.4 times higher than that of the central post mixer at a longitudinal length of 1900 μm. Fig. 6 shows mixing-index variations with the vortex index for different Peclet numbers (100 ∼ 1500). For a fixed Peclet number, the mixing index data collapse onto a single line, indicating that vorticity dominates fluid mixing, regardless of the mixer type. As long as the values of the vortex index are the same despite different flow geometries, the degrees of mixing remain similar. In addition, Fig. 6 indicates that the mixing index approaches zero more rapidly for a given mixer as the Peclet number decreases.

Based on the mixing index variations, we can define a functional form of the mixing index dependence on the vortex index and the Peclet number as

$$M = A \exp(-B\Omega), \tag{6}$$

where the coefficient A is identical to the value (0.5) of

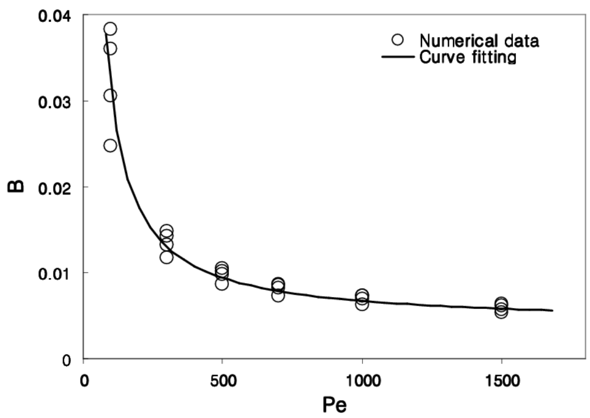

Fig. 7. Variations of coefficient B with Peclet number.

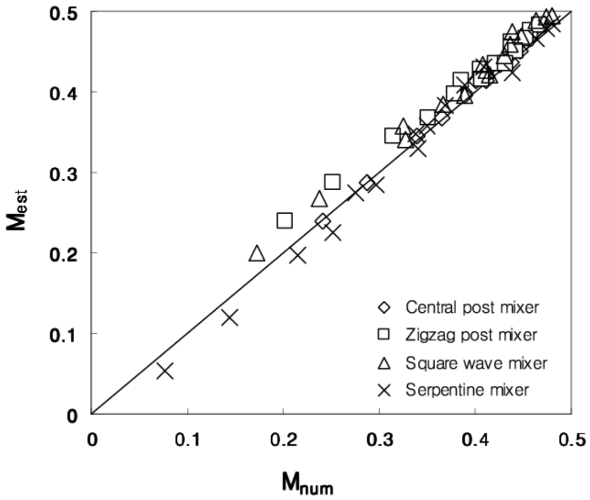

Fig. 8. Comparison of the mixing indices from estimates and numerical calculations.

the mixing index at the inlet because the vortex index is zero at the inlet. The coefficient B is a function of the Peclet number, and it can be determined by fitting all the data of Fig. 6 for different Peclet numbers. The fitting results are plotted in Fig. 7, and the functional relation between B and the Peclet number is

$$B = \frac{2.7}{Pe} + 0.004. \tag{7}$$

Therefore, the mixing index can be modeled as

$$M = 0.5 \exp\left(-\left(\frac{2.7}{Pe} + 0.004\right)\Omega\right). \tag{8}$$

This model can be used to readily estimate the performance of a passive mixer that utilizes diffusion and chaotic advection without solving the coupled diffusion and momentum equations.

IV. DISCUSSION

In order to examine the accuracy of the model, we compare the mixing index (M_{est}) estimated using Eq.

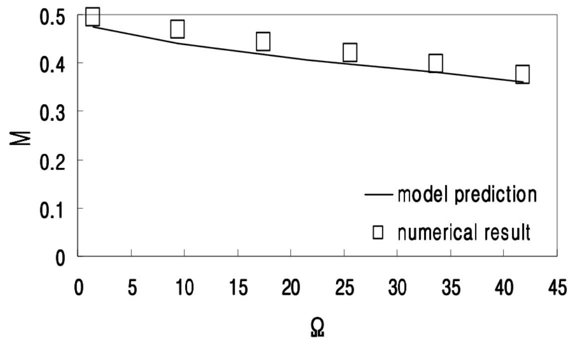

Fig. 9. Prediction of the mixing performance using the model for a square-wave mixer.

(8) to the mixing index (M_{num}) calculated from the numerical results obtained by solving the coupled diffusion and momentum equations. As Fig. 8 shows, most estimates are close to the numerical values, and the maximum discrepancy among the data is 8 % near $M_{num} = 0.2$.

This model is also tested to check if it can accurately estimate the mixing performance of a square-wave mixer with an elongated channel. The channel length is increased by factor of two compared to that of the previous case. The model's estimate is in good agreement with the mixing index calculated from the numerical results within 5 % error at most. This is evidence that this model can be used to estimate the mixing performance of a passive mixer operating over a practical range of Reynolds number and Peclet numbers.

V. CONCLUSIONS

The performance of a passive mixer was predicted by simply considering the Peclet number and the vorticity of the flow. To quantify the degree of mixing and the effects of vorticity on the mixing, we defined a mixing index and a vortex index based on the physical characteristics of fluid mixing. Numerical analyses were performed to develop a model that determined the functional relation between the mixing index, the vortex index and the Peclet number. The model could accurately predict the performance of passive mixers operated in the Peclet number range of 100 to 1500 and the Reynolds number range of 0.1 to 1000 at least.

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