Novel index for micromixing characterization and comparative analysis

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The most basic micromixer is a T- or Y-mixer, where two confluent streams mix due to transverse diffusion. To enhance micromixing, various modifications of T-mixers are reported such as heterogeneously charged walls, grooves on the channel base, geometric variations by introducing physical constrictions, etc. The performance of these reported designs is evaluated against the T-mixer in terms of the deviation from perfectly mixed state and mixing length (device length required to achieve perfect mixing). Although many studies have noticed the reduced flow rates for improved mixer designs, the residence time is not taken into consideration for micromixing performance evaluation. In this work, we propose a novel index, based on residence time, for micromixing characterization and comparative analysis. For any given mixer, the proposed index identifies the nondiffusive mixing enhancement with respect to the T-mixer. Various micromixers are evaluated using the proposed index to demonstrate the usefulness of the index. It is also shown that physical constriction mixer types are equivalent to T-mixers. The proposed index is found to be insightful and could be used as a benchmark for comparing different mixing strategies. © *2010 American Institute of Physics.* [doi:10.1063/1.3457121]

I. INTRODUCTION

Efficient micromixing is required for fast analysis in biomicrofluidic laboratory-on-a-chip applications, such as biochemical analysis,[1] complex enzyme reactions,[2] etc. The mixers used in microdevices can be categorized into active and passive mixers.[3] Active mixers utilize external energy—via pressure, electrokinetic disturbance, etc.—to induce transverse flows. On the other hand, diffusion and chaotic advection are the dominant mixing mechanisms in passive mixers. An excellent review of electrokinetic mixing techniques[4] and various micromixer types along with their comparison[3] can be found elsewhere. The simplest passive micromixer is a T- or Y-mixer, where two reagents flow adjacently and mixing is primarily due to transverse diffusion. Many variations of T-mixer are reported for improved mixing performance such as obstacle based micromixing,[5–8] heterogeneous charged walls,[9] grooves/patterning on channel base,[10,11] etc. Other electrokinetic mixing techniques include ac electro-osmosis based batch-mode micromixers[12] where enhanced micromixing is demonstrated in a reservoir[13] and in a microcavity.[14]

Often improved mixing is achieved at the expense of reduced flow rate[4–10] and there exists a tradeoff between mixing and transport.[15] However, the effect of reduced flow rate is not considered in micromixing characterization. Most of the reported studies evaluate micromixers based on the deviation from perfectly mixed state[5–11] or length required to achieve perfect mixing but species residence time is not accounted. In this study, a new mixing index is proposed for micromixing characterization and comparative analysis. The proposed index accounts for residence time

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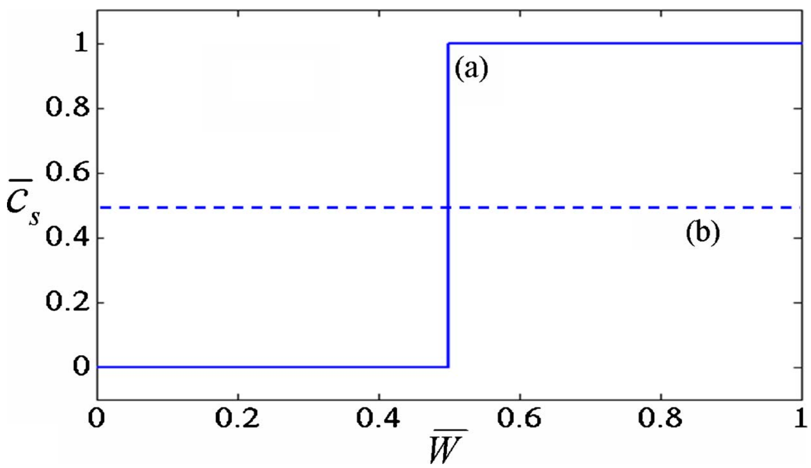

FIG. 1. Cross-sectional concentration profiles for η values (a) $\eta=0$ correspond to perfectly unmixed state (inlet condition for T-mixer); (b) $\eta=1$ corresponds to perfectly mixed state.

and hence identifies the "true" nondiffusive mixing improvement for any given design over T-mixer. The proposed index is defined in the theory section followed by its graphical interpretation. Various case studies are presented to demonstrate the usefulness of proposed index in results section.

II. THEORY

In a T- or Y-mixer, two different solutions flow adjacently in the same direction and mixing is primarily due to transverse diffusion. The inlet condition for T-mixer can be represented by step input, as shown in Fig. 1(a). Mixing performance, for such parallel flow type mixers, is quantified using the following mixing index,[5–11,16] which evaluates the deviation from perfectly mixed state (Fig. 1):

$$\eta = \left[1 - \frac{\sqrt{1/N\Sigma_1^N(\bar{c}_s - \bar{c}_s^*)^2}}{\sqrt{1/N\Sigma_1^N(\bar{c}_s^0 - \bar{c}_s^*)^2}} \right]. \tag{1}$$

In the above equation, N is the number of points in the cross-section used for estimation of the mixing index. The variable $\bar{c}_s$ represents the scaled concentration value at that point, while $\bar{c}_s^0$ and $\bar{c}_s^*$ are the scaled concentration at each point if the solutions are unmixed and the concentration with perfect mixing (i.e., 0.5), respectively. Also, it should be noted that the variable $\bar{c}_s^0$ takes on a value of 0 or 1 at any point across the channel width, resulting in a constant denominator value of 0.5 in Eq. (1). Based on the mixing index definition [Eq. (1)], the theoretical limits for η is between zero and one. The cross-sectional concentration profiles corresponding to η values of zero and one are plotted in Fig. 1. Typically, the above index is evaluated at the channel exit and it has been extensively employed for comparative analysis between various micromixer designs. As stated earlier, the mixing index η estimates the deviation from perfectly mixed state and does not account for reduced flow rates or variation in residence time τ among different designs.

When comparing two different mixer designs, the residence time τ should be considered as it directly relates to the time available for diffusive mixing. Thus mixing performance evaluation based on η alone is insufficient and could lead to a false sense of improvement, as shown in Sec. IV. To accommodate the residence time in comparative analysis, a comparative mixing index (CMI) is proposed below,

$$\alpha_{A,B} = \frac{(\eta)_A|_{(L_c,\tau)}}{(\eta)_B|_{(L_c,\tau)}}. \tag{2}$$

In the above equation, $\alpha_{A,B}$ is the CMI, which essentially evaluates the η values for designs A and B for same residence time. If any design A is evaluated against T-mixer, then the above index can be written as

$$\alpha_{A,\text{T-mixer}} = \frac{(\eta)_A|_{(L_c,\tau)}}{(\eta)_{\text{T-mixer}}|_{(L_c,\tau)}}. \tag{3}$$

Based on the mixing index definition [Eq. (3)], the theoretical limits for $\alpha_{A,\text{T-mixer}}$ is between one and infinity. For given design A, values of CMI close to unity indicate its equivalency to T-mixer whereas higher values suggest better mixing performance with reference to T-mixer. Also, the term, $\alpha_{A,\text{T-mixer}}-1$, identifies the nondiffusive mixing component for design A. Further any two arbitrary designs can be compared by benchmarking their mixing performance with respect to T-mixer using Eq. (3).

It is evident from Eqs. (1)–(3) that proposed index would be useful in analyzing micromixing designs where residence time effects are significant. In particular, the proposed index would be beneficial for continuous, parallel flow type micromixers where static mixing element (conducting/nonconducting obstacles, heterogeneous charged walls) also acts as a resistance to fluid flow. If improved micromixing is achieved via increase in interfacial contact area [sequential injection strategy,[16] pulsed flow techniques,[1,17] using periodic electro-osmotic flow[18] without significantly affecting residence time or resistance to fluid flow then CMI and η would provide similar results. For better understanding, the graphical illustration for the proposed index CMI is presented below.

III. GRAPHICAL INTERPRETATION

Consider Fig. 2, where η and τ are plotted with respect to electric field for T-mixer and any arbitrary design A. It is observed, especially in the case of electrokinetic micromixers,[5–10] that higher η values are obtained at the expense of reduced flow rate, i.e., higher residence time (Fig. 2). Most of the reported studies[5–10] compares mixing performance at a particular applied field without considering the residence time. Therefore, for a given field E_1, only points A and B are considered (Fig. 2) and the difference is identified as mixing improvement over T-mixer. However, T-mixer requires a smaller applied field E_2 ($E_2 < E_1$) for same residence time as of design A. Hence, the proposed index considers points C and D (Fig. 2) for comparative analysis for design A and T-mixer. It is evident that from Fig. 2 that comparison based on η is inadequate and may mislead in terms of improvement in mixing performance over T-mixer (also demonstrated in Sec. IV).

IV. RESULTS AND DISCUSSION

The proposed index is used for characterization in the following mixer types: (1) Physical constriction or obstacle based micromixer, (2) heterogeneous charged walls (symmetric and staggered configuration), and (3) conducting obstacle or induced charge electro-osmotic (ICEO) mixer. All the micromixers are numerically modeled using Smoluchowski's slip velocity approach[19] for thin electric double layer and induced zeta potential for ICEO mixer is determined using correction potential method.[20] The detailed numerical model can be found in the ICEO mixer study reported earlier[21] and simulation parameters are listed in Table I.

A. Physical constriction/obstacle based mixer

Previous studies have identified increment in mixing performance with multiple nonconducting obstacles embedded in microchannel wall.[3,4] These studies have suggested that physical constriction reduces diffusion length around the obstacle which in turn enhances mixing. However, these obstacles offer hydraulic resistance to flow and reduce the overall flow rate, which is not

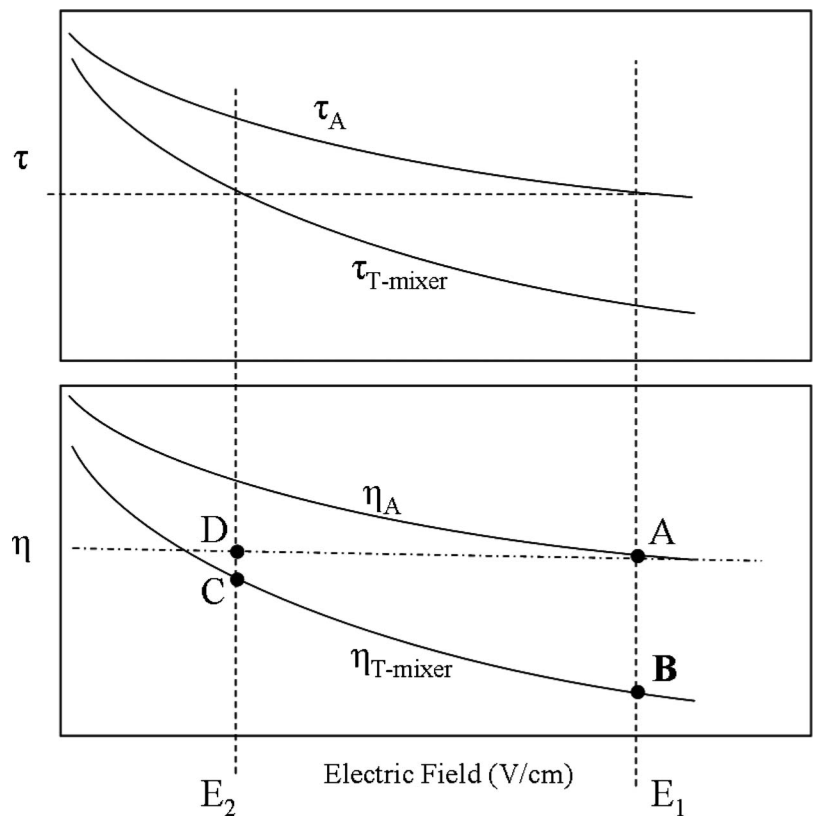

FIG. 2. Graphical interpretation for the proposed index. The proposed index considers residence time and hence identifies the true improvement over T-mixer.

considered in micromixing characterization. In this study, micromixer with nonconducting semicylindrical obstacle is analyzed. The velocity arrow plot and species concentration surface plot for semicylindrical obstacle mixer is shown in Fig. 3(a). The CMI values for this mixer are close to unity [Fig. 4(a)], which indicates equivalent performance as a T-mixer. It suggests that nonconducting obstacles cause equal increment in diffusive flux and hydraulic resistance (also shown below using simple analysis).

In a parallel flow type micromixer, if there are no flow circulations, η is dependent on transverse diffusive flux $(j_D)_y$ integrated over channel length L_c. Therefore, η and hydraulic resistance R_h for T-mixer can be written in terms of channel width w as follows:

TABLE I. Simulation parameters (default values).

Parameter	Value	Description
W	100 μm	Width of the microchannel
L	1 mm	Length of microchannel
ς_f	−50 mV	Fixed zeta potential on channel walls
D_s	5×10^{-11} m^2/s	Diffusivity of species to be mixed
a	25 μm	Radius of nonconducting obstacle [Fig. 3(a)]
p	100 μm	Heterogeneous charged surface patch length [Figs. 3(b) and 3(c)]
L_1, L_2	25 and 50 μm	Dimensions of conducting rectangular obstacle [Fig. 3(d)]

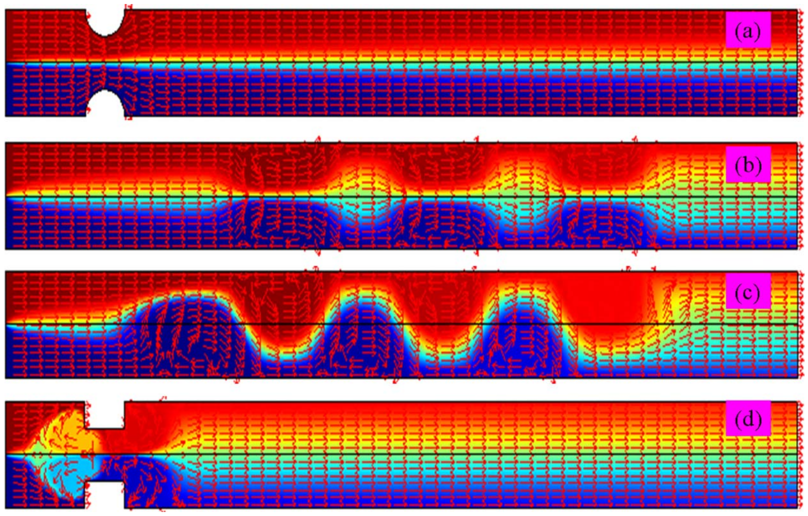

FIG. 3. Species concentration surface plot and velocity arrow plot are shown for various micromixer types at E =100 V/cm. (a) Nonconducting obstacle mixer; (b) heterogeneous charged walls (symmetric arrangement); (c) heterogeneous charged walls (staggered arrangement); (d) ICEO mixer.

$$\eta_{\text{T-mixer}} \propto \int_0^{L_c} (j_d)_y \sim D\frac{\Delta c}{w}L_c,$$
$$(R_h)_{\text{T-mixer}} = \frac{\mu}{\varepsilon\varsigma}\frac{L_c}{w}. \tag{4}$$

For obstacle/physical constriction micromixer, the variation in channel width can be accounted as follows:

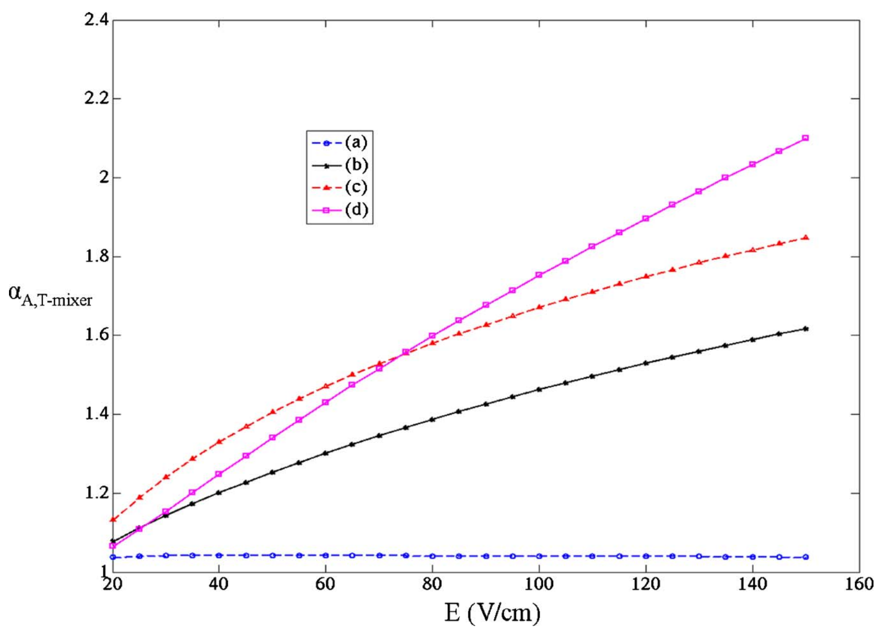

FIG. 4. Various micromixers are evaluated using CMI vs electric field plot. (a) Nonconducting obstacle mixer; (b) heterogeneous charged walls (symmetric arrangement); (c) heterogeneous charged walls (staggered arrangement); (d) ICEO mixer.

$$\eta_{\text{obs-mixer}} \propto \int_0^{L_c} (j_d)_y \sim D\Delta c \int_0^{L_c} \frac{dx}{w(x)},$$
$$(R_h)_{\text{obs-mixer}} = \frac{\mu}{\varepsilon\varsigma} \int_0^{L_c} \frac{dx}{w(x)}. \tag{5}$$

Using Eqs. (4) and (5), it can be shown that variation in width (obstacle) affects mixing performance and hydraulic resistance in same manner, i.e.,

$$\frac{\Delta\eta}{\eta_{\text{T-mixer}}} = \frac{\eta_{\text{obs-mixer}} - \eta_{\text{T-mixer}}}{\eta_{\text{T-mixer}}} = \frac{(R_h)_{\text{obs-mixer}} - (R_h)_{\text{T-mixer}}}{(R_h)_{\text{T-mixer}}} = \frac{\Delta(R_h)}{(R_h)_{\text{T-mixer}}}. \tag{6}$$

Using the proposed CMI, it is shown that physical constriction type mixer does not offer any significant mixing benefits as compared to T-mixer as identified by previous studies[3,4] as well. Although the analysis is carried out for single obstacle, the results are equally valid for multiple obstacle case[3,4] provided that there are no flow circulations in the vicinity of obstacle.

B. Heterogeneous charged walls mixer

Microvortices can be generated using heterogeneous charged walls which, in turn, enhances micromixing.[9,15] The analysis is carried out with three patches (with equal and opposite zeta potential) on each wall for (a) symmetric arrangement (axial location of patches are same on each wall) and (d) staggered arrangement (patches on opposite walls have an offset equal to patch length). The flow profile and species concentration surface plot are shown for both arrangements in Figs. 3(b) and 3(c). The proposed index, CMI, is found to be insightful and beneficial over η for heterogeneously charged wall mixer. For example, at E=20 V/cm, the η values for T-mixer and staggered heterogeneous mixer are 0.55 and 0.95, respectively. Therefore, comparison based on η alone would suggest almost a twofold increase in mixing performance whereas CMI value at same electric field strength is equal to 1.15 [curves (b) and (c) in Fig. 4]. The low CMI value suggests that residence time effects are important at low electric fields (E=20 V/cm). At such fields, flow circulations do not enhance micromixing but significantly increase the resistance to fluid flow.

The CMI dependence on electric field can be understood using scaling analysis presented below. The CMI can be alternatively written as follows:

$$\alpha_{A,\text{T-mixer}} = 1 + \frac{(\eta)_A|_{(L_c,\tau)} - (\eta)_{\text{T-mixer}}|_{(L_c,\tau)}}{(\eta)_{\text{T-mixer}}|_{(L_c,\tau)}} = 1 + \left.\frac{\Delta\eta}{\eta_{\text{T-mixer}}}\right|_{(L_c,\tau)}. \tag{7}$$

The above equation relates the CMI to the relative increase in η value at same residence time. In the diffusion dominant conditions (at smaller fields), η_A, $\eta_{\text{T-mixer}}$ can be empirically related to the Péclet number (Pe) as

$$\eta \sim \frac{a_1}{\text{Pe}^m} \sim a_1\left(\frac{D}{u_x w}\right)^m. \tag{8}$$

Here m is the exponential factor representing the lumped effect of spatial concentration distribution and effective width (due to physical constriction and/or vortices) and a_1 is a constant (could be related to the interfacial contact area). For any arbitrary design A and T-mixer, η decreases with an increase in electric field E; however, the CMI dependence on E is governed by the exponential factor m. In any improved mixer design, the mixing performance decays slowly compared to T-mixer due to reduced diffusion width or transverse velocity components in improved design. For instance, η decay is slower for heterogeneous charged wall mixer (both arrangements) as compared to a T-mixer ($m_{\text{hetero}} < m_{\text{T-mixer}}$), resulting in an increase [positive $\Delta\eta$ in Eq. (7)] in CMI value with electric field.

In the convective dominant regime (at higher electric fields), η would depend on the dimensionless ratio of transverse velocity to axial velocity (u_y/u_x) as mass transport in transverse direction is governed by convection. Therefore, Eq. (7) can be rewritten for convection regime as follows:

$$\alpha_{A,\text{T-mixer}} \sim 1 + a_2\left[\frac{\Delta u_y}{u_x}\right] \sim 1 + a_2\left[\frac{(u_y)_A}{u_x}\right] \quad [\because (u_y)_{\text{T-mixer}} = 0]. \tag{9}$$

Based on Eqs. (8) and (9), the CMI dependence on electric field can be analyzed for various micromixer types. The staggered arrangement appears better than symmetric arrangement as suggested by the CMI plot [curves (b) and (c) in Fig. 4]. For a given electric field, the flow rates (i.e., resistance to fluid flow/residence time effect is identical) and transverse convection are same for both arrangements. The higher CMI values for staggered arrangement can be attributed to the structure of the velocity field (wavy interface), which results in higher contact surface area [Fig. 3(c)] than symmetric arrangement [Fig. 3(b)], i.e., a_1 is higher for staggered arrangement while pre-exponential factor m is same for both arrangements. Further, in both arrangements, the transverse velocity as well as axial velocity scale linearly with electric field i.e., $(u_y/u_x \sim \mathrm{E}/\mathrm{E} \sim \mathrm{E}^0)$. Therefore, at higher fields, CMI value should flatten out for both types of heterogeneously charged walls micromixer, as observed in Figs. 4(b) and 4(c).

C. ICEO/conducting obstacle mixer

Recent studies have demonstrated the use of ICEO for micromixing.[7,8,20,21] The proposed index is used to characterize a rectangular conducting obstacle micromixer, which is modeled using correction potential method. Due to induced charges on obstacle surface flow circulations are generated near the obstacle. The corresponding velocity arrow plot and concentration surface plots are shown in Fig. 3(d). The CMI plot [curve (d) in Fig. 4] suggests better mixing performance at higher fields, which is due to the quadratic dependence of velocity on electric field.[22] For ICEO micromixers, the ratio of transverse velocity to axial velocity scales linearly with electric field, i.e., $(u_y/u_x \sim \mathrm{E}^2/\mathrm{E} \sim \mathrm{E}^1)$ explaining the linear dependence of CMI on electric field [using Eq. (9)], as shown in Fig. 4(d).

V. CONCLUSIONS

A new CMI is proposed for micromixer performance evaluation. The proposed index identifies the true mixing benefits compared to the T-mixer by normalizing the effect of species residence time or reduced flow rate. The equivalency of T-mixer and physical constriction type micromixer is shown using the proposed index. Various case studies demonstrate the advantage of the proposed index over existing mixing index as it clearly identifies the nondiffusive mixing improvement. The proposed index could be used for comparative analysis of various micromixing techniques and characterizing new mixing strategies.

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