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Three-objective optimization of a staggered herringbone micromixer

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ABSTRACT

Shape optimization of a staggered herringbone micromixer (SHM) was performed using the three-dimensional numerical analysis of fluid flows and mixing of two fluids, surrogate modeling, and a multi-objective genetic algorithm. Two design variables related to dimensions of the grooves, i.e., depth and width, were chosen for optimization. Three performance parameters, i.e., the mixing index at the exit of the micromixer, overall friction factor, and mixing sensitivity, which is the mixing index at a specified axial location in upstream part of the micromixer, were employed as the objective functions. Surrogate modeling was performed for the objective functions using response surface approximation. Multi-objective genetic algorithm was used to find the Pareto-optimal solutions. Representative Pareto-optimal designs were analyzed using numerical analysis and a particle tracking method. The optimization results indicate that wide and deep grooves are desirable to promote faster mixing with a low pressure drop inside the SHM.

1. Introduction

Microfluidic systems such as lab-on-a-chip and micro-total analysis systems have gained widespread importance in many applications such as sample preparation and analysis, drug delivery, and biological and chemical synthesis [1–4]. Microfluidic systems exhibit certain inherent advantages over their large scale counterparts, such as lower energy consumption, higher throughput, and lower manufacturing costs. However, the small channel size limits the Reynolds number (*Re*), which makes the flow laminar. Therefore, the mixing processes inside these microfluidic systems are diffusion-dominated, unless a mean to perturb the flow is incorporated. In the last few years, researchers have determined various methods to perturb the flow using geometrical modifications (passive micromixers) and external energy/stimulus (active micromixers) to enhance the mixing at the microscale. Passive micromixers exploit the micromixer's geometry to produce complex flow fields that enhance the mixing of the fluid samples, whereas the active type relies on external agitation. This agitation can be from a pressure disturbance, change in temperature, magnetic energy, or electrical energy.

Design optimization coupled with computational fluid dynamics (CFD) based on the three-dimensional (3-D) Navier–Stokes equations has become a reliable tool for design of micromixers due to the rapid increase in computing power. The objective function(s) for the optimization of a micromixer can be selected among the performance parameters such as mixing efficiency, pressure loss, and residence time, etc. [5–8]. The staggered herringbone groove micromixer (SHM), which was developed by Stroock et al. [9], has been used by many researchers to create well-posed design optimizations. The micromixer was developed by placing specially designed grooves on one or more surfaces of the channel. The volume of fluid is exposed to a repeated series of rotational and extensional local flows, which leads to an enhanced mixing performance. Many researchers have studied the groove shape to understand the underlying mechanisms and mixing performance of the micromixer. Aubin et al. [10] carried out a qualitative study on a diagonally grooved micromixer and SHM using a particle tracking approach and CFD. Later, they determined the effects of the geometrical parameters on mixing inside the SHM and developed a mean to quantify the mixing performance for various combinations of the geometrical parameters [11]. A similar study was conducted by Wang et al. [12] on a SHM. Using CFD simulations and particle tracking technique, Poincare maps were generated to study the chaotic flow. Using surrogate models such as radial basis neural network (RBNN) and response surface approximation (RSA), Ansari and Kim [5,6] optimized the shape of a SHM with grooves applied to a bottom wall. The optimizations employed the mixing index as the objective function and used two or three design variables. Yang et al. [13] determined the effects of various geometrical parameters on mixing performance, flow rate, and pressure drop of a SHM using the Taguchi method and numerical simulations. Cortes-Quiroz et al. [7] optimized a SHM for *Re* between 1 and 10 using CFD, a surrogate model, and a multi-objective genetic algorithm (MOGA). The

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Taguchi method was used as a design-of-experiment technique. The degree of mixing and pressure drop were used as the performance parameters for the micromixer. A Pareto-optimal front was established with an optimized tradeoff, i.e., maximum mixing index with minimum pressure loss.

For the study of micromixers, designers may be interested in assessing the trade-off among various objectives. However, previous optimization studies were limited to either one- [5,6] or two- [7] objective optimizations. In contrast to single-objective optimization (one optimal solution), multi-objective optimization provides many optimal solutions subjected to a set of objective functions and constraints. The goal of present work is to develop a multi-objective optimization procedure that can be applied to the optimizations of micromixers containing more than two objectives using MATLAB Optimization Toolbox [14]. A three-objective optimization of a SHM [9] was conducted using surrogate modeling and MOGA. The width and depth of the grooves inside the SHM were used as the design variables for the optimization. The performance parameters, i.e., mixing index, friction factor, and mixing sensitivity, were the objectives for the optimization. The mixing efficiency is a critical performance parameter related to the mixing performance of the device. The pressure loss is directly related to the pumping power required to drive the fluids through the micromixers, while the mixing sensitivity determines the susceptibility of the mixing phenomenon subjected to the design constraints. The RSA method was used as a surrogate model to approximate the objective functions combined with the MOGA.

2. Problem formulation

Fig. 1 shows the geometry of the SHM used by Ansari and Kim [5]. For the present study, the geometric variables related to the groove dimensions, the ratio of groove width to groove pitch (W_d/Pi) and ratio of groove depth to channel height (d/h), were selected as the design variables for optimization (Fig. 1). The pitch (Pi) is $2\pi/q$. The following variables were held constant: 0.077 mm average channel height (h), 0.2 mm channel width (W), $2\pi/100\ \mu\text{m}^{-1}$ principal wave vector (q), 45° ridge orientation, and 2/3 asymmetry factor (P) [9]. The length of the micromixer was set to 0.01 m with 10 grooves per half-cycle. The channel was parallel to the x-axis. Inlet channels (Inlets 1 and 2) with cross sectional dimensions of 0.20 mm × 0.10 mm were merged with the main channel using a T-joint.

2.1. Flow and mixing analysis

To analyze flow and mixing inside the micromixer, the 3-D Navier–Stokes and mass conservation equations were solved using ANSYS CFX-12.1 [15], a commercial CFD package based on the finite volume method. A multi-component model was used to study mixtures composed of different species as in the previous works [5–7]. The model assumes that the various fluid species are mixed at the molecular level and mass transfer takes place by convection and diffusion. The bulk motion of the fluids was modeled using a single velocity and pressure, but each component had its own conservation of mass equation. The relative mass flux terms govern the motion of the individual components. Since the concentration gradient is the sole source of the relative motion, the relative mass flux term is modeled as a diffusion-like term. Thus, the conservation of mass equation for each species results in an advection–diffusion type equation for the concentration field:

$$(\vec{V}\cdot\vec{\nabla})C_i = \alpha\nabla^2 C_i, \tag{1}$$

where α is the diffusivity coefficient and C_i is the concentration of species i [16]. Eq. (1) was used to calculate the mass fraction of each component.

The specified velocity was given at each inlet with pure ethanol at Inlet 1 (mass fraction equal to 1) and pure water at Inlet 2 (mass fraction equal to 0). At the outlet, zero static pressure was specified, while no-slip condition was applied at the walls. The properties of the working fluids, ethanol and water, were measured at 20 °C. The densities of water and ethanol were 9.97×10^2 and 7.89×10^2 kg/m^3, respectively. The dynamic viscosities of water and ethanol were 0.9×10^{-3} and 1.2×10^{-3} kg/m s. The diffusivity coefficient for the water–ethanol pair was assumed to be 1.2×10^{-9} m^2/s.

In a recent study on the accuracy of the numerical schemes for scalar mixing, Liu [17] showed that higher-order discretization schemes are less susceptible to numerical diffusion. Upwind differencing schemes are likely to introduce numerical discretization errors. However, higher-order upwind (second- and third-order accurate) schemes are known to reduce the numerical diffusion [18]. Thus, the present work employed a high-resolution second-order approximation scheme to discretize the advection terms in the governing equations. The SIMPLEC algorithm [19] was used for the pressure–velocity coupling. The linearized algebraic system of equations resulting from the discretization were solved using a multigrid accelerated incomplete lower–upper (ILU) factorization procedure for faster convergences. The criterion for convergence of each equation was a root mean square (RMS) residual value of 10^{-6}.

To evaluate the SHM mixing performance, a variance-based method was employed. The variance of the species was determined on the cross-sectional plane perpendicular to the x-axis. The variance of the mass fraction of the mixture on a cross-sectional plane normal to the flow direction can be expressed as

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(c_i - \bar{c}_m)^2}, \tag{2}$$

where N is the number of sampling points on the plane, c_i is the mass fraction at sampling point i, and $\bar{c}_m$ is the optimal mixing mass fraction. The values at the sampling points were interpolated based on values at adjacent computational nodes. The number of sampling points must be higher than the number of nodes for accuracy. A value of $N = 900$ was found to exhibit good accuracy. Finally, the mixing index at any cross-sectional plane perpendicular to the axial direction is defined as

$$M = 1 - \sqrt{\frac{\sigma^2}{\sigma_{\max}^2}}, \tag{3}$$

where $\sigma_{\max}$ is the maximum variance over the data range. The mixing index varied from 0 (no mixing) to 1 (complete mixing). An M value close to 1 indicates a more homogeneous concentration and better mixing performance.

2.2. Particle tracking

ANSYS FLUENT-12.1 [20] was used to calculate the trajectories of the massless fluid particles inside the flow using a Lagrangian particle tracking method. The solver predicts the particle paths after post-processing the flow field. Movement of massless particle inside the flow is determined by integrating the vector equation of motion for each particle:

$$\frac{d\boldsymbol{x_p}}{dt} = \boldsymbol{V_p}(x). \tag{4}$$

For the massless particles, the particle velocity is equal to the velocity of the continuous phase. Hence, the trajectory of each particle can be obtained using the particle velocity $\boldsymbol{V_p} = \boldsymbol{V}$, where $\boldsymbol{V_p}$ and $\boldsymbol{V}$ are velocities of the particle and continuous phase, respectively.