OPTIMAL DESIGN AND OPERATION ON CONVERGENT-DIVERGENT NOZZLE TYPE NO-MOVING-PART VALVES (NMPV) IN MICROCHANNEL

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ABSTRACT

The no-moving-part valve (NMPV) pump design has been proven to be a better micro pump design for its easier fabrication, cost-effective and no destroying flow particle. Previous literatures often used a diffuser design with a divergent angle for NMPV studies. Different from previous studies, we apply a convergent-divergent (C-D) nozzle with convergent half angle $\theta_1$ and divergent half angle $\theta_2$ for NMPV design in this study. By using the dipole value ($P_{iD}$) of current C-D nozzle type NMPV as an objective function in “Design of Experiments” (DOE) and “Response Surface Modeling” (RSM) optimization methods, C-D nozzle type NMPV with convergent half angles near $\theta_1 = 46^\circ - 54^\circ$ and divergent half angles $\theta_2 = 113^\circ - 116^\circ$ has a maximum peak region for $P_{iD}$ value. It is found that the optimal design with the convergent half angle of $\theta_1 = 60^\circ$ and the divergent half angle of $\theta_2 = 110^\circ$. The operational Reynolds numbers raging from 20 to 30 are suggested for the optimal design and operation condition for the current C-D nozzle type NMPV. It is also verified that the C-D nozzle type NMPV pump design has a better performance than the typical diffuser type NMPV pump design. These findings would be useful to the design and operation for C-D nozzle type NMPV micropump.

Keywords: No-moving-part valve, Micropump, Optimal design.

1. INTRODUCTION

Numerous fluidic applications in such areas as medicine, chemistry, environmental testing and thermal transport have potential to be scaled down for reasons of sample size, device cost or portability. Cost-effective and reliable fluidic components, including pumps are required for such scaled-down systems. Current pump designs are typically based on valves that open and close in series. Such valves tend to be direct applications of designs that work in macroscopic devices but not necessarily are the best choice for micropump applications. Micropumps have been developed by many research groups based on various principles of actuation and various types of valves [1-4]. For a typical micropump, it requires an actuation component with two microvalves. The actuation structure like piston or membrane components is commonly used to generate driving force for fluid in micropumps. The microvalves [5-7] used in micropumps applications can

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be classified into two categories, active and passive microvalves. The active microvalves are actuated by using external forces to open or close the valve seats. The first active microvalve system was proposed by Ohnstein et al. [8]. They reported an electrostatic type microvalve that can actively control the opening and closing of the valve. The device was integrally fabricated on a silicon wafer by a sequence of thin-film depositions and consisted of an array of single cantilever electrostatic actuators positioned over inlet ports. Flow control was achieved by applying a voltage between the actuator diaphragm and substrate.

On the other hand, the passive microvalves are designed with or without moving parts. For the passive microvalves with moving parts, the valve acts like a one-way valve that opens in one flow direction and closes in the other flow direction. In contrast, the passive microvalves with no moving parts do not actually open and close the valve seats like normal valves. No-moving-part valves (NMPV) produce the net volume flow due to the difference of flow resistance between forward and reverse flow within a microchannel structure. Both active microvalves and passive microvalves with moving parts are expensive and complicated in their production and maintenance. One of the problems should be noticed here is the active/passive valves with moving part will easily cause damage to the biological particles in the fluid if the pumps are used in transport of biological samples. Compared with active/passive valves with moving parts, NMPV micro-pumps are of interest because of their simplicity, reliability, ease of manufacture, and potential for being able to transport biological particles without damage. These advantages allow them can be easily applied in numerous applications like medicine, chemistry, and environmental testing.

The working principle of microvalves with no moving part was utilizing asymmetric character of flow fields to produce a different flow resistance for different direction of a channel flow. A net flow mass would then be obtained by different pressure drop and become into a similar effect of one-way valve. There are many types of NMPV design. The Tesla valve [9] was often used in industry. Another design of micro-pump with diffuser NMPV design embedded in the inlet and outlet positions of the channel was reported [10,11]. The flow has lower flow resistance along the diffuser direction and larger flow resistance along the convergent nozzle flow direction for a diffuser valve with an angle less than 20°. That is to say, the flow would have bigger pressure drag along the reverse flow direction because of the contraction of channel. Another similar design and function of diffuser valve with angle more than 70.5° was addressed by Gerlach et al. [12,13] in 1994. Previous literatures [14,15] often used a diffuser NMPV design. In diffuser NMPV design, the only design parameter in NMPV optimization studies is the divergent angle. Different from previous studies, a convergent-divergent (C-D) nozzle with convergent half angle θ₁ and divergent half angle θ₂ is applied for a new NMPV design in this study. Additional design parameter introduced here is expected for a better NMPV pump performance. Here, the optimal design of C-D nozzle type NMPV, as well as its performance for a NMPV micropump, would be investigated and addressed in the study.

2. NUMERICAL METHOD AND GEOMETRIC MODEL

In this study, the simulation was performed with the CFD–ACE+ software (CFD Research Corporation, Huntsville Alabama), a multi-physics package based on the Finite-Volume methods. The program would be run on a 2.4GHz Pentium IV processor with 1GB of RAM memory. The mesh-independent test runs were made before the study of NMPV micropump. Although operated in the laminar flow regime, a rather fine mesh was needed to account for the detailed features of the pumping mechanism. The time for each run spanned from 2 hours up to 12 hours. On the mesh process, a triangular structured grid preventing the singular point of geometry effectively was made. The total numbers of cell were 16000 and 497000 for 2D and 3D flow simulation respectively. The convergent condition of the iteration is $10^{-4}$. The velocity and pressure limits for truncate error are ±10$^{-10}$ for the numerical results.

In order to get on real case for the research and confer the properties of NMPV, a finite volume was applied to the solution domain; the continuity equation and Navier-Stokes equations were used with the moderate boundary conditions.

A flow model in CFD–ACE+ software will be addressed and used in the simulation.

(1) Flow model

The governing equations for the flow model represent mathematical statements of the mass and momentum conservation laws of physics for flow. These two laws can be used to develop a set of equations (known as the Navier-Stokes equations) for CFD–ACE+ to solve numerically.

(a) Mass Conservation

Conservation of mass requires that the time rate of change of mass in a control volume must be balanced by the net mass flow into the same control volume (outflow-inflow). This can be expressed as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0$$

(1)

where $\rho$ is the density of fluid and $\vec{V}$ is velocity vector of the flow field.

(b) Momentum Conservation

Newton’s second law states that the time rate of change of the momentum of a fluid momentum equation is found by setting the rate of change of $x$, $y$, and $z$-momentum of the fluid particle equal to the total force in the $x$, $y$, and $z$-direction on the element due to surface stresses plus the rate of increase of $x$, $y$, and $z$-momentum due to sources. The Navier-Stokes equations can be simply expressed as:
\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = \frac{\partial (\rho \tau_{xx})}{\partial x} + \frac{\partial (\rho \tau_{yy})}{\partial y} + \frac{\partial (\rho \tau_{zz})}{\partial z} + S_m
\]

\[
\frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = \frac{\partial (\rho \tau_{xy})}{\partial x} + \frac{\partial (\rho \tau_{yx})}{\partial y} + \frac{\partial (\rho \tau_{yz})}{\partial z} + S_m
\]

\[
\frac{\partial (\rho w)}{\partial t} + \nabla \cdot (\rho \vec{w} \vec{w}) = \frac{\partial (\rho \tau_{xz})}{\partial x} + \frac{\partial (\rho \tau_{zx})}{\partial x} + \frac{\partial (\rho \tau_{zy})}{\partial z} + S_m
\]

where \( \vec{V} = u\hat{i} + v\hat{j} + w\hat{k} \), \( u, v, w \) are velocity vectors in \( x, y, \) and \( z \) direction. \( \tau_{ij} \) is stress tensor, \( p \) is pressure and \( SM \) is the external source term.

In the current studies, both steady state and unsteady simulations are performed. For steady state simulations, boundary conditions of fixed velocity at inlet and fixed pressure \( (P = 0) \) at outlet are used. The inlet velocity boundary conditions will be presented as Reynolds number at C-D nozzle throat in the paper. In the end of the paper, three-dimensional unsteady simulation to imitate the realistic operation of NMPV Pump, the boundary conditions are described as following:

The membrane deformation \( (D_{p-p}) \) is governed by the equation as:

\[
D_{p-p} = 10^{-5} \times \sin(2\pi \times f \times T) \times \cos(50 \times \pi \times r)
\]

where membrane radius is 0.01m and \( r = 0 \) is at the center of membrane. The maximum peak to peak deformation of the membrane is 20\( \mu \)m and the vibration frequency \( (f) \) is from 10Hz to 100Hz. For unsteady NMPV micropump simulation, boundary conditions for inlet and outlet of NMPV pump are fixed pressure at \( P = 0 \).

The 2-D and 3-D numerical model for C-D nozzle type NMPV addressed in the study was shown in Fig. 1. The total length of the NMPV was 10mm and the width of channel \( (W) \) was 1mm. The C-D nozzle type NMPV included both convergent half angle \( (\theta_1) \) and divergent half angle \( (\theta_2) \) parameters in design. In the first place, confer the C-D nozzle angle effect. To change the angle of \( \theta_1 \) from 10\(^0\) to 80\(^0\) and angle of \( \theta_2 \) from 30\(^0\) to 150\(^0\). The throat width \( (D) \) of C-D nozzle is set as 300\( \mu \)m, 400\( \mu \)m and 500\( \mu \)m. The normalized throat widths (throat width/channel width) are \( D/W = 0.3, 0.4 \) and \( 0.5 \). The flow direction along the positive \( X \) axis was set as the forward flow and vice versa. In this study, the water at room temperature was taken as the fluid model in the simulation.

The basic principle of NMPV micropump that can produce a net volume flow is mainly due to the difference of flow resistances between forward flow and reverse flow conditions. Steady state flow simulations with boundary conditions of fixed velocity at inlet and fixed pressure \( (P = 0) \) at outlet are used for the calculation of forward flow pressure \( (\Delta P_f) \) and reverse flow pressure \( (\Delta P_r) \) required. The fixed velocity at inlet boundary condition is presented as Reynolds number parameter at throat in this paper. The Reynolds number is defined as:

\[
Re = \frac{\rho \cdot U_{ave} \cdot D}{\mu}
\]

where \( \rho \) and \( \mu \) is the density and viscosity of fluid. \( U_{ave} \) is the average velocity at the throat and \( D \) represents the width of the throat.

The ratio between \( \Delta P_f \) and \( \Delta P_r \) is called dipole \( (D_p) \) of the NMPV and define as:

\[
D_p = \frac{\Delta P_f}{\Delta P_r}
\]

If the value of \( D_p \) equals to one, the net volume flow of a NMPV micropump will be zero. For a useful NMPV, the \( D_p \) value of NMPV is greater than one. The higher the dipole \( (D_p) \) value, the larger the flow rate \( (Q) \) of NMPV pump [14]. Therefore, the dipole \( (D_p) \) value is used as objective function for the optimization design of no-moving-part valve. For the dipole \( (D_p) \) of C-D nozzle type NMPV studies, the dipole value for different \( \theta_1 \) and \( \theta_2 \) angles are evaluated when Reynolds numbers range from 0.01 to 200.

For C-D nozzle type NMPV design, asymmetric flow patterns are characterized by the difference of separation bubble lengths for the forward and reverse flow. Therefore, the length ratio between separation bubbles in the forward and reverse flow is defined as:

\[
\xi^r_s = \frac{\Delta S^r_f}{\Delta S^r_f}
\]

where \( \Delta S^r_f \) means the separation bubble length for the forward flow and \( \Delta S^r_f \) used for reverse flow. The separation bubble length ratio between forward and reverse flow are used as index for the degree of asymmetric flow.

3. RESULTS AND DISCUSSIONS

The main purposes of this study are attended to investigate the optimal design and operational condition...
for C-D nozzle type NMPV. Hence, the optimal design included throat width ($D$) of C-D nozzle, convergent half angle ($\theta_1$) and divergent half angle ($\theta_2$) of C-D nozzle, and aspect ratio ($AR$) would be investigated in this study. Aspect ratio ($AR$) is defined as

$$AR = \frac{H}{D}$$

(7)

where $H$ is channel height and $D$ is width of throat.

In Fig. 2 the dipole values ($D^p_i$) versus the Reynolds number are plotted at different C-D nozzle type NMPV with normalized throat widths of $D/W = 0.3$, 0.4 and 0.5, respectively. The convergent half angle $\theta_1$ and divergent half angle $\theta_2$ in Fig. 2 are $\theta_1 = 20^\circ$ and $\theta_2 = 90^\circ$. It shows that the dipole value ($D^p_i$) is greater than 1 for $Re > 10$ independent any kinds of the C-D nozzle throat width. For a laminar channel flow, higher Reynolds number (or higher flow rate) means higher pressure loss. Therefore, forward and reverse flow resistance becomes asymmetric ($D^p_i > 1$) only when pressure loss of flow system is high enough. The simulation results also indicate that the dipole ($D^p_i$) value of the C-D nozzle with throat width $D/W = 0.3$ is higher than C-D nozzle with throat widths of $D/W = 0.4$ and 0.5. Since C-D nozzle NMPV with throat width $D/W = 0.3$ has higher pressure loss under the same Reynolds number, it can be also concluded that the dipole value ($D^p_i$) will be higher if the pressure loss is higher. Hence, NMPV pump with throat width $D/W = 0.3$ would be expected to have a larger net flow rate, but also come with higher pressure loss [16]. The results of Fig. 3 show that the $D^p_i$ value is larger than 1 for $Re > 10$. And in order to approach the reality, the operational condition of Reynolds number is assumed smaller than 100. However, the C-D nozzle angle of $\theta_1 = 60^\circ$ and $\theta_2 = 110^\circ$ is found to be a better choice because a maximum value of $D^p_i$ appears in the Fig. 3. In order to further confirm the relation between diffuser angles ($\theta_1$, $\theta_2$) and $D^p_i$, “Design of Experiments” (DOE) [17] and “Response Surface Modeling” (RSM) [18] optimization methods are applied for the optimal analysis of C-D nozzle angles in this study. According to the results of Fig. 4, it is shown that the C-D nozzle angles based on the maximum value of $D^p_i$ also exist at $\theta_1 = 60^\circ$ and $\theta_2 = 110^\circ$ and did confirm the previous results of Fig. 3 again. However, this result could be realized well by the flow image for the flow model. Figure 5 showed the forward and reserve flow image for the separation region of the C-D nozzle channel. Some results of Fig. 5 would be addressed as following. The flow separation occurred at $Re > 10$ and the asymmetric flow phenomenon appeared. The results shown in Table 1 indicate that $\varepsilon^s_{55}$ for $\theta_1 = 60^\circ$ and $\theta_2 = 110^\circ$ is larger than the other case and a larger dipole ($D^p_i$)
value also appears. This evidence indicates that the variation of separation bubble length will affect the \( D_p^o \) value. Roughly speaking, the larger the \( \xi^T S \) value is, the higher the \( D_p^o \) value.

Concerning the realistic requirement of NMPV design, offering an optimal design of C-D nozzle angle is important to NMPV. Figure 6 indicated that the constant contours of \( D_p^o \) map versus different \( \theta_1 \) and \( \theta_2 \) at \( D/W = 0.5 \) and \( 20 < \text{Re} < 75 \). The optimal \( \theta_1 \) and \( \theta_2 \) would be suggested in the range of \( \theta_1 = 46^\circ \sim 57^\circ \) and \( \theta_2 = 110^\circ \sim 116^\circ \). In addition, the optimal angles for C-D nozzle type NMPV suggest by Fig. 7 are within the range of \( \theta_1 = 40^\circ \sim 54^\circ \) and \( \theta_2 = 113^\circ \sim 120^\circ \) for \( D/W = 0.3 \) when Reynolds number is between 10 and 30. If one overlaps the NMPV optimal angle region and operation condition between the results of \( D/W = 0.3 \) and \( D/W = 0.5 \), the angles of \( \theta_1 = 46^\circ \sim 54^\circ \) and \( \theta_2 = 113^\circ \sim 116^\circ \) and operational Reynolds numbers ranging from 20 to 30 are suggested for both \( D/W = 0.3 \) and \( D/W = 0.5 \) cases. In the realistic microfluidic condition, the aspect ratio (AR) of C-D nozzle will influence on the efficiency of micropump operation. Therefore, the effect of aspect ratio (AR) on the value of \( D_p^o \) would be taken into account.

In Figure 8, \( D_p^o \) values become larger than 1 for \( \text{Re} > 10 \) corresponding to different aspect ratios are similar to results of 2D flow the value of aspect ratio, the higher the net volume flow rate. In Fig. 8, \( D_p^o \) value approach to the corresponding 2D value for \( AR > 6 \) regardless of Reynolds number. It means the side-wall effect can be neglected if \( AR > 6 \).

To imitate the realistic operation of piezoelectric buzzer driving force system, a sine wave with the different frequency was applied to test the pumping performance at different C-D nozzle angles. Two cases of convergent half angle \( \theta_1 \) and divergent half angle \( \theta_2 \) at \( (\theta_1, \theta_2) = (50^\circ, 115^\circ) \) and \( (60^\circ, 80^\circ) \) would be selected as an optimal C-D nozzle NMPV micropump design and a similar diffuser NMPV micropump design respectively. Here the similar diffuser NMPV micropump design means that the divergent half angle \( \theta_2 \) equals \( 80^\circ \) which is very close to the divergent half angle \( \theta_2 = 90^\circ \) value for a typical diffuser NMPV pump design. The results of Fig. 9 show that the volume flow rate for case of \( (50^\circ, 115^\circ) \) is better than the case

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**Table 1 Different angle of \( \theta_1 \) and \( \theta_2 \) versus the values of \( D_p^o \cdot \Delta S_T^f \cdot \Delta S_T^r \) and \( \xi^T S \), respectively**

<table>
<thead>
<tr>
<th>( \theta_1 )</th>
<th>( \theta_2 )</th>
<th>( D_p^o )</th>
<th>( \Delta S_T^f )</th>
<th>( \Delta S_T^r )</th>
<th>( \xi^T S )</th>
</tr>
</thead>
<tbody>
<tr>
<td>60°, 110°</td>
<td>500μm</td>
<td>0.9061</td>
<td>13.16</td>
<td>14.4</td>
<td>1.09422</td>
</tr>
<tr>
<td>80°, 30°</td>
<td>300μm</td>
<td>0.9562</td>
<td>11.78</td>
<td>11.28</td>
<td>0.95755</td>
</tr>
</tbody>
</table>

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**Fig. 5** The flow separation region versus two cases of \( \theta_1 \) and \( \theta_2 \). (\( \text{Re} = 50, D/W = 0.5 \))

**Fig. 6** The constant contours of \( D_p^o \) map versus different or \( \theta_1 \) and \( \theta_2 \) at \( D/W = 0.5 \) and \( 20 < \text{Re} < 75 \)

**Fig. 7** The constant contours of \( D_p^o \) map versus \( \theta_1 \) and \( \theta_2 \) at \( D/W = 0.3 \) and \( 10 < \text{Re} < 30 \)

**Fig. 8** The values of \( D_p^o \) versus Reynolds numbers at aspect ratios ranging from 0.1 to 6 and 2D simulation for \( D/W = 0.5 \) \( (\theta_1 = 50^\circ \) and \( \theta_2 = 115^\circ) \)
of (60°, 80°). It can be concluded that C-D nozzle NMPV micropump design has a higher performance than the diffuser NMPV micropump design under the same operation condition. In addition, the higher the pumping frequency \( f \), the larger the volume flow rate \( Q \). The relationship between the pumping frequency \( f \) and the volume flow rate \( Q \) are

\[
Q = -0.13228 + 0.017406 f - 0.0003973 f^2 + 1.1988e^{-3} f^3
\] (8)

for \( \theta_1 = 50° \) and \( \theta_2 = 115° \) case and

\[
Q = -0.91485 + 0.12222 f - 0.0045338 f^2 + 8.389e^{-3} f^3
\] (9)

for \( \theta_1 = 60° \) and \( \theta_2 = 80° \) case.

4. CONCLUSIONS

Some significant parameters being helpful to C-D nozzle type NMPV design and operation are obtained by numerical simulation method and shown as follows:

First, the Reynolds number must be larger than 10 to confirm the value of \( D^* \) being larger than 1 in name of existence of net mass flow. Second, the optimal geometry parameters of C-D nozzle type NMPV are found at the angles of \( \theta_1 = 60° \) and \( \theta_2 = 110° \) based on the maximum value of \( D^* \). Third, the width of throat at \( D/W = 0.3 \) has a higher dipole value, but come with a higher pressure loss, among current three C-D nozzle throat widths in this study. By overlapping the optimization regions of both \( D/W = 0.3 \) and 0.5 cases, the angles within \( \theta_1 = 46° \sim 54° \) and \( \theta_2 = 113° \sim 116° \) and the operational Reynolds numbers ranging from 20 to 30 are suggested for the optimal design and operation condition for a C-D nozzle type NMPV. It is also verified by unsteady pumping simulation that C-D nozzle type NMPV micropump design can have larger volume flow rate than a typical diffuser NMPV micropump design under the same operation condition. The side-wall effect would be neglected for \( AR > 6 \). These findings would be useful to the design and operation for a C-D nozzle type NMPV.

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