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CFD as a Design Tool for a Conducting Polymer Micropump

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Abstract

This paper demonstrates the use of computational fluid mechanics as an effective tool in the design of a microfluidic pump. The pump is being fabricated from conducting polymer materials. In the first design fluid motion in a channel is achieved by a travelling wave propagating along the channel wall. These displacements are at a micron scale and CFD provides insight into the potential for improved pump performance via surface modification of the solid walls of the channel (i.e. creation of slip). The second design uses a similar concept and relies on compression of a flexible tube wrapped in a conducting polymer fibre. In this case the computational model solves for both fluid motion and the solid deformation in the tube walls. In the third design a trilayer strip of conducting polymer is oxidized and reduced to create a flapping motion insider a fluid reservoir. This displaces fluid through an outlet. CFD modelling was used to optimize the design of the fishtail device and show that flow rates through the device would be maximised if the frequency was kept in an intermediate range. This device relies on the production of counter-current vortices.

Introduction

Micropumps have a variety of uses which include implantable drug delivery devices and lab-on-chip technology. This paper explores the design of a micropump fabricated from conducting polymer materials. Conducting polymers [2] such as polypyyrole undergo significant volume changes when they are oxidised or reduced. This motion can be in the form of out-of-plane swelling of a film, length-wise strains in the case of a polymer fibre, or a bending motion in the case a polymer strip. Fabrication of micro devices is difficult so CFD is a valuable tool for evaluating design options and selecting which options should be built as prototypes. All CFD calculations presented in this paper were performed using COMSOL [3]. All analyses were performed by solving the incompressible form of the Navier-Stokes equations. The Arbitrary Lagrange-Eulerian (ALE) formulation is used in all cases to handle the mesh motion associated with the displacements oocuring in each of the pump designs. The fluid being pumped in each case is assigned the viscosity and density of water.

Microchannel Design

Out of plane swelling has been observed in polymer films [4]. Local thickness changes of over 20% have been observed. Such thickness changes can be exploited to create an actuation motion by connecting a series of electrodes to a conducting polymer film. By controlling the voltages at these electrodes the polymer can be made to swell (out of plane) along its length. This deformation remains in place until the electrical voltage is reversed. If the polymer film is placed along the bottom (or top) of a closed microchannel then the swelling in the polymer will displace fluid along the channel. Figure 1 depicts the motion of the polymer film for the case of a 20 μm wide channel, in which a polymer film swells by 2 μm. Figure 2 shows the volume flowrate associated with this displacement. The CFD model for this case uses an actuation velocity for the polymer material of consistent with laboratory data. The case depicted in Figure 2 achieves an average flow rate of 4.5 nl/min.

All solid-liquid boundaries in this model were assigned no-slip boundary conditions. However in the manufacture of the microchannel structure it would be possible to use surface science techniques to make the surface of the channel hydrophobic, therefore relaxing the no-slip boundary condition. To assess the impact of surface modification on fluid flow the CFD model for this case was re-run with a slip length of 100 nm assigned to all solid boundary (i.e. the solid channel walls, but not the conducting polymer film which coats the top or bottom of the channel). This slip length is large and would imply there is significant slip at a nanofluidic scale. However the scale of this device (i.e. within a 20 μm channel) the effect of the slip was relatively modest,

Though relatively straightforward to fabricate this design is not currently being pursued further. Practical application of this pumping mechanism would require the use of a one-way valve at the outlet of the device to prevent backflow while the swelling in the polymer was being reversed between during the oxidation/reduction cycle.

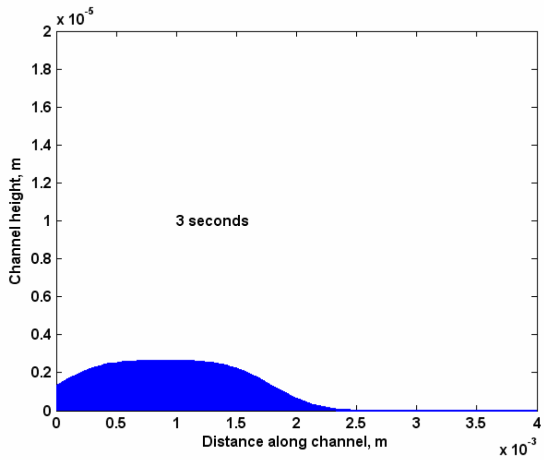


Figure 1. Deformation of a polymer film causing flow along a microchannel.

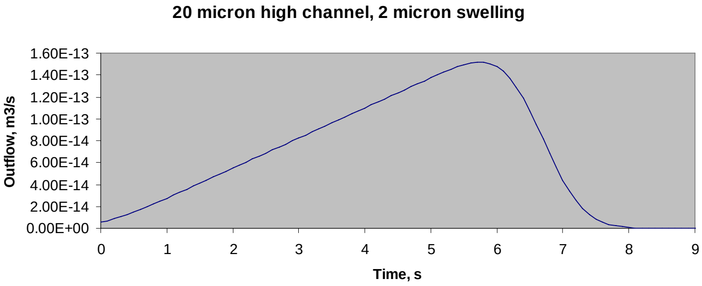


Figure 2. Volume flow rate along a microchannel., average flow rate is 4.5 nl/min.

Tubular Design

The next design evaluated in this project is based on the deformation of a solid tube which contains the fluid being pumped. The tube is wrapped in segments of a coiled fibre of conducting polymer material. When a voltage is applied to the conducting polymer material it contracts producing a length-wise strain in the fibre and in turn compressing the tube. The performance of this design was evaluated using a couple fluid-solid mechanics model with axial symmetry about the centreline of the tube. The force distribution along the tube was modelled as a Gaussian distribution which travelled along the tube in the direction of flow. The computational model then evaluated the stress and deformation in the solid walls of the tube. This was then coupled to fluid flow calculations to relate the volume flow rate achieved to the applied force.

Figure 3 shows example output from the fluid mechanics model. This device would be relatively straightforward to fabricate since suitable conducting polymer fibres are commercially available. The performance of the device is very dependent on the thickness and stiffness of the tube material, however suitable tubes could be fabricated. To ensure unidirectional flow through this device a one-way valve would be required at the outlet. This is seen as a drawback for this design and it is not currently being developed into a prototype.

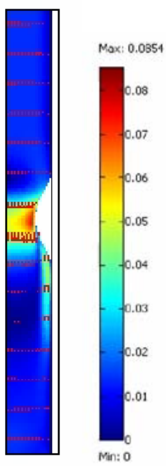


Figure 3. Velocity distribution in the tubular model. Tube has a radius of 5mm and a length of 30mm. Velocity shown in m/s.

Triilayer Strip Design

Background

The third design being evaluated in is a "fishtail" design. The fishtail design was inspired from a magnetically-driven pump [1]. That pump consisted of an iron bar pinned close to one end. This bar rotated about its pinned joint by 35 degrees in each direction. The oscillation was in a specific frequency range chosen so that the bar would generate vortices in the surrounding fluid. The generation of these counter rotating vortices pumps fluid through the reservoir. Counter rotating vortices are observed in the wake of a swimming fish and are associated with their efficient propulsion.

The fishtail structure being analysed in this project is a trilayer structure consisting of a layer of DBS (dodecyl benzene sulfonate) sandwiched between two layers of polypyrrole. The actuation of the polypyrrole is the result of reduction/oxidization between the polymer and an electrolyte induced by an applied voltage. Expansion of the polymer occurs in the reduction process where a cation is gained. When oxidised, the process is reversed and the polypyrrole contracts.

A schematic diagram of a pump based on a fishtail actuator is shown in Figure 4. Experimental data showing the relationship between the maximum displacement of the tip of the fishtail and the oscillation frequency is shown in Figure 5.

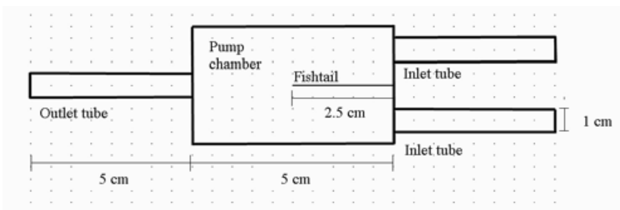


Figure 4. Diagram of the trilayer strip "fishtail" actutator.

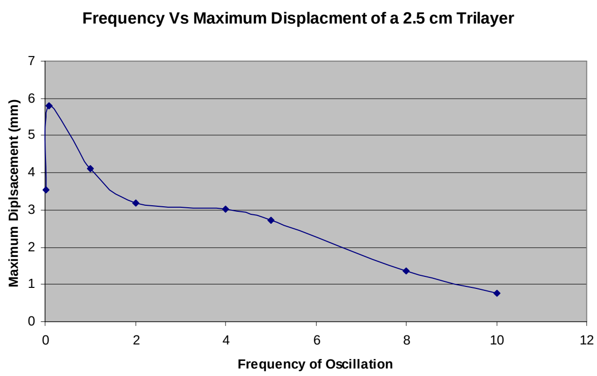


Figure 5. Experimental data depicting the maximum deflection of the tip of the fishtail as a function of the oscillation frequency (Hz).

Mesh Motion

Lab experiments have been conducted to supply data describing the amplitude of the fishtail motion which can be achieved for particular frequencies. The motion of the fishtail was modelled via a moving mesh (ALE) formulation with velocity boundary conditions imposed along the length of the fishtail (equation 1).

$$\frac{dx}{dt} = 2\pi f \frac{1}{\sqrt{1-(\frac{A\sin(2\pi ft)}{L})^2}} \frac{A\cos(2\pi ft)}{L} \cdot$$
$$(-X\sin(\sin^{-1}(\frac{A\sin(2\pi f)}{L})) + Y\cos(\sin^{-1}(\frac{A\sin(2\pi ft)}{L})))$$
$$\frac{dy}{dt} = 2\pi f \frac{1}{\sqrt{1-(\frac{A\sin(2\pi ft)}{L})^2}} \frac{A\cos(2\pi ft)}{L} \cdot$$
$$(X\cos(\sin^{-1}(\frac{A\sin(2\pi f)}{L})) - Y\sin(\sin^{-1}(\frac{A\sin(2\pi ft)}{L}))) \tag{1}$$

When implemented in this manner inverted mesh elements frequently occur near the tip of the fishtail, as shown in Figure 6. To overcome this problem a large box was placed around the fishtail in the geometry (see Figure 7). This box had no impact on the fluid flow solution, however in the ALE solution for the mesh velocities equation (1) was imposed as a boundary condition on all sides of the box. This efficiently avoided difficulties with inverted mesh elements and produced fluid flow results which were very comparable to those obtain with the original ALE setup (and use of frequent remeshing to avoid errors to due to inverted mesh elements).

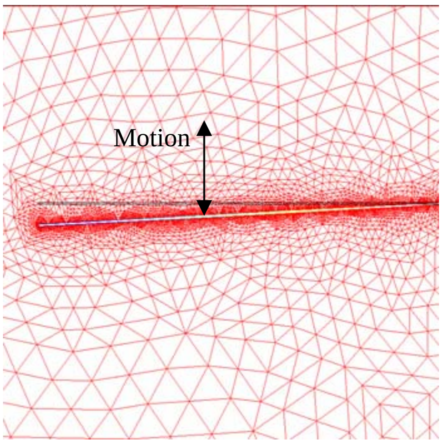


Figure 6. Mesh geometry. Inverted mesh elements during the fishtail motion tend to occur at the top of the fishtail.

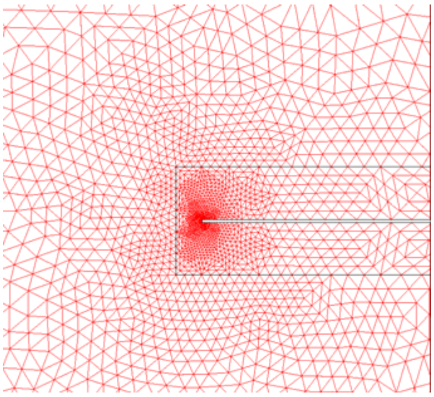


Figure 7. Use of a moving box to avoid inverted mesh elements.

Vortices

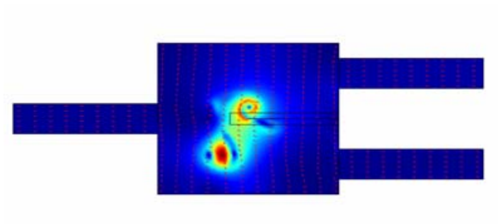
We are interested in analyzing the production of vortices and their impact on the pumping efficiency of the system. According to Sfakiotakis [5] the production of vortices occurs in a Reynolds number between $40 < Re < 2x10^5$ (where the Reynolds number is defined as $Re=\rho UL/\mu$). Atencia [1] claim vortex production occurs in the range $30 < Re < 2x10^3$, where the Reynolds number is defined in terms of the frequency, length and depth of the magnetic oscillating bar in their device.

$$\mathrm{Re} = \rho h(2\pi fL)/\mu$$

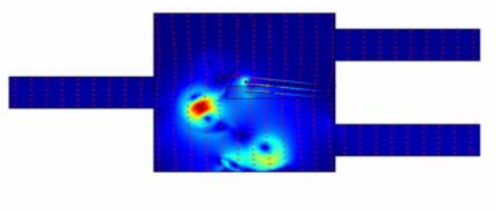
where
Re Reynolds number
f Frequency of oscillation
L Length of the fishtail
h Thickness of the fishtail
μ Dynamic viscosity
ρ Density

(2)

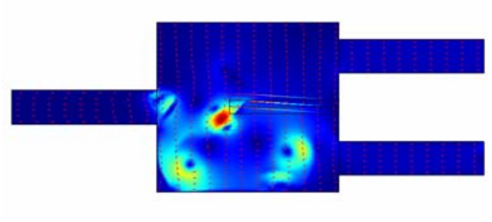
An example of the vortices which are created by the flapping motion of the fish tail depicted in Figure 8.



Time 0.5s



Time 0.7s



Time 0.9s

Figure 8. Velocity field plots for a trilayer oscillating at 4Hz with a maximum displacement of 0.003m for various time steps.

Outlet Design

Unidirectional flow through the outlet is a desirable feature for the pump being developed. In the first two designs presented in this paper this could only be achieved via the additional of a one-way valve (or possibly careful design of the timing of segments of the motion to create a peristaltic motion). In the fishtail design unidirectional flow was achieved by adding two inlet tubes to the pump chamber (instead of the single tube which was initially envisaged). The inflow rates through each of these tubes are out of phase however with slightly different magnitudes, which guarantees and overall net outflow from the pump chamber as shown in Figure 9.

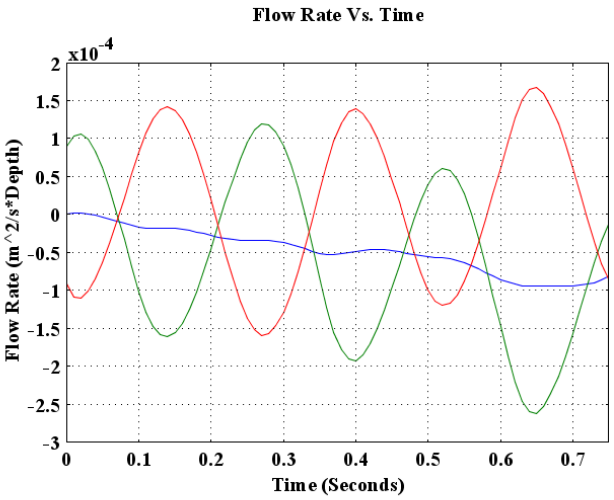


Figure 9. Blue – outlow rate, red inflow rate through upper inlet tube, green inflow rate through lower inlet tube.

The performance of the pump shows some sensitivity to the placement of the inlet tube as shown in Figure 10. Four cases were considered (A) inlets symmetrically placed with as much separation as possible between them, (B) inlets symmetrically placed but closer together, (C) inlets asymmetrically placed, (D) inlets above and below the pump chamber (instead of to its right). The flow rate achieved in case D is 20% lower (at certain points in the pumping cycle) than the flow rate achieved in case A. The performance of the pump is also sensitive to the frequency of the oscillation of the fishtail.

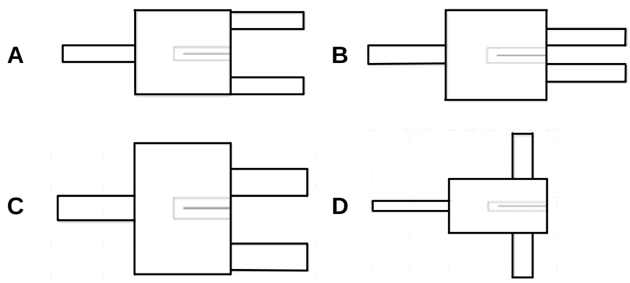


Figure 10. Pump inlet configurations considered.

Conclusions

This paper has introduced three concepts for the design of a microfluidic pump from conducting polymer materials. The first design was pumping by generation of out of plane strains along a microchannel. In this design CFD modelling predicted fluid flow rates and the impact of creating slip at the solid-liquid interfaces. The second design was assessed using a coupled fluid-solid mechanics model of flow in a deforming tube. The force required to create this displacement was supplied by the contraction of a conducting polymer fibre. To ensure one way flow in these designs a one-way valve would be required (or careful creation/timing of a peristaltic mechanism).

A novel design for a fishtail actuator has also been presented. CFD modelling has shown that a configuration with two inlets to the pump chamber can create uni-directional flow at the outlet. All models presented use an ALE finite-element formulation to handle moving meshes. Techniques to avoid inverted mesh elements were discussed.

References

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Acknowledgments

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