2009

DESIGN AND OPTIMIZATION OF PERISTALTIC MICROPUMPS USING EVOLUTIONARY ALGORITHMS

Ravi Bhadauria
Virginia Commonwealth University

Follow this and additional works at: https://scholarscompass.vcu.edu/etd
Part of the Engineering Commons

© The Author

Downloaded from
https://scholarscompass.vcu.edu/etd/1944
DESIGN AND OPTIMIZATION OF PERISTALTIC MICROPUMPS USING EVOLUTIONARY ALGORITHMS

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Mechanical and Nuclear Engineering
at Virginia Commonwealth University

by

RAVI BHADAURIA
B. Tech., Indian Institute of Technology Kanpur, India, 2007

Co-Chairs of Supervisory Committee
Dr. Mohamed Gad-el-Hak
Caudill Professor, Mechanical Engineering

Dr. Ramana M. Pidaparti
Professor, Mechanical Engineering

Virginia Commonwealth University
Richmond, Virginia
August, 2009
Acknowledgment

It has been quite a journey so far. Trying again, failing again, failing better. And then at the end embracing a revelation worth writing. In these moments full of challenges and hardships, there were many people who kept faith and pushed me to this point. At first, I would like to sincerely thank Dr. Gad-el-Hak and Dr. Pidaparti for their invaluable suggestions and advise. I cannot imagine myself writing this document without their nurturing guidance and support. I would also like to mention Dr. Longest here, who on several occasions, proved to be an excellent resource of knowledge. Thanks to Dr. Peters for being in my committee. Secondly, I would like to attribute special thanks to Dr. Mossi for her wonderful and encouraging counseling during my stay at VCU.

People of the department, especially students, have always been my favorite. Thanks to Kittisak and Poorna for their help and support in my research. Thanks to Alex, Jingsi, Jugal, Poorna, Sonya, Steven, and Vivek for all the fun we had while learning together.

A special section of acknowledgments is reserved for my roommates Advait and Yonathan, who are responsible for my mental–metamorphosis and corruption to help me understand social sciences. Without them, integrating science and society would have just been a dream for me. Kudos to us for our discussions over everything. Thanks to Koyal for her care and help.

If something ever disheartened me passing these barriers of support, there were two of them in this planet who gave me extraordinary strength everytime I needed it; my parents. My primary engines who kept me propelling everytime I lost faith in myself. Thank you Mom, thank you Dad... I love you. Ode to both of you.
To my parents

Urmila Singh

and

Mahendra Pratap Singh

who waited so long for this

And to the memory of my grandmother

Shanti Singh
Table of Contents

List of Figures v

List of Tables vi

Abstract viii

CHAPTER 1 Introduction 1
  1.1 Motivation ........................................ 1
  1.2 Applications of micropumps .......................... 2
    1.2.1 Clinical applications ............................ 2
    1.2.2 Microelectronics cooling ......................... 3
    1.2.3 Chemical and biological analysis .................. 4
    1.2.4 Space applications .............................. 5
    1.2.5 Fuel cells ..................................... 5
  1.3 Problem statement ................................ 6
  1.4 Organization of chapters ........................... 7

CHAPTER 2 Literature review 8
  2.1 Classification of micropumps ....................... 8
  2.2 Displacement micropumps ............................ 10
    2.2.1 Piezoelectric actuation ........................ 12
    2.2.2 Electrostatic actuation ........................ 15
    2.2.3 Electromagnetic and magnetic actuation .......... 15
    2.2.4 Thermal actuation ................................ 17
    2.2.5 Pneumatic, composite/polymer and irreversible actuation ... 17
# List of Figures

1.1 Reciprocating displacement micropump with three pump chambers in series developed by Jan Smits .......................................................... 2

2.1 Classification chart of micropumps .................................................. 9

2.2 Classification chart of displacement micropumps .............................. 11

2.3 Vibrating diaphragm micropump in an (a) undeflected position, (b) expansion and (c) contraction stroke ............................................. 12

2.4 Pressure dependence on dome radius on a dome shaped diaphragm transducer micropump .......................................................... 13

2.5 Electromagnetic micropump structure schematic .............................. 16

2.6 SEM images of the PDMS replication from Kim et al. (2005). (a) Overall structure of the replicated PDMS layer of the micropump. (b) Thermopneumatic chamber and membrane ................................................. 19

2.7 Structure and operation of a peristaltic micropump ......................... 20

2.8 Structure and operation of nozzle-diffuser valves ............................ 22

3.1 Dimensions of micropump .............................................................. 24

3.2 Master flowchart of Simulation Strategy .......................................... 26

3.3 Fluid segregate solver solution overview ......................................... 27

3.4 Boundary conditions of fluid domain ............................................. 28

3.5 Displacement of membrane in rotated co-ordinates ......................... 29

3.6 Elements of a neural network ....................................................... 33

3.7 A neural network as a black box ................................................... 34
4.1 Deflections of membrane 1 in geometry 1 in (a), (b) shows the actual deflections against normalized lengths in geometry 1 . . . . . . . . . . 40
4.2 Geometry of 2d validation model . . . . . . . . . . . . . . . . . . . 43
4.3 Validation velocity profile comparison at $x/L = 0.25$ and $t/T = 0.5$ . 44
4.4 Validation velocity profile comparison at $x/L = 0.75$ and $t/T = 0.5$ . 44
4.5 Geometry for the validation problem . . . . . . . . . . . . . . . . . . 45
4.6 Comparison graph of outlet flow for validation . . . . . . . . . . . . 46
4.7 Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude;
   (d) vorticity at $t/T = 0.25$ . . . . . . . . . . . . . . . . . . . . . . . . . 49
4.8 Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude;
   (d) vorticity at $t/T = 0.5$ . . . . . . . . . . . . . . . . . . . . . . . . . 50
4.9 Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude;
   (d) vorticity at $t/T = 0.75$ . . . . . . . . . . . . . . . . . . . . . . . . . 51
4.10 Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude;
    (d) vorticity at $t/T = 1.0$ . . . . . . . . . . . . . . . . . . . . . . . . . 52
4.11 Time history of mass flow rate at 1 Hz. . . . . . . . . . . . . . . . . . . 54
4.12 Locations of rakes in the geometry . . . . . . . . . . . . . . . . . . . 54
4.13 x-velocity at (a) $x = 6.475$ mm; (b) $x = 10.45$ mm; (c) $x = 15.45$ mm;
    (d) $x = 20.425$ mm . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 55
4.14 Parametric curve of average flow rate versus actuating frequency . . . 56
4.15 Convergence plot of training ANN . . . . . . . . . . . . . . . . . . . . 58
4.16 Validation plot of ANN . . . . . . . . . . . . . . . . . . . . . . . . . . 59
4.17 Convergence plot of Genetic algorithm . . . . . . . . . . . . . . . . . 60

D.1 Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude;
    (d) vorticity at $t/T = 0.125$ . . . . . . . . . . . . . . . . . . . . . . . . . 87
D.2 Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude;
    (d) vorticity at $t/T = 0.375$ . . . . . . . . . . . . . . . . . . . . . . . . . 88
D.3 Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude;
   (d) vorticity at $t/T = 0.625$ .................................................... 89

D.4 Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude;
   (d) vorticity at $t/T = 0.875$ .................................................... 90

E.1 Optimized geometry 1 ......................................................... 91
E.2 Optimized geometry 2 ......................................................... 92
E.3 Optimized geometry 3 ......................................................... 93
List of Tables

4.1 Lengths for different geometries ............................................. 38
4.2 Maximum deflections (in mm) for different geometries ................. 39
4.3 Parameters $a$, $b$, $X$, $Y$ (in mm) for four parameter gaussian fit. Subscripts represent geometry number. ............................................. 41
4.4 Comparison of flow rates from numerical simulations with genetic algorithm. Lengths are in mm, frequency in Hz and flow rate in kg/sec. 59
Abstract

DESIGN AND OPTIMIZATION OF PERISTALTIC MICROPUMPS USING EVOLUTIONARY ALGORITHMS

by RAVI BHADAURIA, M.S.

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Mechanical and Nuclear Engineering at Virginia Commonwealth University

Virginia Commonwealth University, 2009

Co-Chairs of Supervisory Committee

Dr. Mohamed Gad-el-Hak
Caudill Professor, Mechanical Engineering

Dr. Ramana M. Pidaparti
Professor, Mechanical Engineering

Micropumps are important and crucial elements of microelectromechanical systems. Extensive studies have been conducted in developing such devices in recent years. Use of an actuating diaphragm is quite common to provide pumping action. Among these pumps, there exists a class that is known as peristaltic micropumps. Pumping action in such devices is achieved by periodic expansion and contraction of walls that mimicks the motion of, for example, oesophagus in human body. Inspite of significant research already accomplished on peristaltic micropumps, negligible efforts have been
made to study the coupled behavior between optimization and inter-field interaction physics of pumping.

The implementation of structure optimization has become an urgent necessity as one of the most viable means with which to achieve improved performance of MEMS devices, for it enables great improvements in device behavior without fundamentally modifying the manufacturing technology steps. Generally one has to follow the routine optimization procedure involving initial guess, FEA, sensitivity analysis, and then consequently updating the design variables. Because of the inter-field interaction in multiphysics, the sensitivity calculation of coupled problems in most cases is really difficult. Alternatively, one can use an evolutionary algorithm, such as genetic algorithms to solve topology optimization problem in which a typical optimization procedure is transformed to a search procedure. Genetic algorithm is based on the principle of survival of the fittest member, which evolves with the generation.

In this study, we are focusing on a design and topology optimization suited for a specific drug delivery rate of a peristaltic micropump and its performance using coupled solid–fluid analysis. A model of the PDMS (PolyDiMethylSiloxane) micropump consisting of four nozzle/diffuser shaped vibrating actuators on the sidewalls is considered for numerical study. These actuators are used to create pressure difference in the four pump chambers. It is the pressure difference that propels the working fluid. The unique operating characteristics (peristaltic motion) of the proposed micropump result from a specific sequence of membrane motion.

The goal of the present work is to design a micropump which can deliver fixed amount of fluid from one point to another. A number of computational fluid dynamics simulations have been performed and then certain flow rates are picked and targeted by changing the geometrical and actuation parameters of the pump. A 95% match between the predicted value of flow rate and its actual value from direct numerical simulations is observed.
CHAPTER 1 Introduction

1.1 Motivation

In recent years, methods to transport small volumes of fluid of the order of 1 cubic cm and even less from one point to another on a lab-on-a-chip system to provide means of conducting laboratory experiments have been of tremendous interest to researchers. There seems to be a never ending demand of these methods in biology and medicine to space exploration and microelectronics cooling and so forth. Since the application of such devices is far more than we can think of today in physical and engineering systems, these devices have always been favorite to many scholars for perusal.

The small fluid volumes in the above mentioned systems are often pumped, controlled and manipulated during operation. Macroscale pumping methods such as axial and centrifugal pumping are not suitable for pumping in such small scales, since the physics in microscale flows is dominated by surface effects (Gad-el-Hak, 1999). An appropriate reasoning of the problem could be discussed in terms of a famous dimensionless flow parameter, the Reynolds number (often represented as $Re$). In a crude sense, Reynolds number can be interpreted as the ratio of inertial forces over viscous forces in the flow. Since the flow in miniature flow devices is highly viscous ($Re \leq 1$), i.e. viscous forces dominate considerably over (or of the order of) inertia forces; macroscale pumping methods such as axial or centrifugal pumping fail to function, since they are dependent upon fluid inertia to perform. In such a scenario, investigation of alternative pumping strategies have become imperative in recent times. Microfluidic transport requirement such as these can sometimes be met by taking advantage of passive mechanisms, most notably surface tension (Hobbs & Pisano, 2003; Su & Lin, 2003), viscosity (Sen et al., 1996). For other applications,
Figure 1.1: Reciprocating displacement micropump with three pump chambers in series developed by Smits (1990). The micropump is made from an etched silicon substrate bonded between two glass plates. Staggered actuation as shown results in net fluid flow from the inlet at left to the outlet at right.

macroscale pumps, pressure/vacuum chambers and valves provide adequate microfluidic transport capabilities (Burns et al., 1998; Blom et al., 2002; Kanai et al., 2003; Selam et al., 1992). Yet for many microfluidic systems, active pump, the size of which is comparable to the volume of the fluid it pumps, is desired. Following is the discussion over the usage of micropump in different applications.

1.2 Applications of micropumps

1.2.1 Clinical applications

Dispensing therapeutic agents into the body has long been a vision and goal for the scientists, especially micropump designers. The idea dates back to early 1980s when
Jan Smits developed the micropump intended for use in controlled insulin delivery systems for maintaining diabetics’ blood sugar levels without frequent needle injections (Smits, 1990) as demonstrated in Figure 1.1. Since then micropump technology has improved dramatically and has flourished leaps and bounds. Today they can pump metered amounts of drug into a microneedle system, which is suitable for delivering modern bio-technological drugs that cannot be delivered by conventional delivery techniques (Poll, 2000). Small size and high precision of micropumps have made them useful for chemotherapy, insulin delivery for diabetic patients, and drug dosing for cancer patients (Smits, 1990). They can dispense engineered macromolecules into tumors or the bloodstream (Dash & CudworthII, 1998; Coll et al., 1999). Though micropumps are incapable of providing high volumetric flow rates, which are not likely to be required of implanted micropumps, it is the precise metering of the drug which makes increases their usage manifold (Dash & CudworthII, 1998; Pickup et al., 1978; Allen, 1986; Hanaire-Broutin et al., 1995).

The pressure generation requirements for implantable micropumps are not insignificant, as the back pressure encountered in vivo can be as high as 25 kPa. Also they have to be reliable, less power consuming and biocompatible with low cost (Dash & CudworthII, 1998; Allen, 1986; Selam, 2001). Because of such limitations and deficiencies, the usage and implantation of micropumps is restricted. Till date, insulin delivery systems make use of static pressure reservoirs which are metered by solenoid-driven valves with over 50 cm³ in size (Selam et al., 1992; Selam, 2001).

1.2.2 Microelectronics cooling

Thermal management of electronic components is of increasing concern in the development of portable and reliable electronic devices. The focus is always to reduce package weight and size of the component while increasing the device functionality and it has received much attention in recent years. Of all the methods and strategies available for thermal management in microelectronic devices, liquid cooling, by far,
is the best. It has the ability to increase power dissipation while also maintaining a small form factor. Many researchers, till date have made efforts to make use of micropump in single- or two-phase cooling of microelectronic devices (Zhang et al., 2002; Jiang et al., 2002; Tuckerman & Pease, 1981). However, the requirement of large pumps to drive the liquid flow and the associated large pumping power (Zhang et al., 2002; Wang et al., 2004) have limited the application of microchannel heat sinks in space-constrained electronics as mentioned in Garimella et al. (2006).

Scaling of such devices also result in greater pressure required to pump the flow. The fundamental scaling law associated with pressure-driven flow points out that high pressures (100 kPa or greater) are required to force high flow rates which are necessary for the action of micro heat sinks. In the laminar regime, most common among the nature of flow in micropumps, an order of magnitude decrease in the hydraulic diameter (the channel cross-sectional area multiplied by four and divided by its perimeter) results in two orders of magnitude of the pressure difference to maintain the constant average flow velocity and flow-rate. Micropumps might directly be integrated into ICs to cool transient hot spots, and therefore their fabrication methods and temporal response characteristics are also the factors one has to model (Laser et al., 2003).

1.2.3 Chemical and biological analysis

Recently, researchers have focused their attention on miniature systems for chemical and biological analysis (Manz & Becker, 1998; Jakeway et al., 2000; Mathies et al., 2002; van der Schoot et al., 1992). These systems are capable to trap, separate, sort, treat, detect and analyze biological materials (van der Schoot et al., 1992). Miniaturization of chemical assay systems result in the reduction of quantities of sample and reagents required for the analysis. Also, manual intervention in such cases is reduced and assays are performed more quickly; portability is also enhanced resulting in reduction of overall cost requirements. Automation of chemical analysis by these
methods leads to very little chemical exposure to operator. Miniaturization of such
devices leads to increased disposability, thus increasing sterility, which happens to be
a very important factor in these micro total analysis (μTAS) systems.

Despite of such promising capabilities, micropumps are found in very few
current generation μTAS systems. Liquid transport is instead often accomplished
through manual pipetting, with external pneumatic sources, or by inducing electroos-
motic flow. The limited use of micropumps in μTAS may be partly due to the lack
of available micropumps with the necessary combination of cost and performance.
Also the presence of particles in fluid may disrupt operation of pumps and valves.
Secondary effects associated with reliability and corrosion include the impact of me-
chanically shearing the sample, chemical reactions, adsorption of analytes and wear
of moving parts.

1.2.4 Space applications

A high number of micropump usages in space explorations have been reported. It
is one of the exciting areas of micropump technologies. Envisioned by Wiberg et al.
(2001), miniature roughing pumps are needed for using mass spectrometer systems
to be transported on lightweight spacecraft. They would require to achieve a vacuum
of approximately 0.1 Pa, which happens to be the level around high vacuum pumps
become active (Watson, 1997). Among the other potential applications of microp-
umps in space, micropropulsion also holds big importance. For the proposed 1–5 kg
‘microspacecraft’, a delivery rate of 1 ml per minute is estimated (Micci & Ketsdever,
2000; Bruschi et al., 2002). For space applications, larger stroke volumes are generally
required as one has to pump gases instead of liquid.

1.2.5 Fuel cells

Micropumps find their application in fuel cell system to enhance the transport of
adequate amount of fuel and removal of carbon dioxide from the fuel cell device.
Direct methanol fuel cells have considered for portable applications. Micropumps for this purpose should be highly efficient in terms of power consumption as compared to the provided flow rate (Zhang & Wang, 2005).

1.3 Problem statement

The objective of the current study is to investigate the complete physics of solid and fluid motion in detail by simulating the solid through finite-element and fluid through computational fluid dynamics tools. These analyses are coupled to model the interaction of the solid and fluid through the interface. Predicting the nature of flow by coupling CFD and FE methods provides a better understanding of complex fluid–structure interaction in the micropump.

One of the major advances in micropump construction has been the development of valveless pumps. Researchers have looked at a number of ways of achieving this from generating standing-waves to varying the frequency and motion of the diaphragm (Richter et al., 2009; Nabavi et al., 2008; Yamahata et al., 2005b). Some of the studies have involved variations in the geometry of the inlet and outlet nozzles (Nguyen et al., 2008). This study was one of the first to look at the geometric construction of components that house the fluid. No extensive studies have been conducted yet to address the effects that the geometry of the pumping chamber wall itself has on pumping performance.

Simulations of diaphragm-based micropumps that use passive valves have been pursued quite extensively in the literature. While finite element (Gong et al., 2000; Gonzalez & Moussa, 2002, Kaltenbacher et al., 1997, Jiang et al., 2000) and boundary element (Kaltenbacher et al., 1997; Zengerle & Ritcher, 1994) methods have been used to study the motion of diaphragm actuators in such pumps, lumped-parameter models have been commonly used to simulate the behavior of complete pumps consisting of diaphragm actuators and check valves. More commonly, lumped parameter descrip-
tions of fluid flow and quasistatic diaphragm motion have been employed (Yao et al., 2007). In this study, the novel structure of our design and its simulation results are also presented, which show good compatibility with the drug delivery requirements.

1.4 Organization of chapters

The first chapter provides an introduction to the micropumps and their importance in many applications. The second chapter provides a comprehensive review of topics pertinent to current study. Since the scope and literature of micropump is vast and extensive, efforts have been made to converge the thoughts on displacement micropump and their principles of operation. Focus on valveless design and peristaltic method of actuation is kept in mind for further investigation. The third chapter talks in detail about the methods of analysis used, the governing equations of the model(s) and solid and fluid physics coupling strategies. The method is also validated against experiments and results from earlier modeling methods. Also, statistical and optimization methods used for optimizing the design of the micropump along with the usage of evolutionary algorithms and artificial neural networks has been discussed. Chapter four presents the results of the current study and their discussions. Chapter five ends this study with summary and conclusions.
CHAPTER 2 Literature review

2.1 Classification of micropumps

Krutzsch & Cooper (2001) were among the first ones to classify traditional pumps. Because of the wide range of applications of micropumps mentioned above, it is very important to categorize them qualitatively, so that one has ease in determining the selection criteria for a particular usage. Since the pumping action is achieved in a wide variety of ways, the first choice of any one would be to categorize them based on pumping mechanisms. This criterion not only discusses the details of pumping mechanism, but also helps the reader to accomplish the objective of selection of appropriate micropump. Several extensive reviews of micropump (Laser & Santiago, 2004; Iverson & Garimella, 2008; Nguyen et al., 2002; Woias, 2005) have classified micropump along the same lines. The classification is broadly categorized into two categories:

1. Displacement (Mechanical) Micropumps—These micropumps exert periodic, oscillatory or rotational pressure forces on the working fluid through a moving boundary. This boundary may be a solid-fluid boundary (vibrating diaphragm, peristaltic, rotary pump) or a fluid-fluid boundary (ferrofluid, phase change, gas permeation pumps). Some cases like pneumatic and phase change actuation methods, the pressure does not necessarily has to be periodic (Laser & Santiago, 2004). Aperiodic displacement pumps typically pump only a fixed volume, which in macroscale can be visualized by a syringe action.

2. Dynamic micropumps—are defined as a class of micropumps which continuously add energy to the working fluid so that it either increases its momentum (cen-
trifugal pumps) or its pressure directly (electroosmotic, electrohydrodynamic, electrowetting, etc.). Because of the continuous energy transfer, these pumps can generate constant/steady flows.

Figure 2.1: Classification of micropumps based on Laser & Santiago (2004), after Krutzsch & Cooper (2001).

Micropumps classified above can be sub-categorized based on their actuation principles. Figure 2.1 shows the extensive classification of micropumps adapted from Laser & Santiago (2004). Also a broad classification of diaphragm displacement micropumps
is shown in Figure 2.2. This study will be focused on displacement micropumps, and their different methods of actuation. Particular attention to the maximum measured volumetric flow rate, $Q_{\text{max}}$, and the maximum measured differential pressure, $\Delta p_{\text{max}}$, will be paid. Also the package size $S_p$ plays an important role where compactness is important. Parameters such as operating voltage and operating frequency will be of interest. Following is the discussion on various types of displacement micropumps.

2.2 Displacement micropumps

Displacement micropumps employ different actuation methods. To date, thermoeelastic, electrostatic, electromagnetic, thermoplastic, bimetallic and smart material, such as shape memory alloy and piezoelectric ceramic, actuated micropumps have been reported by Lintel et al. (1988) and Benard et al. (1998). Displacement type micropumps have different structures and they use different materials for providing the necessary pressure differential inside the fluid housing.

The schematic of the displacement micropump is shown in Figures 2.3(a)–(c). The micropump consists of a pumping chamber connected to inlet and outlet for flow rectification. Diaphragm deflection results in a change in the chamber pressure in real time. During the expansion stroke, when the diaphragm expands, the volume of the chamber increases resulting to a decrease in chamber pressure; as a result fluid comes inside in the chamber with the action of opening of inlet valve. During the compression stroke, the volume of the chamber decreases with the moving diaphragm, causing the chamber pressure to increase leading to opening of the outlet valve and liquid is discharged outside. Diaphragm actuation mechanisms and valve types used are described in following text.
Figure 2.2: Classification of displacement micropumps based on methods of actuation reported in Iverson & Garimella (2008).
2.2.1 Piezoelectric actuation

Piezoelectric actuation is the most common and most widely used mechanism for driving the flow in displacement micropumps. Piezoelectric materials generate an internal mechanical stress under the action of applied electric potential. This phenomenon, known as the converse piezoelectric effect, has been used widely by micropump designers to provide the necessary actuation for movement of diaphragm. The piezoelectric material is glued to, deposited on or embedded into the diaphragm for the actuation and the applied alternating voltage drives the piezo for the expansion and contraction.
strokes as the voltage signal changes its polarity. This leads to a periodic increase and decrease in the pump chamber, which opens up the inlet and outlet valves. Piezoelectric actuation is also highly efficient as it is able to provide large deformation magnitude and relatively better pressure generation. The complementary things for this type of actuation mechanism are the choice of diaphragm material, pump geometry, geometry of the valves. Also, the shear orientation used and the type of piezoelectric material play a dominant role in the resulting net volumetric flow rate.

Though flat-diaphragm shaped geometries are easy to fabricate, researchers like Feng & Kim (2005) have demonstrated that with novel molding process resulting in a dome shaped diaphragm, results in higher pressures generated for small radii pump chambers, which have corresponding larger curvatures. The reason for this is
that flat diaphragms are less efficient in converting plane-strain generated by piezoelectric material to volumetric deflection as compared to dome shaped diaphragms. Figure 2.4 shows the typical variation of chamber pressure with dome radius. It is clear from the graph that with larger radius i.e., smaller curvatures, the pressure exerted decreases.

Flow rectification is necessary since the displacement of the diaphragm is symmetric hence resulting flow has equal tendency to move on either side of micropump. Flow rectification is provided through valves which can take different forms and shapes thus featuring active or passive flow control. An asymmetry in design of rectifier elements in piezoelectrically actuated valveless micropump (PAVM) causes a unidirectional flow as reported in Iverson & Garimella (2008). This approach of flow rectification is advantageous over active check valves, which can clog during operation. Most common methodology is to include passive valves which are, in common, nozzle/diffuser type of elements, which have more resistance to fluid motion in one direction as compared to another. However, valveless micropumps show very low net flow rate, which could be enhanced by optimizing the parameters (Morris & Forster, 2000) of the micropump. In addition to these passive flow rectification devices, active diaphragm valves can also be used as shown by Doll et al. (2005) in which piezoelectrically actuated diaphragms are used not only for the pump chamber but also to open the inlet and the outlet valves in synchronization with the chamber expansion and compression stroke.

Recently, Nguyen et al. (2006) have reported an improvement to the traditional piezoelectric actuators by using Lightweight Piezoelectric Curved Actuator (LIPCA). This actuator is manufactured by co-curing layers at an elevated temperature, one of which is epoxy. Experimental results show that displacement per unit length, also called the fractional stroke of LIPCA based actuators are 0.35% as compared to conventional actuators which have in range of less than 0.2%.
2.2.2 Electrostatic actuation

This method uses the electrostatic forces generated by the electrodes to drive the pump diaphragm (Zengerle et al., 1992). The diaphragm membrane in this case acts as an electrode. As an electrical voltage is applied between diaphragm membrane and another electrode, they act as a capacitor and the membrane deflects to vary the capacitance, towards the counter electrode. As soon as the voltage signal changes its polarity, the membrane deflects away from the counter electrode, resulting in a periodic motion. This periodic motion of the membrane, in turn, changes the volume, hence the pressure inside the micropump which causes the fluid to propel in one direction. Directional preference is achieved through similar flow rectification techniques as that used in piezoelectric micropump. The capacitance between the diaphragm and electrode can be calculated by

$$C = \frac{\epsilon \pi d^2}{4l} \quad (2.1)$$

The force acting to pull the two plates together is given by

$$F = \frac{1}{2} \frac{\partial C}{\partial l} V^2 = -\frac{\epsilon \pi d^2}{8l^2} V^2 \quad (2.2)$$

where \(V\) is the voltage applied between the plates, \(\epsilon\) is the permittivity of the medium, \(d\) is the counter electrode diameter and \(l\) is the separation distance between the two plates. Since the force also depends upon the medium, choosing a medium with appropriate high permittivity facilitates the usage of electrostatic actuation even when the plates are far apart, since the force generated will be enough to pump the fluid.

2.2.3 Electromagnetic and magnetic actuation

When a electric current is passed through a wire under the action of a magnetic field, Lorentz forces come into action. Electromagnetic actuation makes use of this phenomenon by attaching a permanent magnet on the diaphragm and passing current in the coil which surrounds the diaphragm. Lorentz forces deflect the diaphragm due to
the interaction of electric field and magnetic field. Since the voltage requirements are very low (\( \sim 5 \) V) and the driver designs are simple as compared to other mechanisms, this method, at times, could be advantageous. Researchers like Chang et al. (2007); Su et al. (2005, 2006) have tried to improve the micropump diaphragm deflections by integrating the permanent magnets and coils directly into the device as demonstrated in Figure 2.5. Yamahata et al. (2005a) developed a permanent magnet cast in which flow rectification was provided by ball valves. Along the same lines, Pan et al. (2005) used magnet attached to DC motor and relatively large induction coils. Maximum flow rates of the order of 0.7–1.0 ml/min were achieved for back pressures up to 30 kPa. Other than these designs, researchers have developed composite diaphragms in which magnetic particles are embedded in the diaphragm (Yamahata et al., 2005b; Nagel et al., 2006), also the designs in which forces between the permanent magnet and steel disks have been used for actuation (Haeberle et al., 2007) have been studied. Lately, magnetic fluids have been used as an additional choice for micropump actuation. The fluids contain a suspension of magnetic particles in a
carrier medium (Sim et al., 2006). These suspensions are stable and can preserve their properties despite of exposure to extreme temperatures and over long periods of time.

2.2.4 Thermal actuation

When heat is applied to a thermally sensitive material, volume expansion takes place to relieve the induced stresses inside the material. Taking advantage of such phenomenon, in context of diaphragm micropumps, thermopneumatic or shape memory alloys (SMA) are used to actuate the diaphragm. These methods are based on the diffusion of thermal energy, they working is limited to low actuation frequencies.

In thermopneumatic actuation, a secondary fluid, other than that of working fluid, is heated by use of a thin film resistive heater, which causes it to expand and deform the pump diaphragm. This phenomenon causes the suction stroke. For the contraction stroke, heater is turned off causing the secondary fluid to cool down and hence regain its original volume. Since this heating and cooling cannot be faster than a certain rate, hence the working frequencies are low. Kim et al. (2005) have developed a cost effective, transparent, PDMS based micropump with nozzle-diffuser elements for flow rectification as displayed in Figures 2.6(a), (b). They have used Indium Tin Oxide (ITO) as conductive heating element.

In addition to fluid heating, single phase gas heating, wax heating (Boden et al., 2006), and shape memory alloys taking advantage of the phase changes (Shin et al., 2005; Zhang & Qiu, 2006) have been reported. While usage of these pumps is promising, the limitation on working frequency has not allowed the greater application of such devices.

2.2.5 Pneumatic, composite/polymer and irreversible actuation

Pneumatic pumps works on the principle of fluctuations in a gas pressure, which are passed on to diaphragm for actuation. Pneumatic valves are actuated in a similar
manner. These types of forces are generally used for peristaltic pumps described later in this chapter. Composite materials like ionic polymer-metal composite (IPMC) are used for large bending deformations over conventional actuators. Irreversible actuation involves no cyclic movement of fluid. These kinds of pumps have many attractive features like negligible power consumption and large pressure generation. A detailed discussion on these pumps can be found in Iverson & Garimella (2008).

2.2.6 Peristaltic actuation

Peristaltic pumps, as the name implies, mimic the motion of periodic expansion and contraction of oesophagus in the human body, which is called as peristalsis. This results in a sequential pumping of fluid from one point to another. This motion is realized by the motion of actuators in series to generate pumping action. Most common peristaltic pump design till date is with three pumping chambers with diaphragms as actuators in series as displayed in Figure 2.7. Many type of actuation schemes are used discreetly for actuation of individual pumping chambers, and nearly same type of transducers are used for this purpose as described above (piezoelectric, pneumatic, etc.). When the first diaphragm is actuated, fluid is pushed towards the second chamber with restriction on the fluid coming out from the inlet, when the second diaphragm is actuated; fluid is pushed towards the third pumping chamber since the first chamber has not been inflated yet. The final stroke pushes the fluid out of the outlet.

One of the major advantages of peristaltic pump is that they can stand high back pressures (Geipel et al., 2007; Jang et al., 2007; Lin et al., 2007). Single-source-actuated peristaltic pumps have been proposed in recent years. The general design consists of several pumping chambers that are connected serially such that the time phased deflection of successive pumping membranes generates a peristaltic effect. An advantages of using such approach is that these membranes can be driven by a single source with some additional components to generate phase difference, thereby reduc-
Figure 2.6: SEM images of the PDMS replication from Kim et al. (2005). (a) Overall structure of the replicated PDMS layer of the micropump. (b) Thermopneumatic chamber and membrane.
2.3 Flow rectification

Since the diaphragm displacement is symmetric, it provides a flow which has no directional preference. Therefore, in order to achieve net flow in one direction, flow rectification of some sort is required. Valves are used as a common method to achieve flow rectification. They can be classified into dynamic- and static-geometry categories. These are further subdivided into active and passive valves.

Dynamic-geometry valves provide flow rectification by deformation, motion or deflection. Almost any of the diaphragm displacement micropumps described above...
can use dynamic valves for flow rectification. These valves operate in sync with diaphragm motion such that the outlet valve is closed before the expansion stroke and inlet valve is closed before the contraction stroke causing the flow becoming directional. Dynamic-geometry valves run the risk of fatigue failure in long-life operation. Stiction can also be detrimental in operation when the valve does not release properly in time from its seat. Also, the dynamic valves have inherent response time associated with them which makes them to work properly under specific range of operating frequencies. One good property of these valves is that they can stand high back pressures since they do not allow for flow-reversal. But they still suffer from clogging and failure of these valves due to various factors listed above restrict their usage in certain demanding applications.

As a remedy to dynamic-action valves shortcomings, static geometry valves are used. These have no moving boundaries or parts which help in achieving flow rectification; instead they take advantage of the geometry to produce directional flow. Most common among these valves are nozzle-diffuser and Tesla valves. This genre of valves is very promising since they have no moving parts and they need no input energy for rectification. But on the other side, because of flow reversals, they cannot generate large back pressures. In that case, other methods of converting the pulsatile flow to continuous stream of flow are adapted.

Nozzle-diffuser valves work on the principle of different resistance offered to fluid by different geometry elements. As demonstrated in Figure 2.8, when the expansion stroke happens, inlet (diffuser action) provides less resistance to fluid moving into the pump chamber as compared to outlet (nozzle action) which results in more mass accumulation from inlet. Similarly, outlet (diffuser action) provides less resistance as compared to inlet (nozzle action) in the contraction stroke. Overall, when these motions happen in tandem, we see a net flow from inlet to outlet.
Figure 2.8: Structure and operation of nozzle-diffuser valves. Courtesy Iverson & Garimella (2008).
CHAPTER 3  Approach and numerical methods

In this chapter, the primary focus is on the methodology and approach used to model the micropump. This chapter is divided into five major sections, viz. Geometry description, which describes the novel geometry of the micropump and the holistic operation of it. The second section describes the solid part of micropump, lists all the relevant equations and the solution techniques used to model the solid which is succeeded by the fluid modeling section. Here all the flow-models, their setup in FLUENT and analysis methods have been discussed in detail. Emphasis has been made on this section since this is the core of the entire problem. Furthermore, some light on Artificial Neural Networks and Genetic Algorithms has been thrown in subsequent sections and their usage in solving the optimization problem has been discussed in some detail. Also, their setup has been discussed in some length. We proceed with the geometry description in the next section.

3.1 Geometry description

In the present study, we focus on pneumatically actuated series of diaphragms, when actuated under a phase difference, generate a peristaltic motion. It is because of this special type of motion; fluid is propelled from one end to the other end of the pump. Figure 3.1 shows the dimensions of the micropump design studied in this work. The lengths $D_1$, $D_2$ and $D_3$ are the ones to be optimized. In the original design considered, their values are 3 mm, 6 mm and 6 mm respectively. A change of these lengths will provide different lengths for the diaphragms, which in turn have different natural frequencies and shapes for oscillations, resulting in a perturbed flow rate. The thickness of the diaphragm is 0.04 mm.
The micropump consists of four diaphragms made of PDMS (PolyDiMethylSiloxane). PDMS is a highly flexible material with density 965 kg/m³, Young’s Modulus 270 kPa and Poisson’s ratio 0.49. These diaphragms are modeled as two dimensional clamped-clamped beams operating under the action of time varying oscillatory loading. The deflection mode and amplitude of the diaphragms’ displacement at any given time will have an effect on the amount of the fluid volume displaced with determines the flow-rate along with other effects such as phase difference of oscillations between two successive diaphragm. The model of clamped-clamped beam under the action of oscillatory load is described in detail in Meirovitch (2001) which provides a reasonable prediction of the first frequency of the actuator.

3.2 Solid modeling

As mentioned before, the solid part of the pump is a flexible PDMS membrane with 0.04 mm in thickness. We consider the response of the beam which is clamped at $x = 0$ and $x = L$, where $L$ is the length of the beam. The resulting governing
The equation of motion is:

\[- \frac{\partial^2}{\partial x^2} \left[ EI(x) \frac{\partial^2 \delta(x,t)}{\partial x^2} \right] + f(x,t) = m(x) \frac{\partial^2 \delta(x,t)}{\partial t^2} \quad (3.1)\]

where E is the modulus of elasticity, I(x) is the area moment of inertia, \( \delta(x,t) \) is the deflection with time, \( f(x,t) \) is the force per unit length and \( m(x) \) is the mass density, \( EI(x) \) is also known as the flexural rigidity of the solid. The above equation is a bi-harmonic equation in \( x \). Therefore the four boundary conditions are listed as:

\[ \delta(x,t) = 0, \quad \frac{\partial \delta(x,t)}{\partial x} = 0 \quad \text{at} \quad x = 0 \quad (3.2a) \]

\[ \delta(x,t) = 0, \quad \frac{\partial \delta(x,t)}{\partial x} = 0 \quad \text{at} \quad x = L \quad (3.2b) \]

The current model is run in ANSYS® where the static simulations are performed and then the deflection data along the fluid–solid interface are mapped into a path and recorded. This data is passed as a boundary condition for the fluid simulations as illustrated in Figure 3.2 and described in the later sections.

### 3.3 Fluid modeling

The pressure fluctuations inside the pump chamber caused by the diaphragms oscillatory volumetric fluid displacement create a pressure difference across the two ends which drives the fluid. We assume that (1) flow is two-dimensional; (2) fluid is isothermal and Newtonian; (3) flow is laminar, incompressible and unsteady. Fluid Modeling is done in FLUENT®, a commercial fluid software which uses a finite volume solver to convert the governing Navier-Stokes differential equations at each node cell into algebraic equations that can be solved through iteration. The solution algorithm is displayed in Figure 3.3. To gain more insight on the fluid modeling, the governing
equations are represented mathematically as follows:

\[ \nabla \cdot \vec{V} = 0 \quad (\text{Continuity}) \quad (3.3a) \]

\[ \rho \frac{D\vec{V}}{Dt} = \rho \vec{g} + \mu \nabla^2 \vec{V} - \nabla P \quad (\text{Momentum}) \quad (3.3b) \]

where \( \rho \) is the density of fluid, \( \vec{V} \) is the velocity vector, \( P \) is the pressure, \( \vec{g} \) is the acceleration due to gravitation and \( \mu \) is the dynamic viscosity of fluid. Boundary conditions are no slip at fluid-wall and fluid–diaphragm interface and pressure inlet at inlet and pressure outlet at outlet as illustrated in Figure 3.4. A moving wall boundary condition is imposed on diaphragm with its motion described in following
subsection. Since the pump is symmetric, a symmetry boundary condition is applied at the lower line.

3.3.1 Moving diaphragm boundary conditions

In this study the instantaneous harmonic profile of the diaphragm is a function of space and time. In what follows, there is a description of the mathematics used to give diaphragm displacement at an inclined and offsetted co-ordinate system.

Consider a rectangular co-ordinate system at \((x_0, y_0)\) as displayed in the Figure 3.5. A beam is inclined at an angle \(\theta\) from the horizontal at a new origin \((x_1, y_1)\) making a new rectangular co-ordinate system \((x', y')\). We are given a displacement...
\( \delta'(x', t) \) of the beam at the inclined co-ordinate system and seek displacement in terms of global co-ordinates \((x(t), y(t))\) with reference to the co-ordinate system at \((x_0 = 0, y_0 = 0)\). The global co-ordinates of the deflected beam are given by:

\[
\begin{align*}
    x(t) &= x_1 + x' \cos \theta - \delta'(x', t) \sin \theta \\
    y(t) &= y_1 + x' \sin \theta + \delta'(x', t) \cos \theta
\end{align*}
\]

For the deflections in the rotated co-ordinates \(\delta'(x', t)\), the first mode of the deflection is considered. The deflections are computed using a static analysis in ANSYS® and then fitted using a four parameter Gaussian curve represented as:

\[
\delta'(x', t) \approx \left[ Y + a \times \exp \left( -0.5 \left( \frac{x' - X}{b} \right)^2 \right) \right] \sin(2\pi ft)
\]

where \(X, Y, a, b\) are the parameters whose values are obtained for individual membranes. This deflection is then transformed back to the global co-ordinates and ap-
Figure 3.5: Co-ordinate systems in membrane deflection. \((x_0, y_0)\) is the global origin, while the displacement is described in shifted and rotated co-ordinate system \((x', y')\).

plied as a boundary condition to the fluid simulations using User Defined Function Macro `DEFINE_GRID_MOTION` in FLUENT® which will be discussed in later sections.

### 3.3.2 Flow rate measurement

Once the transients have died out after sufficient number of iterations, mass flow rate is calculated using the following formula:

\[
m_{\text{avg}} = \frac{1}{T} \int_{0}^{T} \dot{m}(t) \, dt
\]  

(3.6)

Where \(T\) is the time period and \(\dot{m}(t)\) is the instantaneous mass flow rate. The integration is done numerically using the trapezoidal rule.
3.3.3 FLUENT setup

The mesh is developed in GAMBIT, a standard state-of-the-art preprocessor for FLUENT and imported into FLUENT, which uses a Finite Volume Based method to solve the Non-linear Partial Differential equations into a system of algebraic equations which are solved numerically through iteration. Values are stored at the cell center and face values are interpolated from the cell center values for the convective term in Navier-Stokes equation. Diffusion terms are discretized using central difference method and are always second order accurate.

The two dimensional, double precision, segregated, unsteady, incompressible solver with dynamic mesh option is chosen which is first order implicit with respect to time which makes it unconditionally stable with time step size. The segregated solver is mainly used for incompressible flow where the resulting algebraic equations are solved sequentially as opposed to the coupled solver that solves the algebraic equations simultaneously due to the inter-dependence of scalars on flow field. This is represented pictorially in Figure 3.3. Since the model is laminar, no energy equation is solved.

FLUENT provides four pressure velocity coupling algorithms: SIMPLE, SIMPLEC and PISO and (for time-dependant flows using the Non-Iterative Time Advancement option (NITA)) Fractional Step (FSM). Pressure Implicit with Splitting of Operators (PISO) is based on the higher degree of the approximate relation between the corrections for pressure and velocity. PISO is recommended for transient calculations. PISO may also be useful for steady-state and transient calculations on highly skewed meshes. One of the limitations of the SIMPLE and SIMPLEC algorithms is that new velocities and corresponding fluxes do not satisfy the momentum balance after the pressure-correction equation is solved. As a result, the calculation must be repeated until the balance is satisfied. To improve the efficiency of this calculation, the PISO algorithm performs two additional corrections: neighbor correction and skew-
ness correction. Because of these corrections momentum and continuity equations are satisfied more closely. Although PISO requires more CPU time as compared to the other three, it greatly enhances the computational transient calculation accuracy as pointed out by Tang & Zhong (2005). This algorithm also significantly reduces convergence difficulties associated with highly distorted skewed mesh with approximately the same number of iterations that would be required for orthogonal mesh. Second order upwind discretization is chosen for momentum equation. Under-relaxation parameters are used to reduce changes during iterations. The default under-relaxation parameters were kept at 0.3, 1.0, and 0.7 for pressure, density and momentum respectively. These default values are set near optimal for the largest possible number of cases.

Remeshing and smoothing are activated and set for the dynamic mesh parameters. For remeshing the size remesh interval is set to 1 to check for remeshing after each time step, the maximum skewness was set through trial and error to 0.6 and the “must improve skewness” option is chosen. The minimum cell area values were chosen to be an order of magnitude smaller than the initial smallest cell to prevent both unnecessary remeshing of smaller cells. The minimum was large enough however to prevent a negative cell volume as the diaphragm moves. The maximum cell area was simply chosen to be any value larger than the largest initial mesh cell area. In the smoothing option a spring constant factor of 0.1, boundary node relaxation of 0.0001, convergence tolerance of 1E-4 and max iterations of 200 is set. Similar to the maximum cell skewness, the smoothing option and spring constant factor were chosen through trial and error.

The three macros available for defining a dynamic mesh with a moving boundary are DEFINE_CG_MOTION, DEFINE_GEOM, and DEFINE_GRID_MOTION. Neither of the first two allow for the motion of each node to be specified independently. The DEFINE_GRID_MOTION macro does allow for the position of each node to be updated independently so that it is possible to specify the relative motion amongst the nodes
that occurs with the deforming diaphragm motion. The user defined function (UDF) written in C with the Gaussian displacement profiles described by Equation 3.5 to specify the oscillatory diaphragms movement with code explanation is attached in Appendix A. The UDF is loaded as a compiled function and attached to the diaphragms. The solution is then initialized at all zones with initial guess of zero. 300 iterations per time step is kept and flow is simulated for 5000 time steps. A time step is chosen based on the actuation frequency \( f \) to allow for 200 time steps per cycle as shown below:

\[
\Delta t = \frac{1}{f \times 200} \tag{3.7}
\]

### 3.4 Artificial neural networks

Neural networks (NNs) are intelligent arithmetic computing elements that can represent complex functions with continuous-valued as well as discrete outputs, and large number of noisy inputs, by learning from examples (Fausett, 2005; Rojas, 1996). The network uses systems of non-linear basis functions to relate the input to the desired output. Because of the use of these non-linear functions and the statistical nature of the model, neural networking can be applied to solve a variety of problems that are not possible with analytical methods. Although the idea of neural networks has been around for some time, it has undergone a recent surge of usage in many fields from medical to material science. Neural Networks consist of arrays of processing elements called neurons or nodes. Each neuron is connected to other neurons by means of directed communication links, called synapses, each with an associated weight. Each synapse is given a weight factor that is determined after the network is trained. Weights are the primary means of long-term storage in neural networks, and learning usually takes place by updating these weights. The weights are adjusted so as to bring the network’s input/output behavior more in line with that of the phenomena being modeled by the network.
Often, it is convenient to visualize neurons as arranged in layers that process that data as its passes through the network as shown in Figure 3.6. Neurons in the same layer behave in the same manner. The arrangement of neurons into layers and connection patterns within and between layers is called the net architecture. They are often classified into single layer or multi layer. The input unit is not counted as a layer, since they perform no computation. The number of layers in the net can be defined to be number of layers of weighted interconnect links between the slabs of neurons. This view is motivated by the fact that the weights in the net contain extremely important information.

Artificial neural networks are used in many cases as a black box: a certain input should produce a desired output, but how the network achieves this result is left
to a self-organizing process. In general we are interested in mapping an \( n \)-dimensional real input \((x_1, x_2, ..., x_n)\) to an \( m \)-dimensional real output \((y_1, y_2, ..., y_m)\) as represented in the Figure 3.7.

3.4.1 Neural network architecture, training and testing

A multi-layer feed-forward ANN with back-propagation learning algorithm is developed to represent the mass flow rate as a function of three lengths \(D_1, D_2, D_3\) and frequency of actuation \(f\) of the micropump. The network is developed with the MATLAB® Neural Network Toolbox using the ‘newff’ function. The learning rate was set reasonably low at 0.05 to ensure convergence of the algorithm. There are many transfer functions available in MATLAB software. After some experimentation, the “logsig” transfer function was chosen for the hidden layers and the output neurons, due to nature of the desired outputs. A schematic of the network is shown in Figure 3.7. The network has 4 input nodes that define the lengths and frequency, and 1 output node for the average mass flow rate \(m_{avg}\) in a cycle. There are 2 hidden layers in the network, both with 12 nodes. This configuration was reached after a few iterations of a single hidden layer network proved to give less than adequate re-
results. Two layer deep nested loops were used in an exhaustive search that varied the number of neurons in the first and second hidden layer, and found the appropriate combination (12-12) that best trained the network. The MATLAB scripts for neural network training and validation with code explanation is attached in Appendix B. Therefore, 4-12-12-1 neural network architecture was developed and trained and tested to validate the model.

3.5 Genetic algorithms

The basic underlying principle of genetic algorithm is the Darwin’s evolutionary principle of genetics and natural selection (Darwin, 1859). A Genetic algorithm (GA) allows a population composed of many members to evolve in a manner and selection rules that maximizes the “fitness”, i.e. minimizes the cost function. The fittest members in each generation survive and are allowed to produce offsprings which form the next generation. This method was first introduced by Holland (1973) of the University of Michigan. GA’s have been since extensively used to solve problems where conventional methods are either inapplicable or inefficient. In context of GA’s, the members of the species may be regarded as candidate solutions to a problem under investigation. Also the concept of species in GA is superficial, having no tangible concept in nonbiological applications. The members are ranked on the basis of how well they satisfy a certain criterion, and the fittest members are most favored to combine amongst themselves to form the next generations of members, which then replace the preceding generation. The idea behind this process is that the fitter members tend to produce even fitter offsprings, which represent better solution to the problem at hand. Since this work is not intended to provide comprehensive discussion on GAs, the reader is advised to refer to works by Holland (1992) and Goldberg (1989). The objective to use GA in this study is to search within a domain of plausible pumping configurations and report the one needed and suited for specific application (by fixing
the flow rate for the application). Hence, it optimizes the geometry of the micropump to target the use for drug delivery applications.

Many practical problems involve the determination of optimal shape. In many cases variational methods can be used to determine the optimal shape, provided an appropriate variational principle exists. Most shape optimization problems of practical interest, however, are not amenable to the method of variational calculus, and a recourse to methods involving more sophisticated and discrete functional, such as one determined by Artificial Neural Network is necessary. Gradient based optimization methods require computations of both the objective functional and its derivatives with respect to each degree of freedom characterizing the shape. This is often not possible in practice and otherwise tends to be CPU intensive when the functional is expensive to compute. Deterioration in performance of gradient/Hessian-based algorithms is often evident as the number of degrees of freedom increases. Another limitation is that the gradient based methods invariably yield a local extremas instead of global extremum or optimum. For shape optimization, the major advantages of GAs are.

- They search from a population not from a single parameter set.
- They are capable of searching for solutions from disjointed feasible domains.
- They are capable of locating global optimum.
- They can operate on irregular and non-differentiable functions including Neural Networks.
- They do not require computations of derivatives and Hessian matrices, hence reducing computational complexity.
- They operate on an encoding of the parameter set not the parameter itself.
GA in the current problem is performed using the `gatool` (Genetic Algorithm Toolbox) in MATLAB. It is a state of the art toolbox which can perform Genetic computations very easily and accurately. The objective functional here is of the form $f = \text{abs}(\text{sim}(\text{net},x)-x_i)$ where $\text{sim}(\text{net},x)$ denotes the value of the flow rate computed from the neural network and $x_i$ is the targetted flow rate. The outputs and inputs are scaled from 0.1 to 0.9 with respect to maximum and minumum values. There are four variables as input and there maximum and minimum scaled values are 0.9 and 0.1 respectively. The population size was set to 20, with the crossover function as Gaussian and crossover fraction as 0.8. The mutation function was chosen to be Gaussian with maximum generations set as 100 and tolerance level as $10^{-6}$. The code is then run and it is terminated as soon as the fitness function is minimized to the value of zero, consequently the flow rate is the desired one and the output table lists the values of the four parameter. Note that since the process is completely random and there could be many solutions possible to the above objective functional, we report only one of the answers provided by GA. Everytime the optimization is done, there is likelihood that the results might be different. MATLAB help provides a comprehensive way to use the genetic algorithm optimization toolbox.
CHAPTER 4  Results and discussion

This chapter presents and discusses the numerical results from Structural (Finite Element), Computational Fluid Dynamics, training and testing of Artificial Neural Networks (ANN) and Genetic Algorithms (GA). Structural results are computed in ANSYS and then mapped into the FLUENT C code for membrane deformation. Five different geometries are simulated for generating the example learning cases for ANN. Their different lengths as demonstrated in Figure 3.1 are presented in Table 4.1. This trained Neural Network is then tested and used for population generation for GA optimization method. In what follows, we shall discuss these results in a step by step manner.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>$D_1$ (mm)</th>
<th>$D_2$ (mm)</th>
<th>$D_3$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geometry 1</td>
<td>3</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Geometry 2</td>
<td>2.85</td>
<td>4.8</td>
<td>6.6</td>
</tr>
<tr>
<td>Geometry 3</td>
<td>2.7</td>
<td>5.7</td>
<td>7.2</td>
</tr>
<tr>
<td>Geometry 4</td>
<td>3.75</td>
<td>7.2</td>
<td>4.8</td>
</tr>
<tr>
<td>Geometry 5</td>
<td>4.5</td>
<td>4.2</td>
<td>7.8</td>
</tr>
</tbody>
</table>

4.1  Structural simulation results

The deflections of the membrane $\delta'$ for 5 different geometries in the shifted and rotated co-ordinate system is recorded as a function of $x'$. As shown in Figure 4.1(a)
this displacement is plotted for the membrane 1 of the first geometry. This data is then fitted using Equation 3.5 which is also presented in the same figure. Maximum value of deflections of the diaphragms are listed in Table 4.2. Figure 4.1(b) shows the deflections of the four membranes in geometry 1 against normalized $x'$ which confirms that the nature of all deflections is highly Gaussian; where the normalized deflections are plotted against normalized length of the beam. Hence, use of Equation 3.5 in modeling all of these deflections is justified. The parameters for obtaining absolute displacements using the Gaussian model are listed in Table 4.3. Static solid displacement results are very similar as described in Meirovitch (2001) for the case of a clamped beam. The deflections resemble the first mode shape of the oscillations of a clamped-clamped excited under harmonic load. Hence the simulation model serves the analytical calculation of the deflections and hence the fitted model of deflection is quite justified to be used as boundary condition to the fluid domain. Fluid section results are discussed in detail in the next section, which is followed by the neural network training and validation results and genetic algorithm results.

<table>
<thead>
<tr>
<th></th>
<th>Membrane 1</th>
<th>Membrane 2</th>
<th>Membrane 3</th>
<th>Membrane 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geometry 1</td>
<td>0.4040</td>
<td>0.8221</td>
<td>0.2794</td>
<td>0.8046</td>
</tr>
<tr>
<td>Geometry 2</td>
<td>0.4822</td>
<td>0.4597</td>
<td>0.4890</td>
<td>1.1890</td>
</tr>
<tr>
<td>Geometry 3</td>
<td>0.5752</td>
<td>0.8221</td>
<td>0.3784</td>
<td>1.7931</td>
</tr>
<tr>
<td>Geometry 4</td>
<td>1.6814</td>
<td>1.0948</td>
<td>0.5790</td>
<td>0.4154</td>
</tr>
<tr>
<td>Geometry 5</td>
<td>0.0758</td>
<td>0.2830</td>
<td>1.2083</td>
<td>2.7300</td>
</tr>
</tbody>
</table>
Figure 4.1: Deflections of membrane 1 in geometry 1 in (a); (b) shows the actual deflections against normalized lengths in geometry 1.
Table 4.3: Parameters $a$, $b$, $X$, $Y$ (in mm) for four parameter gaussian fit. Subscripts represent geometry number.

<table>
<thead>
<tr>
<th>Membrane 1</th>
<th>Membrane 2</th>
<th>Membrane 3</th>
<th>Membrane 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_1$</td>
<td>0.5</td>
<td>1.025</td>
<td>0.35</td>
</tr>
<tr>
<td>$b_1$</td>
<td>1.1</td>
<td>1.5</td>
<td>1.3</td>
</tr>
<tr>
<td>$X_1$</td>
<td>2.1</td>
<td>2.9</td>
<td>2.5</td>
</tr>
<tr>
<td>$Y_1$</td>
<td>−0.1</td>
<td>−0.2</td>
<td>−0.075</td>
</tr>
<tr>
<td>$a_2$</td>
<td>0.6</td>
<td>0.575</td>
<td>0.525</td>
</tr>
<tr>
<td>$b_2$</td>
<td>1.1</td>
<td>1.4</td>
<td>1.4</td>
</tr>
<tr>
<td>$X_2$</td>
<td>2.1</td>
<td>2.7</td>
<td>2.7</td>
</tr>
<tr>
<td>$Y_2$</td>
<td>−0.1</td>
<td>−0.1</td>
<td>−0.1</td>
</tr>
<tr>
<td>$a_3$</td>
<td>0.7</td>
<td>1.3</td>
<td>0.475</td>
</tr>
<tr>
<td>$b_3$</td>
<td>1.1</td>
<td>1.5</td>
<td>1.4</td>
</tr>
<tr>
<td>$X_3$</td>
<td>2.2</td>
<td>2.9</td>
<td>2.6</td>
</tr>
<tr>
<td>$Y_3$</td>
<td>−0.125</td>
<td>−0.2</td>
<td>−0.075</td>
</tr>
<tr>
<td>$a_4$</td>
<td>0.2</td>
<td>1.35</td>
<td>0.725</td>
</tr>
<tr>
<td>$b_4$</td>
<td>1.0</td>
<td>1.6</td>
<td>1.4</td>
</tr>
<tr>
<td>$X_4$</td>
<td>1.8</td>
<td>3.0</td>
<td>2.8</td>
</tr>
<tr>
<td>$Y_4$</td>
<td>−0.05</td>
<td>−0.25</td>
<td>−0.125</td>
</tr>
<tr>
<td>$a_5$</td>
<td>0.1</td>
<td>0.35</td>
<td>1.5</td>
</tr>
<tr>
<td>$b_5$</td>
<td>0.9</td>
<td>1.3</td>
<td>1.6</td>
</tr>
<tr>
<td>$X_5$</td>
<td>1.6</td>
<td>2.5</td>
<td>3.1</td>
</tr>
<tr>
<td>$Y_5$</td>
<td>−0.0138</td>
<td>−0.06</td>
<td>−0.22</td>
</tr>
</tbody>
</table>
4.2 Fluid simulation results

The scope of the fluid modeling in this entire work is very high, since it is the core of the entire model. The solid diaphragm results provide a boundary condition for the fluid model, which is then formulated in form of a mathematical equation which is a function of space and time. In this section, fluid results for the first geometry are presented and discussed in detail. The results section of fluid is divided into two parts, validation and the current work.

4.2.1 Validation

Validation of the FLUENT solver is done by solving two problem. For the first problem, an analytic model of viscous flow in a 2 dimensional channel driven by deforming boundaries is developed. This model is then compared with the CFD results predicted by FLUENT. For the second problem, a three dimensional valveless micropump as described in Tsui & Lu (2008) is simulated and the time history is of flow rate is compared. In the following text, the two problems are described and results are presented.

Validation first problem

The first problem of validation is done by developing a mathematical model of a 2D flow driven by the top and bottom wall actuation. The fluid is assumed to be Newtonian, the flow is assumed to be unsteady laminar; and highly viscous. The geometry is presented in Figure 4.2 where the displacement at walls \( y = \pm H \) is given by

\[
\delta(x,t) = \pm A_{max} \sin\left(\frac{\pi x}{L}\right) \sin(\omega t)
\]

where \( \omega \) is the circular frequency, \( A_{max} \) is the applied displacement and \( L = 4\text{mm} \) is the length of the channel. The formulation of mathematical problem and its solution
is described in detail in C. The x-velocity turns out to be of the following form

\[ u(x, y, t) = \frac{\omega A_{max}}{2k} \Re \left[ \alpha \frac{(\cos(\alpha H) - \cos(\alpha y))}{\alpha H \cos(\alpha H) - \sin(\alpha H)} e^{i(kx - \omega t)} \right. \\
\left. + \frac{\alpha (\cosh(\alpha H) - \cosh(\alpha y))}{\alpha H \cosh(\alpha H) - \sinh(\alpha H)} e^{i(kx + \omega t)} \right] \]  

(4.2)

where \( \alpha = \sqrt{\frac{\omega}{\nu}} \), where \( \omega \) is the circular frequency, \( H = 150\mu m \) is the half channel width, \( k = \frac{\pi}{L} \) is the wave number; while \( \Re \) denotes the real part of the complex number. The actuating frequency \( f \) is 1 Hz. Velocity profiles are plotted at \( x/L = 0.25 \) and \( x/L = 0.75 \) for \( t/T = 0.5 \) and the results of analytical solution displayed in Figure 4.3 and Figure 4.4 closely matches with the CFD predictions.

**Validation second problem**

A three dimensional valveless micropump as described in Tsui & Lu (2008) is solved using FLUENT. The authors have used a fully conservative finite volume method using unstructured mesh which they have developed. Since FLUENT also uses finite volume solver, the validation procedure tests the accuracy of the solver by comparing the time history of the flow rate from one opening of the geometry. The following subsection discusses the problem description and setup. The geometry under investigation for the validation problem is displayed in Figure 4.5. The pump consists of a
Figure 4.3: Validation velocity profile comparison at $x/L = 0.25$ and $t/T = 0.5$

Figure 4.4: Validation velocity profile comparison at $x/L = 0.75$ and $t/T = 0.5$
diaphragm which oscillates with time in a trapezoidal profile as:

\[ h(r, t) = h_{\text{max}} \cdot \text{Max} \left( 1, \frac{r_0 - r}{r_0 - r_1} \right) \cdot \sin(2\pi ft) \]  

(4.3)

where \( h(r, t) \) is the deflection of the diaphragm as a function of radial distance from the center of the diaphragm and time, \( h_{\text{max}} \) is the maximum height that the diaphragm can deflect, \( r_0 \) is the radius of the diaphragm, \( r_1 \) is the radius of the piezoelectric disc sitting on top of the diaphragm and \( f = 2200 \text{ Hz} \) is the actuating frequency. The flow rectification is achieved by attaching a nozzle and diffuser to the pump chamber.

There is no pressure difference between the inlet and the outlet openings. The flow rate from the outlet is compared and is displayed in Figure 4.6. The FLUENT model underpredicts the maximum by 4.3\% and hence the validation is reasonable.

4.2.2 FLUENT results

The element size of the mesh is chosen to be 0.0002 in GAMBIT after mesh independence study. Figure 4.7(a) to Figure 4.10(d) display the contours of many primitive
Figure 4.6: Comparison graph of outlet flow. Control case is from Tsui & Lu (2008).
and derived variables in the pump at different times for operating frequency as 1 Hz. These times are chosen to be every quarter step of the pumping cycle. The choice is based on the reasoning that every quarter step of the complete cycle, there is a significant change in the wall motions of the four membranes since they are at a phase lag of 90 degrees. From the contours, it is clear that when the localized chamber pressure becomes less than the working pressure, which is the atmospheric pressure; the walls move inside the fluid chamber to compensate the pressure drop. In other words, the pressure is higher when the wall moves outside the fluid chamber, and is less, both relative to the atmospheric pressure, when the walls move inside the fluid chamber.

Figure 4.7(a) shows the iso-pressure contours at $t/T = 0.25$. It is this time when diaphragm 1 is in expansion mode, diaphragm 3 is in contraction mode; while diaphragms 2 and 4 are undeflected but have velocities in opposite direction. It is due to high pressure around diaphragm 1 and low pressure around diaphragm 3. From the contours of x-velocity displayed in Figure 4.7(b) and contours of speed in Figure 4.7(c), it is evident that the highest wall velocity magnitude is experienced around the fourth diaphragm and the x-velocity is maximum at the outlet. Vortices displayed in Figure 4.7(d) shows the presence of recirculation zones close to diaphragm 4.

At $t/T = 0.5$, diaphragm 1 and 3 come to neutral undeflected position with velocities in opposite direction; while diaphragm 2 and 4 reach their maximum deflection position with zero velocity. Although the local pressure decreases around diaphragm 3, which is in contraction stroke and relatively high pressure is built around diaphragm 2; however, the maximum pressure is still around diaphragm 1 in the entire pump chamber as represented by Figure 4.8(a). The openings are at relatively higher pressure than the atmospheric pressure, which results in fluid coming into the pump chamber. High wall velocity is confirmed at diaphragm 1 and 3 by Figure 4.8(c), and the vortices confirm the fluid coming inside the pump chamber with some recirculation zones close to diaphragm 1.
At $t/T = 0.75$, the entire pump is at 180 degrees phase difference from the $t/T = 0.25$ instant. Diaphragms 1 and 3 switch their positions from expansion mode to expulsion mode and vice-versa. Figure 4.9(a) displays the total pressure contours at this time instant, there is a high pressure zone at diaphragm 3 and low pressure zone at diaphragm 1. Highest velocity magnitude is at the fourth diaphragm as displayed in Figure 4.9(c). Although the flow is very streamlined at the openings represented by x-velocity in Figure 4.9(b), presence of complicated flow patterns in the pump chamber are confirmed by vortices near diaphragm 4 in Figure 4.9(d).

The last set of pictures are for the instant $t/T = 1.0$, when the frequency cycle is completed. Diaphragm 1 and 3 are in neutral position while the diaphragm 4 and diaphragm 2 are deflected. Highest pressure occurs in the vicinity of diaphragm 4 displayed in Figure 4.10(a) while the highest velocity magnitude is present near the first diaphragm as displayed in Figure 4.10(c). Flow vortices are strongly observed near diaphragm 1 which are plotted in Figure 4.10(d).

The consecutive high and low pressure indicate that the flow patterns should be very complicated, which in turn are confirmed by the iso-velocity contours and streamlines. The iso-pressure contours also display that the flow is pulsatile, therefore the flow rates oscillate from the inlet and the outlet openings, but there is a net flow when they are integrated over the complete cycle. The flow rate time history for frequency 1 Hz. is displayed in Figure 4.11. The inlet and the outlet mass flow rates exhibit the periodic nature of the flow with the time period same as that of actuating diaphragms. More contour plots at different time steps are presented in D.

Furthermore, four positions in the geometry represented in Figure 4.12 are picked and the x-velocity, being one of the primitive variables in the Navier-Stokes equations, is plotted against the height from the symmetry line. It is seen from the graphs that the x-velocity in many of the cases, either represent a change in sign or they have a stationary point, consequently indicating the existence of complicated recirculation zones in the interior of the pump chamber. Especially at membrane 3
Figure 4.7: Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude; (d) vorticity at $t/T = 0.25$
Figure 4.8: Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude; (d) vorticity at $t/T = 0.5$
Figure 4.9: Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude; (d) vorticity at $t/T = 0.75$
Figure 4.10: Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude; (d) vorticity at $t/T = 1.0$
mid rake, the presence of recirculation zones at each quarter part of the cycle is clearly evident. Figure 4.14 shows the parametric result of average mass flow rate per second from the micropump with actuating frequency. The peak in this curve indicates that the flow rate increases till the optimum frequency, then it decreases with the increase in the actuating frequency.

The other four geometries show the same nature of the flow, the primitive variables such as pressure show the same phenomenon of decrease and increase in their values as compared to the atmospheric pressure due to the wall motion. The velocity shows the same complex nature, and the recirculation zones are present in different parts of the pump chamber. These results are not presented in this work for avoiding repetition of information and maintaining brevity. The inlet and outlet flow rates represent the periodic nature in all other four geometries and the presence of peak in every parametric curve of flow rate versus actuating frequency is confirmed. Hence, the conclusion that minor perturbations do not disturb the physics of the flow can be drawn. Only the time averaged flow rates over a cycle are affected due to the change in geometry. This is utilized in designing the micropump which can deliver, in exact amount, the fluid required to move from one point to another.

In the following portion of this chapter, results and discussion on Artificial Neural Network training, validation and usage is presented. Later, Genetic Algorithm is used to solve the optimization problem of finding the appropriate lengths and frequency of the operation and then these results are compared with a direct numerical simulation to test the integrity of the procedure.

4.3 Artificial neural network results

In this section, training and validation of the neural network used for the learning of relationship between the flow rate and the four parameter viz. three lengths and the actuating frequency are discussed. The data is sorted in terms of maximum to
Figure 4.11: Time history of mass flow rate at 1 Hz.

Figure 4.12: Locations of rakes in the geometry.
Figure 4.13: x-velocity at (a) $x = 6.475$ mm; (b) $x = 10.45$ mm; (c) $x = 15.45$ mm; (d) $x = 20.425$ mm
Figure 4.14: Parametric curve of average flow rate versus actuating frequency.
minimum and then scaled from 0.1 to 0.9. It is introduced to the network again and again so that the trained network is accurate and robust. The error for training of the “newff” function in MATLAB is set to be 5e-6. Figure 4.15 displays that after 640 iterations, convergence is met. Now the network is ready for validation. For validation purpose, 13 cases are considered which were not introduced while training of the network and the values of the flow rate are predicted using the network by providing it the input parameters. Then these simulated values are compared against the FLUENT simulated values. These results are displayed in Figure 4.16. The predicted values match the actual values with a root mean square error of 0.0083. In other words, the results are 99.17% accurate or the $R^2$ value of the regression is 0.9835. Since this value is very good, we choose the 4-12-12-1 configuration neural network as a reasonably accurate model for the prediction of flow rate.

4.4 Genetic algorithm results

In this section, results of optimization search procedure for finding out a particular value of flow rate are presented and discussed. Three values of flow rates are selected and a global search for the values of input parameters is performed using GA. A typical convergence plot of Genetic algorithm is presented in Figure 4.17. The results are presented in Table 4.4. The geometry of the three optimized designs are presented in E.

From the table, it is evident that the GA prediction matches closely with the FLUENT simulated results. The error in prediction of flow rate is less than 5%. Hence, we have demonstrated that Genetic Algorithms can be successfully used for the topology optimization. However, GA being completely random picks up only one solution out of all possibilities that satisfy the criterion. So, the results are supposed to be different in every run of GA. This can be avoided by choosing the same state
A study of minimizing the energy input to the pump could also be considered. This will become a multiobjective optimization problem with the same constraints in the current problem. This solution should be unique since there will be only one design which pumps the desired flow rate and then has the minimum energy input.
Figure 4.16: Validation plot of ANN.

Table 4.4: Comparison of flow rates from numerical simulations with genetic algorithm. Lengths are in mm, frequency in Hz and flow rate in kg/sec.

<table>
<thead>
<tr>
<th>$d_1$</th>
<th>$d_2$</th>
<th>$d_3$</th>
<th>$f$</th>
<th>$GA$</th>
<th>$NS$</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.3</td>
<td>3.3</td>
<td>5.7</td>
<td>78</td>
<td>0.5691</td>
<td>0.5646</td>
<td>Microelectronics cooling</td>
</tr>
<tr>
<td>3.6</td>
<td>4.3</td>
<td>6.55</td>
<td>12.5</td>
<td>0.0528</td>
<td>0.0532</td>
<td>Drug delivery</td>
</tr>
<tr>
<td>4.1</td>
<td>6.6</td>
<td>5.9</td>
<td>44</td>
<td>0.0481</td>
<td>0.0487</td>
<td>Drug delivery</td>
</tr>
</tbody>
</table>
Figure 4.17: Convergence plot of Genetic algorithm.
CHAPTER 5 Conclusions and recommendations

5.1 Summary

In this study two-dimensional numerical simulations of a pneumatically actuated peristaltic micropump have been performed. The numerical modeling was utilized using a moving wall boundary condition with deflection profiles taken from the solid displacement. This displacement profile was applied to four different diaphragms when operated in a specific phase difference; mimic the peristaltic motion of the oesophagus in the human body. The idea was to design a pump targeted to produce specific flow rates by only changing geometrical parameters, such as certain lengths and only frequency of actuation. The code was validated against a control case from earlier design of a valveless micropump by comparing the time history of the flow rate coming out from the openings.

The actuator modeled here was pneumatically actuated under the action of pressure. The modeling equation used was the Euler-Bernoulli beam equation for the solid and incompressible, laminar, isothermal options for the fluid model. Water was used as a working fluid. The boundary conditions needed for the displacement were obtained from finite element structural dynamics solver and then provided to the fluid solver with a sinusoidal wave input.

Many cases with perturbations in length (up to 30%) were solved using the CFD solver and then the input and output results were used for the training and validation of an Artificial Neural Network modeled in MATLAB using the “newff” transfer function. The idea was to find a complex model which can capture the relationship between the input and output parameters as accurately as possible; which will assist in modeling the cost function for computational genetically assisted op-
timization procedure. ANN prediction was very good with a $R^2$ value greater than 98%.

The search for finding the appropriate input parameters which would result in a particular (fixed) value of flow-rate was accomplished with the help of an evolutionary algorithm, namely Genetic Algorithm (GA). The cost function was designed to be in a manner that the difference between the targeted flow rate and population computed flow rate was close to zero. Genetic Algorithms gave results with above 95% accuracy. The result of this study shows that genetic algorithms can be used for topology optimization purposes and that a design and optimization of a peristaltic pump with no alteration in input pressure was performed.

5.2 Recommendations

The results from genetic algorithms, although closely accurate with the direct numerical simulation, are not unique. A study on the power requirements of the micropump and minimizing that power requirement could lead to a uniqueness in the input parameters. Secondly, a fully coupled fluid–structure interaction model, although computationally intensive, will help understand the physics of the problem more clearly and accurately. Last but not the least, an optimization study utilizing the phase difference of oscillation between the successive diaphragms could lead to very interesting results, perhaps even more efficient in terms of power consumption.
Bibliography
Bibliography


FAUSSETT, L. 2005 *Fundamentals of Neural Networks*. Pearson Education.


Laser, D.J., Myers, A.M., Yao, S., Bell, K.F., Goodson, K.E., Santiago, J.G. & Kenny, T.W. 2003 Silicon electroosmotic micropumps for integrated cir-


APPENDIX A

A.1 User Defined Function for wall motion

#include "udf.h"
#define freq 1.0
#define x1 5.0e-3
#define x2 7.95e-3
#define y1 6.0e-3
#define y2 2.85e-3

/**************************************************************************/
/* Membrane 1 motion */
/**************************************************************************/

DEFINE_GRID_MOTION(mem1, domain, dt, time, dtime)
{
    Thread *tf = DT_THREAD (dt);
    face_t f;
    Node *node_p;
    double alpha, x, y, xprime, yprime;
    int n;
    double l1, ang1, tangent1;
/* Set/activate the deforming flag on adjacent cell zone, which */
/* means that the cells adjacent to the deforming wall will also be */
/* deformed, in order to avoid skewness. */
SET_DEFORMING_THREAD_FLAG (THREAD_TO (tf));

/* Compute angular frequency: */
alpha = 2 * freq * M_PI * CURRENT_TIME;

/* Compute inclination */
l1 = sqrt(pow((x2-x1),2.0) + pow((y2-y1),2.0));
tangent1 = (y2-y1)/(x2-x1);
ang1 = atan(tangent1);

/* Loop over the deforming boundary zone’s faces; */
/* inner loop loops over all nodes of a given face; */
/* Thus, since one node can belong to several faces, one must guard */
/* against operating on a given node more than once: */
begin_f_loop (f, tf)
{
    f_node_loop (f, tf, n)
    {
        node_p = F_NODE (f, tf, n);

        /* Update the current node only if it has not been */
        /* previously visited: */
        if (NODE_POS_NEED_UPDATE (node_p))
        {
            /* */
/* Set flag to indicate that the current node's */
/* position has been updated, so that it will not be */
/* updated during a future pass through the loop: */
NODE_POS_UPDATED (node_p);

x      = NODE_X (node_p);
y      = NODE_Y (node_p);
x = x - x1;
y = y - y1;
xprime = (x * cos(ang1)) + (y * sin(ang1));
yprime = 0.0;
if (xprime>0.0 && xprime<l1)
{
yprime = -0.0004 + 0.0024*exp(-0.5*pow(((xprime-0.0021)/0.0011),2.0));
if (yprime<0.0)
{
yprime=0.0;
}
}
else
{
yprime=0.0;
}
yprime = yprime*sin(alpha)/4.0;
x = (xprime * cos(ang1)) - (yprime * sin(ang1));
x = x + x1;
y = (xprime * sin(ang1)) + (yprime * cos(ang1));
y = y + y1;
NODE_X (node_p) = x;
NODE_Y (node_p) = y;
}
}
end_f_loop (f, tf);
}

APPENDIX B

B.1 Matlab script to repeat data for training of neural network

clear; clc;
a = dlmread('4walleddata.dat');
a = a';
b = a;
for i=1:1:1090
    k = 1+(109-1)*rand();
    t = int32(k);
    b = [b a(:,t)];
end
b = b';
dlmwrite('repeat.dat', b, 'delimiter', '\t');
B.2 Matlab script to scale data for training of neural network

function [trainInputs trainTargets] = ANN_data()

global slope_d1 slope_d2 slope_d3 slope_frq slope_flow;
global inter_d1 inter_d2 inter_d3 inter_frq inter_flow;

% read data
mydata = dlmread('repeat.dat');

d1 = mydata(:,1);
d2 = mydata(:,2);
d3 = mydata(:,3);
frq = mydata(:,4);
flow = mydata(:,5);

% Find Max and Min of each column

d1_max = max(d1);
d2_max = max(d2);
d3_max = max(d3);
frq_max = max(frq);
flow_max = max(flow);

d1_min = min(d1);
d2_min = min(d2);
d3_min = min(d3);
frq_min = min(frq);
flow_min = min(flow);

%Get slopes and intercepts

slope_d1 = 0.8/(d1_max-d1_min);
slope_d2 = 0.8/(d2_max-d2_min);
slope_d3 = 0.8/(d3_max-d3_min);
slope_frq = 0.8/(frq_max-frq_min);
slope_flow = 0.8/(flow_max-flow_min);

inter_d1 = (0.1*d1_max-0.9*d1_min)/(d1_max-d1_min);
inter_d2 = (0.1*d2_max-0.9*d2_min)/(d2_max-d2_min);
inter_d3 = (0.1*d3_max-0.9*d3_min)/(d3_max-d3_min);
inter_frq = (0.1*frq_max-0.9*frq_min)/(frq_max-frq_min);
inter_flow = (0.1*flow_max-0.9*flow_min)/(flow_max-flow_min);

%d1_norm = slope_d1*d1 + inter_d1;
d2_norm = slope_d2*d2 + inter_d2;
d3_norm = slope_d3*d3 + inter_d3;
frq_norm = slope_frq*frq + inter_frq;
flow_norm = slope_flow*flow + inter_flow;

% Categorize data

trainInputs = [d1_norm d2_norm d3_norm frq_norm]';
trainTargets = flow_norm';
B.3 Training of neural network

clear; clc;
global slope_d1 slope_d2 slope_d3 slope_fq slope_flow;
global inter_d1 inter_d2 inter_d3 inter_fq inter_flow;
fid = fopen('rms.dat','wt');
erms_best = 0.09;

% Number of layers for loop

for NL1 = 10:1:30
    for NL2 = 10:1:30

% Train Backpropagation network
[trainInputs trainTargets] = ANN_data();
[rowtar columntar] = size(trainTargets);
net = newff(minmax(trainInputs),[NL1 NL2 rowtar],{'logsig' 'logsig' 'logsig'});
net.trainParam.epochs = 1200;
net.trainParam.goal = 5e-6;
net.trainParam.show = 1200;
[net,tr] = train(net,trainInputs, trainTargets);
trainOutputs = sim(net, trainInputs);

% ----------------------Testing the network--------------------------------

% read data

mydata = dlmread('validation.dat');
d1 = mydata(:,1);
d2 = mydata(:,2);
d3 = mydata(:,3);
frq = mydata(:,4);
flow = mydata(:,5);

% Form the normalised data set

d1_norm = slope_d1*d1 + inter_d1;
d2_norm = slope_d2*d2 + inter_d2;
d3_norm = slope_d3*d3 + inter_d3;
frq_norm = slope_frq*frq + inter_frq;
flow_norm = slope_flow*flow + inter_flow;
validata = [d1_norm d2_norm d3_norm frq_norm]’;

% Simulate the data using the formed network

flowsim = [];
for j = 1:1:length(mydata)
    val = sim(net, validata(:,j));
    flowsim = [flowsim; val];
end
% figure
% plot(flowsim, flow_norm);
erms = sqrt(mean((flowsim-flow_norm).^2));

if (erms<erms_best)
    erms_best = erms;
fprintf(fid, '%f\t %f\t %f\n', NL1, NL2, erms);
save flow_net.mat net;
end

fclose(fid);
APPENDIX C

C.1 Objective

Objective of this work is to develop an analytic model of stokes flow between two oscillating plates. The fluid is assumed to be Newtonian, the flow is assumed to be isothermal, low Reynolds number flow, and unsteady in nature. The geometry is presented in Figure 4.2 where the displacement at walls \( y = \pm H \) is given by

\[
\delta(x, t) = \pm A_{\text{max}} \sin\left(\frac{\pi x}{L}\right) \sin(\omega t) \tag{C.1}
\]

C.2 Flow equations

The flow is described by set of fluid continuity and momentum conservation equations. Since the flow is highly viscous and laminar, we drop the convective terms from the Navier–Stokes equations and write the equations for incompressible Newtonian, unsteady, laminar, highly viscous and isothermal flow. The equations are given by

\[
\begin{align*}
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} &= 0 \tag{C.2a} \\
\rho \frac{\partial u}{\partial t} &= -\frac{\partial p}{\partial x} + \mu \left[ \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right] \tag{C.2b} \\
\rho \frac{\partial v}{\partial t} &= -\frac{\partial p}{\partial y} + \mu \left[ \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right] \tag{C.2c}
\end{align*}
\]

By performing an order of magnitude analysis as explained in Kundu and Cohen (2008) and neglecting terms in y-momentum equation since the Womersley number is large (>> 10) is this case, we deduce that

\[
- \frac{\partial p}{\partial y} = 0 \tag{C.3}
\]
and
\[ \frac{\partial^2 u}{\partial x^2} \ll \frac{\partial^2 u}{\partial y^2} \]  
(C.4)

so x-momentum equation reduces to
\[ \rho \frac{\partial u}{\partial t} = - \frac{\partial p}{\partial x} + \mu \frac{\partial^2 u}{\partial y^2} \]  
(C.5)

At this point, it is just to choose the following form of the pressure

\[ p(x, t) = p_o + \Re \left[ \hat{p}_1 e^{j(kx - \omega t)} - \hat{p}_2 e^{j(kx + \omega t)} \right] \]  
(C.6)

The kernel of exponential \( e^{j(kx \pm \omega t)} \) represents a pressure wave travelling in \( \pm x \) direction respectively. Subtracting them, we get a standing wave in pressure where the end values are \( p_o \). Similarly, \( u \) and \( v \), being \( x \) and \( y \) velocities; have the form

\[ u(x, y, t) = \Re \left[ \hat{u}_1(y) e^{j(kx - \omega t)} - \hat{u}_2(y) e^{j(kx + \omega t)} \right] \]  
(C.7)

\[ v(x, y, t) = \Re \left[ \hat{v}_1(y) e^{j(kx - \omega t)} - \hat{v}_2(y) e^{j(kx + \omega t)} \right] \]  
(C.8)

where \( \Re \) denotes the real part of the complex form of primitive variables. Since the problem is linear, we can decompose the solution into two parts

\[ u(x, y, t) = u_1(x, y, t) + u_2(x, y, t) \]  
(C.9)

where

\[ u_1(x, y, t) = \Re \left[ \hat{u}_1(y) e^{j(kx - \omega t)} \right] \]  
(C.10)

\[ u_2(x, y, t) = \Re \left[ -\hat{u}_2(y) e^{j(kx + \omega t)} \right] \]  
(C.11)

and similarly for \( p \) and \( v \).

C.3 Solution

Substituting the values of \( u_1 \) and \( p_1 \) in equation C.5 we have

\[ -j\omega p\hat{u}_1(y) = -jk\hat{p}_1 + \mu \frac{d^2 \hat{u}_1(y)}{dy^2} \]  
(C.12)
rearranging variables and comparing it to the standard form of type

\[
\frac{d^2 \hat{u}_1(y)}{dy^2} + \alpha^2 \hat{u}_1(y) = Q
\]  
(C.13a)

\[
\alpha^2 = \frac{j \omega \rho}{\mu}
\]  
(C.13b)

\[
Q = \frac{j k \hat{p}_1}{\mu}
\]  
(C.13c)

Since these equations have a forcing term \( Q \) on the right, the solution is the sum of homogeneous and particular solutions. Homogeneous solution is given by

\[
\hat{u}_{1h}(y) = A \cos(\alpha y) + B \sin(\alpha y)
\]  
(C.14)

Since the forcing function is a constant, we assume that the particular solution \( \hat{u}_{1p}(y) \) will be a constant and hence the total solution is given by

\[
\hat{u}_1(y) = \hat{u}_{1h}(y) + \hat{u}_{1p}(y)
\]  
(C.15)

Substituting the total solution back into the ODE given by equation C.13a we get

\[
\hat{u}_{1p}(y) = \frac{k \hat{p}_1}{\omega \rho}
\]  
(C.16)

hence the solution is

\[
\hat{u}_1(y) = A \cos(\alpha y) + B \sin(\alpha y) + \frac{k \hat{p}_1}{\omega \rho}
\]  
(C.17)

Boundary conditions are

\[
\hat{u}_1(y)|_{y=\pm H} = 0
\]  
(C.18)

Solving for \( A \) and \( B \), we get

\[
A = -\frac{k \hat{p}_1}{\omega \rho \cos(\alpha H)}
\]  
(C.19a)

\[
B = 0
\]  
(C.19b)

hence final solution is

\[
\hat{u}_1(y) = \frac{k \hat{p}_1}{\omega \rho} \left[ 1 - \frac{\cos(\alpha y)}{\cos(\alpha H)} \right]
\]  
(C.20)
Substitute this value into continuity equation to obtain
\[
\frac{d\hat{v}_1(y)}{dy} = -j k \hat{u}_1(y)
\] (C.21)

integrate and get
\[
\hat{v}_1(y) = \frac{j k^2 \hat{p}_1}{\omega \rho} \left[ \frac{\sin(\alpha y)}{\cos(\alpha H)} - y \right] + C_1
\] (C.22)

where \( C_1 \) is the integration constant. We have two variables to solve for, namely \( \hat{p}_1 \) and \( C_1 \) and two boundary conditions for \( \hat{v}_1 \).

\[
\hat{v}_1\big|_{y=H} = \frac{j \omega A_{max}}{2}
\] (C.23a)

\[
\hat{v}_2\big|_{y=-H} = \frac{j \omega A_{max}}{2}
\] (C.23b)

Solving them we get

\[
C_1 = 0
\] (C.24a)

\[
\hat{p}_1 = \frac{A_{max} \rho \omega^2}{2k^2 \left( H - \frac{\tan(\alpha H)}{\alpha} \right)}
\] (C.24b)

and \( k = \frac{\pi}{L} \) by comparing the kernel of exponential in boundary conditions. Substituting \( \hat{p}_1 \) to solve for \( \hat{u}_1(y) \); we get

\[
\hat{u}_1(y) = \frac{\alpha A_{max} \omega}{2k} \frac{(\cos(\alpha H) - \cos(\alpha y))}{(\alpha H \cos(\alpha H) - \sin(\alpha H))}
\] (C.25)

where \( \alpha = \sqrt{\frac{j \omega}{\nu}} \); \( \nu \) is the kinematic viscosity. Similarly we can solve for \( \hat{v}_1(y) \).

Proceeding in the same way for \( \hat{u}_2(y) \) and solving the second part of the linear problem, we get

\[
\hat{u}_2(y) = -\frac{\alpha A_{max} \omega}{2k} \frac{(\cosh(\alpha H) - \cosh(\alpha y))}{(\alpha H \cosh(\alpha H) - \sinh(\alpha H))}
\] (C.26)

Therefore the total solution is given by

\[
u(x, y, t) = \frac{\omega A_{max}}{2k} \Re \left[ \frac{\alpha \left( \cos(\alpha H) - \cos(\alpha y) \right)}{\alpha H \cos(\alpha H) - \sin(\alpha H)} e^{i(kx - \omega t)} + \frac{\alpha \left( \cosh(\alpha H) - \cosh(\alpha y) \right)}{\alpha H \cosh(\alpha H) - \sinh(\alpha H)} e^{i(kx + \omega t)} \right]
\] (C.27)
APPENDIX D

Figure D.1: Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude; (d) vorticity at $t/T = 0.125$
Figure D.2: Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude; (d) vorticity at $t/T = 0.375$
Figure D.3: Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude; (d) vorticity at $t/T = 0.625$
Figure D.4: Contours of (a) total pressure; (b) x-velocity; (c) velocity magnitude; (d) vorticity at $t/T = 0.875$
APPENDIX E

Figure E.1: Optimized geometry 1.

All dimensions in mm
Figure E.2: Optimized geometry 2.
Figure E.3: Optimized geometry 3.
Vita

Ravi Bhadauria is a Graduate student in the Virginia Commonwealth University, Department of Mechanical Engineering after completing his Bachelor of Technology in Mechanical Engineering from Indian Institute of Technology Kanpur in 2007. He is an inducted member of Phi Kappa Phi Honor Society since 2008 and also holds the Graduate School Phi Kappa Phi 2009 Scholarship.

In addition to these, he has presented his work in many conferences including International Conference on MEMS, Indian Institute of Technology Madras, 2008, Virginia Academy of Science 87th annual meeting, Richmond, Virginia and 10th US Congress on Computational Mechanics, Columbus, OH. He has also worked as a Teaching Assistant for Advanced Engineering Mathematics, Fluid Mechanics and Computational Fluid Dynamics.