

EXPERIMENTAL AND NUMERICAL STUDIES ON GAS FLOW THROUGH MICROCHANNELS WITH BENDS

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OCTOBER 2022**

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by

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Submitted

In fulfilment of the requirements of the degree of Doctor of Philosophy
to the



INDIAN INSTITUTE OF TECHNOLOGY DELHI

OCTOBER 2022

DEDICATED TO
MY PARENTS, MY BELOVED WIFE AND
MY DAUGHTER SHIVAKSHI

CERTIFICATE

This is to certify that the thesis entitled, “**Experimental and Numerical Studies on Gas Flow through Microchannels with Bends**”, being submitted by **Mr. Hariom Saran Singh** to the Indian Institute of Technology Delhi, India, for award of degree of **Doctor of Philosophy** is a record of bonafide research work carried out by him. He has worked under my guidance and supervision and has fulfilled the requirements for the submission of this thesis, which to my knowledge has reached the requisite standard.

The results contained in the thesis have not been submitted, in part or full, to any other university or institute for the award of any degree or diploma.

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ACKNOWLEDGEMENT

In Indian spiritual-cultural beliefs the very attempt to thank may not be a good idea especially those who have a major imprint on you in shaping your life. That is done by more intense yet subtle means by carrying out what is expected of you in more meaningful contributions. Those are the ones elated on your achievements and that's what expects you work generously for the welfare of the entire creation. By acknowledging those I mean it be ingrained in my thoughts and actions forever.

I shall be wanting to remain indebted forever to my guide in this endeavor, Prof. P.M.V. Subbarao, for believing in me, for encouragement, support, and tenacity to guide me to this point of final culmination of this research work.

I would like to sincerely thank my co-supervisor Dr. Saakshi Dhanekar for helping me in microfabrication of microchannel device. I wholly respect her sincerity and dedication towards the work. Her life style is truly followable.

May I express my deep gratitude to all those who advised me overcome hurdles, helped me through difficulties and encouraged me in slowdowns.

To Prof. M.R. Ravi, Prof. Amit Gupta, Dept. of Mechanical Engineering, and Prof. Murali R. Cholemari, Centre for Applied Mechanics, all Members of SRC.

I would like to greatly appreciate Dr. Samaresh Das (CARE), for his tremendous support in fabricating microchannel systems. I am very much thankful for giving me full freedom to work in Microelectronics laboratory. His cheerful smile and positive approach were always rememberable.

I would also like to acknowledge the Center for Applied Research in Electronics (CARE), Nano Research Facility (NRF) IIT Delhi and Center for Nano Science and Engineering (CeNSE) IISC Bangalore for letting us use their fabrication facilities.

Fellow researchers, Dr. Chinmay Mishra, Dept. of Mechanical Engg.; and Dr. Vandit Vijay, Center for Rural Development and Technology.

Mr. Devershi Mourya, Mr. Thochi Seb Rengma, Mr. Shubham Kumar, Mr Abhinav Chatterjee, Mr Jaswant Hiewani and Dr. L.D Kala, Dept. of Mech. Engg for their support.

Mr. Amresh Kumar who shared tenacious moments while experimenting, Mr. Jitendra Prasad, Mr. Rajender Singh, all of Dept. of Mechanical Engineering.

The Department of Mechanical Engg, Indian institute of Technology Delhi. I apologies for any order that has crept in my going down the memory lane and it does not make any instance less important than the other.

My colleagues, friends and my family who are always there behind me even without naming them, and to the Divine Nature.

ABSTRACT

Gas flow through microchannel has fundamental application in micro electromechanical systems (MEMS). Advancement in microfabrication technology has enabled the fabrication of simple and complex microdevices which include straight as well as complex interlinked microchannels. Present investigation involves experimental and numerical study of gas flow through straight microchannel and most often used complex microchannel i.e with 90° bend(s).

In the straight microchannel, validity of the continuum approach from slip to early transition regime was studied with general second-order boundary conditions. The flow characteristic through a microchannel having aspect ratio of 0.002 was studied along with the computational validation. Unlike conventional microchannels, analysis of rarefied flow in a microchannel requires the combination of experimental and numerical methods. The three-dimensional numerical simulation for the trapezoidal cross-sectional straight channel was carried out using Ansys fluent 18.1. The exact second order slip model was derived and implemented on the top and bottom walls of the channel. Also, first order and no-slip boundary conditions were implemented, and inlet pressure was calculated for comparison of simulation results. Further to model the rarefied gas flow, slip coefficients are required which were predicted using neural network analysis. Input and target data sets are required to train a neural network. The input data set contains different combinations of slip coefficients C_1 and C_2 . The target data set consists of deviations in the known experimental value of microchannel inlet pressure and the values of inlet pressure obtained using simulations assuming different combinations of C_1 and C_2 . To obtain the simulation inlet pressure, second order slip velocity profile based on slip coefficients was generated and implemented in fluent with mass flow rate as inlet and pressure as outlet boundary conditions.

This trained network was used to predict the best slip coefficient corresponding to minimum deviation in pressure. It was found that for Knudsen numbers ranging from 0.0667 to 0.405, the slip coefficient C_1 was varying between 1.13 to 1.15, which is approximately constant. The value of C_2 for Knudsen number 0.0667 was 0.24, and then it became approximately constant as 0.09. The slip coefficients obtained for Knudsen number 0.405 were further validated with their values using iterative method proposed by Srinivasan et al. (2017). It was found that the results based on ANN predicted slip coefficients are closer to the experimental values. Now, based on ANN, predicted slip coefficient modelling was performed and it was found that for maximum Knudsen number 0.405, the average deviation in inlet pressure is 0.84%

In the second part of present work, a microdevice consisting of multiple microchannels with two 90° bends was fabricated and flow behavior through it was studied experimentally and computationally. Mass flow rate through a single microchannel has same order of magnitude as range of commercially available mass flow meter. So, to reduce uncertainty in mass flow rate and to cover wide range of Knudsen number, a set of 20 channels with double 90° bends having common inlet and outlet plenums was fabricated.

In the present case, two 90° bends are required because it is difficult to fabricate an equal length multi microchannel device with single 90° bend. Bends were located in at suitable locations in each microchannel. The suitable locations are selected based on two conditions, namely equal length of all channels and bends are located far from inlet and outlet plenums. To check the effect of bend location, no slip condition simulation was performed for three different microchannels. Two channels on either extreme and one channel in middle were selected since those contained maximum variation in location of bends. The mass flow rate was calculated using pressure as inlet and outlet boundary conditions and it was found that mass flow rate in each channel was same for those three microchannels. Based on this result, each channel was allowing same mass flow rate for given inlet outlet pressures and hence, only

middle channel was selected for further numerical analysis. The microchannel was etched using KOH etchant and anodic bonding was performed from channel side. The channel had an aspect ratio of 0.0026. The mass flow rate through the microchannel was obtained for varying pressure ratios of 1.30 to 1.55, covering the slip regime from Knudsen number from 0.0662 to 0.0805. To check the slip effect in the measured flow, experimental mass flow rate was compared with no-slip boundary condition mass flow rate. One interesting point seen in the present analysis is that with the increase in Knudsen number, the deviation in slip and no-slip condition mass flow rate reduces continuously. For Knudsen 0.0662, the average deviation was 29.13%, and for Knudsen number 0.0805, it was 17.66%.

Further to analyze the rarefied flow behaviour, numerical simulation was performed based on the implementation of first order slip boundary conditions on the channel walls. The present microchannel is a complex microchannel, and there exist no analytical solution for flow. Three-dimensional simulation was performed for flow through microchannel with 90° bends, and inlet pressure of the microchannel was predicted. For the initial slip regime Knudsen numbers 0.0662 and 0.0682, the model overpredicts the inlet pressure and the average deviations in inlet pressure of microchannel were 1.32% and 0.73%, respectively. For Knudsen number 0.0694, it closely resembles the experimental data with deviation of 0.17%. Further increase in Knudsen number led to under prediction of inlet pressure and for Knudsen number 0.0805, deviation was 3.38%. This over prediction of inlet pressure might be the peculiar behavior of flow through bends.

A special variable, namely, mass flow rate ratio (M_b/M_s) with Knudsen number for flow through microchannel with 90° bends. Where, M_b is mass flow rate through microchannel with bends and M_s is analytical mass flow rate through a same length straight channel (literature assumed $TMAC=1$). In this behaviour of mass flow rate ratio (M_b/M_s) was further investigated for the $TMAC=1.0$ and 0.93 (actual value of $TMAC$ for early slip regime). It was found that

for For T_{MAC}=1 Knudsen numbers 0.0662, 0.0682, and 0.0694, the values of M_b/M_s were higher than unity. For T_{MAC}=0.93, the values of M_b/M_s were higher than unity only for Knudsen numbers 0.0662 and 0.0682. Moreover, plots of streamline through microchannel showed corner vortex in the concave corner for all the simulations regarding present experimental data. Equivalent straight length per bend was also calculated for all Knudsen numbers for pressure ratio 1.55. From the calculation, it was found that with the increase in Knudsen number, the equivalent straight length increases that indicates that at higher Knudsen number, there is more momentum loss. However, with the reduction in Knudsen number equivalent length of the straight channel even smaller than the microchannel with 90° with bends. It indicates that for the Knudsen numbers 0.0662 and 0.0668, presence of bend enhanced the mass flow rate. Present work contributes new knowledge to the field of microchannel flows.

सार

माइक्रोचैनल के माध्यम से गैस प्रवाह का माइक्रो इलेक्ट्रोमैकेनिकल सिस्टम (एमईएमएस) में मौलिक अनुप्रयोग है। माइक्रोफैब्रिकेशन तकनीक में प्रगति ने सरल और जटिल माइक्रोडिवाइस के निर्माण को सक्षम किया है जिसमें सीधे और साथ ही जटिल इंटरलिंकड माइक्रोचैनल शामिल हैं। वर्तमान जांच में सीधे माइक्रोचैनल के माध्यम से गैस प्रवाह का प्रयोगात्मक और संख्यात्मक अध्ययन शामिल है और अक्सर जटिल माइक्रोचैनल यानी नब्बे डिग्री मोड़ के साथ उपयोग किया जाता है।

सीधे माइक्रोचैनल में, स्लिप से प्रारंभिक संक्रमण शासन तक सातत्य दृष्टिकोण की वैधता का अध्ययन सामान्य द्वितीय-क्रम सीमा स्थितियों के साथ किया गया था। 0.002 के पहलू अनुपात वाले माइक्रोचैनल के माध्यम से प्रवाह विशेषता का कम्प्यूटेशनल सत्यापन के साथ अध्ययन किया गया था। पारंपरिक माइक्रोचैनल के विपरीत, एक माइक्रोचैनल में दुर्लभ प्रवाह के विश्लेषण के लिए प्रयोगात्मक और संख्यात्मक तरीकों के संयोजन की आवश्यकता होती है। समलम्बाकार क्रॉस-अनुभागीय सीधे चैनल के लिए त्रि-आयामी संख्यात्मक सिमुलेशन ऐन्सिस धाराप्रवाह 18.1 का उपयोग करके किया गया था। सटीक दूसरे क्रम का स्लिप मॉडल चैनल के ऊपर और नीचे की दीवारों पर व्युत्पन्न और कार्यान्वित किया गया था। इसके अलावा, पहले आदेश और नो-स्लिप सीमा शर्तों को लागू किया गया था और सिमुलेशन परिणामों की तुलना के लिए इनलेट दबाव की गणना की गई थी। इसके अलावा दुर्लभ गैस प्रवाह को मॉडल करने के लिए, स्लिप गुणांक की आवश्यकता होती है जिसका अनुमान तंत्रिका नेटवर्क विश्लेषण का उपयोग करके लगाया गया था। तंत्रिका नेटवर्क को प्रशिक्षित करने के लिए इनपुट और लक्ष्य डेटा सेट की आवश्यकता होती है। इनपुट डेटा सेट में स्लिप गुणांक C_1 और C_2 के विभिन्न संयोजन होते हैं। टैरागेट डेटा सेट में माइक्रोचैनल इनलेट दबाव के ज्ञात प्रयोगात्मक मूल्य और सी 1 और सी 2 के विभिन्न संयोजनों को मानते हुए सिमुलेशन का उपयोग करके प्राप्त इनलेट दबाव के मूल्यों में विचलन शामिल हैं। सिमुलेशन इनलेट दबाव प्राप्त करने के लिए, पर्ची गुणांक के आधार पर दूसरा क्रम पर्ची वेग प्रोफाइल उत्पन्न किया गया था और आउटलेट सीमा स्थितियों के रूप में इनलेट और दबाव के रूप में बड़े पैमाने पर प्रवाह दर के साथ धाराप्रवाह में लागू किया गया था।

इस प्रशिक्षित नेटवर्क का उपयोग दबाव में न्यूनतम विचलन के अनुरूप सर्वोत्तम पर्ची गुणांक की भविष्यवाणी करने के लिए किया गया था। यह पाया गया कि नूडसेन संख्या के लिए 0.0667 से 0.405 तक, पर्ची गुणांक C_1 1.13 से 1.15 के बीच भिन्न था, जो लगभग स्थिर है। नूडसेन संख्या 0.0667 के लिए C_2 का मान 0.24 था, और फिर यह 0.09 के रूप में लगभग स्थिर हो गया। नूडसेन संख्या 0.405 के लिए प्राप्त पर्ची गुणांकों को श्रीनिवासनेट एट अल द्वारा प्रस्तावित पुनरावृत्त विधि का उपयोग करके उनके मूल्यों के साथ और अधिक मान्य किया गया था। यह पाया गया कि एएनएन अनुमानित पर्ची गुणांक पर आधारित परिणाम प्रयोगात्मक मूल्यों के करीब हैं। अब, एएनएन के आधार पर, अनुमानित पर्ची गुणांक मॉडलिंग की गई थी और यह पाया गया कि अधिकतम नूडसेन संख्या 0.405 के लिए, इनलेट दबाव में औसत विचलन 0.84 प्रतिशत है।

वर्तमान कार्य के दूसरे भाग में, दो नब्बे डिग्री मोड़ों के साथ कई माइक्रोचैनलों से युक्त एक माइक्रोडिवाइस का निर्माण किया गया था और इसके माध्यम से प्रवाह व्यवहार का प्रयोगात्मक और कम्प्यूटेशनल रूप से अध्ययन किया गया था। एकल माइक्रोचैनल के माध्यम से द्रव्यमान प्रवाह दर में परिमाण का एक ही क्रम होता है जो व्यावसायिक रूप से उपलब्ध द्रव्यमान प्रवाह मीटर की सीमा के रूप में होता है। इसलिए, बड़े पैमाने पर प्रवाह दर में अनिश्चितता को कम करने और नूडसेन संख्या की विस्तृत श्रृंखला को कवर करने के लिए, सामान्य इनलेट और आउटलेट प्लेनम वाले डबल नब्बे डिग्री मोड़ वाले बीस चैनलों का एक सेट तैयार किया गया था।

वर्तमान मामले में, दो नब्बे डिग्री बेंड की आवश्यकता है क्योंकि सिंगल नब्बे डिग्री बेंड के साथ एक समान लंबाई वाले मल्टी माइक्रोचैनल डिवाइस को बनाना मुश्किल है। बेंड प्रत्येक माइक्रोचैनल में उपयुक्त स्थानों पर स्थित थे। उपयुक्त स्थानों का चयन दो स्थितियों के आधार पर किया जाता है, अर्थात् सभी चैनलों की समान लंबाई और मोड़ दूर इनलेट और आउटलेट प्लेनम में स्थित होते हैं। बेंड लोकेशन के प्रभाव की जांच करने के लिए, तीन अलग-अलग माइक्रोचैनल के लिए कोई स्लिप कंडीशन सिमुलेशन नहीं किया गया था। चरम पर दो चैनल और बीच में एक चैनल का चयन किया गया था क्योंकि उनमें मोड़ के स्थान में अधिकतम भिन्नता थी। इनलेट और आउटलेट

सीमा स्थितियों के रूप में दबाव का उपयोग करके द्रव्यमान प्रवाह दर की गणना की गई और यह पाया गया कि प्रत्येक चैनल में द्रव्यमान प्रवाह दर उन तीन माइक्रोचैनल के लिए समान थी। इस परिणाम के आधार पर, प्रत्येक चैनल दिए गए इनलेट आउटलेट दबावों के लिए समान द्रव्यमान प्रवाह दर की अनुमति दे रहा था और इसलिए, आगे के संख्यात्मक विश्लेषण के लिए केवल मध्य चैनल का चयन किया गया था। पोटेशियम हाइड्रोक्साइड वगैरह का उपयोग करके माइक्रोचैनल को उकेरा गया था और चैनल की ओर से एनोडिक बॉन्डिंग की गई थी। चैनल का पहलू अनुपात 0.0026 था। माइक्रोचैनल के माध्यम से द्रव्यमान प्रवाह दर 1.30 से 1.55 के अलग-अलग दबाव अनुपातों के लिए प्राप्त की गई थी, जिसमें स्लिप शासन को नुडसेन संख्या से 0.0662 से 0.0805 तक कवर किया गया था। मापा प्रवाह में पर्ची प्रभाव की जांच करने के लिए, प्रयोगात्मक द्रव्यमान प्रवाह दर की तुलना नो-स्लिप सीमा स्थिति द्रव्यमान प्रवाह दर से की गई थी। वर्तमान विश्लेषण में देखा गया एक दिलचस्प बिंदु यह है कि नुडसेन संख्या में वृद्धि के साथ, पर्ची और नो-स्लिप स्थिति में विचलन द्रव्यमान प्रवाह दर लगातार कम हो जाती है। नुडसेन 0.0662 के लिए, औसत विचलन 29.13 प्रतिशत था, और नुडसेन संख्या 0.0805 के लिए, यह 17.66 था।

इसके अलावा दुर्लभ प्रवाह व्यवहार का विश्लेषण करने के लिए, चैनल की दीवारों पर फोरस्ट ऑर्डर स्लिप सीमा शर्तों के कार्यान्वयन के आधार पर संख्यात्मक अनुकरण किया गया था। वर्तमान माइक्रोचैनल एक जटिल माइक्रोचैनल है, और प्रवाह के लिए कोई विश्लेषणात्मक समाधान मौजूद नहीं है। माइक्रोचैनल के माध्यम से प्रवाह के लिए नब्बे डिग्री मोड़ के साथ त्रि-आयामी सिमुलेशन किया गया था, और माइक्रोचैनल के इनलेट दबाव की भविष्यवाणी की गई थी। प्रारंभिक पर्ची शासन के लिए नुडसेन संख्या 0.062 और 0.0682, मॉडल इनलेट दबाव की अधिक भविष्यवाणी करता है और माइक्रोचैनल के इनलेट दबाव में औसत विचलन क्रमशः 1.32 और 0.73 प्रतिशत थे। नुडसेन संख्या 0.0694 के लिए, यह 0.17% के विचलन के साथ प्रयोगात्मक डेटा के समान है। नुडसेन संख्या में और वृद्धि के कारण इनलेट दबाव की भविष्यवाणी की गई और नुडसेन संख्या 0.0805 के लिए विचलन 3.38 प्रतिशत था। इनलेट दबाव की यह भविष्यवाणी मोड़ के माध्यम से प्रवाह का अजीब व्यवहार हो सकता है।

एक विशेष चर, अर्थात् मास फ्लो रेट रेशियो (एमबी/एमएस) जिसमें नब्बे डिग्री बेंड्स के साथ माइक्रोचैनल के माध्यम से प्रवाह के लिए नुडसेन संख्या होती है। जहाँ, M_b बेंड के साथ माइक्रोचैनल के माध्यम से द्रव्यमान प्रवाह दर है और M_s समान लंबाई वाले सीधे चैनल के माध्यम से विश्लेषणात्मक द्रव्यमान प्रवाह दर है (साहित्य मान लिया गया टीएमएसी=1)। मास फ्लो रेट रेशियो (एमबी/एमएस) के इस व्यवहार में टीएमएसी = 1.0 और 0.93 (ईली स्लिप रिजिम के लिए टीएमएसी का वास्तविक मूल्य) के लिए और जांच की गई। यह पाया गया कि टीएमएसी = 1 नुडसेन संख्या 0.0662, 0.0682, और 0.0694 के लिए, M_b/M_s के मान एकता से अधिक थे। टीएमएसी = 0.93 के लिए, M_b/M_s का मान केवल नुडसेन संख्या 0.0662 और 0.0682 के लिए एकता से अधिक था। इसके अलावा, माइक्रोचैनल के माध्यम से स्ट्रीमलाइन के भूखंडों ने वर्तमान प्रयोगात्मक डेटा के संबंध में सभी सिमुलेशन के लिए अवतल कोने में कोने के भंवर को दिखाया। दबाव अनुपात 1.55 के लिए सभी नुडसेन संख्याओं के लिए बराबर सीधी लंबाई प्रति मोड़ की भी गणना की गई थी। गणना से, यह पाया गया कि नुडसेन संख्या में वृद्धि के साथ, बराबर सीधी लंबाई बढ़ जाती है जो इंगित करती है कि उच्च नुडसेन संख्या में, अधिक गति हानि होती है। हालांकि, नुडसेन संख्या में कमी के साथ सीधे चैनल की बराबर लंबाई नब्बे डिग्री के साथ माइक्रोचैनल से भी छोटी है। यह इंगित करता है कि नुडसेन संख्या 0.0662 और 0.0668 के लिए, मोड़ की उपस्थिति ने द्रव्यमान प्रवाह दर को बढ़ाया। वर्तमान कार्य माइक्रोचैनल प्रवाह के क्षेत्र में नए ज्ञान का योगदान देता है।

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NOMENCLATURES

ar ($=H / W$)-Aspect ratio (non-dimensional)	$\tilde{v}$ -Non-dimensional normal velocity
C_1 and C_2 -Second order slip coefficients	$\bar{u}$ -Average flow velocity (m s^{-1})
H - Microchannel depth (m)	$\vec{v}$ -Vector notation of flow velocity (m s^{-1})
L -Length of microchannel (m)	W -Microchannel width (m)
Kn -Local Knudsen number (non-dimensional)	$\tilde{x}, \tilde{y}$ -Non-dimensional distance along x and y
Kn_o -Knudsen number based on the channel outlet	τ -Shear stress (N m^{-2})
l -Characteristic dimension of the system (m)	p_o -Channel outlet pressure (N m^{-2})
$\dot{m}$ - mass flow rate	$\tilde{p}$ -Non-dimensional pressure w.r.t outlet pressure
M_b -mass flow rate through microchannel with bends	R -Specific gas constant ($\text{J kg}^{-1} \text{K}^{-1}$)
M_s -mass flow rate through straight channel	T -Gas temperature (K)
MFRR- mass flow rate ratio (M_b/M_s)	$\tilde{u}$ -Non-dimensional streamwise velocity
p -Gas pressure (N m^{-2})	$\tilde{u}_s$ -Non-dimensional slip velocity at the walls
P -Pressure ratio = p_i / p_o (non-dimensional)	$\tilde{u}_w$ -Non-dimensional wall velocity
p_i -Channel inlet pressure (N m^{-2})	
Greek symbols	
λ -Mean free path of the gas (m)	μ - Molecular viscosity of the gas (Ns m^{-2})
Φ - Momentum of gas molecules	ρ -Density of the gas (kg m^{-3})
σ -Tangential momentum accommodation coefficient	∇ -Grad operator

Subscripts

i-Inlet

o-Outlet

s-Surface

t-Tangential

w-Wall