

DEVELOPMENT AND APPLICATIONS OF A GENERIC QUASI-INCOMPRESSIBLE FRAMEWORK FOR MISCIBLE FLUID FLOWS

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CERTIFICATE

It is certified that the work contained in the thesis entitled “**Development and applications of a generic quasi-incompressible framework for miscible fluid flows**”, by **Preetirekha Borgohain** has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

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ABSTRACT

The field of miscible fluid flows finds its way into a large number of household and industrial applications in both macro and micro scales. Existence of this type of flows can be observed in a variety applications ranging from our day-to-day life such as, mixing of milk or alcohol into water, mixing of smoke into gases in the atmosphere to that of industrial applications such as in the field of enhanced oil recovery, transportation of crude oil in the pipe lines. In this type of flows, multiple fluids/species involved in the process eventually mix to produce a homogeneous mixture having no distinct interfaces among them. In a broader aspect, mixing can be described as a process that leads to transport of species, temperature and phases to reduce inhomogeneity. The degree of mixing is one of the primary measures that determines how well the species mix into each other. Mixing of certain species can also be accompanied by reactions. The field of combustion that involves mixing of reacting species rely to a great extent on a rapid mixing of the reactants. Mixing of liquids at micro scale has also gained significant attention in microfluidic applications profound in many biotechnological and pharmaceutical industries. As such, this research area covers a wide domain that extents from micro to macro scale and non-reacting to reacting flows.

Different approaches are available to numerically model a problem that basically depend on the nature of the problem, viz., incompressible, quasi-incompressible or compressible. Even though the Mach numbers are low, variable density miscible flows are characterized by non-solenoidal divergence which necessitates a quasi-incompressible assumption and therefore has been adopted in this work. This approach is applicable for situations wherein density cannot be considered to be constant even though the Mach number is less than 0.3 which is typical for flows involving multiple species. The density of the mixture can vary both spatially as well as temporally with no specific constraint on the density ratio (ρ_{max}/ρ_{min}). This doctoral thesis primarily focuses on the development of a generic and robust finite volume based quasi-incompressible numerical framework for non-reacting and reacting miscible flows on arbitrary hybrid unstructured meshes and its applications to laminar mixing and combustion.

The solver which is capable of handling both orthogonal and non-orthogonal meshes (in two- and three-dimensions) in an efficient manner has been indigenously developed with an emphasis on application to problems involving a wide range of density ratios. A collocated grid arrangement that also uses unstructured data is adopted making it capable of handling hybrid unstructured meshes, which can be necessary when dealing with complex geometries. The temporal discretization is done using implicit Euler time stepping whereas diffusive fluxes are computed using central differencing scheme. However, for the convective fluxes, different flux schemes with both first and second order accuracy, such as first order upwind (FOU), Khosla-Rubin and the high resolution CUBISTA scheme have been implemented in the present solver. The pressure-velocity decoupling typical of incompressible solvers is avoided by using momentum interpolation.

A detailed analysis of truncation error and discretization errors has been performed by using the method of manufactured solutions to quantify the numerical errors associated with a particular convective scheme and to establish a relation between the truncation and discretization errors. The truncation errors may be computed apriori and provide a fair indication of the discretization errors which are aposteriori determined. We attempt to devise some guidelines on the choice of convection schemes based on these observations. Rigorous verification and validation studies have been performed for a series of problems starting from simple lid-driven cavity flow to mixing of gases as well as liquids in macro and microchannels. The computed results are found to be in good agreement with previous computations and/or experiments. The solver is shown to have nominal second order accuracy and is then applied to simulate a few pertinent problems related to laminar mixing.

A major shortcoming of mixing of liquids in microfluidic devices is the poor mixing capability because of the omnipresence of high Peclet number (Pe). Therefore, to make the mixing faster in these diffusion dominated flows, where the typical Reynolds numbers (Re) is less than 10, it is imperative to enhance the mixing ability by using either active or passive techniques. We conceptualize of a novel passive micromixer by incorporating thin curved ribs (as flow obstacles) to induce additional transverse convection and explore its mixing ability, both in terms of mixing efficiency (M) and pressure drop for the case of a two dimensional cross-T microchannel. Comparison of the mixing indices for micromixers with curved obstacles to that of the conventional straight ribs shows that the use of curved ribs lead to marginally higher value of mixing efficiency ($M = 45\%$) than that obtained with straight ribs ($M = 43.4\%$). However, the key observation is that this can be achieved with a significantly lower pressure drop than obtained with straight obstacles. Furthermore, a complete set of parametric studies are performed showing the effects of different geometric and flow parameters on the mixing ability of the micromixer such as number of modules (N_m), angle of inclination (θ) of the obstacles, axial spacing between obstacles (s), its size (l) and inlet Re . Studies reveal that M

increases with increasing the number of modules as well as the size of the obstacles, while negative angles lead to much higher pressure drop than compared to that of their positive angle counterparts although both render nearly same mixing efficiency.

Motivated by the superior mixing performance observed in a two-dimensional cross-T microchannel by using the newly devised curved ribs, we extend the work to a more realistic three-dimensional configuration. However, for the three-dimensional channel, a substantial enhancement in mixing efficiency has been observed with the values of 61.3%, 47.6% and 24.3% for microchannels with $h = H = 140 \mu\text{m}$, $\theta = 45^\circ$, $l = 0.2 \text{ mm}$ and $N_m = 4$ for curved obstacles, straight obstacles and without obstacles, respectively, where h and H are the heights of the ribs and main channel, respectively. Not surprisingly in this case also the superior mixing is obtained with lesser pressure drop for curved ribs than straight ribs. Results showed that the extent of mixing attained is determined by the strength of the secondary flows. It has been found that the magnitude of the transversal velocities (v and w) are higher for the channels with curved ribs than that of straight ribs, which however, is almost negligible for plane channels. For the effects of different geometric parameters, it has been found that M is proportional to the number of modules. Unlike intuitive expectations, the mixing process does not show a monotonic trend for angle of inclinations. On the other hand, an increasing-decreasing trend of mixing indices is observed for size and height of obstacles.

A study on gaseous mixing in corrugated channels is also carried out. We discuss the mixing behavior of a binary, non-reacting gaseous mixture of argon and air in a counterflowing horizontal channel with waviness imparted along the channel walls and the dominant mechanism of mixing is brought out through extensive numerical simulations. Results show that wavy channels lead to enhanced mixing compared to that of a plane channel. The vortex patterns which arise out of asymmetries in the wavy geometry seem to manifest in the mixing efficiency. The use of asymmetric channels i.e. with 0° phase difference (PD) showed better mixing capability ($M=97\%$) than their symmetric counterparts with 180° PD ($M = 74\%$) for otherwise same configuration. A closer look reveals that the 180° PD channel has a symmetric recirculation pattern (involving clockwise and counterclockwise vortices) during a single period while the 0° PD channel exhibits an asymmetric pattern of recirculation in one period. The numerical results reveal that the alternate recirculation zone patterns in the former causes higher transverse velocities which combine with diffusion to enhance mixing. Detailed parametric studies are performed for the effects of wavelength (λ), amplitude (a), Re and Pe on the mixing performances of asymmetric wavy channels. It is found that M is maximum (97%) for the case of 16 waves having $\lambda = 0.718h$ among the different wavelengths studied ranging from $2.3h$ to $0.328h$. It has also been found that mixing efficiency increases with increase in amplitude and decreases with increase in Re .

As a final step, attempts have been made to extend the approach to simulate high density ratio flows such as mixing of gaseous reacting species. The presence of reactions in itself makes this a challenging endeavor and this study, therefore, must be considered as a preliminary work involving only laminar gaseous diffusion (non-premixed) flames. Before attempting the reacting flows, first, validation studies for high density ratio non-reacting natural convection flows are performed. It is then followed by implementing the numerical approach, based on the flame sheet concept, for reacting flows wherein a global single step reaction mechanism may be assumed for the chemistry modelling. The complete chemical state is determined by solving only one source-free conservation equation for the mixture fraction (Z) which is a conserved scalar. The mass fractions of all reactants and products are deduced from Z . A validation study involving laminar methane-air diffusion flame with benchmark solutions demonstrates the efficacy of the quasi-incompressible framework.

This doctoral thesis thus presents a comprehensive numerical framework for miscible flow interactions largely in a non-reacting environment and its applications to laminar mixing which is an indigenous contribution to the field. The thesis concludes with a summary of the main findings and some recommendations for future research that can further improve the potential of the numerical framework.

Dedicated to my Parents





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Nomenclature



English Symbols

Symbol	Definition
a	Amplitude of wave
c_p	Specific heat at constant pressure (J/kg.K)
c_v	Specific heat at constant volume (J/kg.K)
D	Diffusivity constant (m^2/s)
F_f	Volume flux at face centroid f
g_i	Gravity in i^{th} direction (m/s^2)
H	Height of main channel (μm)
h	Height of obstacle placed in the main channel (μm)
l	Chord length of curved rib (μm)
L	Length of main channel (μm)
M	Mixing index
Ma	Mach number
mc	Mixing cost
mec	Mixing energy cost
MW_k	Molecular weight of the species k (kg/mol).
N_m	Number of modules
Nu	Nusselt number
p	Total pressure (Pa)
$\bar{P}$	Thermodynamic pressure (Pa)
Pe	Peclet number
Pr	Prandtl number
Q	Heat release per unit mass of fuel (J/kg)
R	Specific gas constant (J/kg.K)
Re	Reynolds number
R_u	Universal gas constant (J/mol.K)
s	Spacing between two consecutive curved ribs (μm)
$\mathbf{S}$	Surface area vector (m^2)
Sc	Schmidt number
t	Time (s)
t_o	Thickness of curved rib (μm)
T	Temperature (K)
u_i	Velocity vector in i^{th} direction (m/s)
u	x -component of velocity (m/s)
v	y -component of velocity (m/s)
V_{co}	Volume of cell co (m^3)
w	z -component of velocity (m/s)
$\bar{W}$	Average molecular weight of a mixture (kg/mol)
W	Width of main channel (μm)
x_i	Spatial coordinate in i^{th} direction

Y_k	Mass fraction of k^{th} species
$\bar{Y}$	Optimum mass fraction
Z	Mixture fraction
Z_{st}	Stoichiometric value of mixture fraction

Subscript

avg	Average
co	Owner cell centroid
f	Face centroid
k	k^{th} species
nb	Neighbor cell centroid

Greek symbols

ϵ	Temperature difference parameter
γ	Deferred constant
Δt	Time step size
λ	Wavelength
κ	Thermal conductivity
μ	Dynamic viscosity of the gas mixture (Pa.s)
ω_k^o	Reaction source term of species k
Π	Hydrodynamic pressure (Pa)
ϕ	General scalar variation
Φ	Conserved scalar ($\rho\phi$)
ρ	Density (kg/m ³)
ρ_k	Density of k^{th} component (kg/m ³)
σ	Standard deviation
$\tau_{i,j}$	Stress tensor
θ	Angle of inclination (°)

Abbreviations

CDS	Central difference scheme
CFD	Computational fluid dynamics
CUI	Cubic upwind interpolation
CUBISTA	Convergent and universally bounded interpolation scheme for the treatment of advection
FDM	Finite difference method
FOU	First order upwind
FVM	Finite volume method
FEM	Finite element method
MHD	Magneto-hydrodynamics
MMS	Method of manufactured solutions
PD	Phase difference
RWP	Rectangular winglet pairs
SAR	Split-and-recombine



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Chapter 1

Introduction

1.1 Background

The field of miscible fluids, whether liquids or gases, finds its way into a large number of scientific and industrial applications both in macro and micro scales. As the name itself suggests, this category of fluids has the ability to mix into one another when they come in contact that results in a homogeneous mixture leaving no distinct interfaces among them. In a broader aspect, mixing can be defined as a process that leads to transport of species, temperature, and phases to reduce inhomogeneity. The degree of mixing is one of the primary measures that determines how well the species mix into each other. Applications are often seen in our day-to-day life such as, mixing of milk or alcohol into water, mixing of smoke into gases in the atmosphere. In regard to the industrial applications, one can see their uses in the field of enhanced oil recovery [1], transportation of crude oil in the pipe lines etc. Mixing leads to secondary effects such as reaction and phenomena such as combustion rely to a great extent on a rapid mixing of the reactants prior to burning in industrial reactors. Another practical field of application where mixing of different liquids has gained substantial attention is in the microfluidic applications. The increasing demand of process industry, pharmaceuticals analysis and biochemistry has been gaining ground in the development of microreactors, particularly for chemical, biological, and medical applications. This has led to miniaturization of one or several laboratory processes down to a chip format, commonly referred to as lab on a chip (LOC) technology. LOC technology has been applied in a wide range of pro-

cesses such as polymerization, organic synthesis, enzyme assay, cell analysis, clinical diagnostics, and drug delivery studies [2]. Keeping a view on the importance of small-scale mixing for all the microfluidic applications, one can easily appreciate the need of a microscale mixer, commonly termed as micromixers. These are basically comprising of channels that are having characteristics length scales of the order of microns, also known as microchannels ¹, typically having the order of dimensions of human hair or less.

As such, one can see that, the field of mixing of miscible fluids has extended over a wide domain ranging from macro to micro scales, liquids to gases, non-reacting to reacting. However, the performance of any mixing process depends on how efficient the mixing process is. The faster the rate of mixing, the better is the process. There are many different mechanisms to provide mixing in macroscale such as molecular diffusion, eddy diffusion, advection, and Taylor dispersion. Eddy diffusion is the transport of large groups of species and generally requires a turbulent flow. However, at microscale level, viscous effect is dominant and hence, inducing turbulence is rather impossible in micromixers. Thus, mass transport via eddy diffusion is not feasible in micromixers and the mixing can be achieved by the other means. For e.g., advection which is the transport phenomenon caused by fluid motion and Taylor dispersion which is advection caused by a velocity gradient. However, the specific Reynolds number (Re) for flows in micro level is very small. At these low Re , fluid streams do not interpenetrate leading to convection to take place only in the direction of flows. As a consequence, mixing relies certainly on molecular diffusion. The transport mechanism of molecular diffusion is characterized by the molecular diffusion coefficient. For gases, the characteristic diffusivity constants are in the order of $10^{-5} \text{ m}^2.\text{s}^{-1}$ whereas for liquids it is in the order of $10^{-9} \text{ m}^2.\text{s}^{-1}$ [3]. Consequently, diffusive mixing itself becomes a very slow process especially for liquids.

To get an idea of mixing time scales in the micromixers, let us take the example of deoxyribonucleic acid (DNA). DNA has diffusivity coefficient, $D = 10^{-10} \text{ m}^2.\text{s}^{-1}$. Therefore a typical mixing time to diffuse in a microchannel of characteristic length

¹The words micromixer and microchannel are used interchangeably and both refer to the same configuration

(l) of $100\ \mu\text{m}$ is

$$t_{diff} = \frac{l^2}{D} = \frac{(10^{-4}\ \text{m})^2}{10^{-10}\ \text{m}^2.\text{s}^{-1}} = 100\ \text{s} \quad (1.1)$$

Considering a velocity of $10^{-3}\ \text{m.s}^{-1}$ (typical for water-based microfluidic system), it would require a distance of about 10 cm to completely diffuse. However, micromixers are intended to fully mix the fluid in the shortest possible distance down the channel, favorably of the order of millimeters rather than centimeters. Demand for longer lengths of the channel defeats the salient purpose of miniaturization. As such, it is not worth to rely on diffusion alone for achieving good mixing. Therefore, efficient mixing techniques are always warranted to enhance the mixing rate.

In the recent past and present, a large volume of research, both experimental and numerical, has been dedicated to analyze the physical aspects of mixing of multiple species and ways to rapidize it. With the advancements in computational facilities that tend to lower the cost of computational simulation relative to experimentation, computational fluid dynamics (CFD) has become one of the most powerful and versatile methods for simulating fluid flow problems. It plays a key role in their development and optimization of any new design. Unstructured finite volume methods (FVM) is one of the several popular approaches, to carry out CFD simulations for fluid flow problems. Furthermore, unstructured framework provides the flexibility of construction of hybrid meshes and it helps in meshing complicated geometries with relative ease. As such, CFD simulations are highly popular within the scientific community.

There are different approaches available in literatures to model a problem numerically. The selection of the approach is basically governed by the physical nature of the problem, i.e., incompressible, quasi-incompressible or compressible. Among these three approaches, the quasi-incompressible approach has been adopted in the present work. This approach is applicable for situations wherein density cannot be considered to be constant even though the Mach number (Ma) is less than 0.2. However, for problems of mixing of multiple species, the mixture density actually varies both spatially as well as temporally. This may give rise to a very high to low density ratio (ρ_{max}/ρ_{min}) for problems such as non-reacting to reacting mixing of species, respectively. The primary causes of density variations are

- gradient of temperature: e.g. natural convection, mixed convection problems.

- species concentration gradient: e.g. non-reacting mixing of liquids as in micromixers.
- combination of both: e.g. reacting flows.

The low Mach number formulation dedicated to quasi-incompressible flows has the ability to capture the flow physics for a wide range of variable density problems. As such, for numerical modelling of quasi-incompressible flows, the low Mach number formulation offers a generic, robust framework for a wide range of variable density problems.

However, numerical modelling of flows involving mixing multiple species is challenging too. For the case of reacting mixing the computational cost becomes a critical parameter if the number of species involved is large enough. For example, oxidization of methane, the simplest hydrocarbon, involves 53 species. This means, one has to solve at least 52 species conservation equations along with the momentum and the continuity equations, to completely characterize the flow field. Another challenge in numerical simulation of mixing of liquids is to ensure that the solutions do not get overly diffused particularly when physical diffusion plays a major role such as in microfluidics due to the numerical error called as false diffusion.

On the basis of the aforementioned considerations, in the past, various methodology for handling variable density quasi-incompressible flows has been developed in the purview of reacting flows. Moreover, new measures, both active and passive, have been proposed with the focus to achieve the best mixing by utilizing a shorter length of channels. In this regard, a detailed literature review has been presented in the following section which is then followed by motivation and research objectives.

1.2 Review of Literature

The primary focus of this doctoral thesis is to develop a generalized three-dimensional numerical framework for non-reacting and reacting miscible fluid flows in the low Ma limit. Moreover, it has already been described in the previous section about the importance of making the mixing process faster for both reacting and non-reacting mixing flows. Substantial works have already been carried out to propose differ-

ent techniques to enhance the mixing behavior of micromixers. In this section, first a detailed literature review has been presented on low Mach number formulation available to model quasi-incompressible flow solver. Some literatures related to verification and validation of a developed numerical solver and for controlling of numerical diffusion are also reported. Thereafter, literatures pertaining to rapidize the mixing capability of micromixers have been discussed in detail, specially focussing on different passive mixing techniques. However, some literatures are also provided for different active mixing techniques for completeness.

1.2.1 Low Mach number formulation

The use of low Mach number model for handling quasi-incompressible or pseudo-compressible flows are found immense attention in the literatures. In this line the first work was carried out by Paolucci [4]. He derived a set of Navier-Stokes equations specially for low Mach number flows by removing the sound waves from the general governing equations without losing much of the physics. These equations which are more general than the Oberbeck-Boussinesq approximations, can be used for the computation of convection in a fluid with large density gradients. Similar formulation has been adopted by LI [5] in his thesis work for numerical simulations of natural or mixed convection in vertical channels. Pember et al. [6] presented an adaptive projection algorithm based on low Mach approximations that consists of evolution equations coupled with a constraint on the divergence of the flow for modelling unsteady, low-Mach reacting flow in an unconfined region. Day and Bell [7] extended the work of Pember et al. [6] by introducing the use of a symmetric operator-split approach that is second-order accurate in time for the simulation of laminar reacting flows with complex chemistry.

Nicoud [8] proposed three dissipation-free finite-difference algorithms to solve a low-Mach number approximation for the Navier-Stokes equations. The key ingredient common to each of the methods presented is a Poisson equation with variable coefficient that is solved for the hydrodynamic pressure. Knikker [9] presented five different algorithms for the simulation of low Mach flows with large temperature variations and made a comparative study of all these algorithms. Ebrahimi-Kebira et al. [10] extended a novel dual-purpose, pressure-based finite-volume algorithm to simulate laminar-mixing and reacting flows in low Mach number regimes. They

reported that their algorithm can improve the capability of any incompressible SIMPLE-based algorithm.

1.2.2 Verification and validation of numerical solver

During the recent decades, CFD has become a powerful and versatile tool for simulating fluid flow problems. However, to ascertain that the computed results are an accurate representation of reality, a rigorous testing of the numerical model is of utmost important. One of the ways to verify the numerical model is by performing the order-of-accuracy study. Roy et al. [11] used the method of manufactured solutions (MMS) to accurately evaluate the discretization error in the numerical solutions obtained from the compressible CFD code Premo. Through global discretization error analyses, they showed that Premo code is free from coding mistakes in the spatial discretization for uniform meshes. Roy [12] in his work provided a broad overview of the two aspects of verification procedures namely, code verification and solution verification for computational simulation. Eca and Hoekstra [13] presented manufactured solutions for code verification of Navier-Stokes solvers for two-dimensional, unsteady flows of an incompressible fluid. They reported that with MMS framework it is possible to study the influence of the two main sources of the numerical error, viz, discretization error and iterative error, on the numerical error of unsteady flow calculations. A comprehensive framework for verification, validation, and uncertainty quantification of scientific computing applications was given by Roy and Oberkampf [14]. Shunn et al. [15] used MMS to verify the convergence properties of a low-Mach number, variable-density flow code with respect to three problems relevant to combustion applications. They showed that linear interpolation of the equation-of-state causes numerical fluctuations that impede convergence and reduce accuracy.

Another aspect of CFD simulations of mixing of liquid species is to accurately resolve the mass transfer rate. For gases with Sc numbers in the order of $O(1)$, mass transfer occurs on the same length scale as the momentum transfer and convective flow, whereas, for liquids with Sc number in the order of $O(1000)$ or even higher, exhibit very short mass transfer length scales [16]. As such, numerical grids for mixing simulation must be very fine to correctly resolve the mass transfer length scale. If not done, it can over predict the degree of mixing due to the inherent drawback

of false (or numerical) diffusion. False diffusion arises because, the numerical approximations for the advective terms in the governing differential equations contain truncation errors that can artificially increase the diffusive transport of species in the numerical solution. It results in smearing of sharp gradients and hence it can overpredict the degree of mixing. For most liquid flows, due to high Peclet (Pe) numbers, false diffusion often masks the molecular diffusion of the fluid, making the solution inaccurate.

Different numerical schemes exhibit such behavior to varying degrees. Liu [17] developed a method to quantitatively measure the effect of false diffusion on scalar decay rate. This method computes an average false diffusivity from a given numerical solution and is not limited to any particular numerical scheme. Bailey [18] examined and quantified the amount of false diffusion associated with the often recommended and versatile second-order upwind method through a series of numerical simulations conducted using a standardized problem on both structured and unstructured meshes. He proposed a procedure for managing false diffusion when simulating steady, liquid micromixing.

1.2.3 Passive mixing techniques

There are two basic techniques exploited to enhance mixing at the microscale. Based on these mixing techniques, micromixers are classified into two categories, viz active and passive, depending on whether mixing is assisted by an external stirring mechanism or not. Stirring means the advection of material blobs subjected to mixing without diffusive action [19]. Passive mixers were the first microfluidic device reported. They do not require any external source of energy other than the pressure head used to drive the fluid flows at a constant rate. Mixing in passive micromixers relies predominantly either on inducing convective transport of the species in transverse directions or by enhancing molecular diffusion itself. The primary way to achieve this is by the geometrical manipulations of the channel to induce transversed advection effects realized to manipulate the laminar flow pattern within the microchannels or to increase the contact area and contact time between the different mixing species. Several review papers on mixing in microchannels provide a comprehensive account of the research in this field [2, 20–23].

These are less expensive and more convenient to fabricate than active micromixers, and can be easily integrated into more complex LOC devices. The passive micromixers can be broadly categorized as basic micromixers, multi-lamination micromixers and chaotic micromixers. The following section provides a detailed review of literature for this category of microfluidic devices.

1.2.3.1 Studies on basic micromixers

T- and Y-shaped micromixers are widely applied for fundamental investigation of mixing processes in micromixers. In the basic T- and Y-mixers, mixing is entirely depends on molecular diffusion, therefore long mixing channels are required to achieve desired mixing efficiency. The fundamental studies of steady diffusion in a T-sensor with rectangular geometry were presented by Kamholz et al. [24]. They explained “the butterfly effect” that corresponds to the shape of the interdiffusion zone between the two input streams Broboana et al. [25] in their work aimed to obtain the description of the “transitory butterfly effect” along the main channel. They numerically modeled the unsteady diffusion process in a symmetric Y-geometry, in particular to determine the evolution of the non-stationary butterfly effect and analyzed the time evolution of the inter-diffusion length at the micro-channel walls.

Depending on Re , different flow regimes have been categorized in the mixing channel, viz., stratified, vortex flow and engulfment flow, [3,26,27]. Engler et al. [27] performed numerical and experimental investigations on T-shape micromixers and proposed a unique identification number for featuring engulfment flow regime. Soleymani et al. [28] also reported on the determination of identification number for the differentiation of flow regimes and its critical value at which transition from vortex flow to engulfment of flow.

Numerical works were carried out to investigate the fluid dynamics and mixing characteristics for gaseous flow inside a T-type microchannel by Gobby et al. [29]. Their results showed that the mixing length was increased with the fluid speed and decreases with the mixer aspect ratio whereas angle between the inlet channels had little affect on the mixing performance. Wong et al. [30] studied micro T-mixer at different cross-sectional dimensions at higher Reynolds number (400-500) of flow. The work of Soleymani et al. [3] reported that unlike gases, for liquids, angle between

the inlet channels had a significant effect on the mixing in addition to aspect ratio and flow rate. They also proposed a TT-mixer which is having much better mixing performance than that of the ordinary T-mixers Hsieh et al. [31] analyzed mixing in passive Y-mixers for different mixing angles, both with and without Joule heating. They found that mixing angles that led to the development of vortices can positively influence mixing performance and effect of Joule heating should be considered for certain values of electric field strength. Ansari et al. [32] studied the effect of the position of fluid stream interfaces on mixing in a rectangular microchannel.

To improve the mixing capability of a conventional T-mixer, Cortes-Quiroz et al. [33] proposed a new configuration of the T-shaped micromixer, called as 3-D T-mixer, that provided a significant enhancement of mixing and lower pressure loss compared to a typical T-mixer for Re in the range 100–500. Sarkar et al. [34] proposed several new 1-1 and 1-2 microfluidic junctions and compared the mixing efficiencies for each design by numerical simulations. They showed three different channel structures to improve microfluidic mixing viz simple-junction-complex-layout, complex-junction-simple-layout and complex-junction-complex-layout. They reported a mixing efficiency of as high as 86% by just manipulating the junction which is normally within the range of 20% for simple junctions.

1.2.3.2 Multi-lamination micromixers

Multi-lamination micromixers work on the principle of decreasing the length of mixing path and thus increasing the contact surface for mixing liquids. Typically multi-laminating micromixers are accomplished by (a) split-and-recombine (SAR) flow arrangement, (b) hydrodynamic focusing, and (c) interdigital flow arrangement.

Split-and-recombine (SAR):

From Eq. 1.1, it has been seen that if molecular diffusion is the only mixing mechanism, then the time required for complete mixing is proportional to the square of the thickness of the lamellar structure. Thus, sequential splitting of the flows of liquids and rearranging them in alternating thin laminae will significantly decrease mixing times. A subdivision of each stream into n laminae leads to n^2 -times faster mixing [35]. In these micromixers, the mixing of fluids takes place in three steps: flow splitting, flow recombination and flow rearrangement [21].

Bessoth et al. [36] splitted each inlet channel into two sub-channels repeatedly until a total of 16 partial flows are generated and then sequentially combining two neighboring channels into one until all partial flows are united in one broad outlet channel. With this, they attained 95% mixing after about 15 ms. Roudgar et al. [37] in their study reported that by splitting the fluid streams at the inlet channels itself gave more mixing than the conventional mixer. They found vertical splitting to be more efficient than horizontal splitting. Kim et al. [38] designed a novel serpentine laminating micromixer with F-shaped mixing units in a basic T-channel that resulted in about 20 times shorter mixing length than compared to the simple T-type micromixer. Another effective yet simple two-dimensional micromixer based on split and recombination theory, named as rectangle-square wave micromixer, was investigated for its mixing capability by Chen [39].

Several other effective but complicated, in terms of design and construction, passive micromixers are proposed and explored numerically and experimentally for their mixing ability such as denoted by Y-Y mixer [40], tear-drop mixers [41], E-shaped [42]. Nimafar et al. [43] presented experimental comparison of two static SAR micromixers, one is based on tear-drop elements and the other is based on O-type mixer elements with that of the basic T-type mixer for low Re range ($0.083 \leq Re \leq 4.166$). Their experimental data showed that the tear drop SAR mixer gave a mixing efficiency of more than 90% which was less than 40% and 10% for the O-mixer and basic T-mixer, respectively. Viktorov and Nimafar [44] introduced two novel 3D SAR ‘chain mixer’ and compare their mixing performance and pressure drop with T, O and tear-drop micromixers. Results showed that an efficiency of up to 98% can be achieved for the chain and tear-drop mixers at the tested Reynolds number ($0.083 \leq Re \leq 4.166$). Moreover, the chain mixers have the advantage of lower required pressure drop than that of tear-drop micromixer. Chen and Shen [42] proposed two design of E-shaped micromixers namely, stacking-E-shape micromixer (SESM) and folding-E-shape micromixer (FESM). Their numerical results showed that both designs significantly increases the mixing index than that of basic T-micromixer; however, the FESM showed better mixing performance than SESM when $Re \geq 30$ and vice-versa.

Hydrodynamic/geometric focusing:

Hydrodynamic focusing is another concept for reducing mixing length in parallel lamination micromixers. The term “hydrodynamic focusing” literary means squeezing the fluid lamella of the inlet flow in the presence of a surrounding flowing medium. A reduction in lamella width down to even submicrometer size can be achieved by pressure-driven flow focusing, owing to the shear forces of the surrounding fluid which was fed into the mixer with a much higher flow rate than the central lamella. At such small length scales, molecules from the side flow rapidly diffuse across the inlet stream, resulting in fast mixing.

These techniques were first developed by Knight et al. [45] to enable ultra-fast mixing in the millisecond range. They showed that their continuous-flow microfluidic mixer was capable of having diffusive mixing times of less than 10 μ s. In addition to lowering the mix time, hydrodynamic focusing also dramatically reduces the volume of sample necessary for continuous flow reaction kinetics experiments. An alternative setup for hydrodynamic focusing was proposed by Veenstra et al. [46] that comprised of a channel that contained a focusing region by simply narrowing down of the channel in which the two lamellae are thinned. This mixer is suitable for mixing slowly diffusing compounds in systems with low flow rates.

Nguyen and Huang [47] theoretically and experimentally investigated a micromixer based on combined hydrodynamic focusing and time-interleaved segmentation. The aim of hydrodynamic focusing is to reduce the transversal mixing path whereas time-interleaved sequential segmentation aims at shortening the axial mixing path. The microchannel comprised of a successive Y-T junction wherein the sheath streams for hydrodynamic focusing are introduced through the two T inlets and the solvent and solute are switched alternately through the Y-inlets so that segments of them are formed in the focused stream. Adeosun and Lawal [48] studied mass transfer enhancement via ‘reorientation and stretching of fluid interfaces’ by imposing some geometric constraints in the form of trapezoid, hexahedral, and octahedral protrusions incorporated on the floor of the multi-channel plate microreactor. Based on the criteria of low pressure drop as well as high mixing performance, the best enhanced-mixing configuration is identified and subsequently optimized.

Zhang et al. [49] studied a focusing-based microfluidic mixer comprised of two Y-

junctions connected serially wherein sheath fluids are introduced through the downstream Y-junction to squeeze the liquid streams to be mixed that are introduced from an upstream Y-junction. They found that mixing depends on the focusing effect, which is dictated by the flow rate ratio of the sheath fluids to the mixing fluids but independent to the device's branch angle of the sheath channel to the main channel. Nasir et al. [50] studied different parameters such as angle of confluence, channel cross-section, fluid momentum, Re etc. that can affect the shape of a hydrodynamically focused stream both in symmetric and asymmetric junctions. They found that curvature in the interface between the sheath and focused fluid, and the resulting cusps of fluid at the channel corners, increased both with increasing Re and the angle of confluence. Similar studies were also reported by Kunstmann-Olsen et al. [51] for the effect of volumetric flow ratio between the main and the side channels, as well as angle between channels on the focusing width.

1.2.3.3 Patterned wall/grooves

In microfluidic systems, creating the three-dimensional flows are rather difficult that are required for manipulating streams in transverse direction to get the benefit of species transport due to transversed convection. To achieve this, one of the commonly used method is to use some patterns such as grooves, waviness, protrusions etc. along the walls of the channel. Pressure driven flows in these channels contain recirculating components that are transverse to the principle direction of flow that are beneficial to mix adjacent streams. Also the transversed components of flow resulted in stretching and folding of volumes of fluid over the cross-section of the channel that reduced the mixing length by decreasing the average distance over which diffusion must act in the transverse direction to homogenize unmixed volumes [52].

Stroock et al. [52] presented a passive method based on chaotic mixing technique for enhanced mixing in microchannels at low Re . They used placing of ridges on the floor of the channel at an oblique angle with respect to the axis of the channel. These ridges generated an axial pressure gradient that is responsible for generating transversed components in the flow that finally results in a helicoidal pattern of the streamlines inside the channel. They also proposed a staggered herringbone mixer (SHM) and compared the mixing efficiency with that of the simple channel with

and without straight ridges. Their results showed significantly higher mixing for the grooved channels with the best results obtained for SHM. Later on, Stroock et al. [53] analytically described how pressure-driven flows over grooved surfaces develop transverse components. They quantified an analytical expression to measure the helicity of the flow and compared it with the experimentally measured values.

Wang et al. [54] studied numerically the mixing in microchannels with grooved surfaces by applying the particle tracking technique. They summarized their results as although the microfluidic mixers with grooved surfaces could not always create chaotic effects, but they always generated the helical flow patterns. Helicity in such microchannels can provide sufficient folding and stretching to fluids that favors mixing. The study of Howell et al. [55] used a combination of two types of grooves namely, straight and chevron-shaped, arranged alternately on both the top and bottom of the channel pointing in opposite directions. It was shown that these double grooves strengthened the lateral velocities that resulted in complex vortex flows and the mixing is greatly enhanced that cannot be created with structures on the bottom alone. Yang et al. [56] numerically investigated the effects of geometric parameters on the mixing performance of a SHM with patterned grooves. They found that the depth ratio and the asymmetry index of the groove are found to be dominant geometric parameters whereas the rate of flow within the groove is verified to be the most significant factor that affects the mixing performance of a SHM.

Yang et al. [57] designed a novel micromixer with grooves crossing multiple sides of the microchannel called it as connected-groove micromixer (CGM). They reported that CGM can induced an intensely transverse field of fluids with a shorter pitch of spiral flow and hence more helical turns providing rapid mixing than patterned grooves on a single side alone. Tsui et al. [58] evaluated the mixing performance of different micromixers by placing patterned grooves (straight or herringbone) and block obstacles on the walls of the channels. Their results showed that block type obstacles are better performer for enhanced mixing but at the cost of higher pressure head. Naher et al. [59] investigated numerically three different microchannel geometries, viz, a plane channel and channels with rectangular blocks and with upward fins along the channel walls with the later showing better mixing. Sahu et al. [60] studied the effect of arrangements of the lateral blocks i.e., symmetric and staggered, and their number on the mixing efficiency. Sarkar et al. [61] studied

the effects of different types of wall protrusions on microfluidic mixing using CFD simulations. They conceptualized two new pattern of wall protrusions and compared their mixing ability to protrusions having standard geometrical shapes, e.g. rectangular, triangular and semicircular. Their results showed that the new designs proposed had better mixing capability than that of the standard designs.

Milotina and Lelea [62] analyzed the mixing phenomena in microtubes having four baffles that create orifice with half and quarter of the cross-section, respectively. The later promotes superior mixing due to the generation of rotational flow conditions that augmented mixing by advection. Fu et al. [63] adopted staggered oriented ridges (SOR) to generate transverse components of flow and to induce chaotic advection. They fabricated two designs of SOR, namely, I and II. They also performed numerical modelling to quantify the efficiency of mixing by computing the amount of lineal stretching of fluid elements which can be used as a measure of chaotic advective mixing and found that SOR-II micromixer is more effective than that of the SOR-I micromixer. The geometric factors that affect the generation of advection flow in this micromixers were identified by Xu et al. [64]. They found that factors like the inflow directions, the ridge height ratio and the ridge asymmetry index had significant effect on the mixing performances.

Shih and Chung [65] proposed a high-efficiency planar micromixer that had three mixing units each contained three baffle obstacles as well as three gaps. They explored the mixing capability of this micromixer for a wide range of Re for the effect of different geometric parameters and ranked them as: Gap ratio > Number of mixing units > Baffle width > Chamber ratio. The advantage of this mixer is that good mixing efficiency can be obtained at relatively low-pressure drop.

1.2.3.4 Serpentine/wavy/zigzag microchannels

The channel with wavy walls is one of the several devices employed for enhancing the heat and mass transfer efficiency of processes having high Peclet numbers [66]. Most commonly used wavy wall channels are those where the top and bottom walls are either at an offset of 0° or 180° . The first case with the channel walls are in phase is commonly referred to as a serpentine or corrugated channel whereas the second type is also known as converging-diverging type of channels [67].

Goldstein and Sparrow [68] were perhaps the first to study fluid flow and heat transfer in a corrugated channel. After that various research studies showed that use of wavy walls is preferable for enhancing the heat transfer. Use of wavy walls for mass transfer enhancements has been well documented for both macrochannels [66, 69–71] as well as microchannels [72–74]. Nishimura and co-workers [66] investigated mass transfer in a serpentine channel focusing on the transitional flow regime. It was found that at low Reynolds numbers the flow is laminar and two-dimensional, whereas for higher Reynolds numbers the flow becomes turbulent and shows an unsteady three-dimensional vortical structure. The unsteadiness of the flow resulted in a significant increase in mass transfer for turbulent flow.

Nishimura et al. [69] studied the effect of wall shapes on the flow and mass transfer characteristics in symmetrical two-dimensional wavy-walled channels for two different wall shapes viz., sinusoidal and arc-shaped, at moderate Re of 20–300. They noticed a new flow structure consisting of a regular three-dimensional flow for the arc-shaped wall that make it to possess a larger mass transfer rate than the sinusoidal wall. Further, they [70] investigated the occurrence of longitudinal vortices in channels with narrow spacing. Forced oscillatory flow in wavy channels was studied by Nishimura [71] for Reynolds numbers between 10 and 500. It was found that a serpentine channel yields better mass transfer and pumping power performance than a converging-diverging channel at low St . At high St , however, a converging-diverging channel yielded higher mass transfer rates.

Mengeaud et al. [72] illustrated the effects of both flow rate and channel geometry on hydrodynamics and mixing efficiency in the mixing process of species in a zigzag microchannel integrating a Y-junction by the use of finite element method. They reported that the transversal components of the velocities generated by the recirculation zones in the channel play a major role in spreading the species from the interface to the walls. Liu et al. [73] carried out numerical investigation to study the influence of difference in the properties of two mixing fluids on the mixing behavior in three micromixers: squarewave mixer, three-dimensional serpentine mixer and a staggered herringbone mixer. They found that among the three channels, serpentine channel performs better and at low Re , the mixing performance varied inversely with mass fraction of glycerol. Similar type of study was also performed by Hossain

et al. [74]. They carried out a comparative study for the mixing performances of three microchannels with different geometries: zig-zag; square-wave; and curved, for a wide range of $Re \approx 0.267$ -267. They found square-wave microchannel as the best candidate for mixing performance for most Re , however, the curved channel exhibits the smallest pressure drop among the microchannels. Microchannels with three different geometries of integrated obstructions are compared for their mixing efficiencies with that of converging-diverging and zigzag type microchannels without obstacles [75]. The simulation results showed that the zigzag type micro-mixer was found to have the best mixing performance.

Chung et al. [76] investigate numerically the fluid mixing of the rhombic micromixer with flat angles and showed high mixing efficiency compared to cross-shape straight microchannel. Over 95% mixing efficiency had been achieved at $Re = 180$ due to enhancement of vortices. Alam and Kim [77] studied the mixing enhancements by providing rectangular grooves along the walls of the serpentine channels. They reported that grooved microchannels produce better mixing performance at $Re > 10$ and the mixing index is sensitive to the width of the grooves but is not sensitive to the depth of the grooves. Parsa et al. [78] proposed a new microchannel with convergentdivergent sinusoidal side walls. They studied the effects of aspect ratio of cross-section and ratio of amplitude to wave length on pressure-drop and mixing index. The results showed that with increasing the aspect ratio of microchannel cross-section, mixing index improved and pressure-drop reduced in all Reynolds numbers. Parsa and Hormozi [79] in their further study noticed that mixing index drastically depends on phase shift (ϕ) and wavelength of side walls and found the best mixing for $\phi = 3\pi/4$ and at a wavelength to amplitude ratio of 3.3.

The objective of the work of Kanaris et al. [80] is to study the effect of the common “building block” of micromixers on the mixing efficiency and on the corresponding pressure drop. For this they selected five types of serpentine micromixer versions of a simple T-intersection viz., simple orthogonal serpentine geometry, two orthogonal serpentine designs with blocks extending on two parallel planes resembling the letter C and L, and a curved serpentine extended either on a single plane or on two parallel planes. They deduced that the geometries that induce a helical flow path offer advantages to enhance mixing which was observed in L-type microdevice. Chen et al. [81] also conducted numerical and experimental studies to

compare the mixing capabilities of different serpentine micromixers. They found the square-wave micromixer to be more efficient for mixing than that of multiwave and zigzag micromixers due to its more sharp turns and longer path of the flow.

1.2.3.5 Embedded obstacles/ridges

Use of flow obstacles placed in the channel is another commonly used passive mixing technique to improve mixing. Placement of obstacles tried to disrupt the flow velocity field altering the flow direction from one fluid to another and thus caused the reduction of the diffusion path [82].

Wang et al. [82] used a 2D numerical method to investigate the micromixer with cylindrical obstacles placed in the channel. It was found that the asymmetric layouts of the obstacles are more favorable rather than the symmetric arrangements. Monaco et al. [83] also reported the same findings by using lattice Boltzmann method. Wang and Hu [84] studied the effect of different parameters such as number, horizontal spacing distance and angle of arrangement for the cylindrical obstacles placed in V-arrangement in Y-type microchannel for improved mixing.

The study of Wang et al. [85] showed that the mixing in a Y-type microchannel can be greatly enhanced by incorporating six rectangular obstacles embedded periodically within the micromixer. Bhagat et al. [86] examined the design of diamond-shaped obstacles within a micromixer experimentally. They also reported simulated results for the flows with circular-shaped, triangular-shaped, diamond-shaped, and stepped diamond-shaped obstacles. Among them, the stepped-diamond shaped obstructions yielded the best mixing.

Kim and Kim [87] studied the mixing enhancements by using rectangular obstacles and reported that properly designed geometric parameters, such as layout, angle of inclination with main flow direction and aspect ratio of obstacles, resulted in improving the mixing performance with only little increase of the pressure drop. Bhagat and Papautsky [88] demonstrated that microfluidic mixers designed for efficient fluidic mixing may not necessarily be efficient for mixing of particle flows. To accomplish this they proposed a micromixer embedded with patterned rectangular obstacles placed at an angle of 45° and showed that their obstruction micromixer exhibits excellent mixing performance for particulate flows.

In recent times enhancement of convective heat transfer from macro-to-microscale by generation of longitudinal vortices (LV) in the flow has received much attention and reported in various research articles [89,90]. The phenomenological similarity between heat and mass transfer opened up the use of longitudinal vortices to increase the mass transfer. These vortices are induced by using either rectangular or triangular shaped vortex generators commonly called as winglets. Kaniewski et al. [91] presented a numerical study of the mixing of two laminar streams of different gases at $Re = 250$ in a large-scale rectangular channel by using a pair of rectangular winglets. They pointed out that a LV needs to be generated with an axis between the two (frequently parallel) streams in mass transfer configurations and reported more than 50% enhancements in mixing with vortex generators than that of without winglets. Hsaio et al. [92] studied the effects of geometrical parameters on the performance of micromixers with micro-scale LVGs are investigated by numerical simulations. Their results showed that the mixing efficiency of the micromixer with divergent RWPs is greater than that of the micromixer with convergent RWPs, with single RW and the micromixer without RWPs for a wide range of Re . They ranked the geometrical parameters according to relative effectiveness as: asymmetry index > angle of attack > winglet height > winglet spacing. Huang et al. [93] extended the work of Hsaio et al. [92] for a full three-stream mixing channel focussing on the effects of the asymmetrical arrangement and the attack angle of the LVGs on fluid mixing.

1.2.4 Active mixing techniques

In this subsection, a glimpse of various literatures available on active mixing enhancement techniques have been reported. Active micromixers are those that use external perturbation to stir the fluid to increase the convective transport of species. Various active mixing techniques can be divided in the following categories, such as, ultrasound, acoustically induced vibrations, electro-kinetic instabilities, pulsing the incoming flow rate, magneto-hydrodynamic action among other means to stir the fluids in order to enhance mixing.

The principle of acoustic/ultrasonic actuation has been used by many researchers to enhance mixing in micromixers [94–101]. Zhu and Kim [94] studied microfluidic

motion by using loosely focused acoustic waves. This technique of heatless acoustic agitation can be advantageous to microfluidic systems where the heating is not desirable. Liu et al. [95,96] presented a novel mixer based on the principle of bubble-induced acoustic microstreaming. Ahmed et al. [98] demonstrated a mixing time as low as 120 ms for a micromixer by trapping air bubbles within the pre-designed grooves on the sidewalls of the Y-shaped channel. Wixforth [99] used surface acoustic waves (SAW) to actuate smallest possible amounts of fluids on the planar surface of a piezoelectric chip. Similar study was also reported by Beyssen et al. [100]. Srithiraran et al. [101] demonstrated the applicability of a SAW-based micro-agitation for conventional, three-dimensional Y-shaped microfluidic systems. In the work of Luong et al. [102], the concept of SAW-induced mixing of continuous flow is applied to fluids having Peclet number as high as 74.4×10^3 .

Electrokinetic forcing, in particular electro-osmosis, serves as an effective means for enhanced fluid mixing [103–108]. Oddy et al. [103] used an electrokinetic process to rapidly stir micro- and nanoliter volume solutions for microfluidic bioanalytical applications. Using the same principle, Huang et al. [106] presented a cross-shaped microfluidic mixer featuring a pair barrier to generate a shedding flow due to electrokinetic instability that resulted in better mixing. Chen and Cho [107] analyzed numerically the effects of the chaotic electrokinetic driving forces on the fluid flow and mixing characteristics within the micromixer. Lim et al. [108] studied the effect of introducing a constriction in a T-type micromixers under periodic electro-osmotic flow.

Magneto-hydrodynamics (MHD) is the study of flow of electrically conducting liquids in electric and magnetic fields. The working principle of magneto-hydrodynamic micromixers is nothing but the Lorentz force. The generated Lorentz force can stretch and fold the liquids in a mixing chamber that is responsible for superior mixing. Micropumps based on the magneto hydrodynamic forces are reported by Jang and Lee [109], Lemoff and Lee [110] etc. Bau et al. [111] described a prototype mixer based on MHD to enhance mixing in micro total analysis systems. Oh et al. [112] utilized magnetically actuated ferrofluid plugs to generate perpendicular periodic pressure oscillation in a T-shaped mixing channel. Tsai et al. [113] reported the mixing phenomena between ferro-nanofluid and water using permanent magnet in a Y-type semi-active micromixer.

The dependency of diffusion constants on temperature is the key parameter for enhanced mixing due to thermal actuation. Mao et al. [114] used a linear temperature gradient across number of parallel channels for achieving micromixing. Tsai and Lin [115] showed that generating thermal disturbance by using a thermal bubble in a Y-shaped mixing channel produced an intrinsically oscillatory flow which can induce a wavy liquid interface that accelerate the mixing process. Kim et al. [116] accomplished micromixing in a biochemical reaction in a microfluidic chamber by using natural convection. Xu et al. [117] analyzed the thermal mixing characteristics in a T-shaped microchannel where hot and cold deionized water (DI water) is injected through the two inlets.

The pioneering work of using pressure field disturbance as a means of active micromixing technique has been reported by Lee et al. [118]. They investigated numerically the mass transfer enhancement by a pulsatile laminar flow in an axisymmetric wavy channel for the range of $50 \leq Re \leq 250$. They reported the generation of circulating vortices that is expected to enhance the mass transfer rate. Equivalent to pressure disturbance, the use of pulsing velocity for attaining enhanced mixing in micromixers at a small Reynolds number has been reported in many literatures.

Glasgow and Aubry [119] studied the effect of pulsing the flow rate in mixing in a simple T-channel intersection numerically. They reported that the best results occurred when both inlets are pulsed 90° out of phase. Studies related to the parameters that can influence the mixing behavior in a microchannel with pulsatile flow has been reported by Glasgow et al. [120]. The work of Hitt and McGarry [121] presented a computational investigation of the interfacial dynamics of pulsatile flows at a microchannel junction with circular and D-shaped cross-section. Mao and Xu [122] performed similar numerical study with 180° phase difference between the two inlets for a T-microchannel and reported that Strouhal number (St) and amplitude significantly effect the mixing performance. Ammar et al. [123] performed a comparative study for the effect of pulsed flow with 180° phase difference on the mixing behavior of different microfluidic junctions. A complete study of using pulsatile flow for mixing enhancement has also been reported by Cheaib et al. [124]. They investigated the dependence of the mixing index on various dimensionless groups.

However, combination of both active and passive mixing techniques have also been found in the literatures. Goullet et al. [125] studied the combined effect of both flow pulsing and the inclusion of features in the channels (ribs in their study). They found that the pulsed flow technique is more effective for mixing than the secondary flow induced by the ribs. However, combining both the methods leads to even better mixing. Chen and Cho [126] proposed a combined active-passive approach in which a wavy-wall section is incorporated within the microchannel along with periodic velocity perturbations applied to the two inlet streams. Their results revealed that mixing performance can be improved by increasing the length of the wavy-wall section and the geometric amplitude of the wavy surface. Miranda et al. [127] also proposed another combination of active-passive mixing approach by combining alternate flow and rectangular obstacles. Their numerical results have showed that mixing increases with the increase of the number of obstacles and frequency. An active-passive mixing technique based on the interaction between the fluids and an obstacle that is heaving in the middle of a channel is studied numerically by Ortega-Casanova [128]. They reported immense enhancement in the mixing efficiency by this method.

Historically, active mixers seem to perform better than passive ones in terms of time and space needed for mixing. However, they suffer from the drawback of fabrication complexities, high cost for active control, typically high power consumption, and difficulties arise in integrating with other devices due to the presence of moving parts. Also, some of the active mixing mechanisms such as ultrasonic waves and high temperature gradients can damage biological fluids making them a poor choice for biological processing. Due to these problems, the use of active mixers is limited on microfluidic devices and hence, passive micromixers are becoming more popular among the microfluidics community.

Considering all the above mentioned literatures, it has now been discussed about the motivations of the present thesis.

1.3 Motivation

By reviewing the available literature in the previous section, it has been noticed that the use of incompressible formulation can be applied for a specific range of variable density problems. For example, for problems involving density variations due to thermal gradients, incompressible Boussinesq approximations can be used when the density ratios remain small enough (≤ 2). This situation is feasible only when the relative temperature difference of less than 10%. However, for flows where the typical density ratio is higher than 8 (such as combustion), the fully incompressible assumption is not at all valid, as these flows do not fall under the Boussinesq limit. From the literature, it is evident that, both the two class of miscible fluids, i.e., reacting and non-reacting, are handled by different formulations although they fall in the low Ma limit. As such, there is a need to develop a single generalized formulation for handling both these two domains of fluid flows problem. To the best of my knowledge, very less attention has been given in this direction to develop a generalized solver over hybrid unstructured meshes that can handle both incompressible and quasi-incompressible limit.

Another important aspect is to enhance the mixing capability, especially for liquid-liquid mixing flows. Previous works reveal that a considerable amount of studies have focused on optimizing the mixing performances. Between the two methods of improving the mixing ability of micromixers, the passive mixing techniques are more popular in the scientific community due to its inherent advantages over the active techniques. Numerous designs of passive micromixers are proposed and investigated by various researchers to achieve efficient mixing. But most of these designs are found to be either suffering from very complex design or from very high pressure drop. Any new design of micromixers that can have the potential of providing higher mixing efficiency but at the cost of lower pressure drop is always appreciated. Thus, in this work, we would like to focus our attention to propose certain new passive mixing techniques that can give higher mixing at lower pressure head loss. However, a more detailed study to exploit the flow physics and the mixing behavior of the newly designed passive mixing techniques is always warranted.

Motivated by the above points, this doctoral thesis is thus devoted to the development of a generic and robust numerical framework for miscible fluid flows on

arbitrary hybrid unstructured meshes and its application to laminar mixing and combustion. Generic in that, the numerical framework adopted should be capable of handling problems with no specific constraint on the density ratio whether low or high.

1.4 Research Objectives

With the primary motivation to put forward a detailed numerical analysis of mixing of multiple fluids in same phase, the objectives of this thesis have been set as follows.

1) **Development and validation of a generic quasi-incompressible flow solver**

The first objective of this doctoral thesis is to develop a robust, generic, three-dimensional mathematical framework for miscible flow simulations using finite volume method over hybrid unstructured grids. We exploit the low Mach number formulation for handling variable density miscible flows with no specific constraint on the density ratio. Extensive solution verification studies are carried out including accuracy studies of the flow solver.

2) **Investigations of truncation and discretization errors**

We study the relation between local truncation and discretization error on different meshes for convective and diffusive problems. A set of guidelines on the choice of mesh and schemes for mixing problems are devised on the basis of these results.

3) **Application of the solver to analyze mixing of liquids in microchannels**

The solver is used to study the laminar mixing of a binary liquid mixture in two-dimensional cross-T type microchannel. A novel passive micromixer with thin curved ribs is devised and parametric studies of its performance, in terms of both mixing efficiency and pressure drop, for ethanol-water mixture are carried out.

4) **To study the performance of a three-dimensional micromixer**

A three-dimensional cross-T micromixer designed exploiting the same two-dimensional configuration studied earlier is analyzed for its mixing performances. Studies are carried out using a commercial solver to understand the effects of obstacle geometry

and layout on mixing index and overall pressure drop.

5) **Application of the solver to study gaseous mixing in corrugated channels**

The flow solver is also employed to study argon-air mixing in macrochannels with wall corrugation. The role of wavelength and amplitude of sinusoidal corrugations on mixing performance is thoroughly analyzed to determine an optimal configuration.

6) **Extension of numerical approach to combustible miscible flows**

As a final step, attempts have been made to extend the approach to simulate mixing of gaseous reacting species. A preliminary study for diffusion (non-premixed) flames is carried out and demonstrates the efficacy of the quasi-incompressible formulations for handling reacting miscible flows.

1.5 Thesis Layout

A general introduction on miscible fluid flows has been presented in Chapter 1. In addition to this, literature survey regarding the different mixing enhancement techniques has also been shown. The chapter is concluded by presenting the objectives of the present thesis. Chapter 2 discusses the governing equations and discretization procedure adopted in the context of developing a generalized formulation that can handle fluid mixing in both incompressible and quasi-incompressible limit. A detailed analysis of the numerical errors, truncation as well as discretization, associated with different convective schemes has been conducted in Chapter 3 to choose the best scheme among them for simulations of mixing flows. Chapter 4 presents the results showing the verification and validations cases for the developed formulation in simulating miscible flows with varying density due to presence of gradients concentrations, for binary liquids and gaseous mixture. Application the developed solver in regard to simulating the mixing performance of a two-dimensional cross-T microchannel with the use of a newly designed obstacle geometry is presented in Chapter 5. Chapter 6 poses the results of the three-dimensional effects of the newly conceptualized obstacle design for mixing enhancements in microchannels. The fo-

cus of Chapter 7 lies in analyzing the mixing characteristics of a binary gaseous mixture in a channel with wavy walls and to study the effect of different parameters on the mixing ability. Chapter 8 presents a preliminary work showing the applicability of the new formulations in simulating the laminar diffusion flames at low Mach number limit. Chapter 9 concludes the present work together with the futuristic scope of the present work.





Chapter 2

Governing Equations and Discretization Procedure

The focus of present work is to develop a generalized three-dimensional mathematical framework for the simulation of miscible flows that can handle simultaneously for flows involving high density ratio (e.g. gaseous combustion) and low density ratio (e.g. microfluidic mixing) over a hybrid unstructured grid at low Mach number limit. The flow regime corresponding to this class is termed as ‘quasi-incompressible’. For the simulation of this kind of flow problems, a popular approach found in the literatures is the low Mach number formulation. In this chapter, a brief discussion on low Mach number formulation has been carried out first. Then the final form of the three dimensional governing equations are presented next followed by the discretization procedure adopted with finite volume method methodology. This is then followed by the solution algorithm and some post-processing technique of the numerical data.

2.1 Low Mach Number Formulation

In fluid dynamics the basic fluid flows problems can be broadly classified into two categories : compressible and incompressible. The parameter which usually differentiates the regimes of incompressible and compressible flows is known as Mach number (Ma). In literature it is reported that the two flow regimes are generally differentiated at $Ma = 0.3$. However, there are situations in which density cannot

be considered to be constant even though Ma is less than 0.3, e.g., combustion in the form of deflagrations. The variations of density field may be due to the presence of gradients of temperature, concentrations of species or both. The terminology associated with these type of flows is low Mach number variable-density flows or quasi-incompressible flows. To investigate such type of flows, Boussinesq approximation may not be appropriate when the relative temperature difference exceeds 10% limit for example combustion problems. As such, for handling of this category of flows i.e., quasi-incompressible flows, an intermediate model between the Boussinesq and the full compressible flow model must be employed. One such intermediate model which is now very extensively used by the scientific community is the “low Mach number formulation” presented briefly in the following section.

The low Mach number formulation adopted in the present work is based on method proposed by Paolucci [4]. The inherent idea behind this approximation is the decoupling between the acoustic speed and the flow velocity. Because it has been found that in some flows particularly with low Mach number, the acoustic waves moves much faster than everything else which is of interest and at the same time carry a minute fraction of energy compared to the part transferred by the flow field. As such the decoupling between the acoustic speed and flow velocity allows substantial relaxation on time step constraint which is limited by Courant-Friedrich-Lewy (CFL) condition which simply states that a sound wave cannot travel more than one computational cell in one time increment. For any computational study the value of time step should be such that one must use the maximum possible value within the stability limit to get the faster results.

This approximation relies on the asymptotic expansion in respect of a small number (Ma) of all the primitive variables like velocity, temperature, pressure and density and properties like density, viscosity and thermal conductivity. The equations are finally reduced by taking the lower order values for the Mach Number. For the derivation of low Mach number equations, the general form of governing equations corresponding to non-reacting, non-radiative single species flows has been taken. Equations 2.1 - 2.3 are the general form of the conservation equations for mass, momentum and energy, respectively whereas Eq. 2.4 represents the equation of state for ideal gas.

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} = 0 \quad (2.1)$$

Momentum Transport Equation:

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + (\rho - \rho_o) g_i \quad (2.2)$$

Energy Equation:

$$\frac{\partial (\rho c_p T)}{\partial t} + \frac{\partial (\rho c_p T u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\kappa \frac{\partial T}{\partial x_j} \right) + \frac{dp}{dt} \quad (2.3)$$

Ideal gas law:

$$p = \rho RT \quad (2.4)$$

where $\rho, u_i, p, T, c_p, \kappa, R$ are density, velocity components in i^{th} direction, total pressure, temperature, specific heat at constant pressure, thermal conductivity and specific gas constant, respectively. These equations are non-dimensionalized by using c_0, T_0, p_0 and ρ_0 as scales of velocity, temperature, pressure and density. Here c_0 represents the speed of sound at initial temperature T_0 , density ρ_0 , and pressure p_0 all evaluated at the reference gravitational potential line. Similar normalization are also done for viscosity, thermal conductivity and specific heat by their initial values μ_0, κ_0, c_{p0} and c_{v0} , respectively. The gravitational vector is non-dimensionalized by their initial magnitude g_0 . In addition length and time are referenced to l and l/U where l is a representative length scale and U represents the characteristic fluid speed. Here p_0 scales the thermodynamic pressure where as $\rho_0 U^2$ scales the dynamic pressure. These normalizations leads to appearance of seven independent dimensionless parameters in the governing equations, which are Mach number Ma , Reynolds number Re , Froude number Fr , Peclet number Pe , the ratio of specific heat γ which are defined by

$$Ma = \frac{U}{c_0}, Re = \frac{\rho_0 U l}{\mu_0}, Fr = \frac{U^2}{g_0 l}, Pe = \frac{\rho_0 c_{p0} U l}{\kappa_0}, \gamma = \frac{c_{p0}}{c_{v0}} \quad (2.5)$$

Using the above non-dimensional parameters the final form of the continuity, momentum, energy, and equation of state are reduced to equations described below

with dimensionless variables written as their dimensional counterparts to prevent overloaded notations.

$$\frac{\partial \rho}{\partial t} + \frac{1}{Ma} \frac{\partial (\rho u_j)}{\partial x_j} = 0 \quad (2.6)$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{1}{Ma} \frac{\partial (\rho u_j u_i)}{\partial x_j} = -\frac{1}{\gamma Ma} \frac{\partial p}{\partial x_i} + \frac{1}{Re} \frac{\partial \tau_{ij}}{\partial x_j} + \frac{Ma}{Fr} \rho g_i \quad (2.7)$$

$$\begin{aligned} \frac{\partial (\rho c_p T)}{\partial t} + \frac{1}{Ma} \frac{\partial (\rho c_p T u_j)}{\partial x_j} = & \frac{1}{Pe} \frac{\partial}{\partial x_j} \left(\kappa \frac{\partial T}{\partial x_j} \right) + \frac{\gamma - 1}{Re} \left(\tau_{ij} \frac{\partial u_i}{\partial x_j} \right) \\ & + \frac{\gamma - 1}{\gamma} \left(\frac{\partial p}{\partial t} + \frac{1}{Ma} \frac{\partial (\rho u_j)}{\partial x_j} \right) \end{aligned} \quad (2.8)$$

$$p = \rho T \quad (2.9)$$

Further we expand the velocity and thermodynamic variables in small parameters Ma as follows:

$$u_i = Ma [u_i^0 + Ma^2 u_i^1 + o(Ma^2)] \quad (2.10)$$

$$T = T^0 + Ma^2 T^1 + o(Ma^2) \quad (2.11)$$

$$\rho = \rho^0 + Ma^2 \rho^1 + o(Ma^2) \quad (2.12)$$

$$p = p^0 + Ma^2 p^1 + o(Ma^2) \quad (2.13)$$

Similar expansions are adopted for properties like μ , κ , c_p . Using the above expansions we obtain the $O(1)$ and $O(Ma^2)$ conservation equation for continuity, momentum, energy equations and perfect gas law.

Continuity Equation:

$$O(1) : \frac{\partial \rho^0}{\partial t} + \frac{\partial (\rho^0 u_j^0)}{\partial x_j} = 0 \quad (2.14)$$

$$O(Ma^2) : \frac{\partial \rho^1}{\partial t} + \frac{\partial (\rho^0 u_j^1 + \rho^1 u_j^0)}{\partial x_j} = 0 \quad (2.15)$$

Momentum Transport Equation:

$$O(1) : -\frac{1}{\gamma} \frac{\partial p^0}{\partial x_i} = 0 \quad (2.16)$$

$$O(Ma^2) : \frac{\partial(\rho^0 u_i^0)}{\partial t} + \frac{\partial(\rho^0 u_i^0 u_j^0)}{\partial x_j} = -\frac{1}{\gamma} \frac{\partial p^1}{\partial x_i} + \frac{1}{Re} \frac{\partial \tau_{ij}^0}{\partial x_j} + \frac{1}{Fr} \rho^0 g_i \quad (2.17)$$

Energy Equation:

$$O(1) : \frac{\partial(\rho^0 c_p^0 T^0)}{\partial t} + \frac{\partial(\rho^0 c_p^0 T^0 u_j^0)}{\partial x_j} = \frac{1}{Pe} \frac{\partial}{\partial x_j} \left(\lambda^0 \frac{\partial T^0}{\partial x_j} \right) + \frac{\gamma-1}{\gamma} \left[\frac{\partial p^0}{\partial t} + \frac{\partial p^0 u_j^0}{\partial x_j} \right] \quad (2.18)$$

$$O(Ma^2) : \frac{\partial(\rho^0 c_p^0 T^1)}{\partial t} + \frac{\partial(\rho^1 c_p^0 T^1)}{\partial t} + \frac{\partial(\rho^0 c_p^1 T^0)}{\partial t} + \frac{\partial(\rho^1 c_p^0 T^0 u_j^0)}{\partial x_j} + \frac{\partial(\rho^0 c_p^0 T^0 u_j^1)}{\partial x_j} + \frac{\partial(\rho^0 c_p^0 T^1 u_j^0)}{\partial x_j} + \frac{\partial(\rho^0 c_p^1 T^0 u_j^0)}{\partial x_j} + \frac{\gamma-1}{Re} \frac{\partial \tau_{ij}^0}{\partial x_j} \frac{\partial u_i}{\partial x_i} \quad (2.19)$$

Ideal gas law:

$$O(1) : p^0 = \rho^0 T^0 \quad (2.20)$$

$$O(Ma^2) : \frac{p^1}{p^0} = \frac{\rho^1}{\rho^0} + \frac{T^1}{T^0} \quad (2.21)$$

From Eq. 2.16 it has been seen that the leading part of the pressure depends only on time where as the motion-induced spatial variation in pressure $p^1 = O(\rho U^2)$ are comparatively smaller than the total static pressure $p^0(t)$. After neglecting the $O(Ma^2)$ terms in the continuity and energy equations and then reintroducing the different scales for the variables and dropping the zero superscript, the final dimensional form from the remaining leading order terms of the governing equations are arrived. The pressure can be expressed as the sum of thermodynamic pressure $\bar{P}(t)$ and dynamical pressure $\Pi(x, t)$ as

$$p(x, t) = \bar{P}(t) + \Pi(x, t) \quad (2.22)$$

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0 \quad (2.23)$$

Momentum Transport Equation:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial \Pi}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + (\rho - \rho_o) g_i \quad (2.24)$$

Energy Equation:

$$\frac{\partial(\rho c_p T)}{\partial t} + \frac{\partial(\rho c_p T u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\kappa \frac{\partial T}{\partial x_j} \right) + \frac{d\bar{P}}{dt} \quad (2.25)$$

Ideal gas law:

$$\bar{P} = \rho RT \quad (2.26)$$

It can be seen that the splitting of pressure into thermodynamic part ($\bar{P}$) and hydrodynamic part (Π) introduces a new unknown. Hence extra equations are required for the calculation of thermodynamic pressure ($\bar{P}$) and the $\frac{d\bar{P}}{dt}$ term appear in the energy equation. These calculations are required only for closed enclosures but not necessary for open systems. Because in the case of open systems the $\bar{P}$ equilibrates with the ambient pressure instantaneously and hence the $\frac{d\bar{P}}{dt}$ vanishes. For closed systems, the expressions for thermodynamic pressure and $\frac{d\bar{P}}{dt}$ are obtained through mass and energy conservation equations, respectively.

2.2 Governing Equations

This section provides the generalized three-dimensional governing equations in differential form for laminar, isothermal (non-reacting), single-phase, miscible flows of fluids following low Mach number model. These equations include conservation equations for mass, momentum and species mass fractions. Assumptions taken for writing the governing equations are as follows:

1. Low Mach number flows.
2. Gravity is neglected.
3. The variations in density and viscosity take place only due to variation in concentration of species.
4. Viscous dissipation, surface tension and radiative forces are neglected.
5. The channel walls are assumed to be smooth, i.e. no roughness present.

Continuity Equation:

The overall continuity equation expressing conservation of mass is

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0 \quad (2.27)$$

Momentum Equations:

The momentum equation expressing the law of conservation of momentum is

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_j u_i)}{\partial x_j} = -\frac{\partial \Pi}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (2.28)$$

where τ_{ij} is shear stress tensor given as

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_p}{\partial x_p} \quad (2.29)$$

and μ is the dynamic viscosity.

Mass Fraction Equations:

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho Y_k u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial Y_k}{\partial x_j} \right) \quad (2.30)$$

where D is the mass diffusivity constant.

Density of the mixture:

For liquid mixtures having k^{th} liquid species, the mixture density is updated as,

$$\rho = \frac{1}{\sum_k \frac{Y_k}{\rho_k}} \quad (2.31)$$

where ρ_k is the density of the k^{th} species.

For a gaseous mixture, density of the mixture is calculated by using the equation of state. The equation of state for a multi-component gas mixture in a flow satisfying the low Mach number assumption is

$$\rho = \frac{\bar{P} \bar{W}}{R_u T} \quad (2.32)$$

where $\bar{W} = \frac{1}{\sum_k \left(\frac{Y_k}{MW_k} \right)}$ is the average molecular weight of the mixture.

Viscosity of the mixture:

The viscosity of the liquid mixture is calculated as a function of the mass fractions of the species by using an expression similar to that used in Sahu et al. [129],

$$\mu = \mu_{min} \exp^{Y_k \ln \frac{\mu_{max}}{\mu_{min}}} \quad (2.33)$$

where μ_{max} and μ_{min} are the viscosities of the species having maximum and minimum value, respectively.

Divergence constraint:

For low Mach number flows, the divergence of the velocity field is non-zero. For multicomponent flows, this constraint on the divergence of velocity field takes two different forms for mixtures of liquids or gases. The complete derivation for the divergence constraint for liquids mixture is shown in Appendix A.1. The final form of the velocity divergence constraint reads as

$$\frac{\partial u_i}{\partial x_i} = -\frac{\partial}{\partial x_j} \left(\frac{D}{\rho} \frac{\partial \rho}{\partial x_j} \right), \quad \text{for liquids} \quad (2.34)$$

However, for a gaseous mixture, the velocity divergence constraint can be derived by differentiating Eq. 2.32 along particle paths and replacing the Lagrangian derivatives by the corresponding governing equations [6]. The detailed derivation is shown in Appendix B.1.

$$\frac{\partial u_i}{\partial x_i} = \frac{1}{\rho} \sum_k \frac{\bar{W}}{MW_k} \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial Y_k}{\partial x_j} \right), \quad \text{for gases} \quad (2.35)$$

This constraint is used to calculate the source term of pressure Poisson equation which is better described in the following section.

In numerical simulations, all these coupled governing partial differential equations are solved by using any one of the numerical techniques. The very first step of implementing the numerical technique is the discretization. The discretization procedure used in the present work has been discussed in Section 2.3.

2.3 Discretization Procedure

In order to carry out numerical simulations, there are primarily three different numerical techniques available, which are finite difference method (FDM), finite vol-

ume method (FVM) and finite element method (FEM). Among these three different numerical techniques, we are using the FVM which is known for its conservative properties to solve the set of partial differential equations. In the FVM, first, the entire solution domain has been sub-divided into a number of non-overlapping cells called ‘control volumes’. This process is referred to as grid generation. In this work, the unstructured grid generation software GAMBIT [130] is used for this purpose. The geometric information pertaining to each control volume such as the volume, face areas and surface normals as well as the centroids, needs to be used in the finite volume framework. The cell shapes could be arbitrary convex polygons but largely consist of tetrahedra, hexahedra, prisms and pyramids or a combination thereof (refer Fig. 2.1). Figure 2.2 shows a typical representation of a hybrid grid where a centrally located tetrahedral cell is surrounded by three prisms and one another tetrahedral cell.

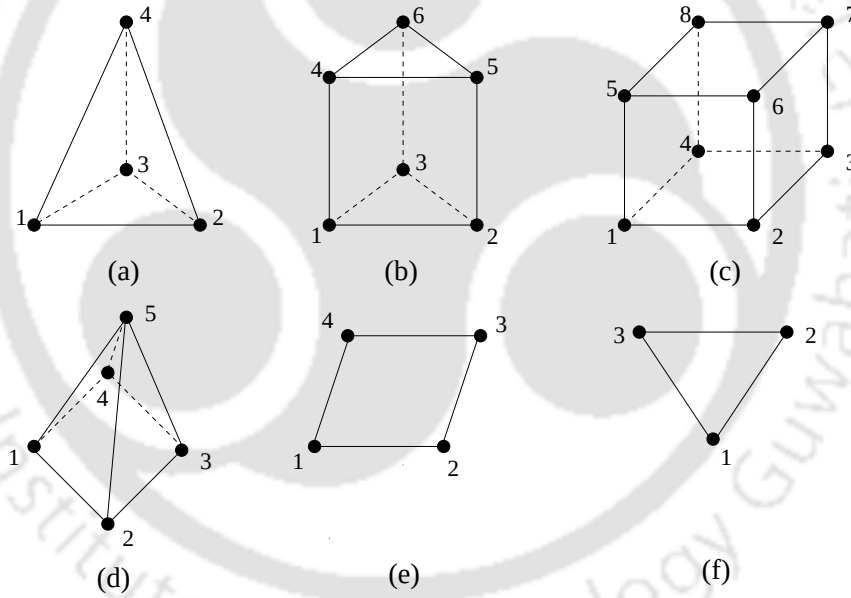


Figure 2.1: Different types of cell: (a) Tetrahedron (b) Prism (c) Hexahedron (d) Pyramid (e) Quadrilateral (f) Triangle

To convert the continuous partial differential equations into discrete form using FVM, the integral form of the governing equations are used. This form of governing equations is obtained upon integrating the differential form of governing equations over the entire control volumes and then applying Gauss divergence theorem. For

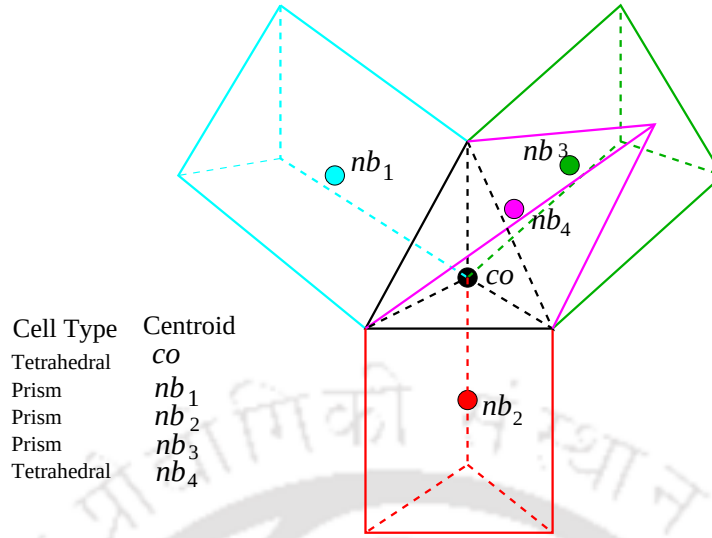


Figure 2.2: Typical representation of a hybrid mesh showing the main control volume along with its neighbor

example, the conservation equation for any variable ϕ in the integral form is shown below.

$$\frac{\partial}{\partial t} \int_V \rho \phi dV + \int_S (\rho \mathbf{u} \phi - \Gamma_\phi \nabla \phi) \cdot d\mathbf{S} = \int_V S_\phi dV \quad (2.36)$$

where Γ_ϕ is the diffusivity constant and S_ϕ is the source term. The numerical approach adopted in this work is similar to the work of Dalal et al. [131]. A collocated grid arrangement has been used where all the dependent variables are defined at the centroid of each individual cell. Consequently, the discrete form of the integral governing equations for each cell may be derived using the following assumptions.

- A cell averaged value is ascribed to the centroid of each control volume.
- A single-point Gauss quadrature is employed for the surface integral and requires only the face mid-point value of all variables.

In FVM generally the governing equations are being solved for conserved variables. As such for any general scalar variable ϕ it has been assumed that $\rho \phi = \Phi$ and all the discretized form are shown in terms of Φ . The detailed discretization procedure of the convective, diffusive and source terms for the generalized transport equation (Eq. 2.36) are shown in the following section.

2.3.1 Temporal term

The temporal term Eq. 2.36, is discretized with Euler implicit time scheme with the assumption that the value of the dependent variable at the centroid is the average over the entire control volume as shown below.

$$\frac{\partial}{\partial t} \int_V \rho \phi dV \approx \frac{(\rho \phi)_{co}^{n+1} - (\rho \phi)_{co}^n}{\Delta t} V_{co} = \frac{(\Phi)_{co}^{n+1} - (\Phi)_{co}^n}{\Delta t} V_{co} \quad (2.37)$$

where subscript co represents the cell centroid of a particular cell, n is the time-step number and $\Phi = \rho \phi$ is the conservative form of variable ϕ .

2.3.2 Convective term

The discretization of convective flux term of Eq. 2.36 is done in following way. Firstly, the approximation for surface integral is done as below

$$\int_S \rho \mathbf{u} \phi \cdot d\mathbf{S} \approx \sum_f \rho_f \phi_f (\mathbf{u} \cdot \mathbf{S})_f = \sum_f \Phi_f F_f \quad (2.38)$$

Now, Φ_f can be found out by utilizing different convective schemes. However, different schemes suffer from different degrees of numerical diffusion. In the present solver, three different convective schemes are incorporated. One is Khosla-Rubin scheme which is a linear combination of upwind and central differencing scheme [132] whereas the other two are high resolution schemes namely Convergent and Universally Bounded Interpolation Scheme for the Treatment of Advection (CU-BISTA) [133] and Cubic Upwind Interpolation (CUI) [134].

Linear combination of upwind and central differencing schemes

Convection dominated flows suffer from unphysical oscillations if the direction of propagation is not accompanied for. In order to implement oscillation free higher order schemes on unstructured meshes with relative cost we adopt a linear combination of Central Difference Scheme (CDS) and first order Upwind Scheme (FOU). The convective fluxes using this scheme can be expressed as,

$$F_f \Phi_f = (F_f \Phi_f)^{\text{FOU}} + \gamma [(F_f \Phi_f)^{\text{CDS}} - (F_f \Phi_f)^{\text{FOU}}] \quad (2.39)$$

where, FOU and CDS represent upwind and central difference schemes, respectively. For calculating the value of variable Φ at face center in case of CDS a volume

interpolation is used where as for upwind scheme the value is taken to be equal to that of upstream cell center. Expanding these terms will result in,

$$F_f \Phi_f = \Phi_{co} [|F_f, 0|] - \Phi_{nb} [| - F_f, 0|] + \gamma \left[F_f \left(\frac{V_{nb}}{V_{nb} + V_{co}} \Phi_{co} + \frac{V_{co}}{V_{nb} + V_{co}} \Phi_{nb} \right) \right] - \gamma [\Phi_{co} [|F_f, 0|] + \Phi_{nb} [| - F_f, 0|]] \quad (2.40)$$

where $[|\alpha, \beta|]$ represents the maximum value between α and β . Subscripts (*co*, *nb*) denote the owner cell and neighbor cell, respectively. The owner and neighbor cells for any face are defined in a consistent manner with the unit normal pointing from owner to neighbor. The factor γ ($0 \leq \gamma \leq 1$) allows the introduction of the numerical diffusion ($\gamma = 0$ means pure FOU, $\gamma = 1$ means pure CDS).

CUBISTA

For implementing the CUBISTA scheme over unstructured meshes, normalized variable approach of Jasak et al. [135] is followed and the final form of the scheme in terms of normalized variable ($\tilde{\Phi} = \frac{\Phi - \Phi_U}{\Phi_D - \Phi_U}$, where subscript *U* and *D* refer to the far upwind and downwind cells) can be written as below.

$$\tilde{\Phi}_f = \begin{cases} \frac{7}{4}\tilde{\Phi}_C, & 0 < \tilde{\Phi}_C < \frac{3}{8} \\ \frac{3}{4}\tilde{\Phi}_C + \frac{3}{8}, & \frac{3}{8} \leq \tilde{\Phi}_C \leq \frac{3}{4} \\ \frac{1}{4}\tilde{\Phi}_C + \frac{3}{4}, & \frac{3}{4} < \tilde{\Phi}_C < 1 \\ \tilde{\Phi}_C, & \text{elsewhere} \end{cases} \quad (2.41)$$

In case of unstructured grid as shown in Fig. 2.3, far upwind point is not clearly defined. Using the approach of Jasak et al. [135], the value at the far upwind point is replaced by the known values of upwind and downwind grid points. They showed that,

$$\tilde{\Phi}_C = \frac{\Phi_C - \Phi_U}{\Phi_D - \Phi_U} = 1 - \frac{\Phi_D - \Phi_C}{2(\nabla \Phi)_C \cdot \mathbf{n}_f} \quad (2.42)$$

CUI

Another popular second order accurate scheme for convective flux calculation is the CUI scheme which is also presented by using the normalized variable approach and is given as

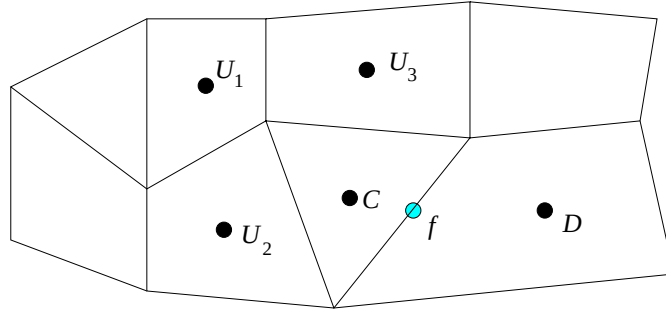


Figure 2.3: Unstructured grid showing upwind (C), downwind (D) and far upwind cells (U) with respect to face f

$$\tilde{\Phi}_f = \begin{cases} 3\tilde{\Phi}_C, & 0 < \tilde{\Phi}_C \leq \frac{2}{13} \\ \frac{5}{6}\tilde{\Phi}_C + \frac{1}{3}, & \frac{2}{13} < \tilde{\Phi}_C \leq \frac{4}{5} \\ 1, & \frac{4}{5} < \tilde{\Phi}_C \leq 1 \\ \tilde{\Phi}_C, & 1 < \tilde{\Phi}_C \leq 0 \end{cases} \quad (2.43)$$

2.3.3 Diffusive term

Integrating over the control volumes and then using Gauss divergence theorem, the diffusive fluxes of Eq. 2.36 is

$$\int_V \nabla \cdot (-\Gamma_\phi \nabla \phi) dV = - \int_S \Gamma_\phi \nabla \phi \cdot d\mathbf{S} \approx - \sum_f (\Gamma_\phi \nabla \phi \cdot \mathbf{S})_f = - \sum_f F_{d\phi f} \quad (2.44)$$

where $\mathbf{S}_f$ is the face area vector with a magnitude A_f and its direction is shown by unit vector $\hat{\mathbf{n}}_f$. For orthogonal grids, the vector $\hat{\mathbf{n}}_f$ co-align to the line joining adjacent cell centroids. However, for non-orthogonal grids, the surface vector is inclined to the line joining adjacent cell centroids. To understand it, let us consider a geometrical arrangement as shown in Fig. 2.4, where a face “abc” is shared by two neighboring cells with centers marked as co and nb . The face unit normal is represented by $\hat{\mathbf{n}}_f$. Projecting the cell centers over the surface normal will result in two more points co' and nb' . Now, we can write

$$\begin{aligned} \overrightarrow{O nb} + \overrightarrow{nb nb'} &= \overrightarrow{O nb'} \\ \overrightarrow{O co} + \overrightarrow{co co'} &= \overrightarrow{O co'} \end{aligned}$$

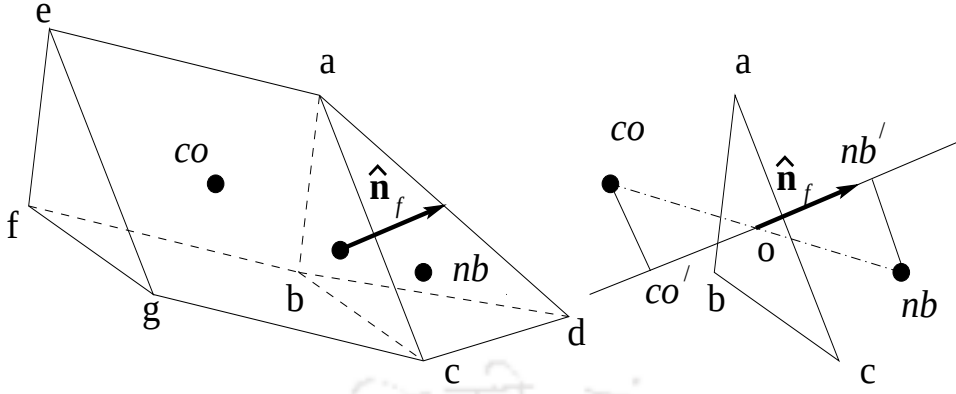


Figure 2.4: Non-orthogonal contribution of diffusive fluxes.

For a particular face, the diffusive fluxes can now be calculated as,

$$(\nabla\Phi)_f \cdot \mathbf{S}_f = A_f (\nabla\Phi)_f \cdot \hat{\mathbf{n}}_f = A_f \frac{(\Phi_{nb'} - \Phi_{co'})}{\Delta n} \quad (2.45)$$

where Δn is the distance between points co' and nb' . Using Taylor series expansion, $\Phi_{nb'}$ and $\Phi_{co'}$ can be expressed as (neglecting higher order terms),

$$\Phi_{nb'} = \Phi_{nb} + \nabla\Phi_{nb} \cdot \overrightarrow{nb \ nb'} \quad (2.46)$$

$$\Phi_{co'} = \Phi_{co} + \nabla\Phi_{co} \cdot \overrightarrow{co \ co'} \quad (2.47)$$

Substituting Eqs. 2.46 and 2.47 in Eq. 2.45, finally we get

$$(\nabla\Phi)_f \cdot \mathbf{S}_f = A_f \frac{(\Phi_{nb} - \Phi_{co})}{\Delta n} + \frac{(\nabla\Phi_{nb} \cdot \overrightarrow{nb \ nb'} - \nabla\Phi_{co} \cdot \overrightarrow{co \ co'}) A_f}{\Delta n} \quad (2.48)$$

The value of $\overrightarrow{nb \ nb'}$ and $\overrightarrow{co \ co'}$ can be obtained by following the procedure as shown below,

$$\overrightarrow{nb \ nb'} = \overrightarrow{O \ nb'} - \overrightarrow{O \ nb}, \quad \overrightarrow{O \ nb'} = (\overrightarrow{O \ nb} \cdot \hat{\mathbf{n}}_f) \hat{\mathbf{n}}_f$$

$$\overrightarrow{co \ co'} = \overrightarrow{O \ co'} - \overrightarrow{O \ co}, \quad \overrightarrow{O \ co'} = (\overrightarrow{O \ co} \cdot \hat{\mathbf{n}}_f) \hat{\mathbf{n}}_f$$

The first part of Eq. 2.48 is the orthogonal component of diffusive fluxes while the second part is mainly appearing due to non-orthogonality of the grids. It is to be noted that for calculating value at the face for any variable Φ , inverse volume

weighted interpolation technique employed by Dalal et al. [131] is used unless otherwise stated.

However, the discretization of the diffusive term of the momentum equation i.e., the second term of RHS of Eq. 2.28 gives rise to a set of source terms which are shown below (derivation is shown in Appendix A.2).

For u velocity

$$\begin{aligned}
 &= \sum_f \mu_f \underbrace{\left(\nabla u \cdot \mathbf{S} \right)_f}_{\text{Ia}} + \underbrace{\sum_f \mu_f \left(\frac{\partial u}{\partial x} S_{fx} + \frac{\partial v}{\partial x} S_{fy} + \frac{\partial w}{\partial x} S_{fz} \right)}_{\text{IIa}} \\
 &\quad - \underbrace{\frac{2}{3} \sum_f \mu_f \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) S_{fx}}_{\text{IIIa}} \quad (2.49)
 \end{aligned}$$

For v velocity

$$\begin{aligned}
 &= \sum_f \mu_f \underbrace{\left(\nabla v \cdot \mathbf{S} \right)_f}_{\text{Ib}} + \underbrace{\sum_f \mu_f \left(\frac{\partial u}{\partial y} S_{fx} + \frac{\partial v}{\partial y} S_{fy} + \frac{\partial w}{\partial y} S_{fz} \right)}_{\text{IIb}} \\
 &\quad - \underbrace{\frac{2}{3} \sum_f \mu_f \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) S_{fy}}_{\text{IIIb}} \quad (2.50)
 \end{aligned}$$

For w velocity

$$\begin{aligned}
 &= \sum_f \mu_f \underbrace{\left(\nabla w \cdot \mathbf{S} \right)_f}_{\text{Ic}} + \underbrace{\sum_f \mu_f \left(\frac{\partial u}{\partial z} S_{fx} + \frac{\partial v}{\partial z} S_{fy} + \frac{\partial w}{\partial z} S_{fz} \right)}_{\text{IIc}} \\
 &\quad - \underbrace{\frac{2}{3} \sum_f \mu_f \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) S_{fz}}_{\text{IIIc}} \quad (2.51)
 \end{aligned}$$

The first terms of Eqs. 2.49 - 2.51 are similar to that shown in Eq. 2.44 and hence the term is handled as shown in Eq. 2.48. The terms II-III of Eqs. 2.49 - 2.51 are zero for purely incompressible flows. Since, in this work, we are using the quasi-incompressible formulation, and hence these terms cannot be neglected and are treated as source terms. Any other source terms present in the governing equations are shown in the next section.

2.3.4 Source terms

The pressure term of Eq. 2.28 comes as a source term in the momentum equation and can be discretized as

$$-\int_S \Pi \cdot d\mathbf{S} \approx -\sum_f \Pi_f S_{fi} \quad (2.52)$$

Where Π_f is the pressure at the face center f and S_{fi} as the i^{th} direction component of the surface vector of face f . For evaluating Π_f volume interpolation is used. Whereas other source terms are integrated over the cell volume as follows.

$$\int_V S_\phi d\mathbf{V} \approx (S_\phi)_{co} V_{co} \quad (2.53)$$

In addition to these, the two terms (terms II to III) of Eqs. 2.49 - 2.51 are also treated as source terms which are already presented in its discretized form in Section 2.3.3.

2.3.5 Pressure velocity coupling

The present solver is based on collocated arrangement of grids. As such, to avoid checker board pressure during iteration of the momentum equation, here we use the momentum interpolation technique which was proposed by Rhie and Chow [136]. For this, in order to calculate the provisional momentum, first, the Navier-Stokes equations are solved by dropping the pressure gradient term. The resultant momentum equation in semi discrete form can be written as,

$$\frac{(\rho \mathbf{u})_{co}^* - (\rho \mathbf{u})_{co}^n}{\Delta t} V_{co} + \sum_f F_f^n (\rho \mathbf{u})_f^* - \sum_f F_{duf}^* = 0 \quad (2.54)$$

Then to get the pressure field, we solve the pressure Poisson equation (PPE), which is obtained by subtracting the provisional momentum equation from the full momentum equation and then taking the divergence. In general the variable coefficient PPE can be written as,

$$\Delta t \left(\frac{\nabla^2 \Pi}{\rho} \right) = \nabla \cdot \mathbf{u}^* - \nabla \cdot \mathbf{u}^{n+1} \quad (2.55)$$

The 2^{nd} term of RHS of Eq. 2.55 i.e., $\nabla \cdot \mathbf{u}^{n+1}$ has been calculated by using the expression given by Eq. 2.34. Since the density is spatially variable, the coefficients of the matrix changes with time rendering the matrix to be asymmetric

which necessitates the use of a preconditioned krylov solver. This linear solver is implemented using the Library of Iterative Solvers [137]. The discretized form of the above pressure-Poisson equation is

$$\Delta t \sum_f \left(\frac{\nabla \Pi^*}{\rho} \right)_f \cdot \mathbf{S}_f = \sum_f F_{0f}^* - \sum_f F_f^{n+1} \quad (2.56)$$

where, $F_{0f} = \mathbf{u}_f^* \cdot \mathbf{S}_f$ is the volume flux due to the mass velocities. Once the pressure field is obtained by solving the PPE then the volume fluxes at each face is corrected by

$$F_f^{n+1} = F_{0f}^* - \Delta t \left(\frac{\nabla \Pi^*}{\rho} \right)_f \cdot \mathbf{S}_f \quad (2.57)$$

Finally, the cell centroid velocities are updated in the following way.

$$\mathbf{u}_{co}^{n+1} = \mathbf{u}_{co}^* - \Delta t \left(\frac{\nabla \Pi^{n+1}}{\rho} \right)_{co} \quad (2.58)$$

The discrete form of all the governing equations generate a system of linear equations, which are iteratively solved by ILU preconditioned krylov solver.

2.3.6 Solution algorithm

The overall solution procedure is as follows.

1. Initialize all variables and all the other parameters to their respective initial conditions.
2. For the start of $(n + 1)^{th}$ time step, assign

$$F_f^* = F_f^n$$

where superscript “n” denotes values at previous time step.

3. Solve the $(k - 1)$ scalar equations for the mass-fraction of the $(k - 1)^{th}$ species using Eq. 2.30 to obtain the corresponding values at $(n + 1)^{th}$ level.
4. Calculate the mass-fraction of k^{th} species as

$$Y_k^{n+1} = 1 - \sum_{i=1}^{k-1} Y_i$$

5. Update the mixture density by using Eqs. 2.31 or 2.32 depending up to the problem under consideration.
6. Solve Eq. 2.54 to get the provisional momentum. Then the provisional velocities (mass velocities) are calculated by dividing the provisional momentum by the latest available density.
7. Provisional volume fluxes at each face are calculated using the values of available mass velocities and iterate the PPE (Eq. 2.56) up to the desired tolerance level to get the pressure field.
8. Update the actual volume flux at each face using Eq. 2.57 and then calculate the cell centroidal velocities at $(n + 1)^{th}$ time level using Eq. 2.58.
9. Check if the momentum and scalars have converged to the required level of accuracy. If not converged then for the next time step calculations, go back to step 3 and repeat the same procedure until stopping criterion is met.

2.4 Post-processing: Quantification of Mixing

The focus of the present thesis is on studying the mixing of miscible fluids of the same phase. For such studies, it is typical to evaluate the extent of mixing through some of the quantitative measures. In order to have a quantitative idea of the goodness of the fluid mixing process, several parameters have been found to be proposed in the earlier studies. Some of the frequently used parameters includes mixing index, pressure drop, mixing cost and mixing energy cost. The mathematical definitions of these parameters are provided in the following sub-sections.

2.4.1 Mixing index

It is the most widely used parameter which is responsible for the quantification of the degree of mixing. In literature, *mixing index*, also called as *mixing efficiency*, is defined on the basis of Danckwerts segregation intensity and is expressed similar to that used in Sarkar et al. [34]

$$M = \left(1 - \sqrt{\frac{\sigma^2}{\sigma_{max}^2}} \right) \times 100 \quad (2.59)$$

where σ^2 denotes the actual variance and of one of the components of the mixture. The actual variance is expressed as

$$\sigma^2 = \frac{1}{N} \sum (Y_i - \bar{Y})^2 \quad (2.60)$$

and N is the number of sampling points taken on a plane perpendicular to the axis of the channel, Y_i is the mass fraction at the sampling point i , $\bar{Y}$ is the optimum mass fraction, and σ_{max}^2 is the maximum possible variance of mass fraction which corresponds to a plane where apparently no mixing has taken place. For flows with equal volumetric flow rates of the streams to be mixed, σ_{max}^2 equals to 0.25 by taking $\bar{Y}$ equal to 0.5 and Y_i is assumed 0 and 1, respectively, for the two halves of the cross-section [34]. For the streams with unequal flow rates, values of $\bar{Y}$ should be suitably adjusted to calculate σ^2 and σ_{max}^2 . The value of N is taken to be 200 for all the cases considered in the present study. It is easy to see that M can have a maximum value of 100 indicating complete mixing and a minimum value of 0 which corresponds to no mixing.

2.4.2 Pressure drop

Another important parameter for analyzing the mixing capability of a passive micromixer is the *pressure drop*. Pressure drop, which is difficult to realize, is routinely overlooked in most of the designs. The pressure drop translates the power required to pump the liquid through the channel and an ideal configuration would demand maximum mixing with low pressure drop across it. However, mixing efficiency and the pressure drop are two competing parameters. As such, enhanced mixing is also likely to be associated with higher pressure drop. In the present study, pressure drop is measured as,

$$\Delta\Pi = \Pi_1 - \Pi_2 \quad (2.61)$$

where Π_1 and Π_2 are the static pressure values at horizontal inlet and outlet of the microchannel, respectively.

2.4.3 Mixing cost

It can however be noted that, combining M and $\Delta\Pi$ together to have a unique parameter will result in a even better option to evaluate the goodness of a micromixing

device. Different options have been proposed in some of the earlier literatures. One of these parameters is termed as *mixing cost* (mc) which was introduced by Chung and Shih [138]. It is defined as the ratio of the mixing efficiency to the pressure drop in the microchannel. Mathematically it can be represented as

$$mc = \frac{M}{\Delta\Pi} \quad (2.62)$$

From Eq. 2.62, it is clear that for a mixer to be efficient, mc should be as high as possible.

2.4.4 Mixing energy cost

Another parameter called *mixing energy cost* (mec) has been introduced by Ortega-Casanova [128] which measures the power needed to get just 1% of efficiency and is defined as

$$mec = \frac{C_p}{M} \quad (2.63)$$

where, C_p is the input power coefficient. In the present study, the input power coefficient has been defined as

$$C_p = \frac{\text{Input power}}{\frac{1}{2}\rho_{avg}u^3A} \quad (2.64)$$

where ρ_{avg} is the average density of the two liquids, u is the inlet velocity and A is the corresponding inlet area. Input power is calculated as

$$\text{Input Power} = \dot{q} \times \Delta\Pi \quad (2.65)$$

In contrast to mc , an efficient mixer would demand as low mec as possible.

2.5 Closure

In this chapter, we have presented about the low Mach number formulation adopted towards the development of a quasi-incompressible flow solver. The details of the numerical framework involving governing equations, discretization procedure, solution algorithm are also presented. Investigations of truncation and discretization errors using the method of manufactured solutions are carried out in the next chapter to quantify the numerical errors associated with a particular convective scheme.

Chapter 3

Analysis of Numerical Schemes for Mixing Problems

Numerical modelling of a given problem is based on the use of different numerical schemes to convert the partial differential equations to their respective discretized equations. The solutions to these discretized equations by using some suitable algorithm finally lead to the solutions to the physical problems. However, as described in the previous chapter, there are various numerical schemes developed with different order of accuracies. Moreover, different schemes suffer from different pros and cons. As such, selection of the best scheme among the all possible available schemes is the primary requirement to carry out numerical simulations.

3.1 Discretization and Truncation Errors

Consistency and convergence are the two main property that any numerical scheme should have. For a numerical scheme to be consistent, the discretized equations must approach the original (continuum) partial differential equations in the limit as the element size ($\Delta x, \Delta y, \Delta z, \Delta t$) approaches zero. Convergence, on the other hand, addresses the issue of the solution to the discretized equations approaching the continuum solution to the partial differential equations in the limit of decreasing element size. Thus, consistency addresses the equations, while convergence deals with the solution itself. Convergence is measured by evaluating (or estimating) the discretization error (DE). The discretization error can be defined as the difference

between the solution to the discretized equations ϕ_k and the solution to the original partial differential equation ϕ_{exact} .

$$\text{DE} = \phi_k - \phi_{\text{exact}} \quad (3.1)$$

where k refers to the mesh level. For a stable numerical scheme, the errors must not grow in the marching direction.

In addition to this, every numerical scheme has a formal order of accuracy. For FDM and FVM, the formal order of accuracy is obtained from a truncation error (TE) analysis. TE is the error made by truncating an infinite sum and approximating it by a finite sum. One approach to evaluate the TE is to start with a Taylor series expansion of the solution variables. However, TE can also be evaluated by the use of order of test which is an one shot calculation.

3.1.1 Order of accuracy test

There are a variety of acceptance criteria for code verification using method of manufactured solutions (MMS). Among them, the “order of accuracy test” is the most rigorous test and is therefore recommended as the acceptance criteria for the accuracy of the developed solver. Every numerical scheme used either for spatial or for temporal discretization has a theoretical formal order of accuracy that can be determined by a truncation-error analysis of the discretized equations. This test assesses whether or not the numerical method reproduce the formal order of accuracy in space and/or time.

The order of accuracy test involves evaluating the numerical solution on a series of nested grids, and with various time steps for unsteady problems. The spatial and temporal discretization errors are monitored to determine if the observed order of accuracy matches the formal order of accuracy. The discretization error will generally decrease as $1/r^p$, where r is the grid refinement factor (i.e., $r = \Delta x_{\text{coarse}}/\Delta x_{\text{fine}}$) and p is the order of accuracy. For example, if the numerical scheme is of second order accurate i.e., $p = 2$, then when the grid is doubled (or $r=2$), then the discretization error should decrease by a factor of four on each successively refined mesh level. In order to examine the global discretization error behavior, both L_2 and L_∞ norms of

the errors can be used

$$L_2 \text{ norm}_k = \left(\frac{\sum_{n=1}^N |\phi_{k,n} - \phi_{exact,n}|^2}{N} \right)^{1/2} \quad (3.2)$$

$$L_\infty \text{ norm}_k = \max |\phi_{k,n} - \phi_{exact,n}| \quad (3.3)$$

where k refers to the discrete mesh level and n varies over all control volumes N in space excluding boundary cells when Dirichlet boundary conditions are applied for which the discretization error is identically zero. Obtaining the formal order of accuracy in the L_∞ norm is generally more difficult than the other error norms as it represents the maximum error over the entire domain. In a similar manner, this order of accuracy test can also be performed for truncations error analysis with the help of MMS.

3.1.2 Method of manufactured solutions

The method of manufactured solutions is a general and very powerful approach in which rather than trying to find an exact solution to a system of partial differential equations, the goal is to manufacture an exact solution to a slightly modified set of equations. The general concept behind MMS is to choose the solution a priori, then operate the governing partial differential equations onto the chosen solution, thereby generating analytical source terms. The chosen (manufactured) solution is then the exact solution to the modified governing equations made up of the original equations plus the analytical source terms. The six steps required for implementing the MMS are:

1. Choose the form of the governing equations.
2. Choose the form of the Manufactured Solution.
3. Apply the governing equations to the Manufactured Solution to generate analytical source terms.
4. Discretize the equations and solve on multiple mesh levels using analytical boundary conditions and source terms from the Manufactured Solution.
5. Evaluate the global discretization error in the numerical solutions.

6. Determine whether or not the observed order of accuracy matches the formal order of accuracy.

If the comparison in Step 6 is favorable, then the coding options exercised are verified. If the comparison is unfavorable, then one generally examines the local discretization error, uses this information to debug the code, then returns to Step 4. MMS can be used to rigorously test the order of accuracy of a numerical scheme. Manufactured solutions should be chosen to be smooth, analytical functions with smooth derivatives. To get a more clear picture of error behavior of different schemes for both convective and diffusive fluxes, the error behavior of these two terms are addressed separately in the following sections.

3.2 Analysis of TE and DE using MMS

The purpose of analyzing the discretization and truncation errors is to numerically establish a relation between the two for a given convective scheme. For linear equations, it is easy to show that the convection of the discretization error is dictated by the truncation error (residual), although numerical studies are still necessary to establish a more conclusive quantitative relation between the two errors. One must realize that the discretization error is *a posteriori* meaning that it can be determined after the solution process is completed and additionally requires an exact solution or a close approximation thereof. Defined in the present manner, the truncation error is *a priori* and exploits the manufactured exact solution with the latter used to calculate the discretization error as well. In this section, the TE and DE are trying to relate with each other so that the best possible conditions can be found as *a priori* to carry out the numerical simulations. In order to do this, the order of accuracy test has been performed to a problem having manufactured solutions.

3.2.1 TE and DE for convective fluxes

As described in Section 2.3.2, in the present solver, three different convective schemes are incorporated. One is FOU, second is the linear combination of FOU and CDS [132] whereas the remaining is the high resolution bounded scheme namely CUBISTA [133]. Depending on the blending factor (γ), full upwind or full CDS scheme can be obtained. However, one can also argue that second order upwind

(SOU) can be a better choice than that of FOU. The reason for not considering SOU is that, unlike FOU and CUBISTA, SOU is not a bounded scheme which might create trouble for problems with high gradient zones such as flames. The general convective-diffusive equation for a variable ϕ has been taken for this study.

$$\frac{\partial(\phi)}{\partial t} + \frac{\partial(\phi u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(D \frac{\partial \phi}{\partial x_j} \right) \quad (3.4)$$

To begin with, it is now considered the case with $D = 0$ such that diffusive fluxes vanishes and we need to address only the convective fluxes. The manufactured solution for this modified equation with no diffusive contribution has been chosen as

$$\phi = x^3 + y^3, \quad \text{with} \quad u = y^2, v = -x^2 \quad (3.5)$$

To find the order of accuracy of TE as well as the DE with respect to each scheme, uniform Cartesian meshes of different grid resolutions ($\Delta x = 0.04, 0.02, 0.01, 0.005$) are being used. For the TE or DE calculation on a particular mesh, exact values of ϕ are initialized at all the cell centroids whereas exact velocities are specified at all the face centroids. Since the convective fluxes are calculated on the faces, the face average values of ϕ_f has been approximated by using different convective schemes. To find out the DE at steady state, a convergence of 10^{-8} has been chosen as the stopping criteria. In order to examine the global TE or DE behavior for each scheme, L_∞ norms of the error are used excluding the boundary cells. The obtained L_∞ norms of TE and DE on each grid are plotted against different grid resolutions for different convective schemes and are shown in Figs. 3.1(a) and (b), respectively.

Figure 3.1(a) shows the variation of TE with grid size for three different schemes viz. FOU, Khosla-Rubin scheme with deferred constant of 0.5 and CUBISTA scheme. In all cases, the errors show a decreasing trend with grid refinement, with the slopes indicating the order of accuracy of the local truncation error. From the figure one can note an interesting point about CUBISTA scheme. Although CUBISTA is devised as a second-order bounded scheme, the truncation errors for CUBISTA scheme are falling at a rate equal to 2 only when exact gradients are used. However, CUBISTA with gradients calculated numerically by Green-Gauss reconstruction (GG), the truncation error for the convection problem decreases at a rate equal to 1. It is believed that this may be attributed to the way the gradients

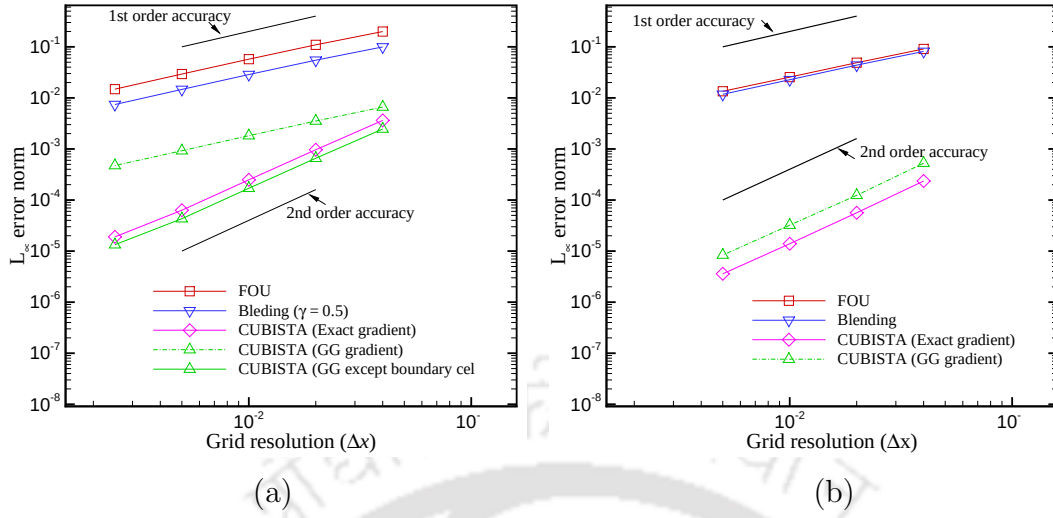


Figure 3.1: Order of accuracy test for different convective schemes as applied to the function $\phi = x^3 + y^3$ with $u = y^2$ and $v = -x^2$ for (a) truncation error and (b) discretization error.

are calculated using the GG reconstruction, particularly at the boundaries. This can be easily verified from Fig. 3.1(a) where it can be seen that when the gradients are calculated using GG for all cells except the cells sharing the boundaries where the exact gradients can be used, the TE decrease at a rate of 2. These issues however show no impact on the discretization error, where CUBISTA shows the lowest errors with the rate of decay of errors showing a slope of 2 (on log-log scale). Another important scheme, which is often overlooked, is the Khosla-Rubin scheme that is obtained as a equi-blend of FOU and CDS schemes. Despite the latter schemes showing first and second-order accuracies on smooth flow problems, the Khosla-Rubin scheme shows an overall first order accuracy, evident both in Figs. 3.1(a) and (b). Importantly, these figures also show that the errors from the blended scheme is no different from the FOU scheme, meaning that there is no real suppression of the false diffusion that plagues first-order upwind schemes when applied to convection problems. These results provide a fair indication that truncation error may be used as an indicator of the discretization error for convective schemes. With the former being apriori, these errors are easily determined without actually solving the problem making it an useful tool to compare different convective flux schemes in a finite volume framework. As far as mixing problems dealt in the following chapters are concerned, we largely employ the CUBISTA scheme for most simulations since they

offer the lowest errors for a given grid resolution and nominal second-order accuracy on structured meshes. One can argue that such an exercise to establish the need for and superiority of bounded high-resolution schemes such as CUBISTA is not strictly valid for laminar mixing problems since the chosen manufactured solution is not exactly representative of the physical problem. While the latter is indeed desirable, the chosen manufactured solution is a smooth function similar to how we would also expect the numerical solutions to fluid mixing to behave as well and justifies the study.

3.2.2 TE and DE for diffusive fluxes

Although the effect of convective term discretization plays a more crucial role in liquid mixing problems in order to limit the false diffusion to an acceptable limit, however, treatment of diffusive terms also plays a role in getting the correct numerical solutions. In this context, the order of accuracy test for the TE and DE of the diffusive terms are explored herein this section. The diffusive terms are discretized with CDS which is devised as a second-order scheme. However, as described in Section 2.3.3, diffusive flux calculations indeed require the gradients of the transported variable involved in the cross-diffusion terms. Moreover, the importance of the treatment of gradients of a variable has also been observed from the TE analysis of convective terms in Section 3.2.1.

A general Poisson equation has been selected for the order of accuracy test of the diffusion term as shown below.

$$\nabla^2 \phi = S \quad (3.6)$$

where S denotes the source term. The manufactured solution and the generated source term for Eq. 3.6 are

$$\phi = \frac{\cos(4\pi x) + \cos(4\pi y)}{4} \quad (3.7)$$

$$S = -4\pi^2 [\cos(4\pi x) + \cos(4\pi y)] \quad (3.8)$$

To find the order of accuracy of TE of the numerical diffusive scheme, three different types of meshes (structured and unstructured), namely, uniform hexahedral,

non-uniform hexahedral and uniform triangulated hexahedral meshes having same grid resolutions of $\Delta x = 0.04, 0.02, 0.01, 0.005$ are used. Figure 3.2 shows the L_∞ error norm for the TE of diffusive scheme with three different gradient schemes for each of the meshes.

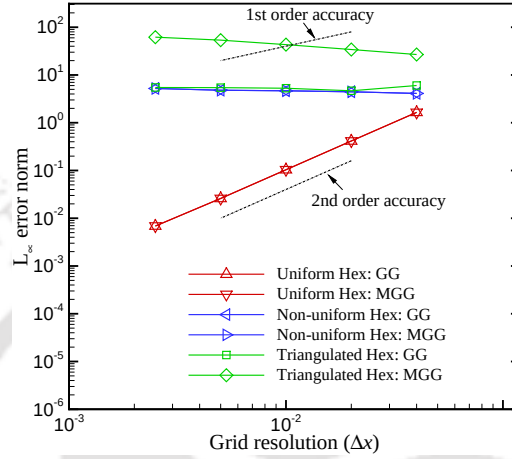


Figure 3.2: Order of accuracy with respect to L_∞ norm of TE for diffusive scheme.

From the figure, it can be seen that the TE decreases at a rate of 2 for uniform orthogonal meshes only. Whereas for other types of meshes the TE does not at fall with grid refinement at the expected rate. To get the reason behind this, it is then decided to check the rate of fall of the error in gradients calculation schemes. For this, two gradient calculation schemes viz, Green-Gauss (GG) and modified Green-Gauss (MGG) are tested. The errors are defined as the difference between the numerical gradients and that of exact gradients. Figure 3.3 shows the error norm for different gradient schemes.

From the figure one can easily see that the errors in gradients are falling approximately at a rate of 1 other than uniform orthogonal meshes irrespective of gradient schemes. These observations confirm that if the gradients are second order accurate, the truncation error will also be so. This happens due to fortunate cancellations. If the gradients are first order accurate, the diffusive fluxes behave as $O(1)$, meaning they do not decrease with grid refinement which can be clearly observed in Fig. 3.2. However, one can also argue that why gradients behave in one way and the diffusive fluxes in other way. This may be because of the fact that diffusive fluxes use the

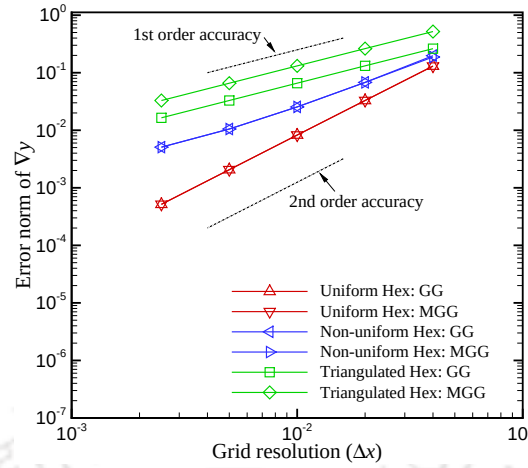


Figure 3.3: Order of accuracy for errors in gradient schemes with respect to different grids.

gradients at the face, which are interpolated from the cell centroids. Even if the centroidal gradients are second-order accurate, the interpolation could reduce its order of accuracy if the line joining the cell centroids is not bisected by the center of the face shared by the two cells. The latter that happens on uniform hexahedral grids are rarely happen on others. As such the calculations of discretization error for the diffusive fluxes are done only for uniform hexahedral meshes and is shown in Fig. 3.4. From the figure it can be seen that the DE for diffusive fluxes are of second-order accurate.

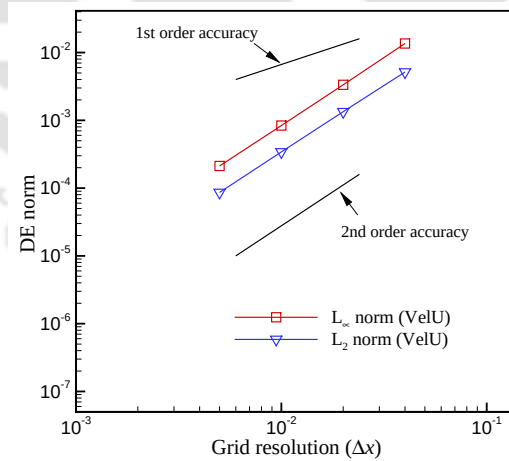


Figure 3.4: DE order of accuracy for diffusion scheme.

3.3 Closure

In this chapter, truncation and discretization error analysis for convective and diffusive fluxes has been performed. Based on these analysis it has been found that a fair indication of truncation error may be used as an indicator of the discretization error for convective schemes. Among the different convective schemes, scheme which produces lesser truncation error is also observed to produce lesser discretization error. Based on this analysis, CUBISTA like schemes have been adopted for problems where physical diffusion plays an important role specially for mixing of liquids. The performances of these schemes are checked by simulating a series of well known benchmark problems and are presented in the next chapter.



Chapter 4

Verification and Validation of the Solver

As stated in the earlier chapter, CFD modelling has enormous potential to impact the design, analysis, and optimization of engineering systems. It is basically the use of any computer application which involves the numerical solution to a system of partial differential equations that govern the flow physics. However, there may always be a possibility of existence of certain sources of errors that may get overlooked sometimes. Hence, to achieve its full potential as a predictive tool for simulating the physical problems, a rigorous testing of the numerical solver is of utmost importance to ascertain that the computed results are an accurate representation of reality.

The two terminologies associated with the determination of accuracy of any numerical solver are *verification* and *validation*. Although, these two terminologies seem to be synonymous; however, in the current perspective, they both have very different meanings which are basically related to the sources of errors in mathematical simulations. Verification deals with mathematics and addresses the correctness of the numerical solution to a given model. Validation, on the other hand, deals with physics and addresses the appropriateness of the model in reproducing experimental data. In other words, it can be said that verification can be thought of as solving the chosen equations correctly, while validation is choosing the correct equations in the first place. This chapter is intended to provide a framework for building the confidence in computational simulation predictions.

4.1 Verification of Numerical Solver

Verification is defined as to insure that a model is correctly implemented according to the developer's conception [11]. Verification can be broken down into two distinct categories: code verification and solution verification. Code verification is the process of ensuring, to the degree possible, that there are no mistakes (bugs) in a computer code or inconsistencies in the solution algorithm. Solution verification is the process of quantifying the numerical errors that occur in every numerical simulation. Examples of these numerical errors include round-off error, iterative error, and discretization error. While code verification is generally performed once and for all for a given set of coding options (at least for smooth problems), solution verification must be performed for each and every simulation that is significantly different than previous simulations. For code verification purposes, it is convenient to define the DE as is defined in Eq. 3.1. Moreover, there must be a certain criteria on the basis of which the code can be verified for its accuracy. Among a variety of acceptance criteria for code verification, the "order of accuracy test" is the most rigorous test. It determines whether or not the discretization error is reduced at the expected rate. This test is equivalent to determining whether the observed order of accuracy matches the formal order of accuracy and is therefore recommended as the acceptance criteria for the accuracy of the developed solver. The classical Taylor-Green (T-G) vortex problem [139] has been considered herein to investigate the order of accuracy of the present solver.

4.1.1 Problem definition: Taylor-Green vortex

In fluid dynamics, the Taylor-Green vortex is an unsteady flow of a decaying vortex, which has an exact closed form solution of the incompressible Navier-Stokes equations in Cartesian coordinates. A 0.5×0.5 domain has been selected for the computations. The analytical solutions for velocities (u, v) and pressure (Π) are given below.

$$u = -\cos(2\pi x)\sin(2\pi y)e^{\frac{-8\pi^2 t}{Re}} \quad (4.1)$$

$$v = \sin(2\pi x)\cos(2\pi y)e^{\frac{-8\pi^2 t}{Re}} \quad (4.2)$$

$$\Pi = \frac{-\{\cos(2\pi x) + \cos(2\pi y)\}}{4} e^{\frac{-16\pi^2 t}{Re}} \quad (4.3)$$

Dirichlet boundary conditions are specified at the boundaries by providing the exact values. The problem has been simulated for $Re = 100$ by using the developed solver with CUBISTA scheme for the convective terms and the implicit Euler scheme for the discretization of the temporal term. The diffusion fluxes are computed with central difference scheme. Simulations are carried out by considering a uniform Cartesian mesh with 100×100 grid resolution with $\Delta t = 5 \times 10^{-5}$ s. The numerical results obtained at $t = 1$ s are compared with the exact solutions at that particular time instant and are shown in Fig. 4.1.

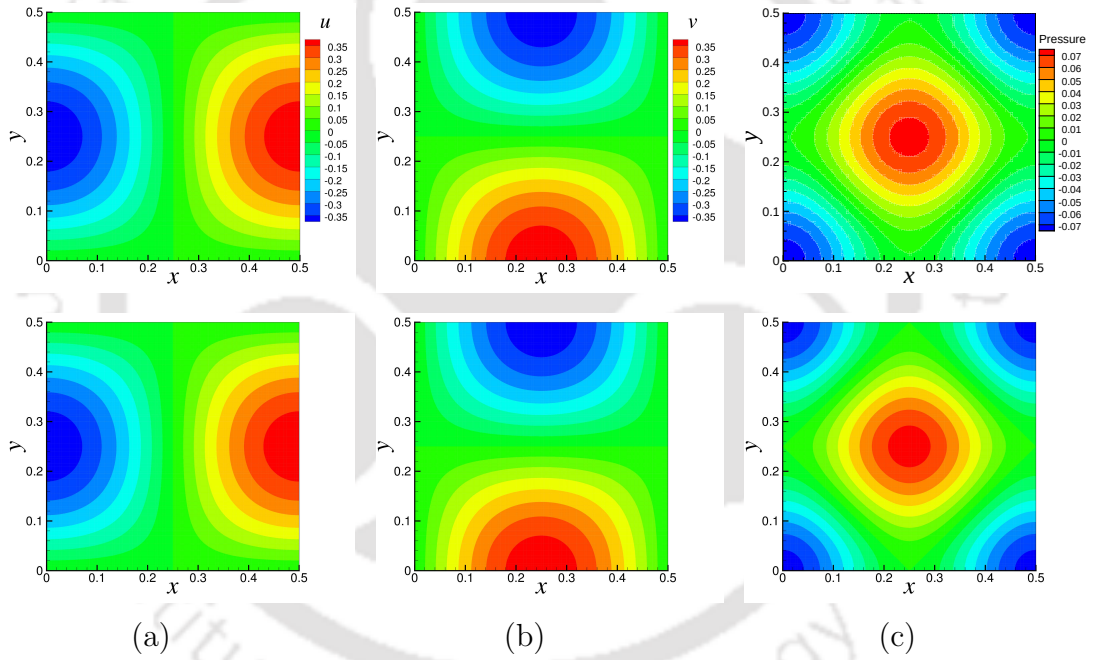


Figure 4.1: Comparison of instantaneous contours obtained from present simulation (top) with that of exact (bottom) for T-G vortex problems at $t = 1$ s: (a) u -velocity, (b) v -velocity and (c) pressure.

Numerical results are found to be in close agreement with that of the exact solutions as can be seen from Fig. 4.1. However, the order of accuracy of test of the solver with different schemes has been carried out in the following section.

4.1.2 Studies on spatial accuracy

In order to study the spatial accuracy of the present solver, T-G vortex problem has been selected. The spatial discretization of the convective terms are carried out by (a) FOU, (b) blending of FOU and CDS with $\gamma = 0.5$ and (c) CUBISTA. To find out the discretization errors with respect to each scheme, uniform Cartesian meshes of different grid resolutions ($\Delta x = 0.04, 0.02, 0.01, 0.005$) with a constant time step $\Delta t = 5 \times 10^{-5}$ are used. The temporal discretization and the diffusive fluxes are calculated in a similar manner as given in Section 4.1.1. In order to examine the global discretization error behavior for each scheme, both L_2 and L_∞ norms of the error are used. The obtained error norms, as a representative of global DE, are plotted against different grid resolutions for each convective scheme which are shown in Figs. 4.2(a)-(c).

From the figures, it can be clearly seen that among the selected convective schemes, a slope of two for the DE vs grid refinement line is observed only for CUBISTA scheme whereas the slope is nearly one for the other two schemes. This means that, only CUBISTA scheme is of second order accurate whereas, both FOU and blending scheme show nominal first order accuracy. Another point to be noted is that between the two 1st order schemes i.e., FOU and blending of FOU and CDS, the absolute values of the DE are less for blending scheme than compared to that of FOU. Thus blending can be viewed as a better choice than compared to that of FOU scheme. These results, however, matches with the formal order of accuracy of the respective schemes. This provides a significant evidence of the accuracy of the solver in regard to the implementation of different numerical schemes.

4.2 Validation of Numerical Solver

This section is intended to address the appropriateness of the developed numerical model in reproducing experimental data to simulate the interaction of multiple species that are non-reacting and miscible in nature. To do that, the developed solver using unstructured variable density formulation described in the previous chapter is used to solve a set of problems involving constant density as well as variable density due to the presence of concentration gradients. Several problems are simulated and the obtained numerical results are validated against the published literature in each

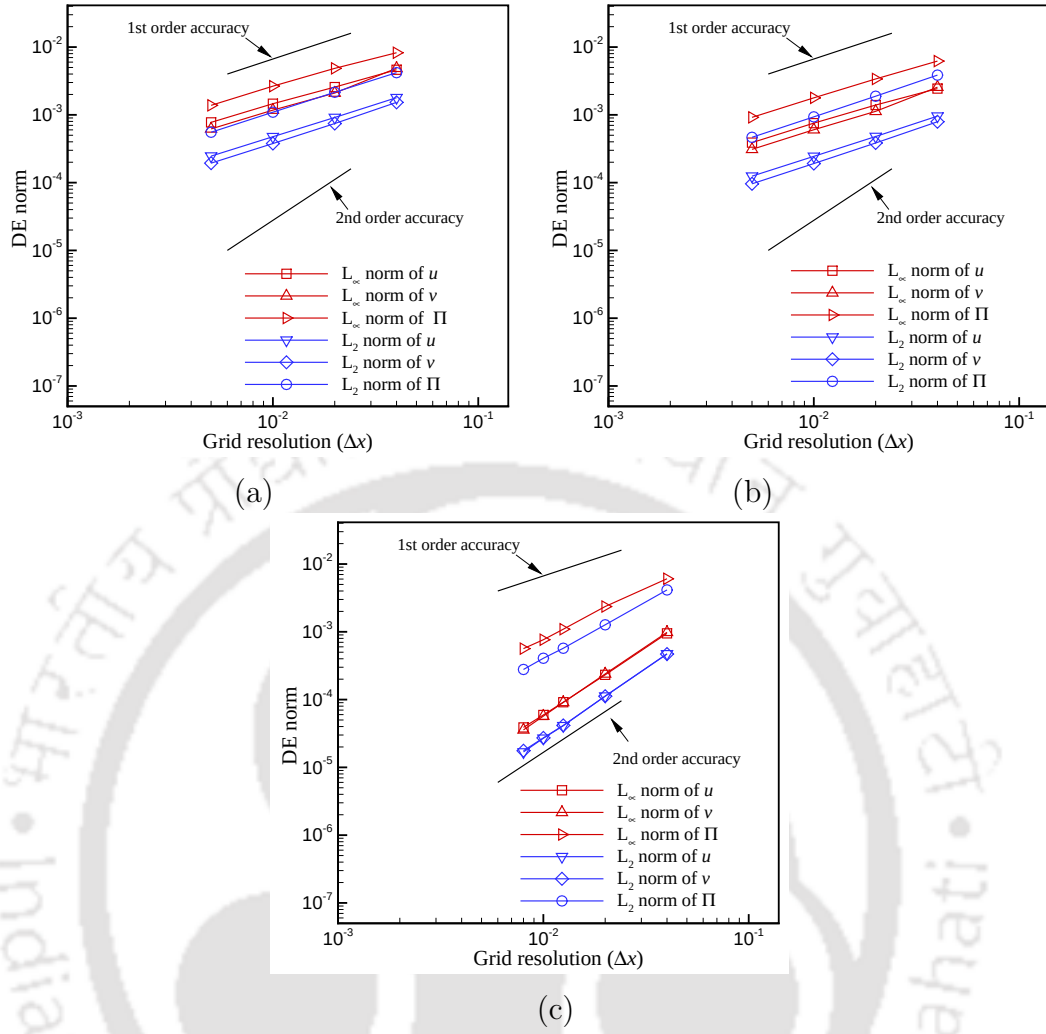


Figure 4.2: Order of accuracy study of the discretization error for T-G vortex problem at $t = 1$ s: (a) FOU, (b) Khosla-Rubin ($\gamma = 0.5$) and (c) CUBISTA.

and every step to check the capability of the solver to simulate flows with single as well as multiple species (gases or liquids), flows in macrochannels and microchannels in both two- and three-dimensional geometries. Among these problems the first problem essentially check the implementation of Navier-Stokes equations for single species. The remaining test cases deal with open domain problems with gas mixtures and liquid mixtures.

The developed solver is inherently three-dimensional. Therefore, to solve two-dimensional problems, one makes use of hexahedral/prismatic elements of one cell

width in the direction normal to the plane of the flow and provide symmetry boundary conditions on the lateral walls to ensure that the simulations are necessarily two-dimensional. Furthermore, problems having steady-state solutions are solved using pseudo-transient manner.

4.2.1 Lid driven cavity

The three-dimensional lid driven cavity flow problem is solved using 2,71,320 tetrahedral cells in a $1 \times 1 \times 1$ cubical cavity with a moving lid at the top and stationary walls at the sides and the bottom. The top lid moves with a non-dimensional velocity of unity and simulations are carried out for Reynolds numbers of 100, 400 and 1000, ensuring a laminar regime for the flows. The velocity variations along the vertical and horizontal centerline of the cavity are compared with that of Ku et al. [140] and shown in Figs. 4.3(a) and (b). It shows very good agreement with the literature.

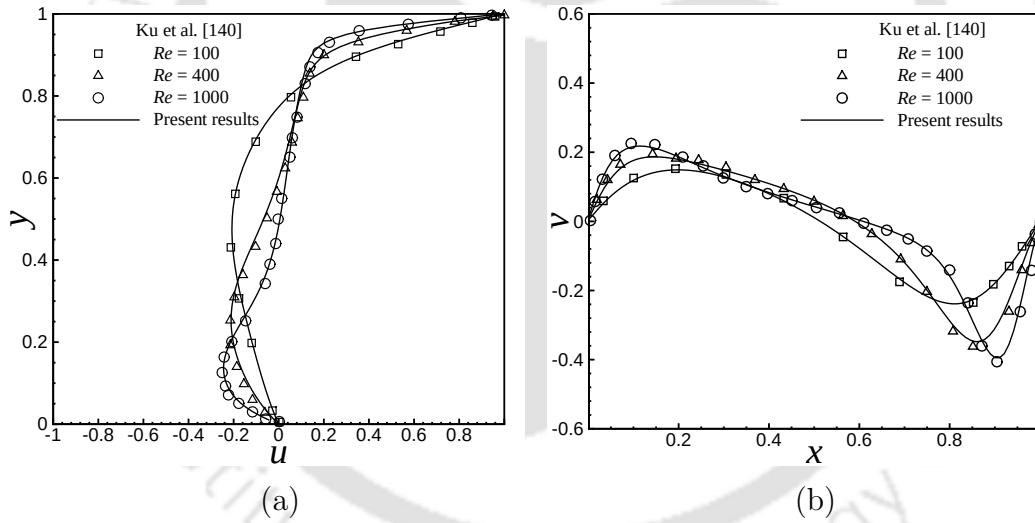


Figure 4.3: Comparison of (a) u -velocity along vertical centerline, (b) v -velocity along horizontal centerline for the 3D lid driven cavity.

4.2.2 Coflow mixing of laminar jets in a horizontal channel

The present code is also validated for mixing of two laminar jets coflowing at different velocities in a coaxial horizontal channel. A schematic layout of the problem

definition is shown in Fig. 4.4. Argon (Fluid 1) flows through the inner channel having radius R_1 while ambient air (Fluid 2) flows through the outer channel having radius R_2 . A radius ratio of 0.25 ($R_1=0.5$ in, $R_2=2.0$ in) and a mixing length $L=30$ in. are considered. Fully developed velocity profiles of both the jets are specified at the entrance to the mixing region. This problem is taken from the experimental work performed by Shavit and Lavan [141]. The Reynolds number (Re) at the inlet of each jet is 1072 and the Schmidt number (Sc) is 0.772. The density ratio (ρ_1/ρ_2) and the viscosity ratio (μ_1/μ_2) of the inner fluid to that of the outer fluid are 1.345 and 1.255, respectively. The numerical simulation is carried out by considering half the domain. Uniform hexahedral cells with 4000 control volumes are used for the computation. Argon concentration profiles along planes perpendicular to the channel axis at various axial lengths from the inlet are plotted and shown in Fig. 4.5. The present results are found to be in good agreement with the experimental work of Shavit and Lavan [141].

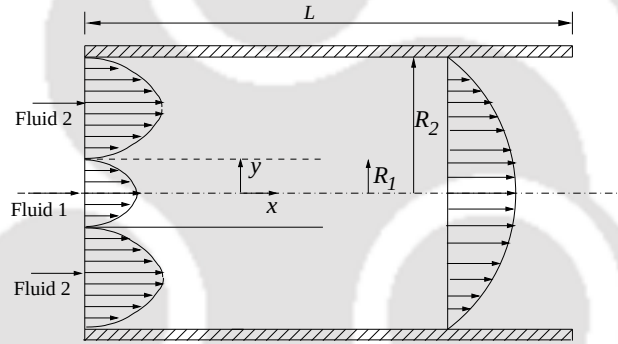


Figure 4.4: Schematic diagram of the coflow mixing of two laminar jets in a horizontal channel.

4.2.3 Counterflow mixing of jets in a confined channel

The numerical model considered in this section is an isothermal, laminar mixing process of two confined non-reacting opposing jets in a parallel channel. The two species enter through two different equi-sized slots positioned exactly opposite to each other creating a counter flow when they meet each other. The fluid mixture then flows out of the channel along a direction normal to the jet axes. Figure 4.6(a) shows the schematic diagram of the problem considered. The widths of the two inlet slots of the channels (D) and the height (h) are equal. Since the geometry is

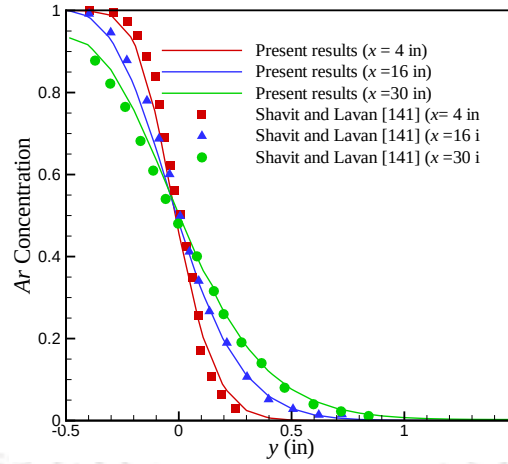


Figure 4.5: Validation with experimental work: Comparison of Argon concentration profiles along planes perpendicular to channel axis at distances of 4, 16 and 30 inches from the inlet.

symmetrical about the axis of the inlet jets (y -axis), one half of the of the physical domain is chosen as the computational domain to reduce the cost of numerical calculations. Figure 4.6(b) shows the numerical model of the problem of study where the widths of the two inlet slots of the channels are $0.5h$ and $L = 12h$ is the length of the computational domain.

The left boundary of Fig. 4.6(b) represents the plane of symmetry while the right boundary represents the outlet of the flow domain. The walls are impermeable. The temperatures of the two impinging jets are assumed to be constant and equal so as to prevail an isothermal mixing situation. In order to maintain equal momentum for both the inlet fluids as that of Gomes and Caldeira [142], we have assumed that the two inlet fluids are having same properties and both fluids are flowing with the same velocity. Fully developed velocity profiles are specified at the entrance to the mixing region. The non-dimensional parameters such as the inlet Re and Pe of 60 and 42, respectively, are based on the average velocity at the inlet and the inlet slot width ($0.5h$). For the numerical simulation uniform hexahedral cells of 24000 numbers are used.

The mass fraction of species entering from the top inlet are plotted along a line perpendicular to the axis of the mixing channel at $x = 0.4h$ from the inlet and compared with the work of Gomes and Caldeira [142]. The comparison is shown in

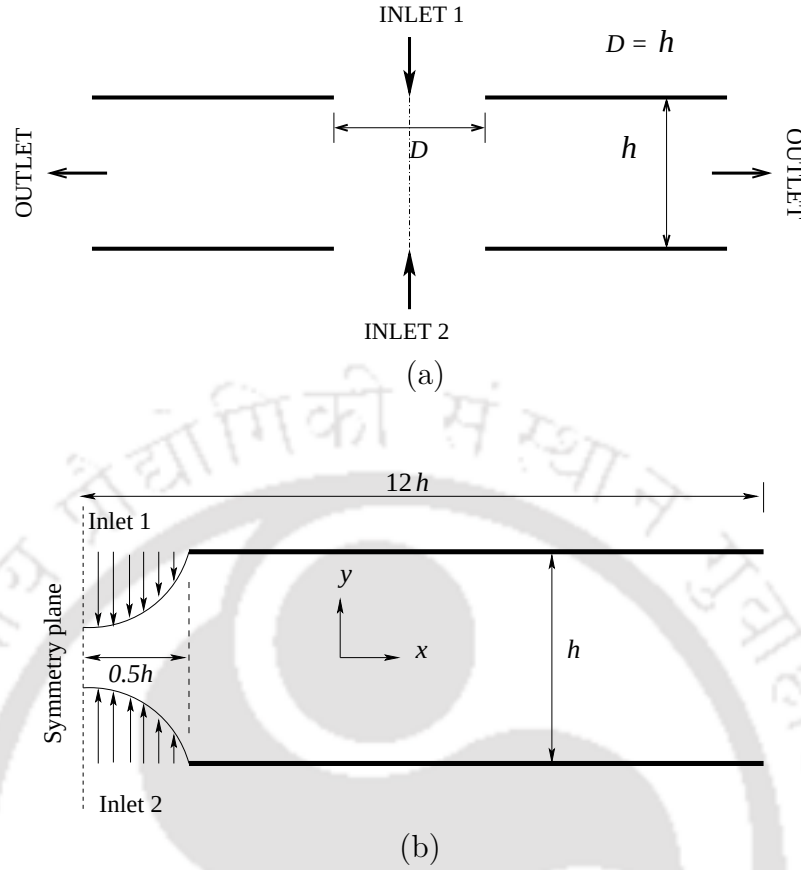


Figure 4.6: (a) Schematic of the flow domain for confined counterflow mixing of jets and (b) representative computational domain adopted for validation study.

Fig. 4.7 which represents a reasonably good match with the published literature.

4.2.4 Two-dimensional mixing of liquids in a T-shaped micromixer with and without obstacles

The validation cases studied in Sections 4.2.1 - 4.2.3 are to demonstrate the capability of the present solver for handling mixing of gaseous species. However, the test problems chosen in the following sections have been selected to validate the developed solver against mixing of liquids in microchannels. This test case has been adopted from the work of Rasouli et al. [143]. The geometry includes a straight microchannel with two inlets that form a T-shaped micromixer. Two fluid streams (Fluid 1 and Fluid 2) with constant mass fractions having ($Y_{k,1}=1$ and $Y_{k,2}=0$ and

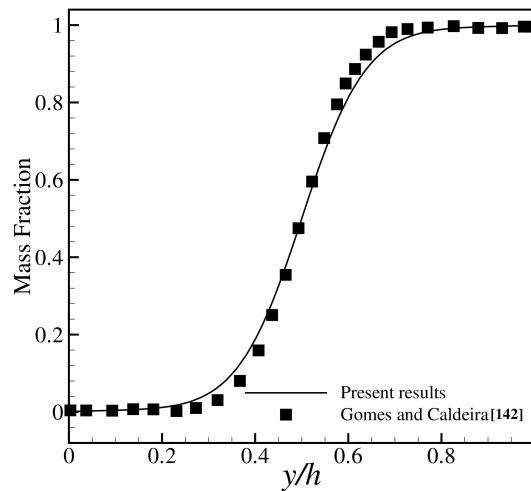


Figure 4.7: Validation results: Comparison of Argon mass fraction profile along a plane perpendicular to channel axis at a distance of 0.4 from the inlet.

vice versa at the two inlets) are assumed to flow into the micromixer through the upper and lower inlets, respectively. When the two liquids come into contact with each other, transfer of mass will take place at the interface and the resulting mixture then flows out of the channel. Figure 4.8 shows the schematic diagram of the basic geometry for the test problem.

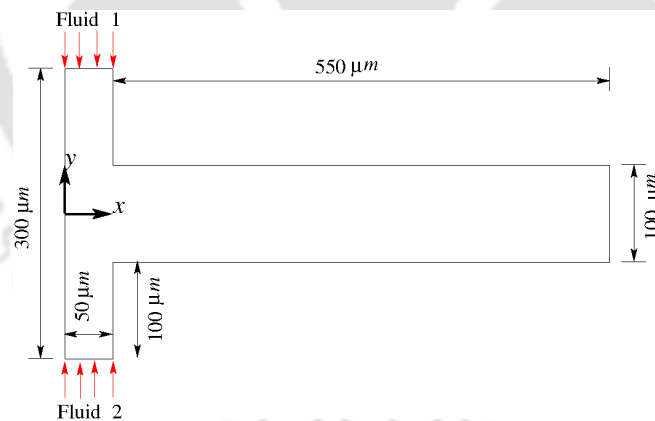


Figure 4.8: Mixing Geometry of the basic two fluids T-shaped micromixer

The boundary conditions for the fluid velocity components at walls are typically no-slip condition and zero flux condition for the species, while pressure outlet boundary condition is applied at the channel outlet and the normal gradients of pressure on the solid walls of the micromixer was considered to be zero. A velocity

boundary condition having a magnitude of 4 mm.s^{-1} , derived from Re (based on the width of inlet channel), has been implemented at both the inlets. The inlet Re and Sc are 0.2 and 200, respectively. It has been assumed that both the incoming fluids are having similar properties that are given in Table 4.1. In order to carry out the numerical simulations, 70882 prismatic cells are being used.

Table 4.1: Properties of the fluids.

Parameters	Values
Density (ρ)	1000 kg/m^3
Viscosity (μ)	0.001 Pa.s
Mass diffusivity (D)	$5 \times 10^{-9} \text{ m}^2/\text{s}$

The second part of this test problem involves the mixing behavior due to the placement of five rectangular obstacles having a width of $20 \mu\text{m}$ and a height of $50 \mu\text{m}$ in the middle of the same T-channel, schematically represented in Fig. 4.9. The boundary conditions are same as that of the base case with the additional no-slip conditions applied on the obstacle walls. For this simulation, 64834 prismatic cells are being used.

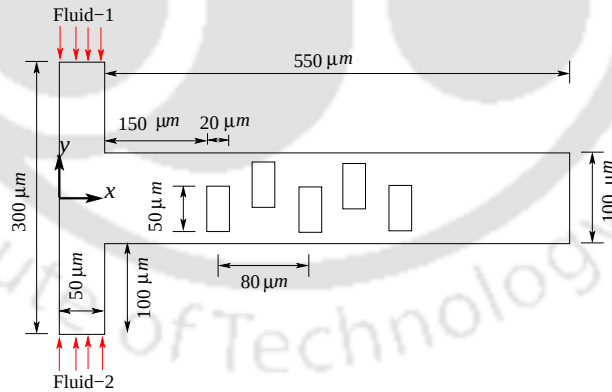


Figure 4.9: Mixing Geometry of two fluids T-shaped micromixer with obstacles

The variation of concentrations with respect to channel width at four different cross sections along the two micromixers (without and with obstacles) has been illustrated in Figs. 4.10(a) and (b). From the figures, it can be seen that at steady

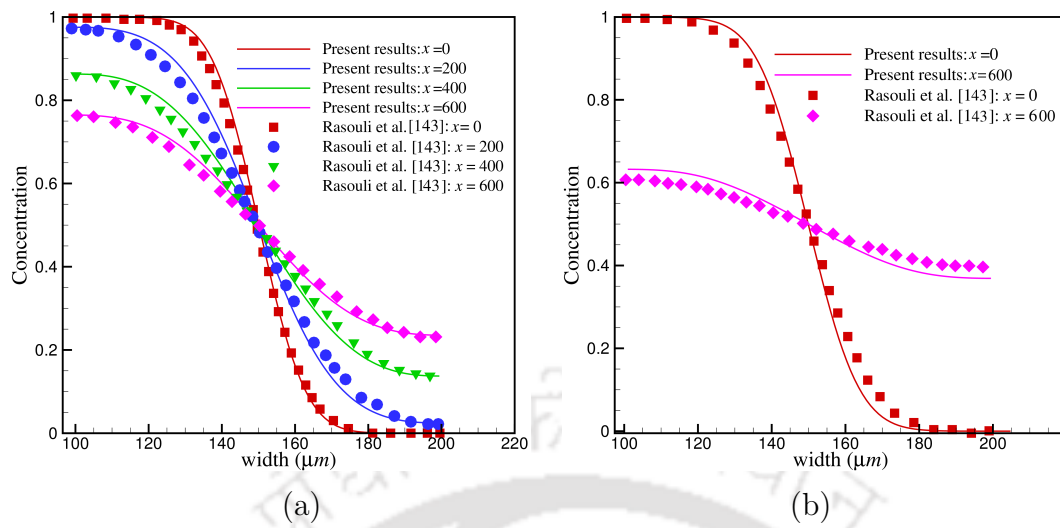


Figure 4.10: Variation of concentration with respect to channel width at four different cross sections for (a) the basic T-shaped micromixer, (b) T-shaped micromixer with obstacles.

state, apparently no mixing has occurred at the left wall and hence the mass fractions will vary from 0 to 1. However, as one move downstream to the mixing channel this variation gradually decreases. The variations obtained in the present work are found to be in good agreement with that of the published literature. Also, the mixing efficiency calculated at the outlet of both the two micromixers are shown in Table 4.2. The corresponding mixing efficiencies are within the acceptable limit of error (maximum 2.5%).

Table 4.2: Mixing efficiency at the outlet of the two micromixers.

Mixer type	Mixing Efficiency, M (%)		$\%Error = \frac{(a)-(b)}{(a)} \times 100$
	Present results	Rasouli et al. [143]	
	(a)	(b)	
Basic T-channel	62.41	61.48	1.5
T-channel with obstacles	84.39	82.45	2.3

4.2.5 Three-dimensional mixing in a T-microchannel

In order to validate the computational approach for a three-dimensional problem, we choose the mixing of liquids in a T-shaped microchannel geometry investigated by Hsiao et al. [92]. The problem definition is shown schematically in Fig. 4.11. Geometrical dimensions are expressed in terms of channel height $H = 130 \mu\text{m}$. The widths of the main channel and the inlet channels are $W_m = 3H$ and $W_i = 1.5H$, respectively, and $L = 78.25H$ is the total length of the straight main channel. The fluids entering from the two inlets are pure DI water and a $33 \mu\text{mole/l}$ solution of Rhodamine B (Fluka, Germany) in DI water with a diffusion coefficient (D) of $3.6 \times 10^{-10} \text{ m}^2.\text{s}^{-1}$. Thus, the fluids entering the two inlets are assumed to possess the properties of water having density and the viscosity equals to 997 kg.m^{-3} and $0.00097 \text{ kg.m}^{-1}.\text{s}^{-1}$, respectively. Equal flow rate at both inlets is considered with uniform inlet velocities corresponding to Re of 0.125, 0.5, 2, 8, 32 and 64. Here, the definition of Re is taken as $Re = \bar{u} d_h \nu^{-1}$ where $\bar{u}$, d_h and ν denotes the characteristic value of flow velocity, the hydraulic diameter of the main channel ($195 \mu\text{m}$) and the kinematic viscosity of the fluid, respectively. The outlet pressure is set to be 1 atm and the no-slip condition is set on the solid walls.

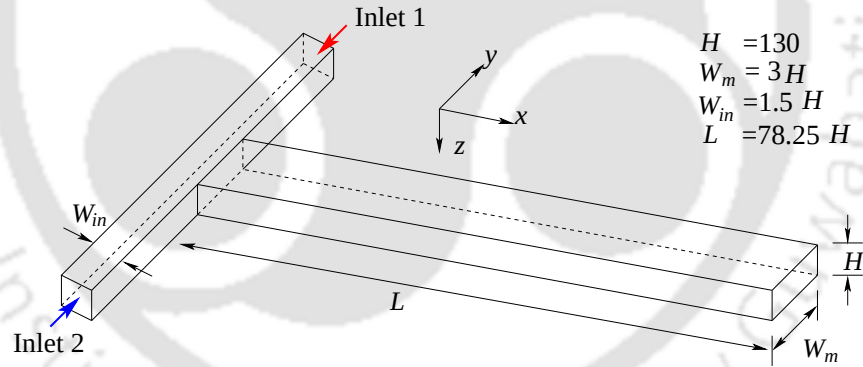


Figure 4.11: Schematic diagram of 3D T-shaped microchannel

The spatial discretization is done by using CUBISTA scheme for the convective terms and CDS for the diffusive terms in all the governing equations. The time step size (Δt) is 10^{-4} s . Convergence is set at 10^{-5} . The problem is also solved by using the commercial solver ANSYS Fluent 14.5. In ANSYS Fluent, the steady-state solver with second order upwind (SOU) scheme has been used for the spatial discretization and to evaluate the mixture density, the volume weighted mixing law has been used. The mixing index obtained at the outlet of the channel and the associated pressure

drop for different Re by using the developed solver and the commercial solver are compared with that of Hsiao et al [92]. The comparison is shown in Figs. 4.12(a) and (b), respectively. From the figure, it can be clearly seen that the numerical results obtained from the developed solver are more closer to that of those reported in Hsiao et al. [92] than compared to that of the ANSYS Fluent.

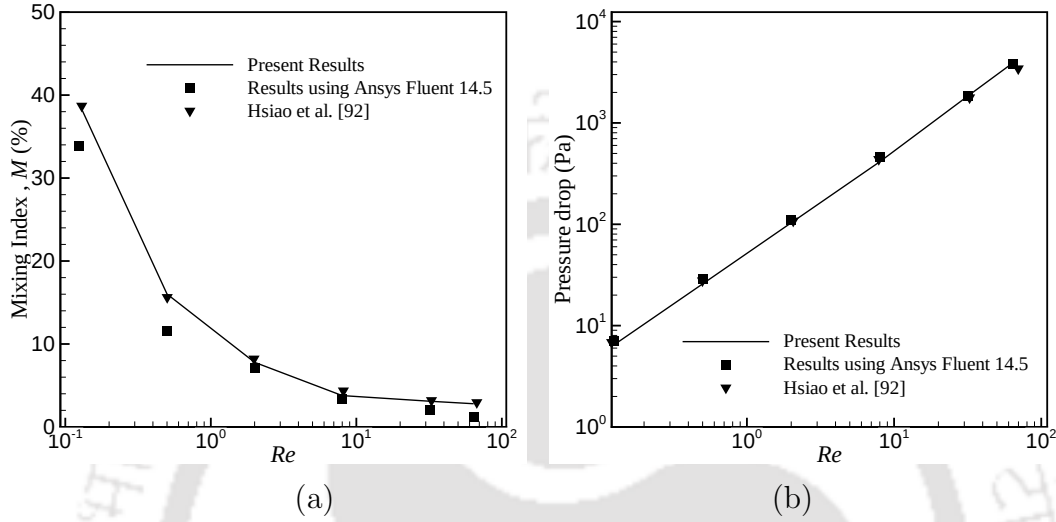


Figure 4.12: Comparisons of the present numerical results with literature and Ansys-Fluent for the 3D T-microchannel at different Re : (a) outlet mixing efficiency, (b) pressure drop between the inlets and the exit of the microchannel.

4.2.6 Three-dimensional mixing in a microchannel with longitudinal vortex generators

In this section, a more complicated three-dimensional mixing problem has been selected. The problem consists of mixing of two liquids in a T-shaped microchannel in the presence of longitudinal vortex generators. This test problem has also been adopted from the work of Hsiao et al. [92]. The problem concerns the mixing behavior of the same T-shaped micromixers (referred in Section 4.2.5), but in the presence of divergent rectangular winglet pairs (RWPs) mounted on the bottom of the main channel. The basic channel dimensions are same as shown in Fig. 4.11. The winglet thickness is $t = 0.3H$, $L_e = 10H$ is the length from the inlet of the straight main channel to the first pair of winglet. The vortex generators with height ($h=0.75H$)

protrude into the flow at an angle of attack ($\theta=22.5^\circ$). The width of the gap between the winglets of a RWP is $w_c = 32.5 \mu\text{m}$, the distance between each winglet of a RWP and its neighboring sidewall is $w_d = 30 \mu\text{m}$ and the number of modules $N_m = 5$. The spacing between the consecutive winglet pairs is $D=1.5W_m$ whereas $d=0.167W_m$ is the asymmetry index. The schematic diagram of the problem is shown in Fig. 4.13.

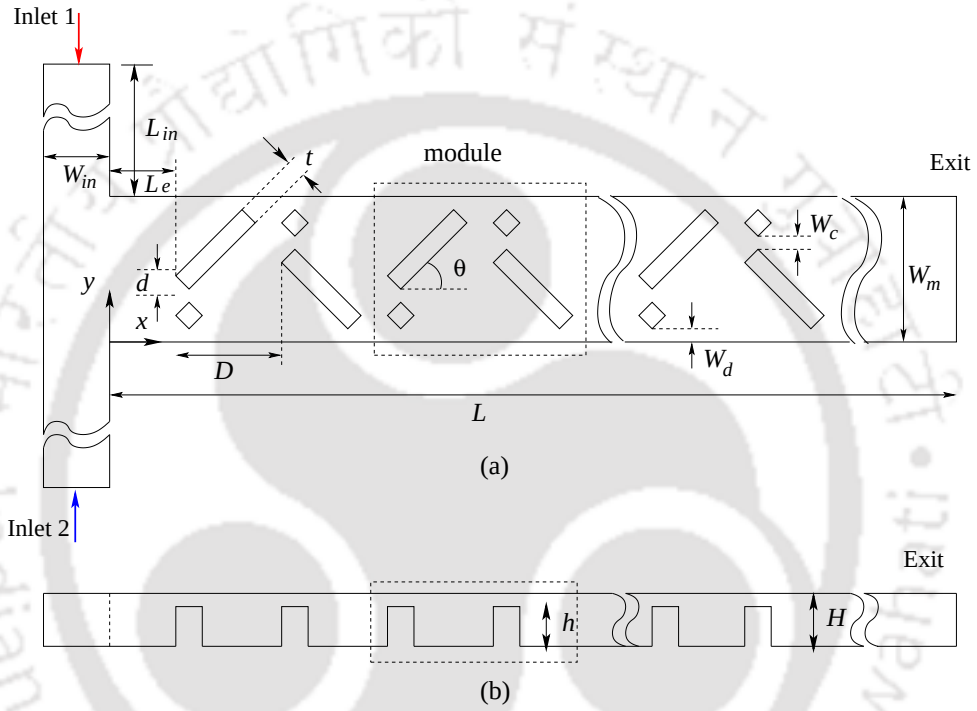


Figure 4.13: Schematic diagram of 3D T-shaped microchannel with LVG (a) top view, (b) side view

Comparison of mixing index calculated at the outlet of the channel from present simulations and the associated pressure drop for different Re are depicted in Fig. 4.14. It is easy to see a reasonably good agreement of the results from the present solver with that of Hsiao et al. [92]. The validation results undercover the ability of the present solver to simulate microfluidic problems with complex flow structure with a good amount of accuracy.

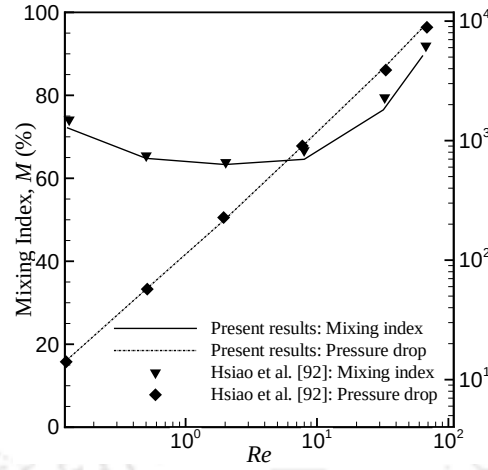


Figure 4.14: Comparisons of the outlet mixing efficiency and the pressures drop of the 3D T-shaped microchannel with LVGs at different Re

4.2.7 Mixing in a three-dimensional micromixer with gaps and baffles

This test case has been adopted from the work of Xia et al. [144]. They studied, both numerically and experimentally, the mass transfer characteristics in a micromixer with gaps and baffles. The schematic diagram of the micromixer has been shown in Fig. 4.15. The specific geometric dimensions are provided in Table 4.3.

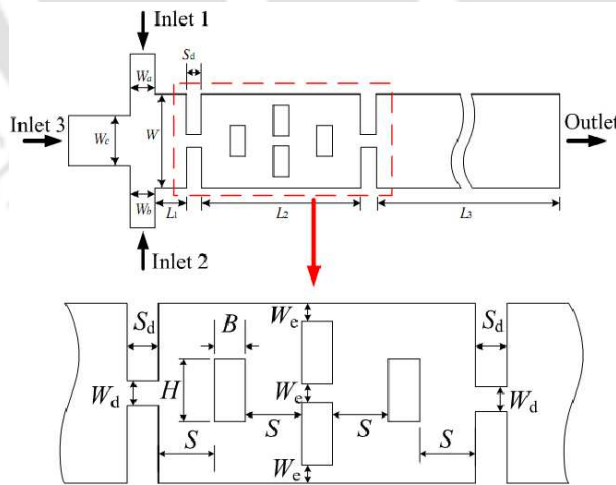


Figure 4.15: Schematic diagrams of the micromixer with gaps and baffles

Table 4.3: The geometric dimensions of the micromixer presented in this study

Parameters	W_a	W_b	W_c	W	W_d	W_e	S_d	S	H	B	L_1	L_2	L_3
Values (μm)	80	80	160	290	40	30	50	90	100	50	100	510	910

The three inlets are set as velocity inlets and the outlet is a pressure outlet where the reference atmospheric pressure is zero. The adiabatic boundary conditions are set at the solid walls. DI water and labeled water are taken as the two working fluids for mixing analysis. In the simulation, the temperature is taken to be 20 °C. The density and viscosity of water are 998.2 kg.m^{-3} and $0.00097 \text{ kg.m}^{-1}.\text{s}^{-1}$, respectively. The diffusivity between water and ink is $3.23 \times 10^{-10} \text{ m}^2.\text{s}^{-1}$. The Reynolds numbers are calculated based on the physical parameters of water and the characteristic length of inlet 3 (horizontal inlet).

The computational mesh comprises of 522800 hexahedral elements. For the spatial discretization of the convective terms, CUBISTA scheme has been used whereas CDS has been used for the discretization of the diffusive terms. The time step size is 10^{-4} s with the steady-state convergence criteria is set at 10^{-5} . Simulations are carried out for $Re = 10$. A velocity of magnitude $6.073 \times 10^{-2} \text{ m.s}^{-1}$ are specified at all the three inlets.

Figures 4.16(a) and (b) represent the visualization of the flow field in the xy -plane at the middle of the channel height obtained from the present numerical results with that of the experimental results performed by Xia et al. [144] for both Re .

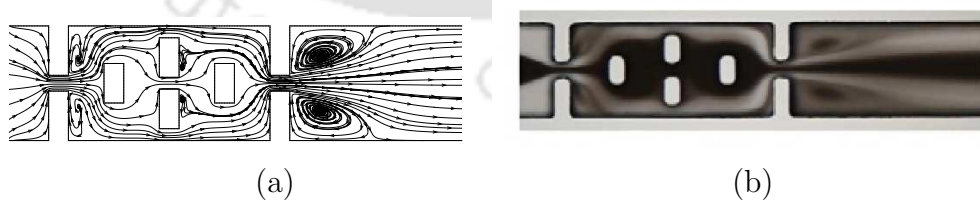


Figure 4.16: Comparison of the characteristics of fluid flow in the xy -plane at the middle of the channel height for $Re = 10$: (a) present simulations, (b) experimental results.

However, for a quantitative comparison, the mixing index values calculated at the outlet are shown in Table 4.4 along with the values reported in the literature. From the table it can be seen that the present results are in better agreement with the experimental results than compared to that of the numerical results obtained by Xia et al. [144]. However, the present numerical results underpredicts the values of mixing index a bit, but the percentage errors are within the acceptable limit.

Table 4.4: Comparison of mixing index

Parameter	Present results	Xia et al. [144]		% Error $(\frac{b-a}{b} \times 100)$
	(a)	Experimental (b)	Numerical	
Re=10	54.2	56.4	61	3.9

4.3 Closure

The present chapter discusses the verification and validation studies for the developed solver. In this chapter, some of the early results for flows with single as well as with multiple species (without phase change) obtained from the in-house quasi-incompressible solver are presented. For problems involving multiple species, all the three aspects of varying density i.e., gradients of temperature, concentration and both, have been explored. For all the cases studied, the results obtained are found to be in good agreement with the available literatures. In the next chapter, the developed solver has been used to study the mixing characteristics of a newly devised passive micromixer for its mixing capabilities.

Chapter 5

Numerical Assessment of Mixing Performances With Curved Ribs

Numerous works were carried out in examining the mixing capability in conventional symmetric micromixers typically, T and/or Y type micromixers. Use of different bluff-body obstacles like circular, triangular, diamond and rectangular shaped showed appreciable amount of mixing enhancement in these symmetric micromixers [82,83,86]. However, to the best of our knowledge, very few of them has focussed on to explore the mixing quality in cross-T type microchannels which renders a simple asymmetric microfluidic junction. Despite of its simple geometry, this type of microfluidic junctions suffer from the disadvantage of demanding a longer channel to get proper mixing. Indeed for a specific configuration of this class, Ansari et al. [32] reported a value of about 17% of mixing efficiency at the outlet when the interface between the fluids is along the centerline of the mixing channel. It has already been mentioned that an ideal configuration would demand maximum mixing with lower possible pressure drop across it. Therefore, an effort has been made in this work to improve the mixing performance as a whole, both in terms of increased efficiency and lower pressure drop, in a simple asymmetric microfluidic junction. We select the microchannel geometry to be comprised of a Cross-T microfluidic junction as referred in the work of Sarkar et al. [34].

The present work considers a measure to enhance the mixing capability in cross-T micromixers by placing a new design of obstacle geometry, in the form of thin

curved ribs. The mixing performance of the micromixer is studied extensively by using the developed numerical solver for low Re flows (<1), typical of microfluidic applications. However, one point to be noted is that the purpose of placing the obstacles is not to generate turbulence in this flow regime which is characterized by a sufficiently low Re , but their effect is to stir the fluid creating transversal mass transport. The principle is very similar to the phenomenon of mixing sugar in a cup of coffee. For example, one has to wait passively for a longer time for the sugar to get mixed evenly into a cup of coffee. But the same mixing process can be accelerated by stirring the mixture with a spoon.

First, the effect of the newly designed obstacle is studied for this asymmetric microchannel. Results have been analyzed thoroughly in terms of the flow field and quantifying the mixing performances to draw the salient conclusions for the mechanism of mixing enhancements. Numerical simulations are also performed to compare, on one to one basis, the mixing capability by using curved ribs with that of conventional straight rib obstacles having the same geometric parameters.

Secondly, a parametric study is carried out with the newly devised curved obstacles to examine the effects of certain geometric as well as flow parameters such as, the number of modules (defined as one staggered pair of ribs), angle of inclination (θ) i.e. the angle between the chord of the obstacle and the horizontal line and size of obstacles (based on chord length l), axial distance between the obstacles (s) and Reynolds number (Re) on the mixing efficiency across various points inside the channel. For all the cases, mixing efficiencies at the outlet of the channel as well the pressure drops are calculated and suitably tabulated ¹.

5.1 Problem Definition

In this section, a two-dimensional study has been presented to investigate the effect of placing a set of curved ribs as the obstacles on the mixing performances in a cross-T shaped micromixer. The selection of obstacles with a curved surface is

¹A substantial portion of this chapter has been published in P. Borgohain, A. Dalal, G. Natarajan and H. P. Gadgil (2018), "Numerical assessment of mixing performances in cross-T microchannel with curved ribs", *Microsyst. Technol.*, vol. 24, pp. 1949-1963

motivated from the success of implementing curved winglet type vortex generators for heat transfer enhancements [145]. The analogy between heat and mass transfer compels us to see its effect in mass transfer enhancement in microchannels.

The base geometry is taken same as that of used by [32]. The geometry is shown schematically along with the dimensions in Fig. 5.1. The width of the mixing channel (W) has been taken as $200\ \mu\text{m}$ and is equal to the widths of the two inlet channels (side and main/horizontal). The lengths of the main mixing channel and inlet channels are fixed at $L=5\ \text{mm}$ and $L_{in}=1.8\ \text{mm}$, respectively. Species considered to be are ethanol and water. The properties of the water and ethanol were taken at 20°C and are given in Table 5.1. The non-dimensional numbers such as Reynolds number (Re) and Schmidt numbers (Sc) are defined based on the reference quantities which are assumed to be associated with the unmixed ethanol stream entering from the main inlet. Thus, in the definition of Re and Sc , properties (such as ρ , μ and D) of ethanol, average velocity at the main inlet ($\bar{u}$) and the width of the main inlet channel (W) are being used.

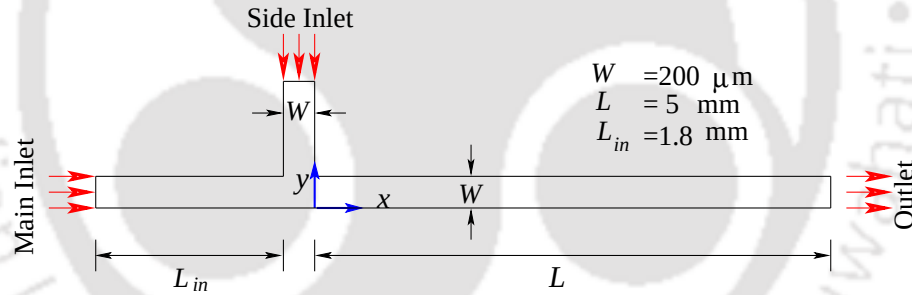


Figure 5.1: Mixing Geometry of two fluids micromixer for the basic cross-T microchannel.

For the obstacle geometry, first a curved surface has been generated by selecting the curvature similar to that of the inner profile of the EPPLER-376 airfoil with a chord length of $l=1\ \text{mm}$. In that curvature, a constant thickness (t_o) of $0.02\ \text{mm}$ has been provided so as to generate a thin curved rib by taking into account of the manufacturing facility. The curved obstacle generated from this profile has been scaled down to a factor of 0.2 to fit inside the channel that corresponds to a chord length (l) and thickness (t_o) of $0.2\ \text{mm}$ and $0.004\ \text{mm}$, respectively. The schematic diagram of the obstacle geometry is shown in Fig. 5.2(a). A staggered

Table 5.1: Properties of the fluids at 20°C.

Fluid	Density, ρ (kg/m ³)	Viscosity, μ (Pa.S)	Mass Diffusivity, D (m ² /s)
Water	999.8	0.9×10^{-3}	1.2×10^{-9}
Ethanol	789.0	1.2×10^{-3}	1.2×10^{-9}

configuration of the ribs placed on either side of the centerline of the mixing channel has been chosen, which is schematically shown in Fig. 5.2(b). The set of one pair of obstacles/ribs are termed as one module. Moreover, the two obstacles comprising a module are chosen such that they represent the mirror image of each other. Inside the main channel the obstacles are placed at an angle of inclination of $\theta = 45^\circ$ which is defined as the angle between the chord of the obstacle and the horizontal line. The distance between the wall of the channel and that of the obstacle (d) is 0.01 mm. The first obstacle is placed at an axial distance (L_{obs}) of 0.225 mm from the start of mixing channel whereas the spacing between two consecutive obstacles (s) is 0.135 mm. The number of modules taken is denoted by N_m which is equal to 4 in Fig. 5.2(b).

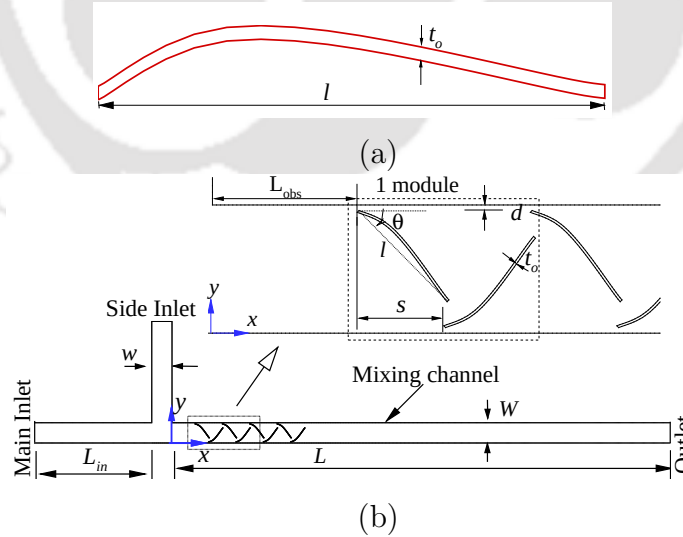


Figure 5.2: Schematic layout of (a) curved ribs employed as the obstacles within the microchannel and (b) the cross-T microchannel with modified curved obstacles.

A uniform and equal velocity profile based on $Re = 0.5$ (which is of 3.8 mm/s) is specified at both the inlets. The walls are assumed to be impermeable with no-slip condition specified for velocity components. At the outlet of the channel, a fixed-pressure boundary condition is applied and the normal gradients of pressure on the solid walls of the micromixer was considered to be zero. CUBISTA scheme [133] is used for the discretization of convective terms whereas CDS is used for the diffusion terms. Time step size is 10^{-4} s and the relative convergence is set at 10^{-5} .

5.2 Grid Independence Study

In this section a grid independent study is performed to choose the mesh resolution for the present simulations. For this, four different grid densities are selected to study the effect of the number of cells on the predicted mixing behavior in the cross-T junction at $Re = 0.5$. Details regarding the obstacle arrangement are: $N_m = 4$ (i.e., 4 staggered pairs of curved ribs), $\theta = 45^\circ$. At both inlets, a uniform velocity boundary condition of magnitude 3.8 mm/s (based on $Re = 0.5$) has been implemented while the no-slip condition is specified at the walls. At the outlet, pressure outlet boundary condition is applied. Hybrid meshes consisting of hexahedral cells and prismatic cells are being used. Prismatic cells are placed in the neighboring regions of ribs and remaining parts are filled with hexahedral cells. A wide ranges of meshes having 23354, 39448, 64172 and 82422 numbers of cells (also referred to as coarse, medium, fine and finest meshes, respectively) were considered for the study.

Figure 5.3 shows the ethanol mass fraction distribution along the width of the channel at the middle of the main channel (i.e. at $x = 2.5$ mm). The mass fraction distributions observed on fine and finest meshes appear to be quite close to each other. Furthermore, the mixing index at the outlet of the channel and the corresponding pressure drop for all four meshes are shown in Table 5.2. One can observe that as the number of volumes is increased, both mixing index and pressure drop tend to converge to a constant value. It is evident that results for mixing index and pressure drop on the fine and finest meshes agree well and therefore are grid-independent. In order to keep computational cost to a minimum, all studies are carried out on a grid resolution comparable to the fine grid having 64172 (approximately) control volumes in this work.

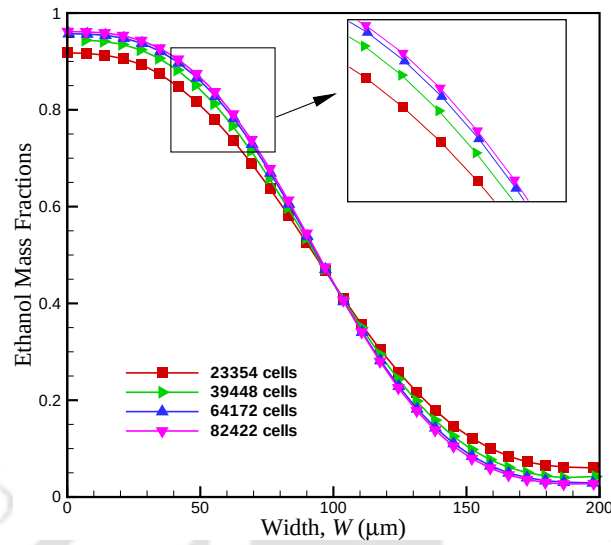


Figure 5.3: Grid independent study: Ethanol mass fraction profile along the width of the mixing channel extracted at the middle of channel i.e., at $x=2.5$ mm from the junction for various numbers of grids.

Table 5.2: Mixing performance with respect to different grid densities.

Sl. no.	Grid density (no. of cells)	Mixing efficiency, M (%)	Pressure drop (Pa)
1	23354	48.4	146
2	39448	45.0	153
3	64172	42.1	156
4	82422	41.5	159

5.3 Results and Discussion

This section presents the results of the numerical simulations for the effect of the obstacles in mixing enhancements. All the results are thoroughly analyzed to draw the salient conclusions for the mechanism of mixing enhancements. It has already been mentioned that the basic reason behind the placement of obstacles is to stir the

fluid to enhance the transversal mass transport. As such, first, the results showing the mixing capability of the new micromixer with the curved obstacles are presented and compared against the standard micromixer having integrated with straight ribs. The results of a complete parametric studies performed for the present work are reported in the subsequent subsections.

5.3.1 Comparison of curved and straight ribs

In order to carry out the comparative study for the mixing capabilities with the two obstacle designs, viz, curved and the conventional straight ribs, an arrangement with $N_m = 4$ with $\theta = 45^\circ$ has been selected (see Fig. 5.2). The distance between the wall of the channel and that of the obstacle (d) is $0.01 \mu\text{m}$. The first obstacle is placed at an axial distance (L_{obs}) of 0.225 mm from the start of mixing channel whereas the spacing between two consecutive obstacles (s) is 0.135 mm .

The developed solver uses a pseudo-transient method to handle the steady-state problems. As such a simple first-order Euler Implicit scheme is employed for temporal discretization. For spatial discretization, the second order accurate CUBISTA scheme [133] and central difference scheme (CDS) are being used for handling the convective and the diffusive terms, respectively. The developed solver is inherently three-dimensional. Therefore, to solve two-dimensional problems, one makes use of hexahedral/prismatic elements of one cell width in the direction normal to the plane of the flow and provide symmetry boundary conditions on the lateral walls to ensure that the simulations are necessarily two-dimensional.

Figures 5.4(a) and (b) show the mass fraction contours for the channels having curved ribs and straight ribs for the same axial locations between $x=0.2-1.6 \text{ mm}$, while Figs. 5.4(c) and (d) show the streamlines patterns for the same, respectively. From the figures, it can be seen that for both the two types of obstacles, i.e., curved as well as straight, the mass fraction contours and the streamline patterns are almost similar.

Table 5.3 shows the comparison of mixing efficiencies at different axial locations along with the pressure drop encountered for both the two configurations of obstacles. From the table, it has been seen that the placement of both the obstacles gives

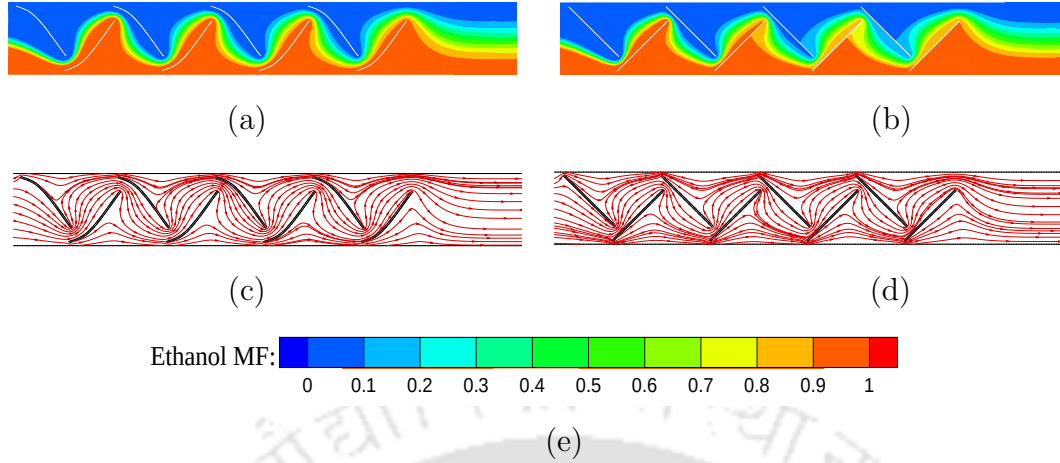


Figure 5.4: Ethanol mass fractions contours across $x=0.2-1.6$ mm for microchannels with (a) curved ribs and (b) straight ribs and streamlines at the same location for microchannel with (c) curved ribs and (d) straight ribs and (e) contour levels for mass fractions.

rise to a significant increase in mixing quality of the cross-T channel compared to that of the base case (i.e., without obstacles). The main reason for this enhancement can be attributed to the fact that the placement of obstacles stirs the fluids in the transverse direction giving rise to species mixing due to lateral convection. But it has also been noticed that a marginally higher enhancement in mixing has been found in terms of the mixing efficiencies for the channel with curved obstacles as compared to that of the straight obstacles. However, the pressure drop occurred in the channel with curved obstacles are significantly low than the corresponding value for the channel with straight obstacles. This observation, which is an outcome of the present study, is also interesting in that the reduction in pressure drop (and hence the power needed to drive the flow) when curved ribs are employed does not degrade the mixing efficiency for the low Re flows investigated in this work. Moreover, the ideal configuration for any passive micromixer is the one where maximum mixing efficiency can be obtained at the cost of minimum pressure drop. As such, the new design of obstacles considered opens up opportunities to design optimal micromixers, which have high mixing efficiencies accompanied by low pressure drops for a range of Re , and to analyze the specific mechanisms that allow the realization of such designs.

Table 5.3: Comparison of mixing efficiency and pressure drop with different obstacle geometry for cross-T micromixer with that of no obstacle case.

Obstacles geometry	Mixing efficiency, M (%)					Pressure drop (Pa)
	$x=0.2$ mm	$x=2$ mm	$x=3$ mm	$x=4$ mm	$x=5$ mm	
Straight obstacles	9.39	33.80	37.10	40.28	43.40	225.2
Curved obstacles	8.71	35.00	38.30	41.50	45.00	153.1
Without obstacles	5.23	13.10	16.6	19.07	21.58	15.8
Without obstacles ([32])	4.3	11.8	14.4	16.9	-	-

5.3.2 Parametric Studies for the curved ribs

As can be seen in Section 5.3.1, the basic advantage of using of curved ribs is the higher mixing efficiency with the lower pressure drop. However, it is also important to note that the design could give good mixing performance at decent pressure drop cost only for a limited range of parameters which may be categorized as geometric and flow parameters. There are a large number of geometrical parameters that can influence the performance of the micromixer. Among these, the following parameters, which are believed to be influential factors, are chosen to study their effect on the mixing performance. The parameters selected for detailed analysis are (1) the number of modules (N_m), (2) the angle of inclinations (θ), (3) axial spacing between curved ribs and (4) size of obstacles. Finally the effect of inlet Re on mixing performance is also investigated.

5.3.2.1 Effect of number of modules (N_m)

In this section, the effects of the number of modules on the mixing behavior of the cross-T type microchannel are studied. The module is defined as a pair of obstacles placed staggeredly on either side of the axis of the channel. Keeping all the parameters same as considered in the study conducted in Section 5.3.1, only the number of modules are varied for the microchannel. The number of modules taken for this study are 1, 4, 5, 6, 8, 10, respectively. The variation of mixing efficiencies calculated along the length of the channel having different number of modules are shown in Fig. 5.5.

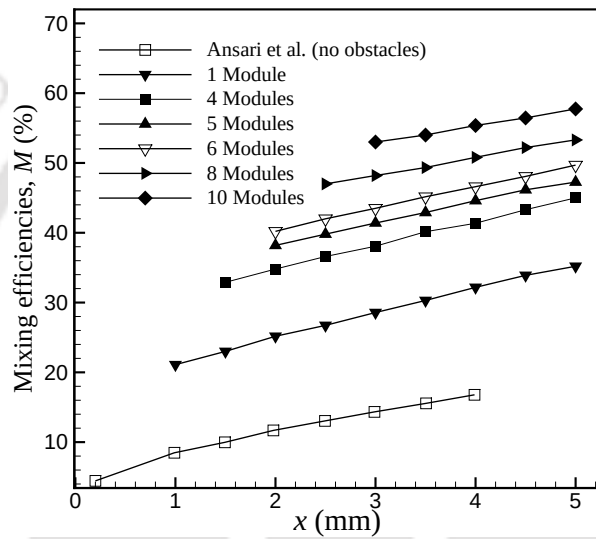


Figure 5.5: Variation of mixing efficiencies along the length of the channel having different number of modules.

From Fig. 5.5, it has been seen that the placement of more number of modules leads to enhanced mixing over the plane channel with no obstacles. In the case of the plane channel, the mixing efficiencies increase almost linearly from the start of the mixing channel till the exit. The first value of mixing efficiency for each line involving a different number of modules corresponds to that location in the channel which is after the last module. For the channels with a progressively higher number of modules, the mixing efficiencies increase to a high value while passing through the modules and after crossing the last obstacle point, the mixing efficiencies follow a more or less linearly increasing pattern. The slope of this linearly increasing pattern is nearly same for all the cases including for the case with no obstacle. This

Table 5.4: Mixing efficiency and pressure drop for different number of modules.

Sl. no.	No. of modules	Mixing Efficiencies, M (%)	Pressure drop, (Pa)
1	1	35.16	44
2	4	45.0	153
3	5	47.26	189
4	6	49.39	225
5	8	53.0	299
6	10	57.5	371

clearly compels us to believe that the enhancements observed in mixing behaviors of the channels is basically due to the placements of the obstacles and more number of modules leads to higher mixing efficiencies. The reason behind this is that the placement of obstacles agitates the transversal motion of the fluids and thus lateral convective transport of the species takes place in addition to diffusive transport. Since mixing efficiency and the pressure drop are two competing objectives, the enhanced mixing has been achieved at the cost of additional pressure drop. The corresponding mixing efficiencies calculated at the outlet for each case and the associated pressure drops are shown in Table 5.4. It has been seen that the increased pressure drop is significantly higher than the corresponding increase in mixing efficiencies. For the 10 module case, the pressure drop is near about 2.5 times more to get an enhancement of 12.5 %, i.e., only 1.27 times more than compared to that of the corresponding values for the 4 module case.

5.3.2.2 Effect of angle of inclination (θ) of the curved ribs

In this section, an effort has been made to see the effect of angle of inclination of the obstacles (θ) on the mixing behavior of the channels under study. Six sets of angles have been taken for the present study including both positive and negative angles. Positive angles correspond to the clockwise rotation of the obstacles whereas negative angles correspond to anticlockwise rotation of obstacles (see Fig. 5.6). The magnitudes of angles considered in the present study are $\pm 30^\circ$, $\pm 45^\circ$ and $\pm 60^\circ$. The basic geometry is same that of studied in Section 5.3.1.

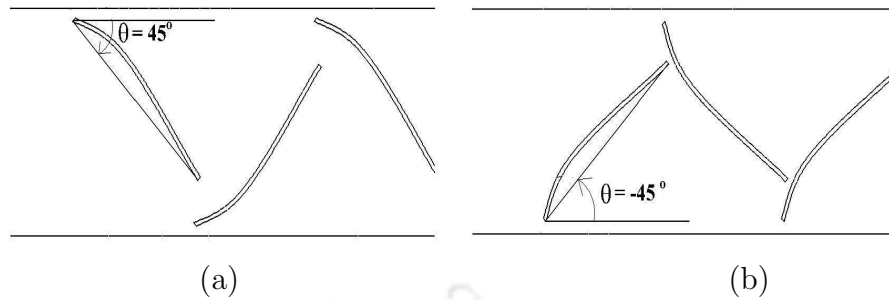


Figure 5.6: Schematic representation of angle of inclination of the obstacles (a) clockwise rotation of obstacles giving +ve angle of inclination and (b) anticlockwise rotation of obstacles giving -ve angle of inclination.

Figures 5.7(a)-(f) show ethanol mass fraction contours for different angle of inclinations. In each sub-figure, the zoomed view of the selected portion of the mixing channel (specified by dotted lines) for the same axial locations of is shown. It can be seen that mixing increases qualitatively with the increase in the angle of inclination irrespective of signs, either positive or negative. However, for the same magnitude of the angle of inclinations, the mixing zone is shifted towards the bottom of the channel for negative angles than compared to that of its positive angle counterparts.

To quantify the degree of mixing, variation of mixing efficiencies along the length of the mixing channel for different angle of inclinations is shown in Fig. 5.8. Also the comparison of mixing efficiencies at the channel outlet along with the pressure drop obtained for different angle of inclinations for the obstacles is shown Table 5.5. From the table it has been seen that with the increase in the value of the angles, both for positive and negative, the mixing efficiencies increases. But at the same time, pressure drop also increases significantly. It has also been seen that for the same value of the angles but with different signs, the value of mixing efficiencies are almost in the same range. However, the channels with the negative angles achieve this mixing at the cost of much higher pressure drop than compared to that of their positive angle counterparts. One of the possible reasons behind this higher pressure drop for the negative angle of inclinations may be the clearance between consecutive obstacles. From Figs. 5.7(a)-(f), one can clearly see that the clearance is more for positive angles rather than the negative angles. Because of the larger clearance,

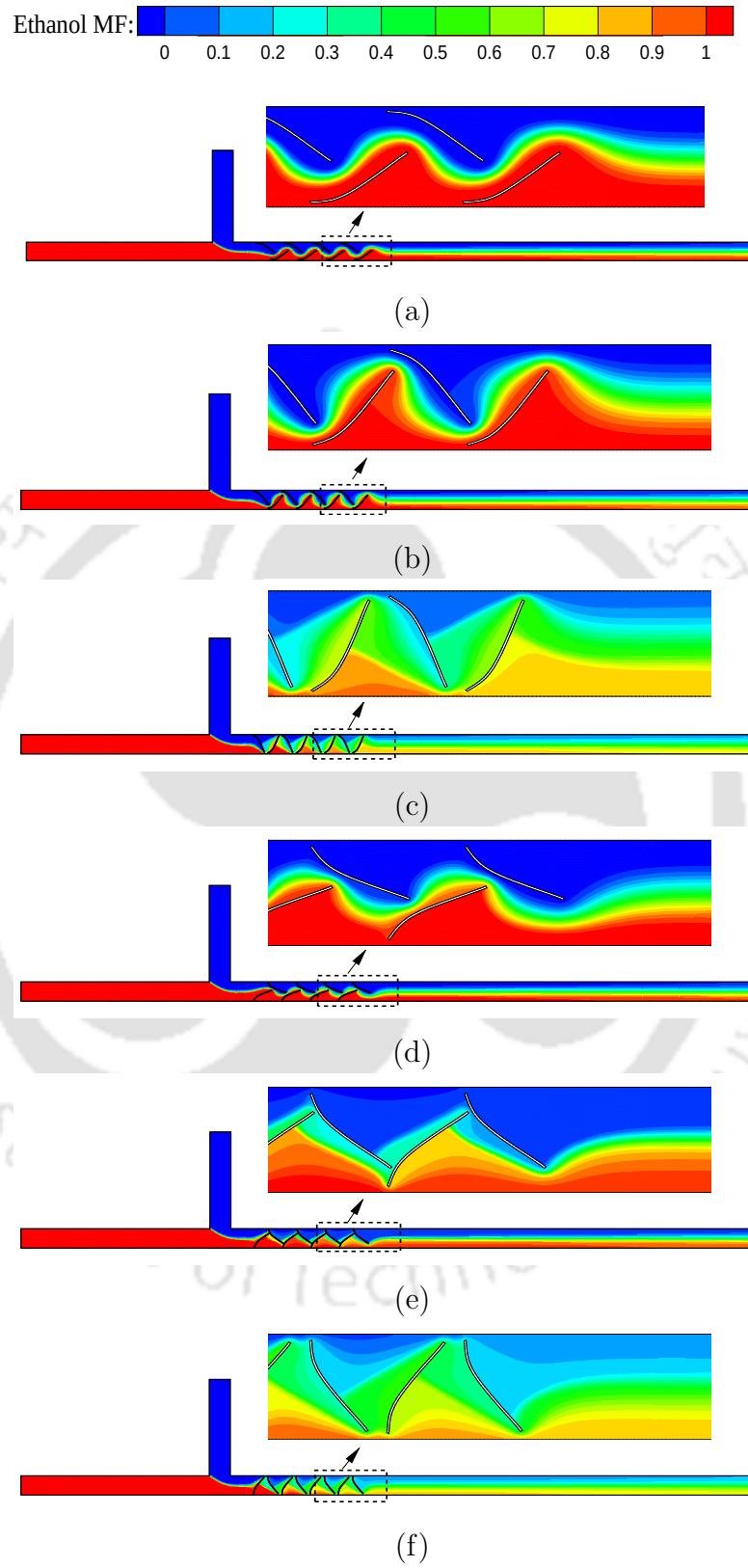


Figure 5.7: Effect of angle of inclination: Ethanol mass fraction contours for angle of inclination of (a) 30° , (b) 45° , (c) 60° , (d) -30° , (e) -45° (f) -60° .

Table 5.5: Mixing efficiency and pressure drop for variation angle of inclination.

Sl no.	Angle of inclination, θ ($^\circ$)	Mixing efficiency, M (%)	Pressure drop (Pa)
1	+30	38.0	52
2	+45	45.0	153
3	+60	62.0	467
4	-30	39.3	149
5	-45	39.5	322
6	-60	62.5	487

the fluid suffers from less resistance to flow through the gap and vice versa. This finally leads to increase in pressure drop for the negative angles of inclinations of the obstacles.

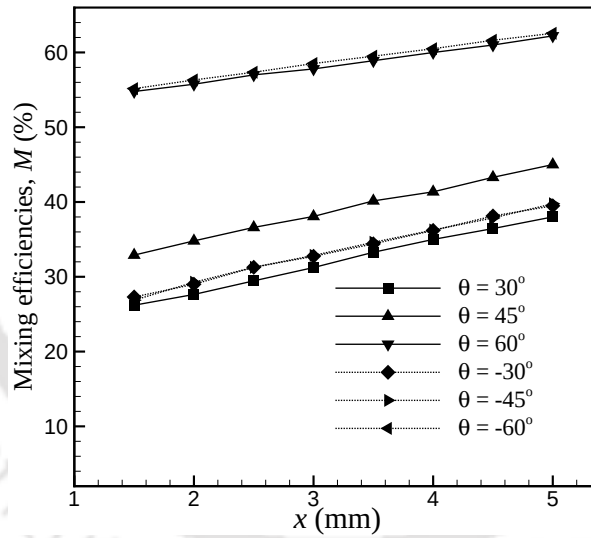


Figure 5.8: Variation of mixing efficiencies along the length of the channel for different angle of inclination of the obstacles.

5.3.2.3 Effect of axial spacing between curved ribs

This section presents the results for the effect of the axial spacing (s) provided between the ribs on mixing behavior of the microchannel. The channel configuration

Table 5.6: Mixing efficiency and pressure drop for different axial spacing.

Sl no.	Axial distance between obstacles, s (mm)	Mixing efficiency, M (%)	Pressure drop (Pa)
1	0.085	40.5	702.9
2	0.135	45.0	153.0
3	0.270	44.7	91.0
4	0.405	42.9	91.73

studied in Section 5.3.1 with 4 modules and 45° angle of inclination is taken as the reference case. In the reference case, the axial spacing between the obstacles is $s=0.135$ mm. In this configuration, the distance between the ribs is varied making it almost halved, twice and thrice (i.e., 0.085, 0.27 and 0.405 mm, respectively) than that of the reference case. The variation of mixing efficiencies along the length of the channel for three different spacing between obstacles are shown in Fig. 5.9. In this figure, the first point for each line corresponds to the axial locations sufficiently downstream of the last module so that the local effect of obstacle placement doesn't come into the picture. Thus, with greater spacing, the first point shifts to a further downstream location. Also, the outlet mixing efficiencies and the pressure drop for the channel having obstacles with different axial spacing are shown in Table 5.6. Comparing the values in the figure and the table, it has been seen that keeping the obstacles very close to each other (i.e., with halved the spacing) did not lead to increase in mixing efficiency but rather it leads to a very huge pressure drop. However, keeping the spacing twice than that of the reference case, the mixing efficiency almost remains same but this time it has been achieved with significantly less pressure drop (almost less than 1.5 times compared to that of the reference case). Any further increase in this distance beyond a limiting value which is 0.27 mm for the present study, the pressure drop almost becomes constant but at the same time mixing efficiency also start dropping. So, it can be concluded that an optimum spacing is required between the obstacles to get the benefit with respect to the combined effects in terms of the higher mixing performance as well as lower pressure drop.

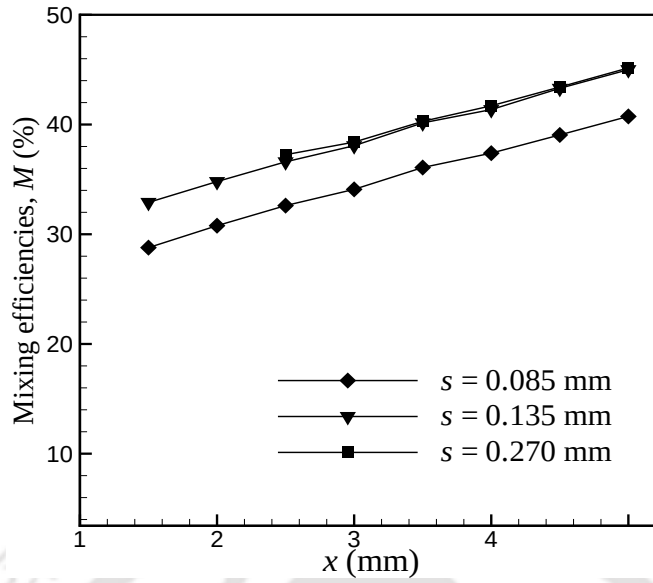


Figure 5.9: Variation of mixing efficiencies along the length of the channel for different spacing between the obstacles.

5.3.2.4 Effect of size of curved ribs

Size of the obstacle is another important factor that can directly affect the mixing performance of the microchannel under study. So it is very much important to have a certain idea of how the size of the obstacles can affect the mixing performance in microchannels. Obstacle configuration with 4 number of modules with an angle of inclination of 45° is taken for this study. For the different sizes of the obstacles, the original curved obstacle with a chord length of 1 mm has been scaled down to different scaling factors such as 0.1, 0.15, 0.175, 0.2 and 0.225 that finally leads to obstacles having dimensions in terms of chord length and thickness (l, t_o) of (0.1, 0.002), (0.15, 0.003), (0.175, 0.0035), (0.2, 0.004) and (0.225, 0.0045), respectively. Ethanol mass fraction contours over the last 2 modules for the channel with different sizes of obstacles are shown in Figs. 5.10(a)-(c) for the scaling factor of 0.1, 0.175 and 0.225, respectively. The figures are plotted for the same axial locations between $x=0.6$ mm to $x=1.6$ mm. From the figures it can be seen that with the increase in the sizes of the obstacles, the two species got more diffused across the interface.

The mixing efficiencies calculated at different axial locations along the length of the channel having different sizes of obstacles are shown in Fig. 5.11. From the figure

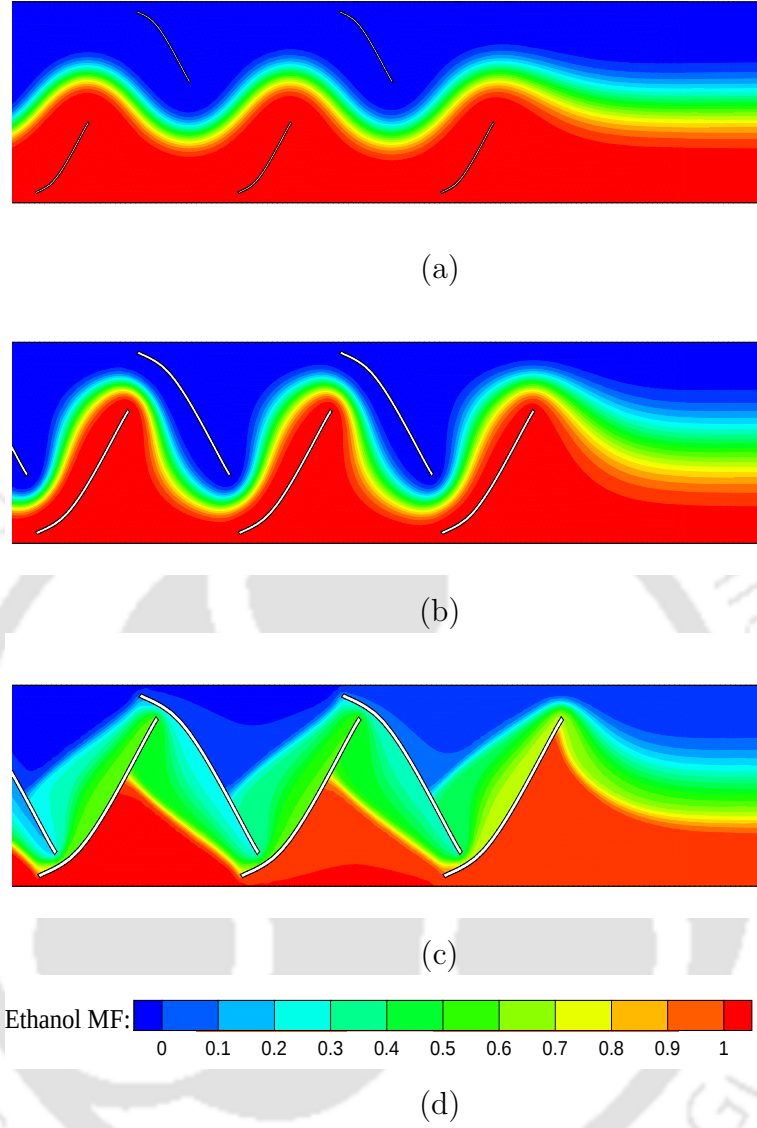


Figure 5.10: Effect of obstacle size: Ethanol mass fraction contours with different sizes of obstacles for cross-T microchannel across the axial locations of $x=0.6$ mm to $x=1.6$ mm for scaling factor of (a) 0.1, (b) 0.175, (c) 0.225 and (d) Contour levels.

it has been seen that the efficiency of the micromixer increases with the increasing size of the obstacles which also supports the mass fraction contours shown in Figs. 5.10(a)-(c). The increments for consecutive higher sizes of the obstacles are also same till a particular size of obstacles which corresponds to the chord length (l) of 0.2 mm for the present study. After this critical size of obstacles, any further increase in the

size of obstacles doesn't lead to any appreciable enhancement in efficiency of the mixer. The quantitative measure of the mixing quality of the present microchannel with different sizes of obstacles are given Table 5.7 in terms of mixing efficiencies at the channel outlet and pressure drop. From the table it can be seen that the increase in efficiency is also counteracted by the significant increase in pressure drop across the channel. And after the critical size of the obstacles, the increase in efficiency by using a bigger size of obstacles is very marginal whereas the increase in pressure drop is significantly high for almost comparable mixing efficiencies. So it is not preferable to use a bigger size of obstacles in regard to pressure drop.

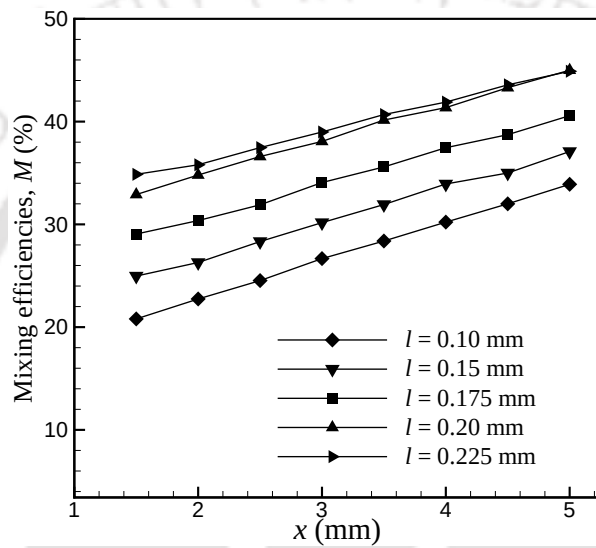


Figure 5.11: Variation of mixing efficiencies along the length of the channel for different sizes of the obstacles.

Table 5.7: Mixing efficiency and pressure drop for different sizes of the obstacle.

Sl no.	Obstacle dimensions	Mixing efficiency, M (%)	Pressure drop (Pa)
1	$l=0.1, t_o=0.002$	33.8	30.0
2	$l=0.15, t_o=0.003$	37.04	44.3
3	$l=0.175, t_o=0.0035$	40.9	71.0
4	$l=0.2, t_o=0.004$	45.0	153.0
5	$l=0.225, t_o=0.0045$	45.08	537.7

5.3.2.5 Effect of Reynolds number (Re)

This section focuses on the effect of the inlet Reynolds number (Re) on the mixing behavior of the microchannel. The Reynolds number is defined as: $Re = \rho_E \bar{u} W / \mu_E$, where ρ_E , $\bar{u}$, W and μ_E are the density of ethanol, average velocity of ethanol in the main inlet, width of the mixing channel and dynamic viscosity of ethanol, respectively. The value of Re is varied from 0.1 to 10. The channel having 4 modules with 45° angle of inclination with a scaling factor of 0.2 is taken as the base case. The degrees of mixing and the pressure drop associated with respect to different Re values are shown in Table 5.8. From the table it can be seen that with the lower value of Re equal to 0.1, higher mixing efficiency (about 86.3%) is achieved even at a comparatively very low pressure drop compared to other channels with different Re values. With the increase in Re , the mixing efficiencies start decreasing with a corresponding increase in pressure drop. One of the possible reasons may be is that at low Re value, the residence time for the fluids is more and since the mixing relies mainly on diffusion at this Re , a comparatively shorter length of the channel is required to achieve the equilibrium mass fraction of 0.5. As the value of Re increases, the flow velocities also get increased having fixed all the other parameters. This results in the reduction of the residence time for the fluids and the fluids get less time to diffuse into each other.

Table 5.8: Mixing efficiency and pressure drop at different Re .

Sl no.	Re	Mixing efficiency, M (%)	Pressure drop (Pa)
1	0.1	86.3	30
2	0.5	45.0	153
3	1	33.1	308
4	5	23.4	1784
5	10	21.7	4494

5.4 Closure

The focus of this chapter lies in the implementation of the developed solver in application to microfluidic devices, such as micromixers. It involves a newly designed obstacle geometry, in the form of thin curved ribs, and its layout in a cross-T microfluidic junction type micromixer to enhance the rate of mixing between different liquids. The performance of the newly designed micromixer is explored thoroughly for its mixing capability via numerical analysis. It has been found that the use of curved ribs is more preferable compared to its straight ribs counterparts for enhancing the mixing capability in terms of the combined effect of increased mixing efficiency with lower pressure drop. Subsequently, a set of parametric studies are also carried out to see the effects of different geometric as well as flow parameters on the mixing capability of the present micromixer.

Nevertheless, these investigations were two-dimensional in nature. However, it led to interesting results. As such, the current analysis has been extended for a more realistic three-dimensional configuration to study the flow and mixing characteristics which is presented in the next chapter.

Chapter 6

Performance of a Three-Dimensional Micromixer with Curved Ribs

The studies carried out in Chapter 5 show some interesting results for the mixing performance in regard to a cross-T micromixer by the use of curved ribs. The newly designed curved ribs employed as the flow obstacles are found to produce enhance mixing typically at lower pressure drop compared to that of using conventional straight rib. However, these investigations were two-dimensional in nature. The present chapter focuses on extending this work for a more realistic three-dimensional configuration to study the flow and mixing characteristics. In particular, investigations have been carried out for the role of three-dimensional effects and obstacle curvature for low to medium Re mixing flows, typical of most microfluidic applications. The enhancements in mixing with the incorporation of thin curved ribs is evaluated in a simple cross-T or perpendicular microfluidic junction through extensive three-dimensional numerical simulations. Simulation results for the influence of some of the important geometrical parameters are also brought out for the selection of an optimum configuration of the obstacle layout. ¹.

¹A substantial portion of this chapter has been submitted to Chemical Engineering Research and Design after first revision

6.1 Problem Definition

The present study focusses on assessing the mixing performance of two liquid streams in a three-dimensional cross-T micromixer with the introduction of thin curved ribs. The basic details of the numerical model is similar to that used Section 5.1. In the present study, however, the obstacles are mounted on one of the side walls (at $z = 0$) of the mixing channel protruding with height (h) into the flow at an angle of inclination designated by θ . The schematic diagram of the model under study is shown in Figs. 6.1(a)-(c). All dimensions of the geometry is provided in Table 6.1.

Table 6.1: Basic dimensions of the geometry under study.

Sl. No.	Parameter	Dimensions	Sl. No.	Parameter	Dimensions
1	$w = W$	$200 \mu\text{m}$	6	l	$200 \mu\text{m}$
2	L_{in}	1.8 mm	7	t_o	$4 \mu\text{m}$
3	L	5 mm	8	θ	45°
4	H	$140 \mu\text{m}$	9	L_{obs}	$225 \mu\text{m}$
5	h	$0.75 H$	10	d	$0.01 \mu\text{m}$

In the present study, we consider the mixing of ethanol and water with the former entering through the main inlet and the later enters through the side inlet. Both the two inlet fluids are entering with the same volume flow rate.

An extensive parametric study is carried out with the newly devised curved obstacles to examine the effects of certain geometric as well as flow parameters on the mixing efficiency of the microchannel. In this work, we choose the obstacle height (h), number of mixing modules (N_m), angle of inclination (θ) and size of obstacles (based on l, t_o) as the geometric parameters to be investigated; while the values of $H, L, L_{in}, W, d, L_{obs}$ are kept fixed. The effect of inlet Reynolds numbers (Re) is also explored to judge the mixing performance over a range of flow conditions. We remark that the non-dimensional numbers reported in this study are defined based on the reference quantities associated with the unmixed ethanol stream, the average velocity of ethanol at the main inlet and the width of the main channel. The value of Sc is equals to 1267.

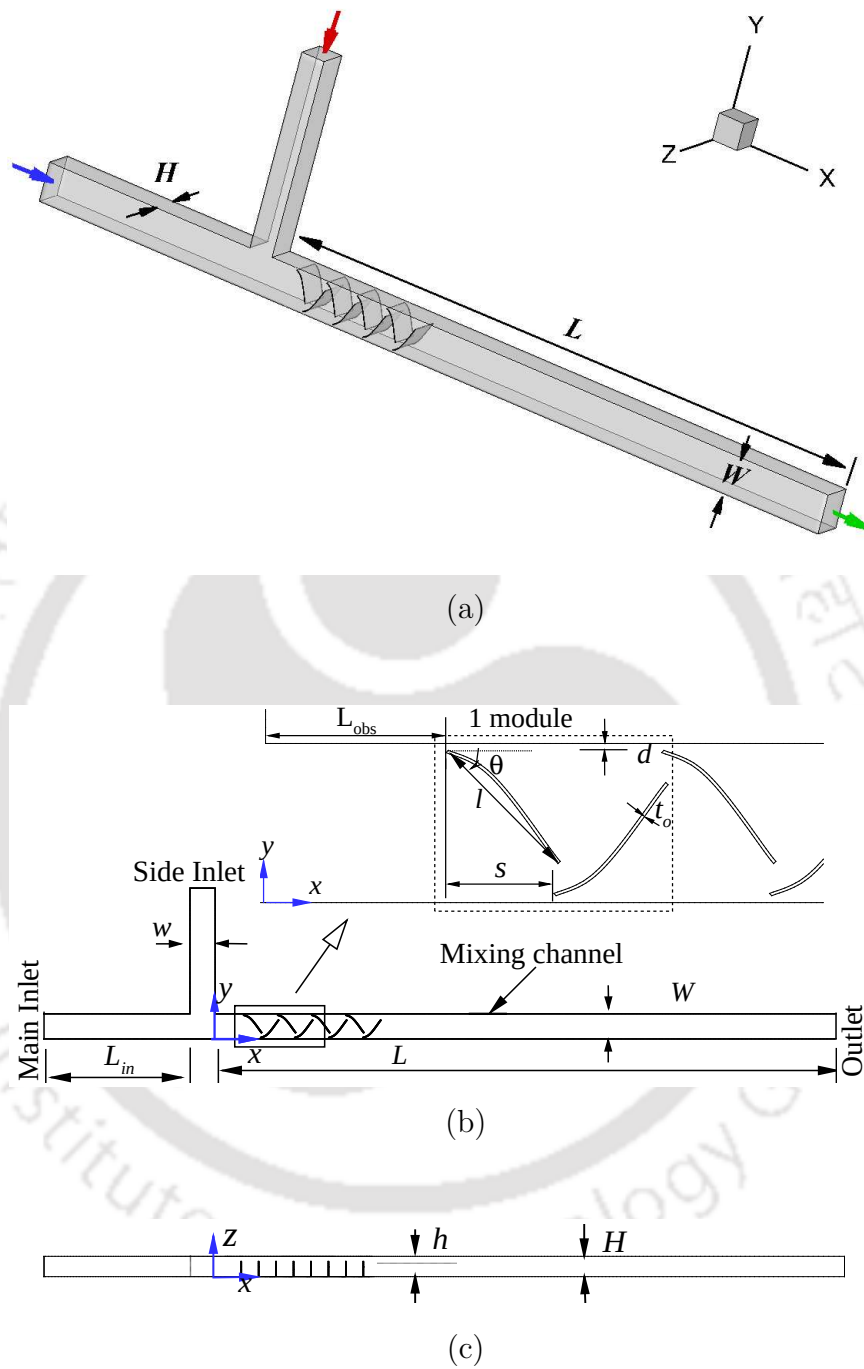


Figure 6.1: Schematic diagram of the complete set up of the microchannel geometry with curved obstacles (a) 3D view, (b) side view and (c) top view (not to scale).

6.1.1 Boundary conditions

Uniform velocities are specified at the inlet based on fluid properties and chosen Reynolds number. The mass fraction of water and ethanol for the main and side inlets are (0,1) and (1,0), respectively. The walls are assumed to be impermeable with no-slip condition specified for velocity components. The applicability of the no-slip condition is justifiable as the Knudsen number (Kn), defined as the ratio of the mean free path (λ) of fluid molecules to a characteristic length (L), is less than 10^{-3} [144]. At the outlet of the channel, pressure outlet boundary condition with a fixed value of 1 atm is applied and the normal gradients of pressure on the solid walls of the micromixer was considered to be zero.

6.1.2 Numerical flow solver

The present study comprises of three-dimensional numerical simulations which incur a high computational cost. To avoid the high computational cost, problems having a steady-state solution is preferably solved by using a steady-state solver. Although the solver developed in this work has been verified to handle three-dimensional problems with a good amount of accuracy, as can be seen in Sections 4.2.5 and 4.2.6, it is based on a pseudo-transient approach to solve steady-state problems. This can further increase the computational cost to a great extent. As such, the commercially available numerical software ANSYS Fluent 14.5 [146], has been used to simulate the flow and mixing in this case.

The steady solver with SIMPLE algorithm is adopted to implement the coupling between pressure and velocity. Second order upwind scheme is used to discretize the convective term of the governing equations [92]. This choice also minimizes false diffusion which could otherwise be detrimental to mixing problems. Solutions are considered to be converged when the relative residual of each variable is less than 10^{-5} .

6.2 Grid Independence Study

Before performing the final numerical simulations, a grid independent study has been carried out to choose the mesh resolution for the present cross-T microchannel

geometry studied in this work. To this end, the following parameters are being selected, viz, $Re=0.5$, $N_m = 4$, $\theta = 45^\circ$ and $l = 0.2 \mu\text{m}$. All the obstacles are placed at an axial distance of $s=135 \mu\text{m}$ from one another. To perform the test, three different meshes having approximately 0.2, 0.4 and 1 million hybrid unstructured cells (also referred to as coarse, medium and fine meshes respectively) are used for the simulations. The results of grid independence test are summarized in Fig. 6.2 which shows the mass fraction distributions at the outlet. The mass fraction distributions observed on medium and fine meshes appear to be quite close to each other.

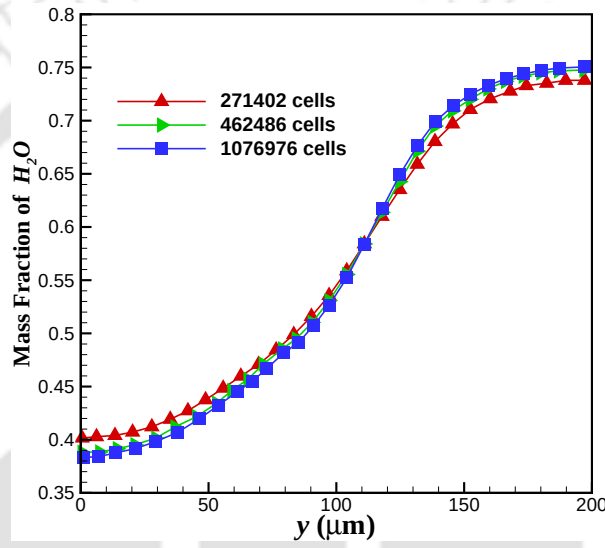


Figure 6.2: Grid independent test: Mass fraction variation along the width of the channel at the $z=100 \mu\text{m}$.

Furthermore, the mixing index at the outlet of the channel and the corresponding pressure drop for all three meshes are shown in Table 6.2. One can observe that as the number of volumes is increased, both mixing index and pressure drop tend to converge to a constant value. It is evident that results for mixing index and pressure drop on the medium and fine meshes agree well and therefore are grid-independent. In order to keep computational cost to minimum, all studies are carried out on a grid resolution comparable to the medium grid of 4.6 lakhs (approximately) control volumes in this work.

In this context, the Grid Convergence Index (GCI) proposed by Roache [147]

Table 6.2: Effect of number of cells used in the simulation on mixing index and pressure drop.

Sl. no.	Number of control volumes	Mixing index, M (%)	Pressure drop, $\Delta\Pi$ (Pa)
1	271402	72.93	110.91
2	462486	70.72	113.02
3	1076976	70.33	114.87

is found to be an another measure of convergence of relevant quantities with mesh refinement. The index is an indicator of the proximity of the solution to its asymptotic value and typically employs three mesh resolutions to estimate the solution in the continuum regime using Richardson extrapolation. Stated mathematically, the GCI may be calculated as,

$$GCI_{21} = F_s \frac{|\epsilon_{21}|}{r_{21}^p - 1} \quad (6.1)$$

where, $F_s = 1.25$ is the factor of safety, $\epsilon_{21} = \frac{M_{\Delta x_1} - M_{\Delta x_2}}{M_{\Delta x_1}}$ with the subscripts 1, 2 and 3 referring to fine, medium and coarse meshes and $r_{21} = \frac{\Delta x_2}{\Delta x_1}$ is the grid refinement ratio. In the present studies, we use the mixing index (M) as the solution functional and assume $p = 2$, since nominally second-order accurate scheme is employed. It must be noted that we do not use the solutions to determine p since the meshes are unstructured and are not generated through uniform refinement. Table 6.3 shows the GCI_{21} and GCI_{32} values for the micromixer configuration. For specific details on computation of GCI, the readers may refer to [147–149].

Table 6.3: Grid convergence study.

Parameter	GCI_{21}	GCI_{32}
Mixing Index (M)	0.923%	9.38%

It can be seen that the GCI_{21} is significantly smaller than GCI_{32} indicating that the dependence of the mixing index on the grid resolution is considerably reduced. Importantly, the smaller value of GCI_{21} is also evidence that the solution is nearly

independent of mesh resolution and no reasonable improvement can be achieved by increasing the number of cells in the domain. This is also reflected in Fig. 6.3 which shows the mixing indices on the three meshes along with the extrapolated value.

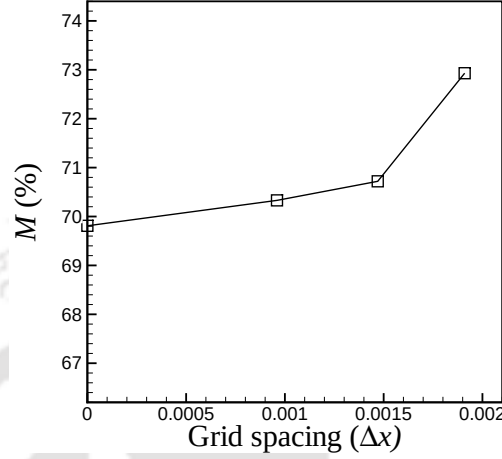


Figure 6.3: Variation of mixing indices on the three meshes along with the extrapolated value.

6.3 Results and Discussion

This section presents the results of the numerical simulations for the effect of the obstacles in mixing enhancements. All the results are thoroughly analyzed to draw the salient conclusions for the mechanism of mixing enhancements. The basic reason behind the placement of obstacles is to stir the fluid that may lead to the generation of transverse velocity components. These transverse convective currents, when combined with diffusion are observed to aid the mixing process. First, the results showing the mixing capability of the new micromixer with the curved obstacles are presented and compared against the standard micromixers. This is then followed by the results obtained from the parametric studies performed for the present work.

6.3.1 Comparison of straight and curved obstacles

In this section, we presented the results obtained for three different microchannels geometries which are as follows,

1. Microchannel with no obstacles placed inside the channel (referred to as the base case),
2. Microchannel integrated with non-curved (straight) rectangular obstacles placed inside the channel and
3. Microchannel with the newly conceptualized obstacles having a curvature along the surface.

The geometrical parameters associated with the obstacle, such as height (h), angle of inclination (θ), size (l), spacing between each obstacle (s), number of modules (N_m) are kept same to make a comparative study of the above three configurations possible. The corresponding values are $h = H = 140 \mu\text{m}$, $\theta = 45^\circ$, $l = 0.2 \text{ mm}$, $s = 0.135 \mu\text{m}$, $N_m = 4$. The value of Re is assumed to be 0.5, typical of many microfluidic applications.

The mass fraction distributions at three different vertical cross sections namely before the first module, after the last module and at the exit of the channel is shown in Figs. 6.4(a)-(c) for the base case and cases with straight and curved obstacles, respectively. It has been seen that among the three microchannels, the mass fractions become more homogenized at the outlet for the channel with curved obstacles.

To get a better insight of the mechanism of mixing in the presence of obstacles, we have observed the flow patterns on different vertical cross sections, viz, before the start of obstacles, after the third and sixth obstacles that corresponds to the planes at $x = 0.2$, 0.6388 and 1.043 mm , respectively. These vector plots are shown in Figs. 6.5(a)-(c) for the base case and for the channels with straight and curved obstacles, respectively. From the Fig. 6.5(a), it has been clearly seen that for the base case the velocity magnitudes are very small compared to that of the channels with obstacles shown in Figs. 6.5(b) and (c). However, for the cases with obstacles, higher magnitude of velocity vectors can be seen and also the velocity field in the cross sections corresponding to subsequent obstacle changes their direction accordingly to mirror the flow field of the preceding obstacle. From these results one can conclude that the presence of obstacles generate additional transverse velocity components. The strength of these secondary flows determines the extent of mixing attained in channels with obstacles.

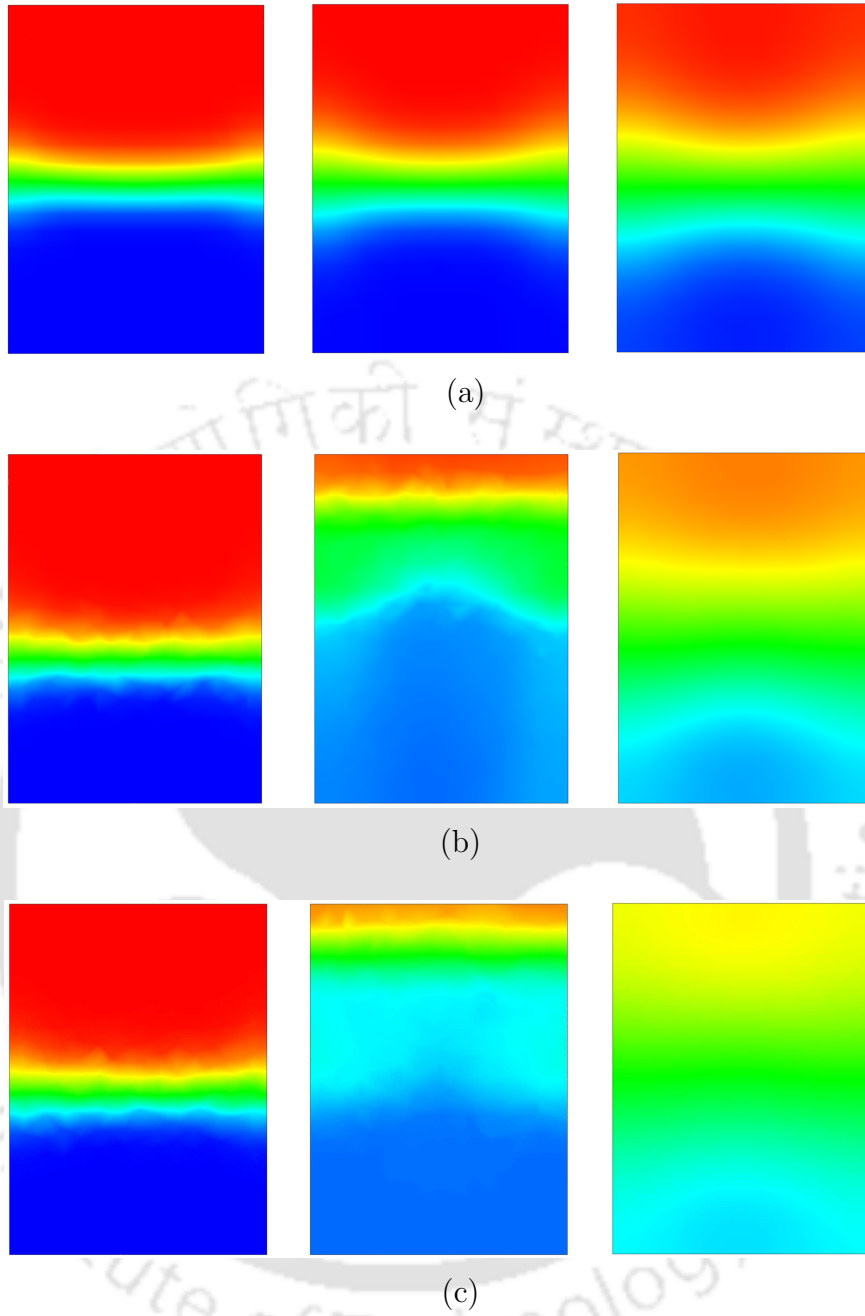


Figure 6.4: Mass fraction distributions on three vertical cross sections namely before the first module (left), after the last module (middle) and at the exit of the channel (right) (a) base case (without obstacles), (b) channel with straight obstacles and (c) curved obstacles.

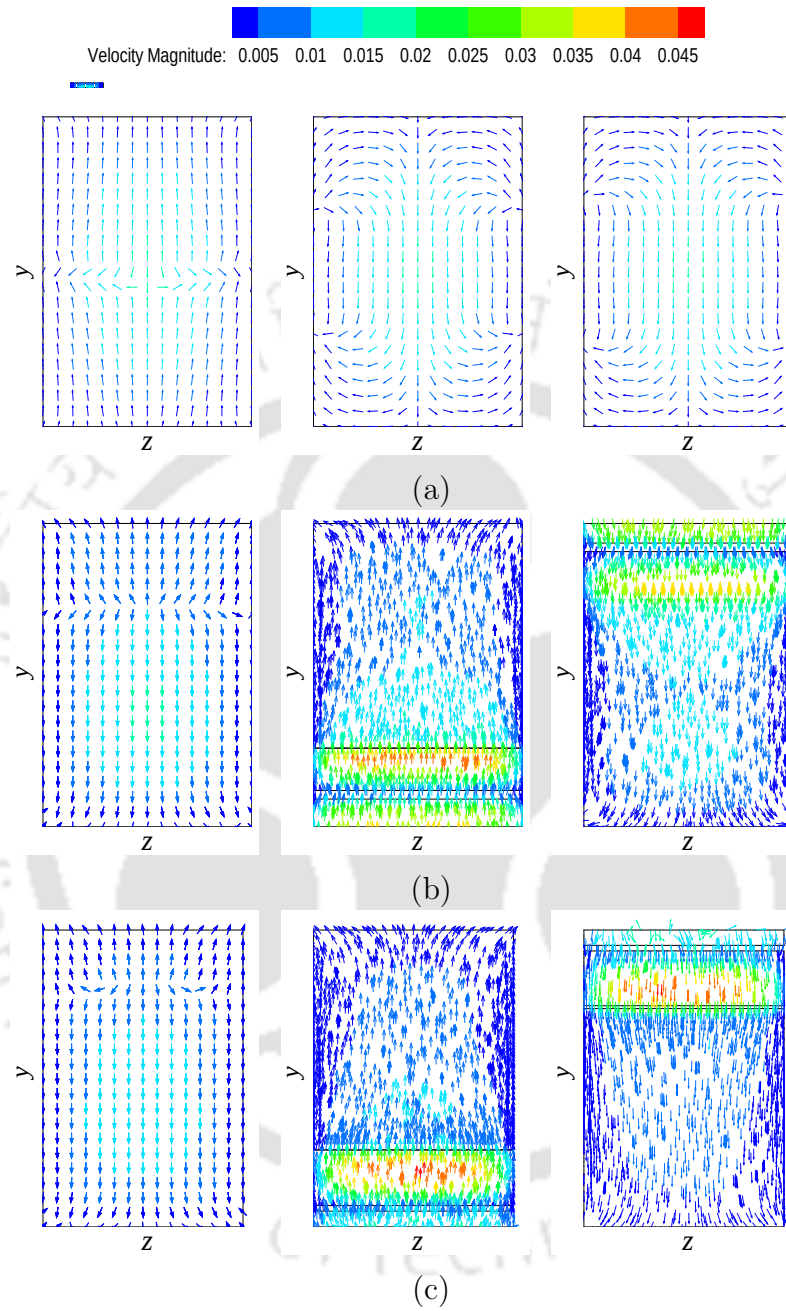


Figure 6.5: Comparison of simulated flow patterns at three different vertical cross sections in the downstream zones (a) before the start of obstacles (b) after 3rd obstacle and (c) after 6th obstacle for base case (top), channel with straight obstacles (middle) and curved obstacles (bottom), respectively.

To get a quantitative measure of the strength of the secondary flows generated due to the presence of obstacles, variations of the transversal velocities (v and w) along the channel height for the plane at $x=0.6388$ mm is presented in Fig. 6.6. From the figure, it can be identified that the transversal velocities (v and w) for the channel without having any obstacle is very poor compared to those with obstacles. Furthermore, curved obstacles lead to generate the greatest transversal velocity, which may result in superior mixing due to greater convective transport of species in these diffusion dominated flows.

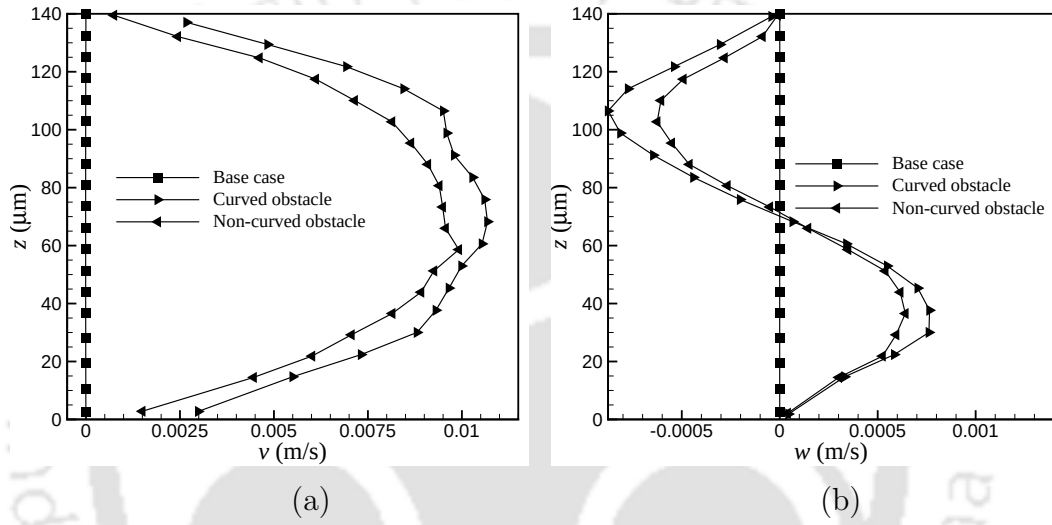


Figure 6.6: Comparison of the transversal velocity along the horizontal center-line of zy plane at $x=0.6388$ mm.

For the quantitative comparison, the mixing indices calculated at the exit of the microchannel and the associated pressure drop for each of the channel as shown in Table 6.4. From the table, it can be seen that the mixing index is very low about 24.3% for the base case whereas the mixing capability is greatly enhanced by the implementation of the obstacles, both straight and curved, giving mixing indices of about 47.6% and 61.3%, respectively. Interestingly, the pressure drop for the channel with curved obstacles is lower than for those with straight obstacles. This is clearly an added advantage for obstacles with curved surfaces since increased mixing index is associated with the lower pressure drop. Thus, it can be concluded that, the cross-T type of microchannel, which is very inefficient on their own, can be made suitable for enhanced mixing by the use of the newly designed curved obstacles.

Table 6.4: Mixing index for microchannels with different obstacles geometry compared to that of its base channel without obstacles.

Sl. no.	Configuration of microchannel	Mixing index, M (%)	Pressure drop, $\Delta\Pi$ (Pa)
1	Base case without obstacles	24.3	52.5
2	Channel with straight obstacles	47.6	276.3
3	Channel with curved obstacles	61.3	193.1

6.3.2 Geometrical variations for the curved obstacles

This section contributes to the studies for the effects of the following parameters which are believed to be the influential factors for the mixing performances of the microchannel. The parameters selected for detailed analysis are (1) height of the obstacles (h), (2) the angle of inclinations (θ), (3) chord length (l) and (4) the number of modules (N_m). Finally the effect of inlet Re on mixing performance is also investigated.

6.3.2.1 Effect of height (h) of the curved obstacle

For this study, six values of obstacle heights ranging from $h = 0$ to $h = H$ through $0.25H$, $0.5H$, $0.75H$ and $0.875H$ has been chosen. All the other geometric parameters are kept constant at $\theta=45^\circ$, $l=0.2$ mm, $s=0.135$ μm , $N_m=4$. Simulations are carried out for Re equals to 0.5.

Figures 6.7(a) and (b) present the transverse components of the velocity along the horizontal center-line of zy plane at $x=0.6388$ mm for different obstacle height. Combining the magnitudes of both the transverse velocity components, one can summarize that there may be an optimum height (around $h = 0.75H$) for the benefit of achieving the greatest transversed convection of species.

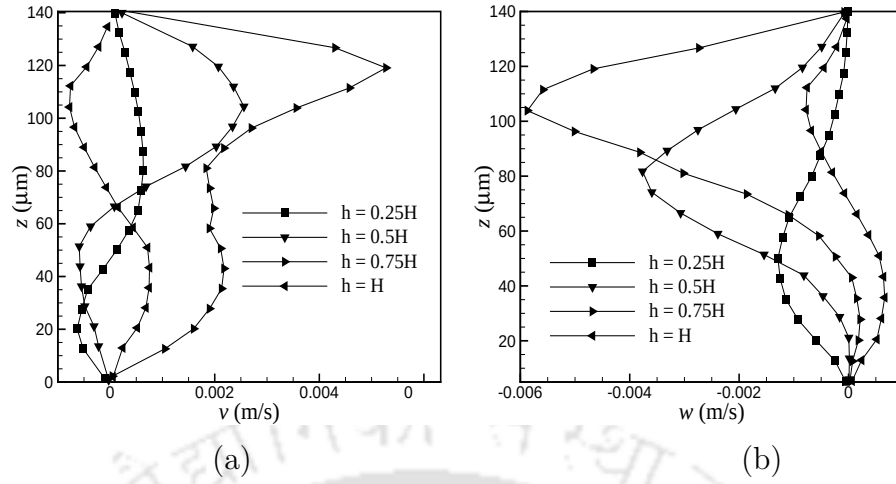


Figure 6.7: Transverse components of velocity along the horizontal center-line of zy plane at $x=0.6388$ mm for different heights of the obstacles.

To quantify the degree of mixing, the variation of mixing indices calculated at different vertical cross sections is plotted along the length of the channel and is shown in Fig. 6.8. From the figure, it can be seen that the mixing indices continuously increase all along the length of the channel with heights of obstacles up to $h=0.75H$. There has been seen little change in mixing indices for $h = 0.75H - 0.875H$. When the obstacle heights are further increased beyond $h = 0.875H$, there has been noticed a drop of mixing efficiencies. Also, it has been evident that major percentage of enhancements has been observed in the region where the obstacles are placed. This is because, in this region convective transport of species dominates over the diffusive transport. Beyond this region the mixing almost follows a linear variations with a slope similar to that of the base case without obstacles (i.e., $h = 0$). Another reason of getting higher mixing may be that with the increase of the heights of the obstacles, the region of influence in z -direction (i.e., along the depth of the channel) for transversal mass transport got increases. Thus, it gives rise to more mixing of fluids due to the evolution of convective transport. However, when the height of the obstacles reaches a point above a certain height i.e., $h = 0.875H$, the throttling by the gap between the obstacle and the side wall decreases and hence it shows a decreasing trend of degrees of mixing for the microchannel.

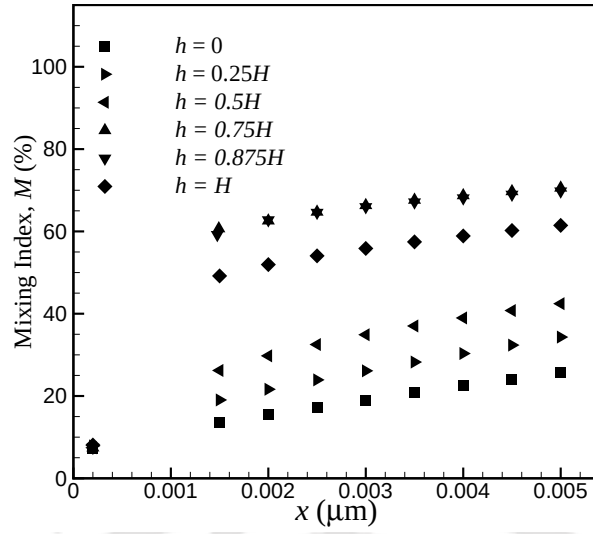


Figure 6.8: Variation of mixing index at vertical cross sections along the length of the microchannel for different heights of the obstacles.

6.3.2.2 Effect of angle of inclination of the obstacles

In this section, efforts are made to analyze the effect of angle of inclination of the obstacles (θ) on the mixing behavior of the microchannel. For this study, we have taken angles ranging from both positive and negative values (Fig. 5.6). The other geometric and flow parameters are $h = 0.75H$, $l = 0.2$ mm, $s = 0.135$ μm , $N_m = 4$, $Re = 0.5$.

Figure 6.9(a) shows the variation of mixing indices along the axial length of the microchannel for all the angles under study while Fig. 6.9(b) shows the variation of outlet mixing index (M_{outlet}) with respect to angle of inclination (θ).

It can be observed that the mixing ability of the channel is greatly influenced by the angle of inclination of the obstacles. Unlike intuitive expectations, the mixing process does not show a monotonic trend. For the positive values of angles, at lower magnitudes ($\theta < 5$), the mixing index at the outlet is slightly greater than that of the base case ($M = 25\%$). For these low values of θ , one can speculate that the fluid streams follow smoothly the curvature of the obstacles and the generated transverse components are possibly not strong enough to enhance the mixing process to a great extent. However, the mixing index then increases with θ showing a maximum at

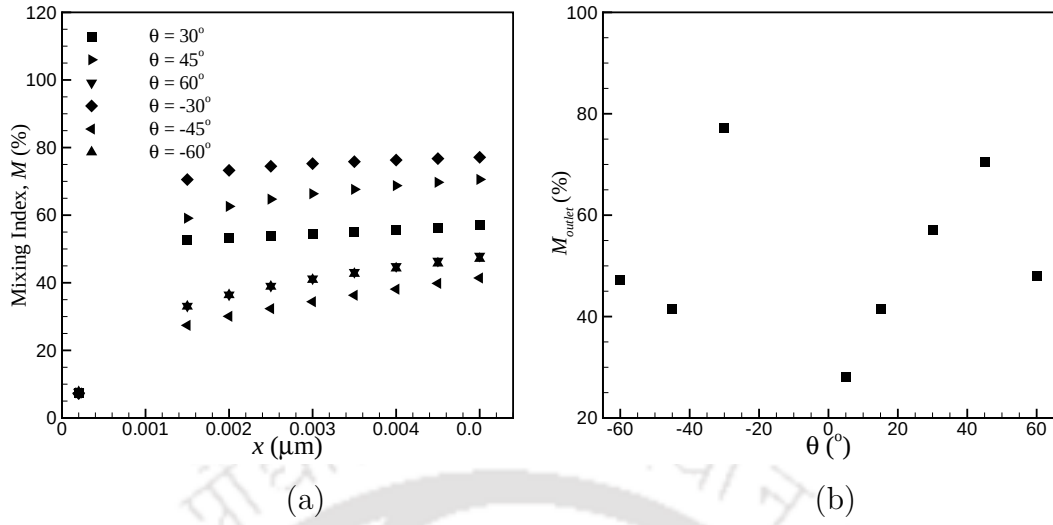


Figure 6.9: Variation of mixing index (a) at vertical cross sections along the length of the microchannel for different angle of inclination of the obstacles and (b) variation of outlet mixing index with respect to angle of inclinations.

$\theta = 45^\circ$ and then decreases with further increase in the inclination angle. However, the case is showing just an opposite trend for the negative angles. For negative angles, mixing capability first decreases reaching a minimum near at $\theta = -45^\circ$ after which it increases as the inclination magnitude increases. Among all the values studied herein, the maximum mixing is achieved with $\theta = -30^\circ$ while the minimum is found at $\theta = -45^\circ$. The justification for the above speculation can be found in Fig. 6.10 which shows the corresponding transverse velocity profiles along the depth of the channel at $y = 100 \mu\text{m}$ of the plane after the end of third obstacle for all the angles. The magnitudes of the v velocity strongly tally with the enhancements i.e., higher the transverse velocity better is the mixing (see Fig. 6.9) except for $\theta = -30^\circ$.

In order to explore the mechanism that makes the channel having $\theta = -30^\circ$ the potential candidate for the best mixing in spite of having the lower magnitude of transverse velocities, the cross sectional vector plots at $x = 0.6388 \text{ mm}$ are plotted and shown in Fig. 6.11. From the figure, it can be observed that among all the angles, only $\theta = -30^\circ$ brings about two circulating flows in different sizes, rotating in opposite directions. For all the other cases, only one circulating fluid zone is established rotating in a particular direction, either upward or downward. Also the staggered pattern of subsequent obstacles alters the directions of these circulations

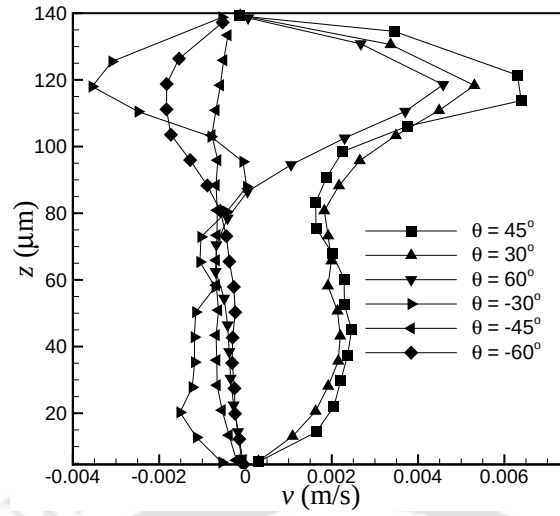


Figure 6.10: Comparison of v velocity along the depth of the channel at $y=100 \mu\text{m}$ for the planes at just at the end of the third obstacles for angle of inclinations.

zones. These alternate counter-rotating circulation patterns may cause the exchange of the fluid from one side of the cross section to the other side more intensely which finally lead the better mixing among all the angles of inclinations.

6.3.2.3 Effect of size of obstacle

Another important geometric parameter related to the obstacles is their size. In this section, the size of the obstacles has been studied for its effect on mixing. We define the size of obstacle in terms of its chord length (l) and thickness (t_o). Five different sizes of obstacles are selected having (l, t_o) of $(0.1, 0.002)$, $(0.15, 0.003)$, $(0.175, 0.0035)$, $(0.2, 0.004)$ and $(0.225, 0.0045) \mu\text{m}$. The height ($h = 0.75H$) and angle of inclination ($\theta = -30^\circ$) of the obstacles are chosen from the Sections 6.3.2.1 and 6.3.2.2, respectively, for which the maximum mixing has been achieved. The distance between the obstacles and the number of modules are fixed at $0.135 \mu\text{m}$ and 4, respectively.

The mass fraction distributions at the outlet plane of the channel are shown Figs. 6.12(a)-(e) for all cases. From the figure, one can observe that the mass fraction contours are more homogenized having a mean value close to 0.5 for $l = 0.2 \mu\text{m}$ (Fig. 6.12(d)).

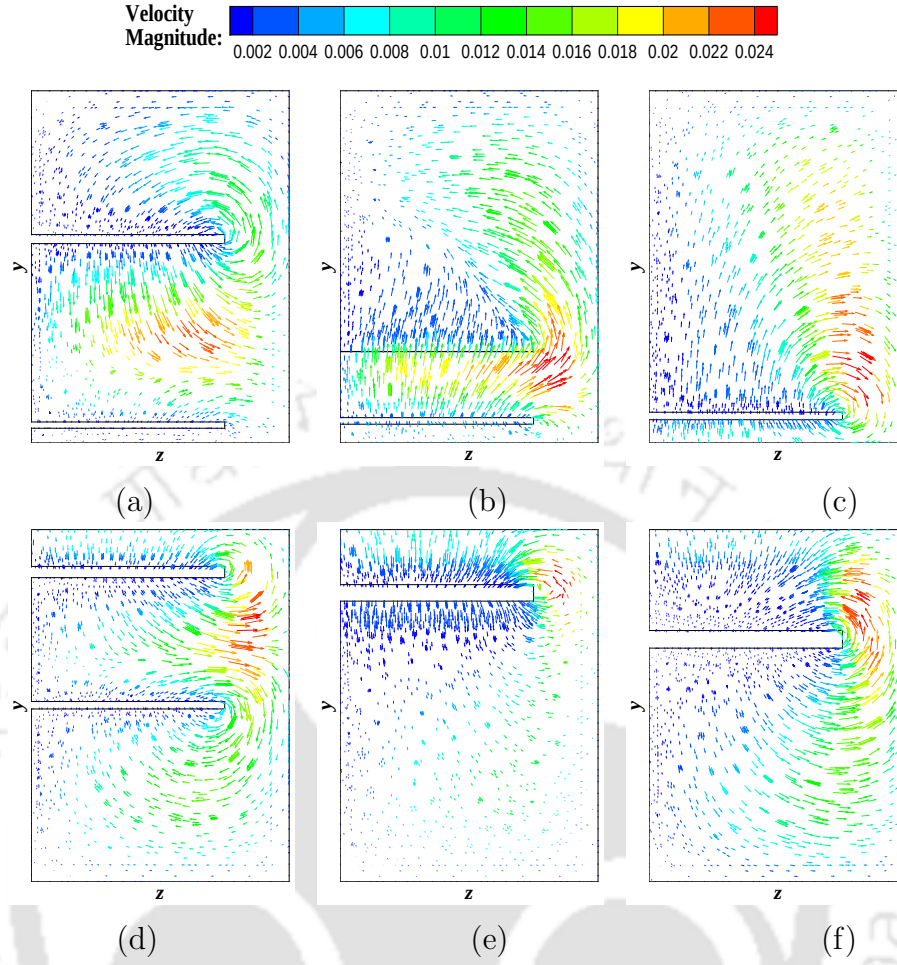


Figure 6.11: Comparison of simulated flow patterns across vertical cross section at $x=0.6388$ mm for (a) $\theta = 30^\circ$ (b) $\theta = 45^\circ$, (c) $\theta = 60^\circ$, (d) $\theta = -30^\circ$, (e) $\theta = -45^\circ$ and (f) $\theta = -60^\circ$, respectively.

For the quantitative estimate of the degree of mixing with respect to different sizes of the obstacles, variation of outlet mixing index and the pressure head required is shown Fig. 6.13. From the figure it can be seen that with smaller the size of obstacles ($l=0.1 \mu\text{m}$), the mixing efficiency of the microchannel is found to be around 33% which is about 8% higher than that of the base case (see Table 6.4). The mixing index and the pressure head required then continuously increases with the increasing size of the obstacles. However, there exists a critical size of the obstacle, beyond which mixing index decreases with further increase in it's size. However, the pressure head goes on increasing beyond the critical size of the obstacle. One of the

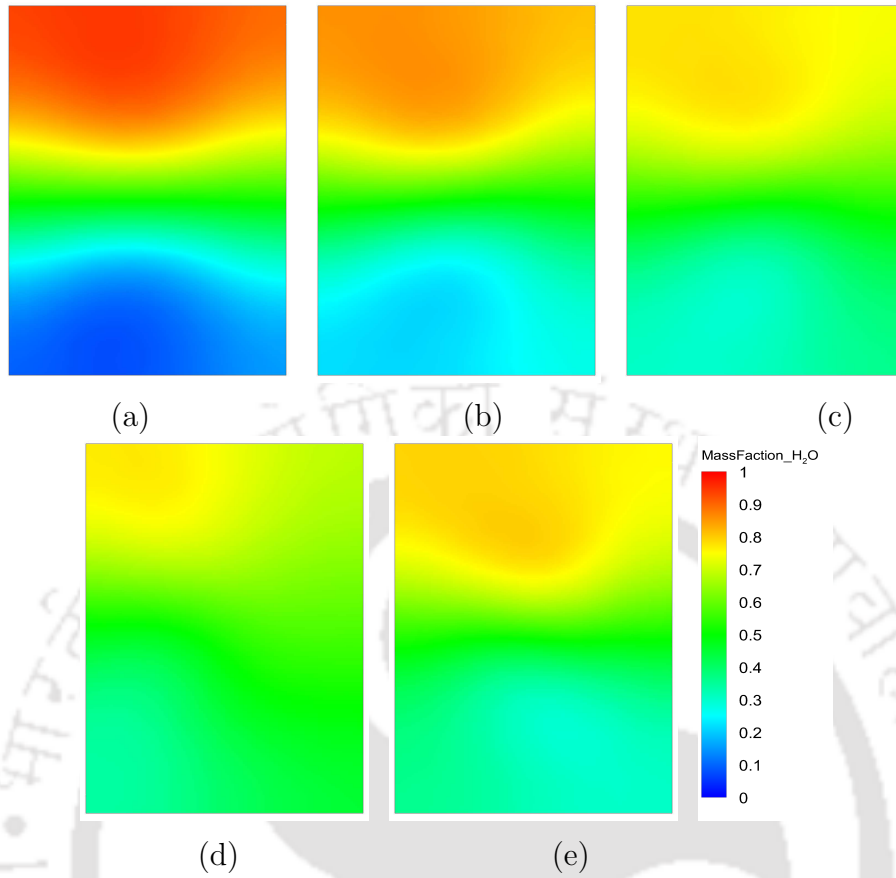


Figure 6.12: Mass Fraction contour plots at the outlet of the microchannel under study at $Re=0.5$ for five different sizes of obstacles having chord length (l) equals to (a) $0.1 \mu\text{m}$, (b) $0.15 \mu\text{m}$, (c) $0.175 \mu\text{m}$, (d) $0.2 \mu\text{m}$, (e) $0.225 \mu\text{m}$, respectively.

probable reason may be that with the increasing size of the obstacles, the strength of the convective transport of species gradually increases. But since the spacing between the obstacles are fixed, the increase in size of the obstacles beyond the critical value restricts the flow passage area between each pair of obstacles. Thus, the advantage of using the bigger size of obstacles to stir the fluid is counteract by the resistance offered to the flow due to its over size. As a result, mixing index reduces but the pressure head increases.

Comparisons of mc and mec with respect to different size of the obstacles are also shown in Fig. 6.14. From the figure it is clearly seen that the obstacle size with chord length of 0.2 mm represents the optimum size of the obstacle among all

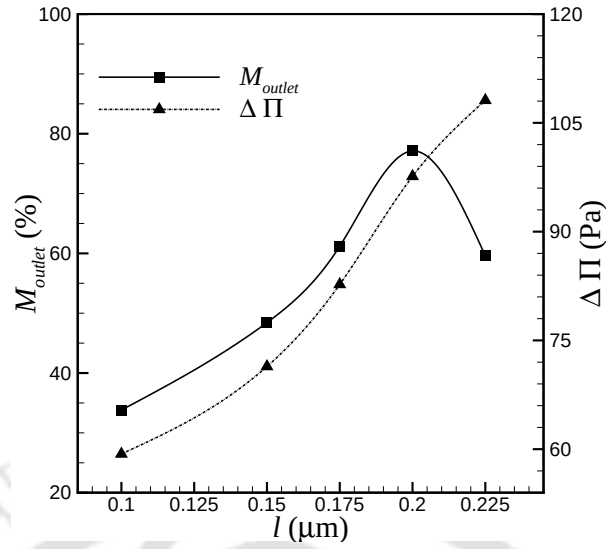


Figure 6.13: Variation of outlet mixing index and the associated pressure drop with respect to different chord lengths of the obstacles.

the sizes with respect to both mc and mec . This conclusion is however found to be consistent with the Fig. 6.13 where it shows that maximum mixing efficiency is also achieved for the channel with chord length of 0.2mm.

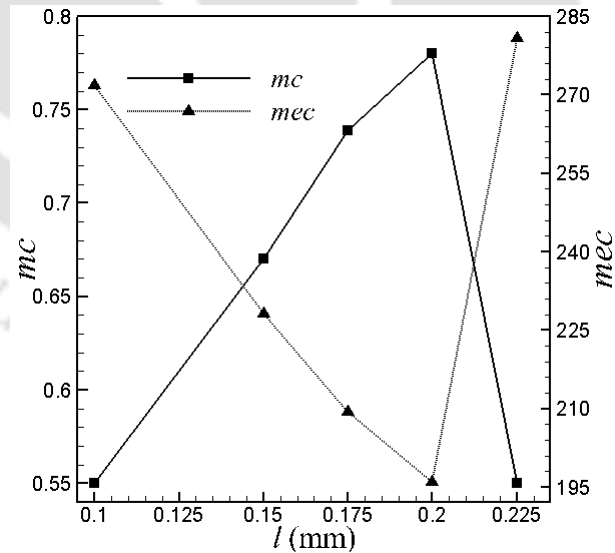


Figure 6.14: Variation of mc and mec with respect to size of obstacles.

6.3.2.4 Effect of number of modules of the obstacle

Simulations are also carried out to study the mixing capability of the present microchannel with the number of modules. For this study, six sets of simulations have been carried out by varying number of modules (N_m), from 1 to 10 in order to explore its effect on the mixing index. The height, angle of inclinations, axial distance between the obstacles, Re are taken to be same as that of in Section 6.3.2.3. The size of the obstacles is fixed at $l = 0.2 \mu\text{m}$ which corresponds to the maximum mixing index among all the sizes (see Fig. 6.13).

Figure 6.15 depicts the variation of outlet mixing index along with the pressure head required to maintain the flow with respect to the number of modules. From the figure, one can observe that the degree of mixing of the two fluids increases with the increase in the number of modules. The maximum mixing index is found to be almost 3.6 times higher than that compared to the conventional simple microchannel. However, it can be seen that beyond four modules, the rate of increase in mixing

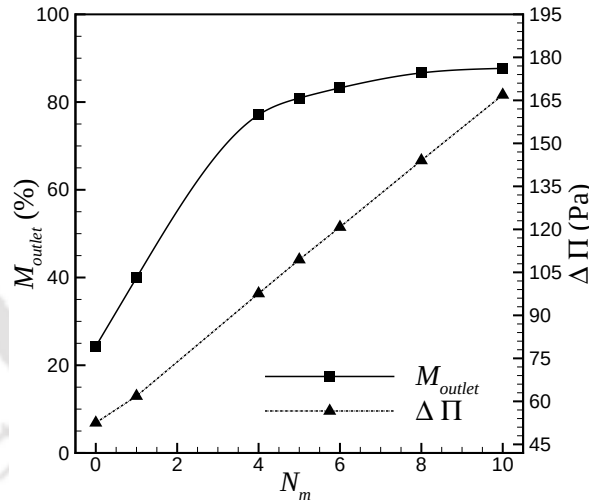


Figure 6.15: Variation of outlet mixing index and the associated pressure drop with respect to number of modules.

efficiency is found to be more gradual for even higher number of modules while the pressure drop increases linearly. In order to analyze the reason behind this, the transverse velocity profiles for both v and w are plotted for channels with different number of modules. Variations of both v and w velocities along the width of the channel (y) after the last module at the mid z -plane are shown in Fig. 6.16(a) and

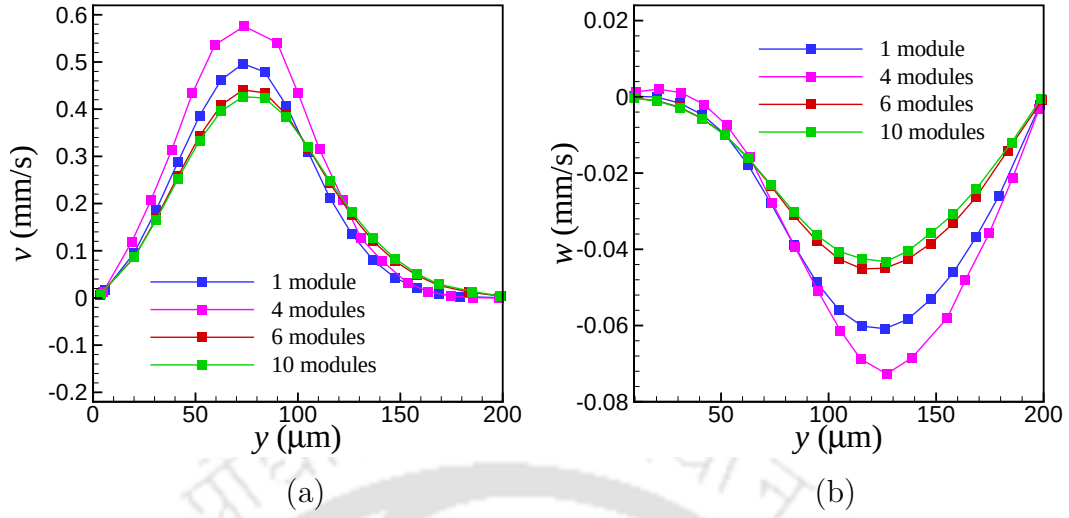


Figure 6.16: Transverse velocity profiles along the channel width for different number of modules: (a) v velocity and w velocity.

(b), respectively. From the figure it can be seen that as the number of modules increases from 1 to 4, the peak transverse velocities increases. However, for the channels with 6 modules, the magnitudes of peak transverse velocities become lower than that of the 4 module channel. Moreover, the induced transverse velocities are seen to be not substantially different when the numbers of modules are increased beyond 6. Since transverse convection is the dominant mechanism in mixing at the conditions studied and its effect is weakened when the number of modules exceeds four, the mixing index shows a much gradual increase than observed when the number of modules is lesser than four.

It must also be noted from Fig. 6.15 that although increasing the number of modules ensures good mixing, this is achieved at the cost of higher pressure drops. This is because every module introduces an added resistance to the flow leading to a nearly linear relation between pressure drop and number of modules. This, however, should not be considered as the disadvantage of the proposed design. The comparison of a simple and a complex microfluidic junction should be done for a desired mixing index. It must also be remembered that achieving a mixing performance similar to 10 modules case using the conventional cross-T type microfluidic junction would necessitate a very long channel and the pressure drop associated with the long length may turn out to be in the range of the pressure drop observed for 10 modules case or so [34].

6.3.2.5 Effect of inlet Re

Mixing at a microfluidic junction is strongly dependent on Reynolds number. Any new design should ensure good mixing over a wide range of Reynolds number. Reynolds numbers reported in this study are based on the width and average velocity in the main inlet channel. This section reports the results from numerical simulations carried out at different Reynolds numbers to check the versatility of the new design of obstacles over a range of Re . This study is performed for the microchannel having parameters for which maximum mixing has been observed in the previous sections, defined by, $N_m = 4$, $h = 0.75H$, $\theta = -30^\circ$, $l=0.2 \mu\text{m}$ and $s=0.135 \mu\text{m}$. The Reynolds numbers are varied ranging from 0.1 to 60.

The variation of mixing indices and the pressure drop associated with each Re value is shown in Fig. 6.17. From the figure it can be seen that, the present design shows a local minimum for the mixing index at $Re = 5.0$ with the mixing index increasing for lower and higher Re . At very low Re , the mixing index is quite high. Low Reynolds number generally defines a stratified flow where the fluid streams do not interpenetrates each other causing mixing to be poor. But at the same time, the

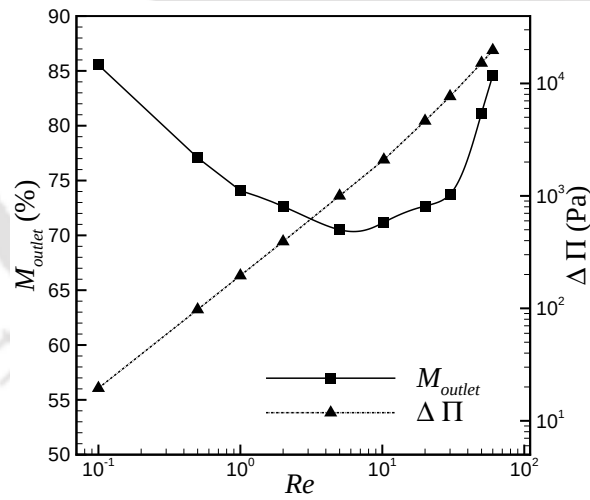


Figure 6.17: Variation of outlet mixing index and the associated pressure drop with respect to Reynolds number.

residence time of fluids is more and also the presence of curved obstacles impart some transversal velocity components that break the flow stratification. The combined effect of both these two factors results in higher mixing at low Re . As Reynolds

number is increased stratified flow still persists but residence time reduces causing mixing to decrease marginally. When Reynolds number is high enough the streams starts interpenetrating each other resulting in better mixing compensating for the reduced residence time. A noticeable aspect with this new design is that even the minimum value of mixing index is significantly greater than that of the base case. One can hence argue that the new design ensure the requirement of achieving good mixing over a wide range of Re for cross-T microchannels.

6.3.3 Comparison of the present micromixer design with earlier micromixer designs

This section presents a comprehensive analysis of the comparison of the mixing performance of the present micromixer with respect to micromixer designs reported in the earlier works. Numerous designs of microchannel geometry have been proposed in the previous literatures to achieve better mixing performances. Therefore, one way to conclude, among them, on which method is better, is to compare all the mixing parameters for different designs of microchannels. This primarily includes comparison of mixing efficiency, pressure drop, mc and mec . In order to perform the comparative study, three microchannel configurations have been selected other than that of the present design of micromixer. A short description and the primary mixing mechanism of each of the microchannels are given below.

1. The first configuration is a planar rhombic micromixer with an asymmetrical structure (constriction elements at the junctions between two rhombi) designed by Chung and Shih [138] for mixing enhancement. The mixing enhancement reported were due to result of multiple mixing mechanisms such as focusing/diverging, recirculation and Dean vortices.
2. The second configuration is a staggered herringbone micromixer (SHM) studied by Tsui et al. [58] who evaluate the mixing performance of different grooved and obstructed micromixers. The primary mechanism that leads to superior mixing is the chaotic mixing.
3. The third configuration consists of a T-microchannel with longitudinal vortex generators studied by Hsiao et al. [92]. The primary mixing mechanism in this design is the generation of longitudinal vortices.

Table 6.5 shows the values of different mixing parameters for the four different micromixer design adopted for comparison.

Table 6.5: Comparison of different micromixer designs for their mixing parameters.

Sl. No.	Micromixer design	Re	M (%)	$\Delta\Pi$ (Pa)	mc	mec
1	Present design with curved obstacles	1	74.8	195.6	0.38	101.3
2	Rhombic micromixer [138]	1	54.8	148.7	0.37	384.0
3	SHM [58]	1	32.4	174.7	0.18	65.8
4	Microchannel with LVG [92]	1	65.4	128.7	0.51	159.1

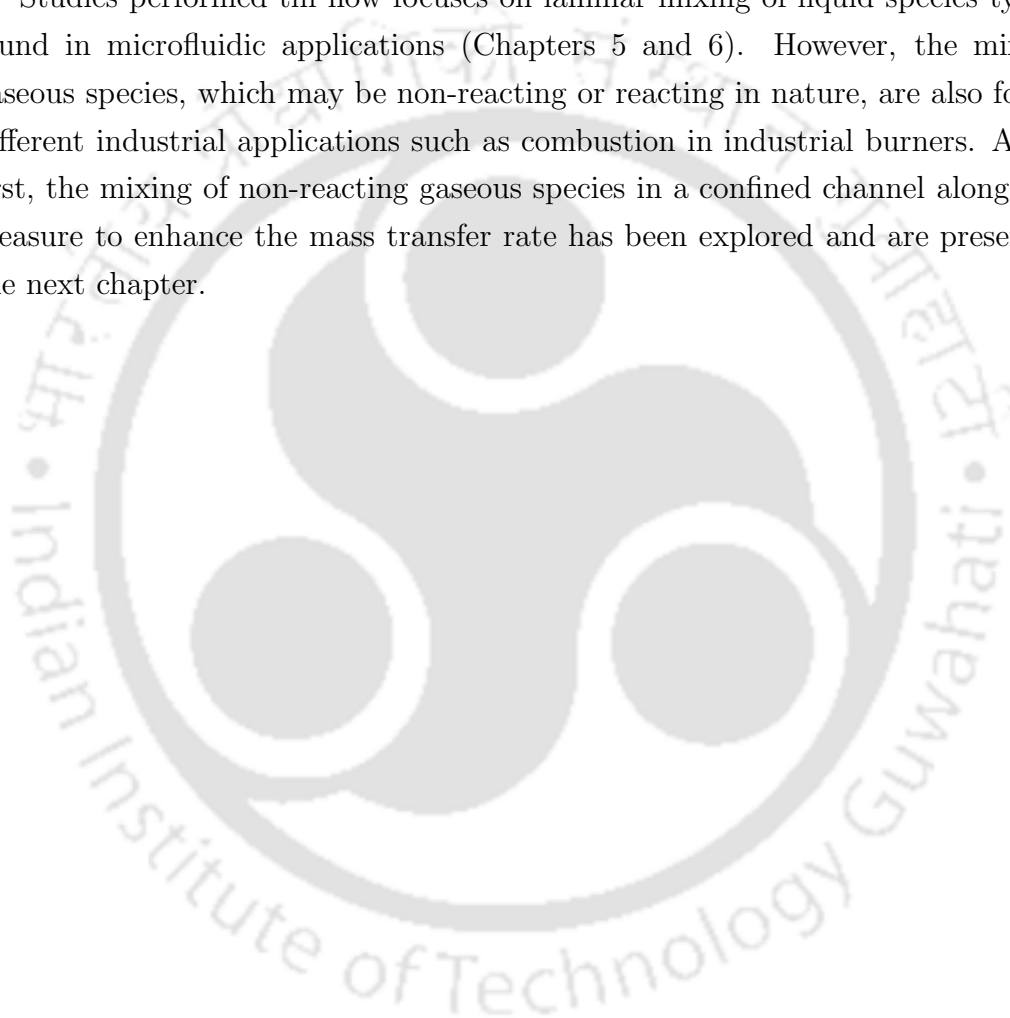
From the table, it can be seen that with respect to mixing efficiency, both micromixer-1 and -4 are comparable with the maximum value among the selected micromixer designs whereas micromixer-3 shows the minimum. However, between micromixer-1 and -4, micromixer-1 is better with respect to mec whereas micromixer-4 is better with respect to mc . Furthermore, micromixer-3 shows the ideal design with respect to mec with the minimum value among all the four, but it is not comparable with respect to mixing efficiency and mc . On the basis of pressure drop, micromixer-2 becomes the second best option, but it requires the highest mec among all. Thus, it has been seen that the present design of micromixer has the capability of producing superior mixing efficiency. However, it is believed that the pressure drop, on the other hand, can be managed to reduce by optimizing the geometric parameters of the channel. It may also be noted that designing a micromixer for best results with respect to all parameters is not an easy job and hence, the selection of the best method and/or design of micromixer can be done depending upon the requirement of the application problem.

6.4 Closure

In this chapter, the performance analysis of a three-dimensional cross-T micromixer has been presented, specially focusing on its mixing characteristics, by the use of

curved ribs. Simulations are also carried out to compare its mixing characteristics to those having obstacles with straight ribs and to those having no obstacle at all. Results showed that the channel having curved obstacles is found to perform superior mixing than compared to those with straight ribs. Furthermore, a full set of parametric studies has also been conducted for the effect of the several geometric properties associated with the obstacle layout.

Studies performed till now focuses on laminar mixing of liquid species typically found in microfluidic applications (Chapters 5 and 6). However, the mixing of gaseous species, which may be non-reacting or reacting in nature, are also found in different industrial applications such as combustion in industrial burners. As such, first, the mixing of non-reacting gaseous species in a confined channel along with a measure to enhance the mass transfer rate has been explored and are presented in the next chapter.





Chapter 7

Mixing Characteristics of Gaseous Mixture in Wavy Channels

The present work deals with the development of a general purpose flow solver to simulate mixing of multi-species flows. A significant amount of work has already been reported in Chapters 5 and 6 that demonstrates the capability of the present solver in simulating mixing of liquid mixtures in microchannels. As such, the present chapter focuses on analyzing the mixing characteristics of gaseous mixtures. The field of gaseous mixing can be divided into two categories: reacting and non-reacting. For both these two categories, rapid mixing of gases plays an important role. However, in this chapter, attention will be given in analyzing the mixing characteristics of non-reacting gaseous mixtures and exploring ways to rapidize the mixing rate. The reacting part will be handled in the next chapter.

The present chapter considers the mixing of a binary, laminar, non-reacting gaseous mixture in a confined horizontal channel. Furthermore, the mixing characteristics of the channel is explored with the introduction of waviness along the channel walls. Also, the dominant mechanism of mixing is brought out through extensive numerical simulations performed by using the developed solver ¹.

¹A substantial portion of this chapter has been published in P. Borgohain, D. Choudhary, A. Dalal and G. Natarajan (2018), "Numerical investigation of mixing enhancement for multi-species flows in wavy channels", Chem. Eng. Process. Process Intensif., vol. 127, pp. 191-205

7.1 Problem Definition

The basic geometry to study the mixing characteristics of gaseous mixture is taken from the work of Gomes et al. [142]. The schematic diagram of the numerical model is shown in Fig. 7.1. Detailed geometric description can be found in Section 4.2.3.

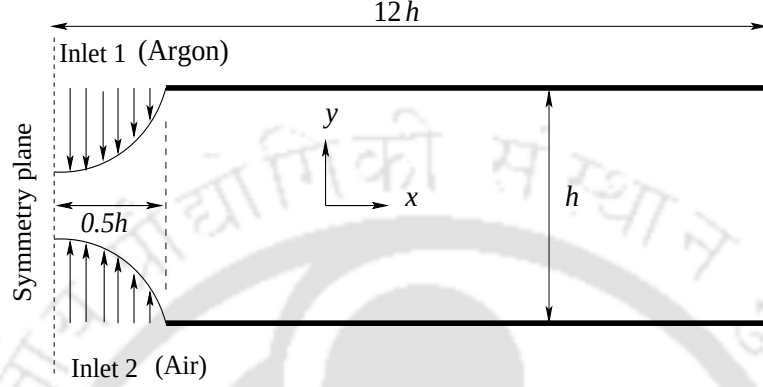


Figure 7.1: Schematic diagram of the horizontal channel selected for the base case

Next, the effect of introducing ridges of sinusoidal nature along the walls of the channel on mixing performance has been presented. For this, in the base geometry represented in Fig. 7.1, waviness in the form of sinusoidal nature are imparted along the walls of the channel. The equation of the sine wave is uniquely defined by $y = a \sin(2\pi x/\lambda)$ where a is the amplitude and λ is the wavelength of the wave. We have selected two configurations of the wavy channel depending upon the phase difference (PD) of the waves on both the walls, i.e., 0° and 180° . The channel with 0° and 180° PD are also commonly termed as asymmetric and symmetric channels, respectively. These two configurations are shown in Figs. 7.2(a) and (b).

The widths of the two inlet slots of the channels are $0.5h$ where h is the height. $L(= 12h)$ represents the length of the computational domain. The value of h is taken to be unity. Species considered for this study are Argon (Ar) and ambient air where the later is entering from the bottom inlet. The use of Ar and ambient air as the working fluids have been adopted from the works of Shavit and Lavan [141]. The density ratio (ρ_{Ar}/ρ_{Air}) and the viscosity ratio (μ_{Ar}/μ_{Air}) of argon to that of air are 1.345 and 1.255, respectively. The Schmidt number (Sc) of the flow is taken to be 0.772. The flow physics is studied for two different Reynolds numbers (Re). In the present work, the non-dimensional numbers (like Re , Sc and Pe) are defined

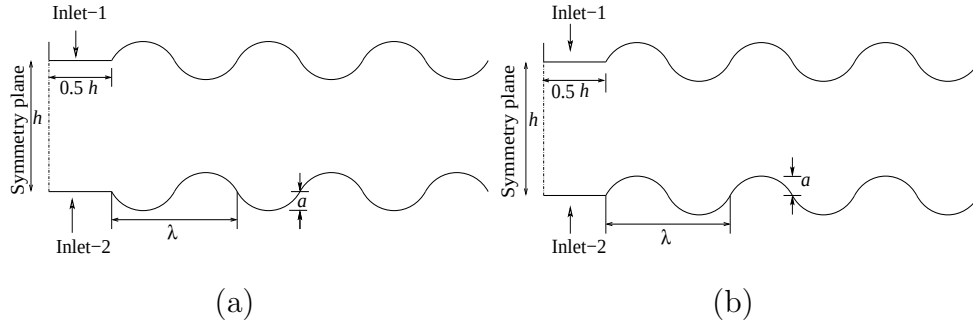


Figure 7.2: Schematic of channels having (a) 180° and (b) 0° phase difference waves along the walls.

based on the reference quantities associated with the unmixed air stream coming from the bottom inlet, its average velocity ($\bar{u}$) and the width of the inlet channel ($0.5h$). Both the two streams are assumed to have equal volumetric flow rate. Fully developed velocity profiles with average velocity ($\bar{u}$) are enforced at the inlet. The walls are assumed to be impermeable with no-slip boundary conditions. At the outlet, pressure outlet boundary condition has been specified.

The developed solver uses the pseudo-transient method to handle the steady-state problems. As such a simple first-order Euler Implicit scheme is employed for temporal discretization. The time step size (Δt) is set at 10^{-3} . For spatial discretization, a blended scheme that uses a weighted average of central difference scheme (CDS) and first order upwind (FOU) schemes [132] are being used for handling the convective terms whereas diffusive terms are handled by second order accurate central difference scheme (CDS). The present study uses symmetric blending of CDS and FOU so as to ensure trade-off between solution accuracy and numerical diffusion. ILU preconditioned BiCGSTAB is used to solve the variable coefficient pressure Poisson equation in Eq. 2.55. Since the density is spatially variable, the coefficients of the matrix changes with time rendering the matrix to be asymmetric which necessitates the use of a preconditioned krylov solver. Solutions are considered to be converged when the relative residual of each variable is less than 10^{-5} .

7.2 Grid Independence Study

Prior to carry out the actual numerical simulations, a grid independent study, which is must, is carried out in this section. For this study, the channel with sinusoidally varying wavy walls having wavelength ($\lambda = 0.575h$), amplitude ($a = 0.1h$) and 0° PD has been chosen. Simulations are carried out for $Re_{air} = 120$ and $Pe_{air} = 92.64$. The corresponding values for argon stream are $Re = 128$ and $Pe = 98.8$. Hybrid meshes consisting of hexahedral cells and prismatic cells have been used. Hexahedral cells are placed in the near wall region and prismatic cells towards the center of the channel. 9130, 16976, 27916 and 35156 numbers of cells were considered for the study. Figure 7.3 shows the variation of Ar mass fraction along a plane perpendicular to the channel axis at a distance of $0.5h$ from the symmetry plane. From Fig. 7.3, one can easily see that the results are mesh independent for more than 27916 number of cells and therefore this mesh has been chosen for all subsequent studies.

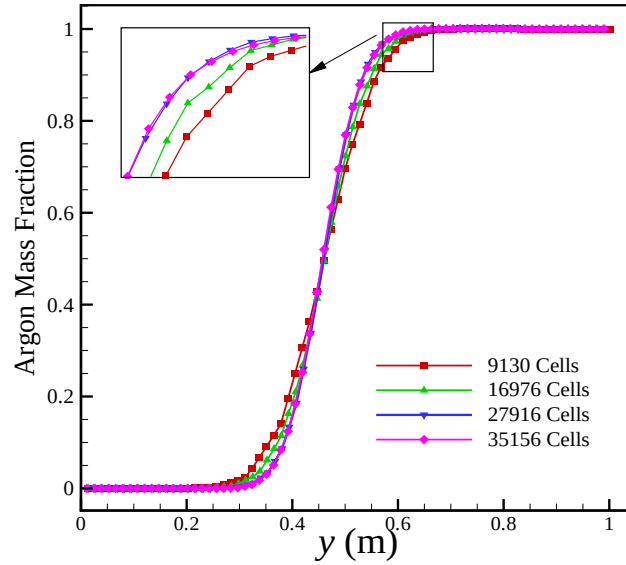


Figure 7.3: Grid independent study: Argon mass fraction contours along a plane perpendicular to the channel axis at a distance of $0.5h$ from the symmetry plane for various numbers of grids.

7.3 Results and Discussion

In this section, the numerical results obtained from the developed in-house solver is analyzed to evaluate the mixing characteristics of a binary gaseous mixture in a plane channel as well as in corrugated channels consisting of sinusoidal waved ridges on the walls. The effect of symmetrical and anti-symmetrical wave patterns (differed by a phase difference of π radian) on the mixing efficiency is investigated and the mechanism of enhanced mixing for the symmetrical wave pattern case is brought out through extensive numerical simulations. A full set of parametric study has also been carried out to examine the effects of some of the important geometric and flow parameters such as, (1) phase difference (PD) of the waves between the walls, (2) wavelength (λ), (3) amplitude of waves (a), (4) inlet Re , and (5) Pe on the mixing efficiency across the channel length. All different configurations are analyzed in terms of both mixing index and pressure drop.

7.3.1 Effect of phase difference (PD)

In this section, we study the effect of phase differences of the sinusoidal corrugation provided along the channel walls. For the sake of better understanding, to begin with, only a single sine wave of amplitude ($a = 0.1h$) and wavelength ($\lambda = 1.15h$) is introduced at the walls near the inlet of the channel and its effect on the mixing efficiency is studied. The channel geometry considered for the present case is similar to Fig. 7.2 except that it considers only one wave instead of multiple waves across the channel walls. Simulations are carried out for $Re = 120$ and $Pe = 92.64$, based on the reference quantities associated with the unmixed air stream.

Figures 7.4(a)-(c) show streamline contours at steady state in case of a plane channel (without wave), and the channels having waves of 180° and 0° phase difference (PD), respectively, with equal amplitudes and wavelengths. It must be noted that the formation of vortex near the Argon inlet in the plane channel case is due to the unequal momentum of the two fluid jets. Although velocities of the fluid jets are same, density of Ar being higher, Ar jet has a higher momentum. Due to turning of the two fluids by 90° , recirculation zones are expected to be produced near both the jet inlets. But as the Ar jet momentum is larger, the lower vortex is suppressed and the air jet turns without any recirculation zone. This also explains why a larger

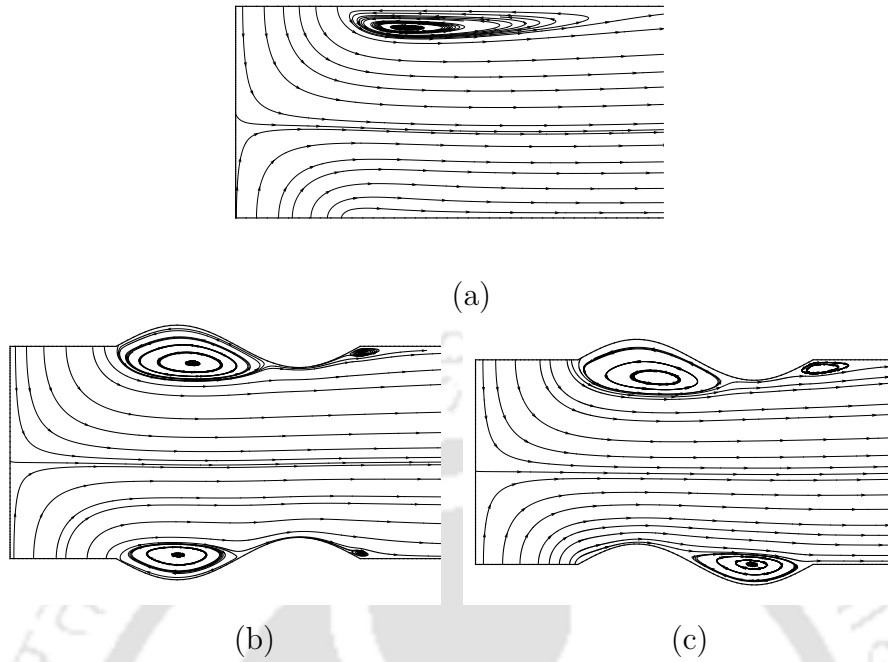


Figure 7.4: Streamline contours for (a) plane channel, (b) channel with single sinusoidal wave having a phase difference of 180° , and (c) channel with single sinusoidal wave having a phase difference of 0° for a length of $2h$ from the inlet (along the wave).

vortex is formed in the crest of the upper wall in case of the sinusoidal walled channel.

Figure 7.5(a) shows the variations of mixing efficiencies along the lengths of the single sinusoidal wavy channels with both 0° , 180° PD and also along the length of a simple plane channel without wall corrugation. It can be seen that the mixing process of both plane channel and channel with 180° PD are very close to each other. The mixing efficiency increases almost linearly and reaches a value of about 14% at the axial location where the wave ends (i.e. at $x = 1.65$ m). On the other hand, the mixing progresses a little faster for the channel with 0° PD and the mixing efficiency is observed to be 19% at the same location of $x = 1.65$ m. The corresponding values of mixing efficiencies at the channel outlet for plane channel, channels with 0° and 180° PD are 60.1%, 63.4% and 60.4%, respectively. This shows an enhancement of nearly 3.3% in mixing efficiency for the channel with 0° PD with a single sinusoidal wavy wall. Also it is seen that 50% mixing is attained earlier in

the 0° phase difference channel at around $x=7.81h$ while for the other two channels, it is attained at around $x=8.84h$. Thus, it can be reported that the introduction of even a single asymmetric sinusoidal wave on the walls of a channel enhances the mixing efficiency over a plane channel without waves. This is due to the fact that, in case of channels having waviness, the combined effect of the crests (troughs) and lower (upper) wall directs the fluid jets towards the core flow region, giving rise to transverse velocities thus enhancing mixing.

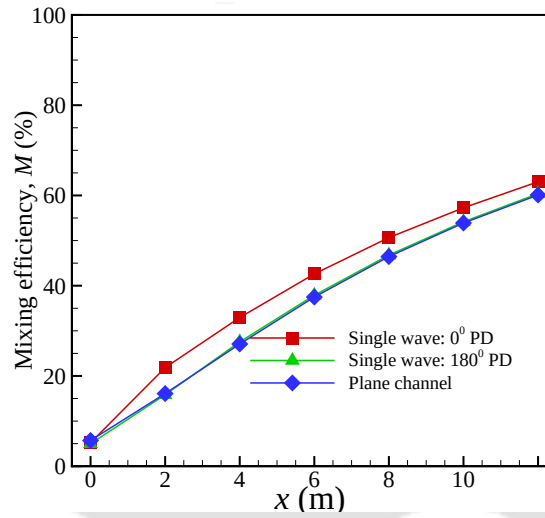


Figure 7.5: Comparison of mixing efficiencies along the axial length for a plane channel and single wave corrugated channels with 180° and 0° PD having same amplitude $a=0.1h$.

Figure 7.5 corresponds to the mixing characteristics of corrugated walls having only one wave along the channel walls. However, in channels having sinusoidal waves all throughout, similar trends for mixing efficiencies follow along the entire channel. Figures 7.6(a) and (b) show the mixing efficiencies of various channels having different number of waves incurred along the walls of the channel for both 0° and 180° PD channels. It can be seen that 0° PD channels always give higher mixing for same number of waves compared to that of the 180° PD channels. For the case of 0° PD channel, 16 waves case is showing the highest mixing efficiency of 88.1% which is about 67.7% for the case of 180° PD channel. This shows an enhancement of about 28% and 7.6%, respectively, for 0° and 180° PD channels compared to that of the plane channel without waviness.

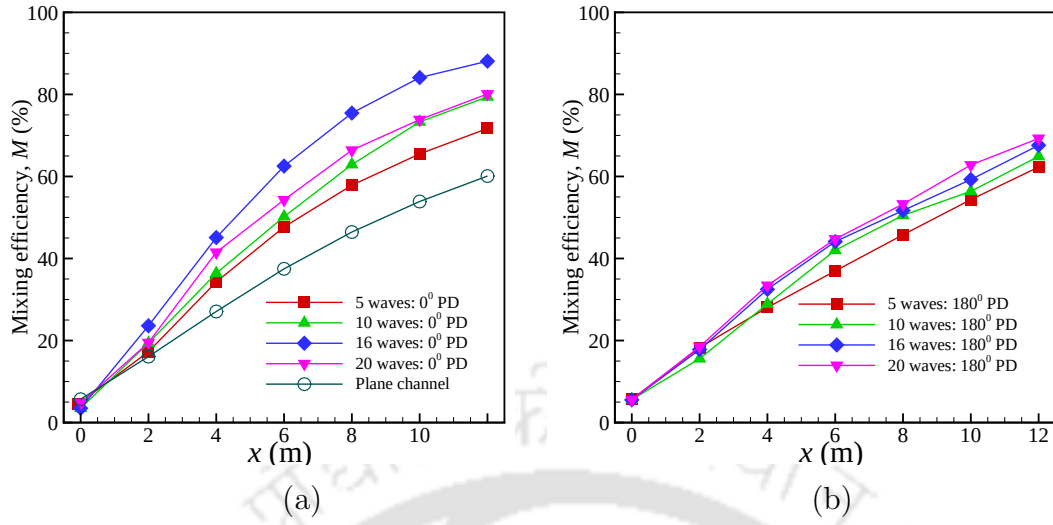


Figure 7.6: Effect of phase difference on mixing: (a) channels having different number of 0° PD waves and (b) channels having different number of 180° PD waves all throughout the length of the channel having $a=0.1h$.

It is interesting to note that the 0° PD channel shows a superior mixing performance when compared to the 180° PD channel for the same number of waves and amplitude. A closer look reveals that the 180° PD channel has a symmetric recirculation pattern (involving clockwise and counterclockwise vortices) during a single period while the 0° PD channel exhibits an asymmetric recirculation in one period as can be seen in Figs. 7.7(a) and (b), which represent the streamline patterns in 16 waves case for 0° and 180° PD wavy channels, respectively.

The differences in the vortex patterns of 7.7(a) and (b) which arise out of asymmetries in the geometry are seen to manifest in the transverse velocities, as shown in Fig. 7.8. It is evident that the magnitudes of transverse velocities are higher for the 0° PD case as opposed to that of 180° PD case. The alternate recirculation zone patterns in the former causes higher transverse velocities which combine with diffusion to enhance mixing. We refer to this mechanism of better mixing performance in asymmetric (0° PD) channels as the “chirality effect”. Consequently, we carry out numerical investigations in the successive sections to follow using only the 0° PD channel.

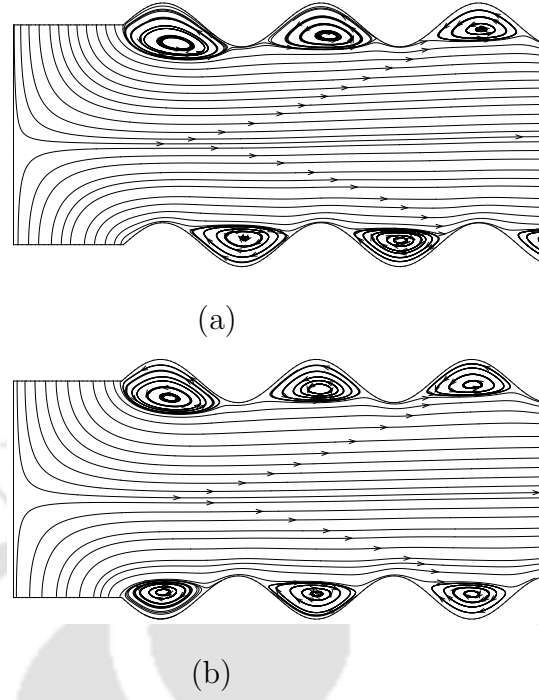


Figure 7.7: Effect of phase difference on the generation of recirculation zones for 16 wave channel ($\lambda = 0.718h$, $a = 0.1h$) with (a) 0° PD and (b) 180° PD.

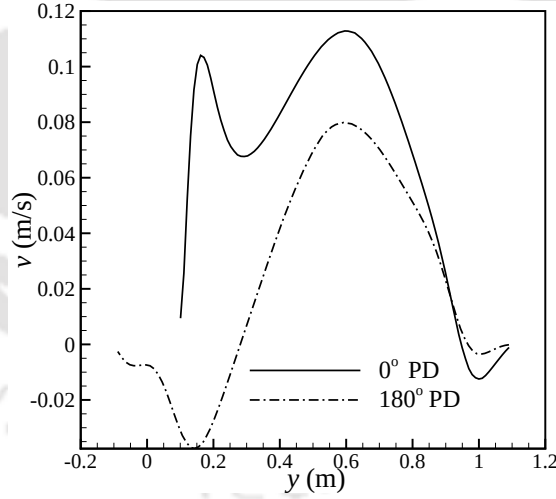


Figure 7.8: Effect of phase difference on transverse velocities: Variation of v velocity along the widths of two channels having 16 waves for 0° and 180° PD, respectively, at the axial location corresponds to the mid-point of the third crest.

7.3.2 Effect of wavelength

Mixing of species in channels having sinusoidally varying wavy walls shows superior performance as it can be seen from section 7.3.1. The focus of this section is to study the effect of wavelength of the walls on the mixing efficiency. Simulations are performed for a wide range of wavelengths ranging from $2.3h$ - $0.328h$ giving rise to a total of 5-35 numbers of waves, respectively. The 0° PD wave has been selected for this study as from section 7.3.1, it shows a better candidate than that of 180° PD wave for mixing enhancement. Simulations are carried out for $Re_{air} = 120$ and $Pe_{air} = 92.64$. The corresponding values for argon stream are 128 and 98.8. The value of a of the waves was also kept constant at $0.1h$. Figures 7.9(a)-(e) show the Ar mass fraction contours and streamlines for the same location of the channel for various cases of wavelengths.

When the number of waves is low, the wave is flatter and the streamlines follow the shape of the channel. No recirculation zones are created near the crests/troughs (Fig. 7.9 (b)). As a result, the fluid jets do not get directed to the core flow region to that extent as that in case of vortex formation. When the number of waves increases, the recirculation zones appear as seen in Figs. 7.9(c) and (d). The Ar mass fraction contours of the 16 waves case are more homogenized (see Fig. 7.9(c)) than the other three cases. However, when the number of waves exceed some critical range (Fig. 7.9(d)), the flow detaches at a very early point in the wave and re-attaches at a later stage, that results in the generation of weak transverse velocities. As a consequence, in such cases, mixing, like in the plane channel case, takes place mostly by molecular diffusion as very little transverse velocities are introduced. Thus mixing efficiency drops.

Figure 7.9(e) shows the comparison of variation of mixing efficiencies along the length of channels having different number of waves. It can be seen that mixing efficiency is low for lesser number of waves. Mixing is improved initially with increasing number of waves up to a certain limit, but then it starts decreasing with further increase in the number of waves. Among the cases studied, the wavy channel having 16 waves shows the highest outlet mixing efficiency of 88.1%.

In order to understand the mechanism that promotes mixing, the profiles of mass

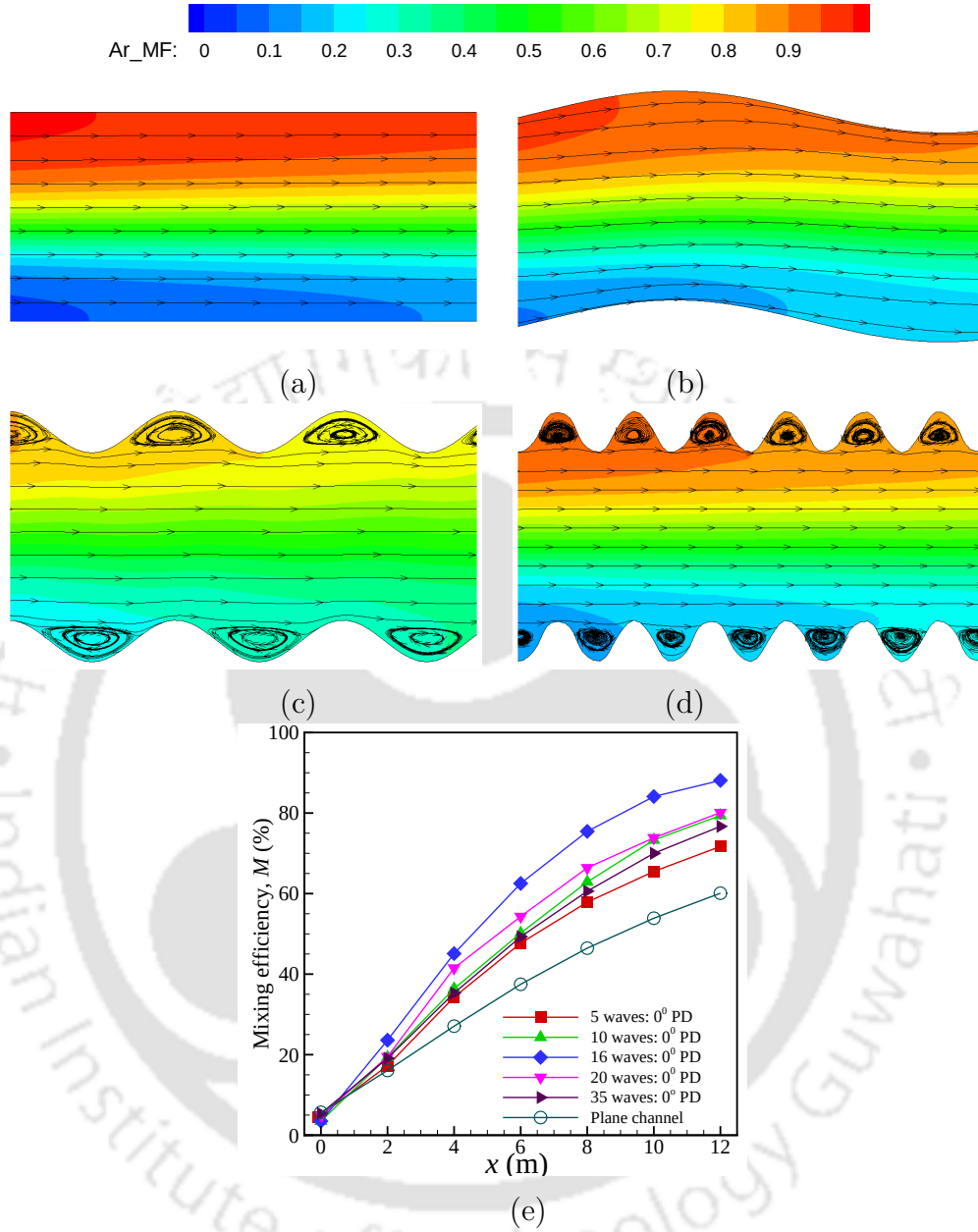


Figure 7.9: Varying wavelength case: Streamlines and Ar mass fraction contours at $Re=120$, $Pe=46$ in sinusoidal channels at the same location between $5h$ to $7h$ having $a = 0.1h$ (a) no waves, (b) 5 waves, (c) 16 waves, and (d) 35 waves. (e) Variation of mixing efficiency with varying wavelengths along axial length of channels having 0° phase difference.

fractions and transverse velocities along the width of the channel at two different axial locations, namely $x = 7$ and $x = 9$, are compared in Figs. 7.10 for 5 waves and 16 waves case.

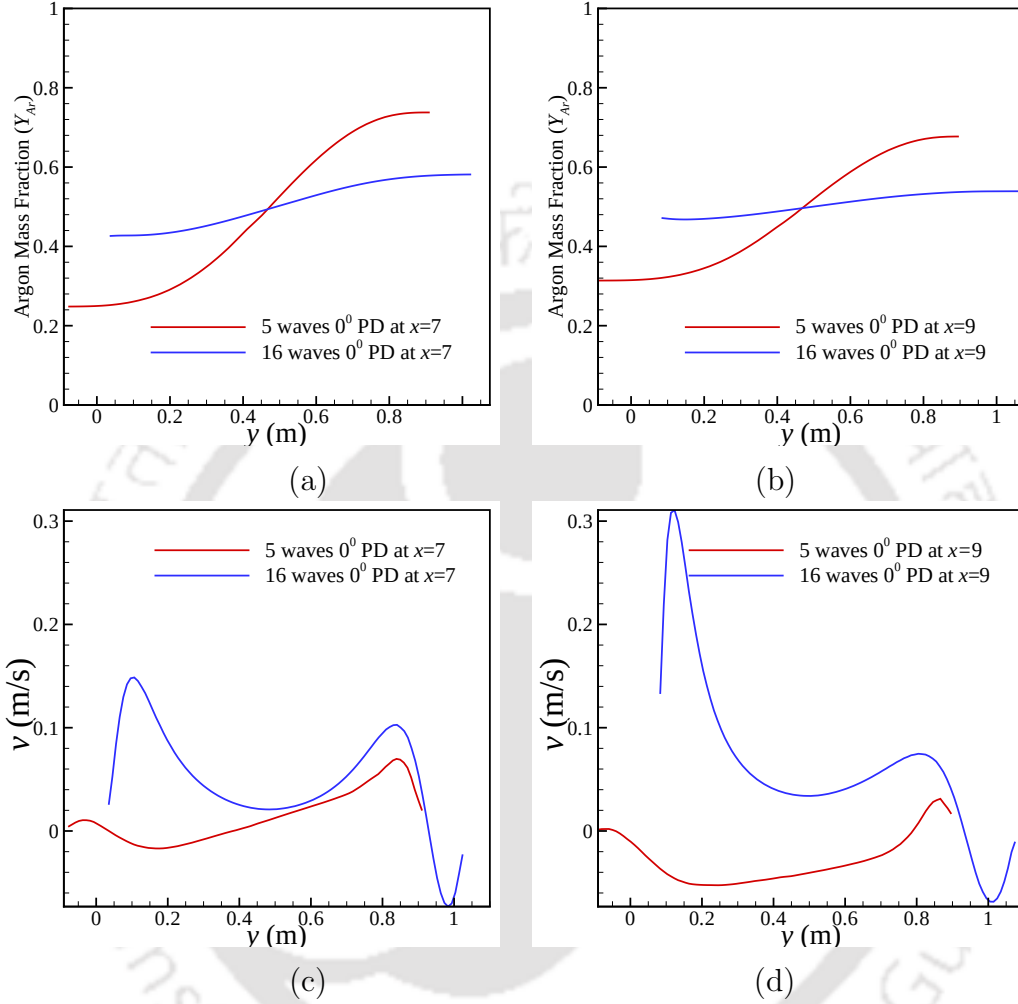


Figure 7.10: Variations of mass fractions at (a) $x = 7$ and (b) $x = 9$ and transverse velocities at (c) $x = 7$ and (d) $x = 9$ for 5 waves and 16 waves cases along the width of the channels having 0° PD.

From Figs. 7.10(a) and (b), one can observe that between corrugated channels, for the channel having 16 waves that shows a greater mixing efficiency as compared to that of 5 waves case, the mass fraction profiles become much flatter for the former than compared to that of the latter. This is not merely due to physical diffusion but also due to a significant amount of transverse convection. This effect is clearly

visible in Figs. 7.10(c) and (d) which shows that the maximum and minimum values of v -velocities at a particular axial location are higher for the 16 waves case than compared to that of the 5 waves case. Thus the combined effect of the transverse velocities generated and the physical diffusion, leads to the enhancement in mixing to a greater extent in corrugated channels. The results for even higher waves are essentially very similar to that of the lower number of waves and therefore we do not discuss it any further.

Furthermore, a comparison between mixing efficiency at the outlet and a measure of pressure drop (in terms of pressure gradient) for channels having different wavelengths in 0° PD waves has been shown in Table 7.1. One can see from Table 7.1 that higher mixing efficiency is typically obtained at the cost of increased pressure drop. However, practical applications would demand a configuration having as high as mixing efficiency possible with low pressure drop.

Table 7.1: Mixing efficiency and pressure gradient for channels having 0° PD waves with different wavelength but with same amplitude ($a = 0.1h$)

Sl No.	Different Channels	Mixing Efficiency, (M %)	Pressure Gradient ($\Delta\Pi$)
1	Plane channel	60.1%	0.14
2	Channel with 5 waves	71.7%	0.36
3	Channel with 10 waves	79.4%	0.53
4	Channel with 16 waves	88.1%	0.76
5	Channel with 20 waves	80.1%	0.63
6	Channel with 35 waves	76.7%	0.60

7.3.3 Effect of amplitude

As like the case with wavelength (section 7.3.2), the mixing efficiency can also be improved by adjusting the amplitude of the sine waves. Simulations were performed for 0° PD channels by keeping λ constant at $0.575h$. Three different amplitudes, viz, $0.05h$, $0.1h$ and $0.2h$ with $Re_{air}=120$ and $Pe_{air}=92.64$ are selected for this study.

The corresponding values of Re and Pe for argon stream are 128 and 98.8, respectively.

Figures 7.11(a)-(c) show the streamlines and Ar mass fraction contours at steady state in all the three amplitudes under consideration for a particular length of the channels ($2h-4h$). It is seen from the contours that the fluid mixture is more homogenized as the amplitude increases.

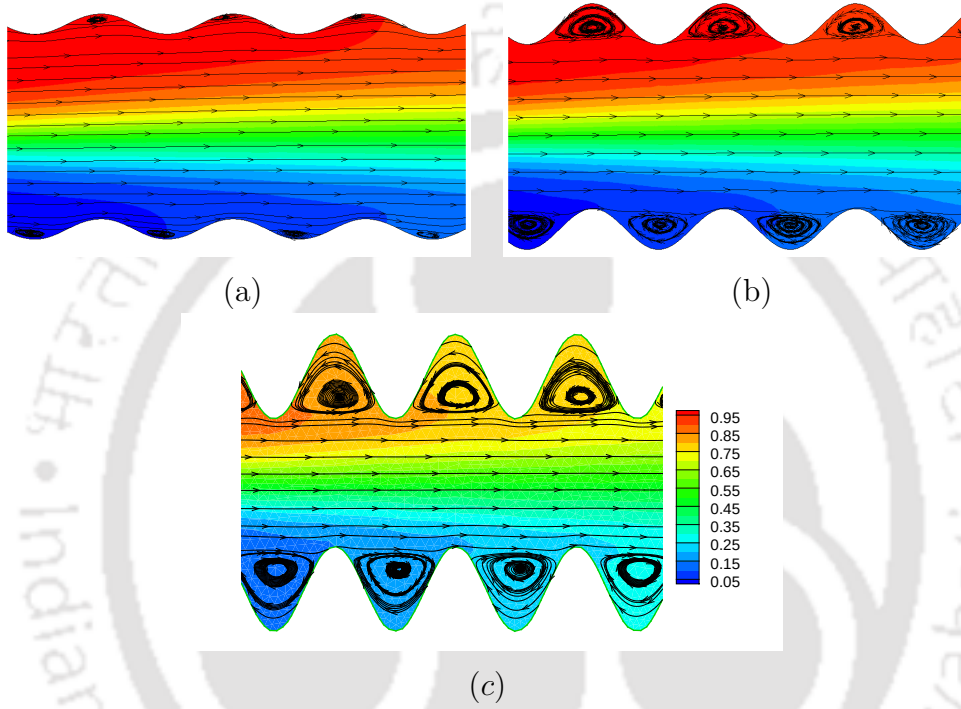


Figure 7.11: Streamlines and Ar mass fraction contours at $Re=120$, $Pe=46$ in sinusoidal channels at the same location between $2h$ to $4h$ having $\lambda = 0.575h$ and $a =$ (a) $0.05h$, (b) $0.1h$, and (c) $0.2h$.

Figure 7.12 shows the variation of mixing efficiency along the channel length for channels having the aforesaid amplitudes. Among the considered amplitudes, the channel having $a=0.2h$ gives the fastest mixing while that having $a=0.05h$ gives the least such that at the outlet, the mixing efficiencies are around 83.4%, 80.1% and 73.7% for channels having $\lambda = 0.575h$ with amplitudes of $0.2h$, $0.1h$ and $0.05h$, respectively.

The explanation for this is similar to that in the varying wavelength case. At a lower amplitude of the wave, the fluid flows close to the channel walls. Thus flow

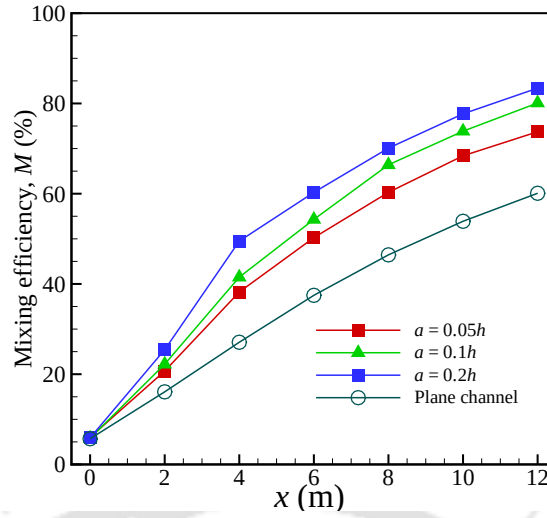


Figure 7.12: Variation of mixing efficiency with varying amplitudes along axial length of channels having 0° phase difference, $\lambda = 0.575h$ at $Re=120$, $Pe=46$.

is mostly uni-directional and the mixing takes place primarily by diffusion. As the amplitude increases, flow begins to separate from the walls and the recirculation zones push the fluid particles towards the core part of the channel. As amplitude increases, these zones increase in size. The amount of fluid flowing unhindered in the core region reduces. Thus the core fluid gets mixed in shorter lengths. It seems that the application of even higher amplitude would be beneficial as far as mixing efficiency is concerned. However, it is very likely that there could be a critical amplitude for which mixing efficiency is maximum.

7.3.4 Effect of Re

The mixing phenomenon in channels having sinusoidal ridges were studied for three different Re , viz, 20, 60 and 120, at constant $Sc=0.772$, $\lambda=0.575h$. The corresponding Pe numbers are 42 and 92.64, respectively. Figure 7.13 shows the comparison of mixing efficiencies along the length of the channel having 0° PD with 20 waves for different Re . It is observed that as Re increases, mixing efficiency drops. The reason for this is that as Re increases, the flow velocities are also increased having the other parameters constant. As a result it reduces the residence time for the fluids and hence a longer length of the channel is required to achieve the equilibrium mass fraction.

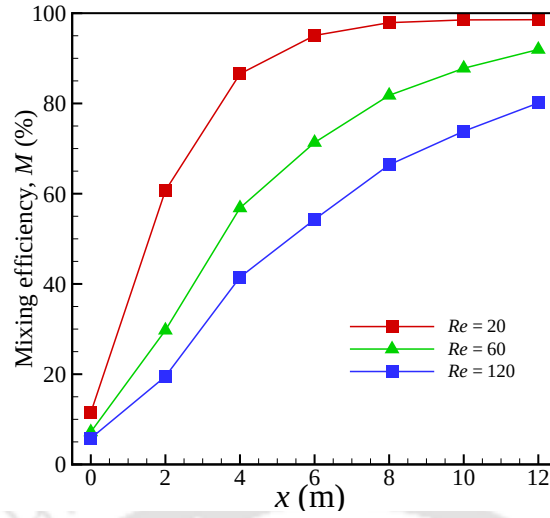


Figure 7.13: Comparison of variation of mixing efficiency along the length of the channel for $Re = 20, 60$ and 120 , for channels having 0° PD with $\lambda = 0.575h$, $a = 0.1h$.

7.3.5 Effect of Pe

In order to check the contribution of convection and molecular diffusion on the mixing process, a study with a low and high Pe (42 and 4200, respectively) at $Re = 60$ is performed. The corresponding Sc numbers are 0.772 and 70, respectively. These values are with respect to the properties of air stream. The corresponding Pe for argon stream will be The results that have already been reported in the previous sections are corresponding to low Pe value case. In this section the Pe has been increased two orders more than that of the low Pe case. Simulations are carried out for two types of wavy channels having 180° and 0° PD, respectively. Keeping $Re_{air}=60$ at inlet, Pe_{air} is now increased to 4200.

Figures 7.14(a) and (b) show the Ar mass fraction contours for the two channels considered in this study for $Pe = 4200$. From the figures it can be clearly seen that for a high Pe , both the wavy channels with 180° and 0° PD behaves in a same manner.

This can also be verified from Fig. 7.15 which shows the comparison of distribution of mixing index along the length of the two wavy channels for the two Peclet numbers. One can also see from the Fig. 7.15 that for $Pe = 42$, the channel with 0° PD shows superior mixing capability to that of the channel with 180° PD, which

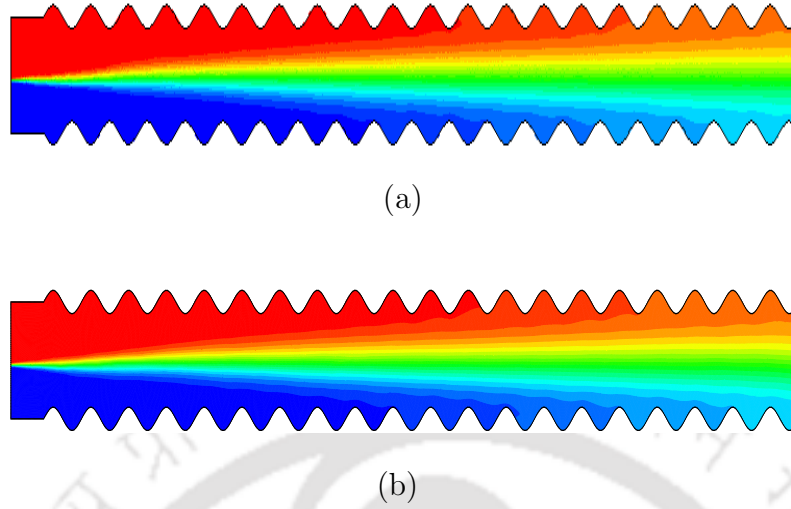


Figure 7.14: Contours of Ar mass fraction for inlet $Re=60$ and $Pe=4200$ for wavy channel having (a) 180° PD and (b) 0° PD for $\lambda = 0.575h$.

is however not observed for the channels at high Pe .

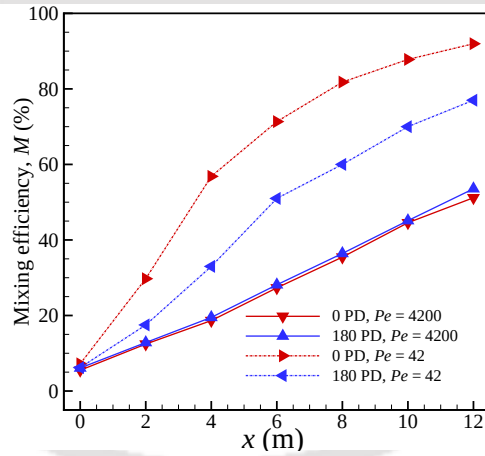


Figure 7.15: Comparison of variations of mixing efficiencies along axial length between $Pe=42$ and 4200 keeping $Re=60$ for 0° PD channel and 180° channel ($\lambda = 0.575h$ and $a = 0.1h$).

One of the probable reasons for this behavior may be that high Pe numbers leads to low molecular diffusion which is the dominant mechanism for mixing. As can be seen from Fig. 7.16, there is hardly any significant difference in the magnitudes of transverse velocities generated in both 0° and 180° PD channels at $Re = 60$. As such

mixing due to advection of the species may be considered to be negligible. Hence, the rate of mixing of the two species is largely determined by the molecular diffusion which is same for both channels.

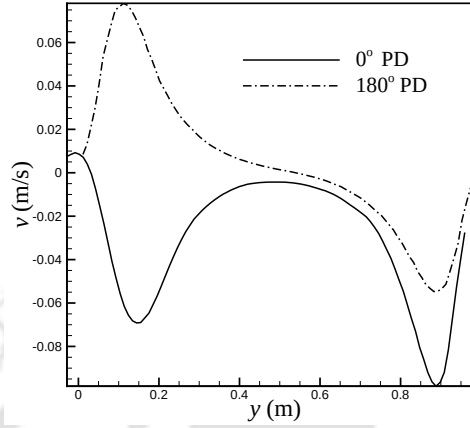


Figure 7.16: Comparison of v -velocity profiles along the width of the channels having 0° and 180° PD for $Pe=4200$ and $Re=60$ ($\lambda = 0.575h$ and $a = 0.1h$) at the middle of the channel.

7.4 Closure

In this chapter, the developed solver has been successfully used to study the mixing performance in a wavy channel compared to its plane channel counterparts. Results show that wavy channels lead to enhanced mixing compared to that of a plane channel. It is basically due to the generation of recirculation patterns that lead to higher transverse velocities. A complete set of parametric studies is subsequently carried out to investigate the effect of the geometric parameters of waves along with Reynolds number, Peclet number for the 0° PD wavy channel.

The results presented warrant the capability of the present solver to analyze the flow field and the mixing characteristics of mixing of gaseous species, particularly non-reacting in nature. Approaching the last objective of the present work, an effort has now been made to extend the numerical approach for handling variable density reacting flows. The detailed mathematical formulations for reacting flows are described in the next chapter.

Chapter 8

Extending the Approach to Mixing of Reacting Flows

In all the previous studies, the interacting species are non-reacting in nature. However, there are applications where mixing of reacting species are involved. In this type of flows, variation in density is taken place due to the simultaneous effects of gradients of temperature and concentrations. Major applications of reacting flows can be found in the field of combustion which is associated with the transforming of chemical energy content of fossil fuels into useful energy in the form of heat. It is defined as a complex sequence of chemical reactions between fuel and oxidizer accompanied by liberation of heat and light. Based on the mixing modes of fuel and oxidizer, the combustion process can be categorized as either premixed or non-premixed. In case of premixed mode, both fuel and oxidizer are mixed prior to actual combustion whereas in non-premixed mode they are not mixed beforehand. The use of combustion technology can be found in different applications such as power generation, household heating (cooking), propulsion and transportation etc.

However, the limiting nature of these fuels in the earth crust and the continuously increasing global energy demand necessitates a detailed analysis of combustion systems so that optimum utilization of the available energy sources can be granted. This require a detailed simulation of the combustion process, both experimentally and numerically, to know the underlying flow dynamics associated with mixing of reacting species. However, the presence of reactions in itself makes this a challenging

endeavor that makes its numerical simulations very challenging too. In this chapter, an initiative has been made to extend the present quasi-incompressible formulation developed for isothermal mixing in Chapter 2 and extensively studied in Chapters 4-7, for problems involving gaseous combustion. However, this study is considered as a preliminary work involving only laminar gaseous diffusion flames (non-premixed flames). The salient details of the numerical approach adopted are discussed in the following sections.

8.1 Challenges in Numerical Modelling of Combustion

The numerical modeling of combustion problems is based on the solution of a set of conservation equations for momentum and scalars, supported by additional auxiliary equations. The science of combustion often involves complex interactions between many constituent disciplines: thermodynamics, chemical kinetics, fluid dynamics, heat and mass transfer, turbulence etc., which makes its simulation is very complex and much challenging. These are basically because of the following reasons:

- Chemical time scales for different reactions are different and are very small compared to that of flow time scales. As such, time step size (Δt) should be sufficiently small to resolve the flow physics at different time interval which, on the other hand, drastically increases the computational cost.
- The increase in the number of species involved in the process further increases the computational cost.
- Handling of chemical source terms needs special attention due to its stiffness.
- The heat released by combustion leads to a temperature rise of the order of thousands of Kelvin. This makes the properties like density, specific heat, thermal conductivity, thermal diffusivity dependent on temperature which must be taken into account.

However, with the development of the computational facilities, a number of computational methods have been developed to numerically model the reacting flows. It gives an insight into flow patterns that are difficult, expensive or impossible to study

using traditional (experimental) techniques. Although numerical modeling does not replace the measurements completely but the amount of experimentation and the overall cost can be significantly reduced.

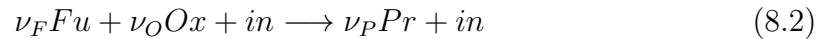
8.2 Modelling of Reacting Flows

This section provides the generalized three-dimensional governing equations in differential form for laminar non-premixed combustion flows. The governing equations involve conservation of mass, momentum and species with the inclusion of source terms due to reaction. The species conservation equation for chemical species k in a system of N species is given as

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho u_j Y_k)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D_k \frac{\partial Y_k}{\partial x_j} \right) + \dot{\omega}_k \quad (8.1)$$

where $\dot{\omega}_k$ is the source term due to production and destruction of species k by chemical reaction. Handling of this term is very complex in nature. Moreover, the traditional method of solving a reacting mixture involves solving of $(N-1)$ number of species equations, which becomes computationally very expensive, if N is very large.

To avoid this, however, there is another approach based on the “flame sheet” concept proposed by Burke and Schumann [150], specifically suitable for the simulation of diffusion flames. This concept is based on the idea that the reaction rates are infinitely fast and limited to a very thin exothermic reaction zone which separates the fuel and oxidizer. This assumption implies that the reaction time is much shorter than the mixing time and no fuel is present on the oxidizer side and vice versa. As such all the intermediate products can be neglected and hence global single step reaction may be assumed for the chemistry modeling. The single step reaction of fuel (Fu) and oxidizer (Ox) in the presence of inert gas (in) to form product (Pr) can be written as,



where ν_F, ν_O, ν_P are the stoichiometric coefficients of the reaction.

This concept allows to determine the complete chemical state by solving only one

source-free conservation equation for the variable called mixture fraction (Z) which is a conserved scalar. The conservation equation for Z is deduced from species conservation equation (derivation is given in Appendix B.2) and is given as

$$\frac{\partial(\rho Z)}{\partial t} + \frac{\partial(\rho Z u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\rho D_Z \frac{\partial Z}{\partial x_j} \right] \quad (8.3)$$

The mass fractions of fuel and oxygen are related to the mixture fraction according to the following relationships [151]:

$$0 < Z \leq Z_{st} : \begin{cases} T = T_{ox}(1 - Z) + \left[\frac{Q}{c_p} Y_{fu} + T_{fu} \right] Z \\ Y_{fu} = 0, \\ Y_{ox} = \left(1 - \frac{Z}{Z_{st}} \right) \cdot Y_{ox,o} \\ Y_{pr} = Y_{fu} \frac{MW_{pr} \nu_{pr}}{MW_{fu} \nu_{fu}} Z \end{cases} \quad (8.4)$$

$$Z_{st} < Z \leq 1 : \begin{cases} T = T_{fu}Z + \left[T_{ox} + Y_{ox} \frac{Q}{c_p} \frac{MW_{fu}}{MW_{ox}} \frac{\nu_{fu}}{\nu_{ox}} \right] (1 - Z) \\ Y_{fu} = \left(\frac{Z - Z_{st}}{1 - Z_{st}} \right) \cdot Y_{fu,f} \\ Y_{ox} = 0 \\ Y_{pr} = Y_{ox} \frac{MW_{pr} \nu_{pr}}{MW_{ox} \nu_{ox}} (1 - Z) \end{cases} \quad (8.5)$$

where Q is the heat release per unit mass of the fuel and Z_{st} is the stoichiometric value given by

$$Z_{st} = \frac{1}{1 + s \left(\frac{Y_{fu,f}}{Y_{ox,x}} \right)} \quad (8.6)$$

where $s = \frac{MW_{O\nu_O}}{MW_{F\nu_F}}$. The mass fraction of the inert component, Y_{in} is given by

$$Y_{in} = 1 - Y_{Fu} + Y_{Ox} + Y_{Pr} \quad (8.7)$$

This conserved scalar concept is particularly useful in dealing with non-premixed mode of combustion. For premixed combustion, the mixture fraction is everywhere uniform, assuming all species have the same diffusivities.

8.3 Quasi-Incompressible Formulation for Reacting Flows

The generalized non-solenoidal divergence constraint for variable density reacting flows is given by Eq. B.15 which reads as

$$\begin{aligned} \nabla \cdot \mathbf{u} = & \frac{1}{\rho c_{p,mix} T} \left[\nabla \cdot (\kappa \nabla T) + \sum_k \rho D \nabla Y_k \cdot \nabla h_k \right] + \frac{1}{\rho} \sum_k \frac{\bar{W}}{MW_k} \nabla \cdot (\rho D \nabla Y_k) \\ & + \frac{1}{\rho} \sum_k \left(\frac{\bar{W}}{W_k} - \frac{h_k}{T c_{p,mix}} \right) \omega_k + \left(\frac{R_u - c_{p,mix}}{\bar{P} c_{p,mix}} \right) \frac{D\bar{P}}{Dt} = \tilde{S} \end{aligned} \quad (8.8)$$

It can be seen from Eq. 8.8 that the divergence constraint of velocity field in reacting flows results due to the presence of both temperature as well as concentration gradients. Moreover, the heat released by combustion leads to rise the temperature to a much higher value that provides the major contribution to the constraint on the divergence of velocity field. Furthermore, larger temperature difference also results in a significant variations in density and hence the use of purely incompressible algorithm can be vulnerable for modelling reacting flows.

However, the system of equations for reacting flows are overdetermined in terms of using continuity (Eq. 2.27) and equation of state (Eq. 2.32). Use of Eq. 2.27 ensures conservation of mass in the discrete level. But in a sequential approach, it is rather impossible to simultaneously satisfy both continuity equation and equation of state (EOS). It has been observed that conservation of mass is more important for problems involving high density ratios. Hence, in the present approach also the mixture density is evaluated by solving Eq. 2.27. In regard to the low Mach number model, it has already been mentioned in Section 2.1 that use of this model introduces new unknowns in terms of thermodynamic pressure ($\bar{P}$) that has to be handled carefully. Handling of these new unknowns are separately discussed in the following sub-sections for closed and open systems.

8.3.1 Handling of close systems for large density ratio

For closed systems, the expressions for $\bar{P}$ is obtained through mass conservation equations. Let m_0 be the mass in the enclosure at time $t = t_0$. Using the ideal gas

law we arrive at the expression for initial mass in a enclosure of volume V as

$$m_0 = \int_V \rho(t_0) dV = \int_V \frac{\bar{P}(t_0) \bar{W}(t_0)}{R_u T(t_0)} dV \quad (8.9)$$

As the total mass remains constant in a enclosure so at any particular time instant t

$$m_0 = \int_V \rho(t) dV = \int_V \frac{\bar{P}(t) \bar{W}(t)}{R_u T(t)} dV \quad (8.10)$$

from the above equation we get

$$\bar{P}(t) = m_0 \frac{R_u}{\int_V \frac{\bar{W}(t)}{T(t)} dV} \quad (8.11)$$

The equation for $\frac{d\bar{P}}{dt}$ can be obtained by integrating Eq. 8.8 over the entire domain Ω and then applying impervious boundary condition. For a non-reacting mixture of gases and assuming specific heat of the species are equal and constant, this expression can be given as

$$\begin{aligned} \frac{d\bar{P}}{dt} = & \frac{\bar{P}}{(R_u - c_p)\Omega} \left\{ \frac{1}{\rho c_p T} \int_V \nabla \cdot (\kappa \nabla T) dV \right\} + \\ & \frac{\bar{P}}{(R_u - c_p)\Omega} \left\{ \int_V \frac{1}{\rho} \sum_k \frac{\bar{W}}{W_k} \nabla \cdot (\rho D \nabla Y_k) dV \right\} \end{aligned} \quad (8.12)$$

8.3.2 Handling of open systems for large density ratio

For open systems, $\bar{P}$ equilibrates with the ambient pressure instantaneously and hence it is independent of both space and time. As such the term $\frac{d\bar{P}}{dt}$ vanishes in Eq. 8.8. But, violation of satisfying EOS discretely may leads to drifting of the thermodynamic pressure ($\bar{P}$) from its actual value say $\bar{P}_0$, that needs to remain constant in open systems. This, effect is however not significant for non-reacting flows where the density ratio is quite small. In such problems, either of the continuity equation or the equation of state can be used to evaluate the mixture density. In order to prevent the algorithm from drifting too far off the equation of state, a pressure relaxation term is added to numerical representation of the divergence

constraint as discussed in the work of Pember et al. [6] and is given as

$$\nabla \cdot \mathbf{u} = \tilde{S} + f \frac{c_{p,co} - R_{co}}{\Delta t c_{p,co} \bar{P}_{ij}} (\bar{P}_{co} - \bar{P}_0) \quad (8.13)$$

where $\bar{P}_{co}$ refers to the instantaneous value of thermodynamic pressure at the cell centroid (co) of each computational cell and f is a constant satisfying $f < 1.0$. For open systems, $\bar{P}_0 = 101325$ Pa which is nothing but the atmospheric pressure.

8.4 Validations

In this section, the results obtained from the developed solver are validated against problems involving high density ratio having benchmark solutions for closed as well as open systems. The first problem considers the natural convection in a closed cavity where the variations in density is due to gradients of temperature only. The second problem considers the same natural convection in a closed cavity but in the presence of multiple species where gradients of both temperature and concentration are involved. The last problem considers the simulation of a laminar diffusion flame.

8.4.1 Two-dimensional natural convection in a square cavity

In this section, the natural convection in a closed square cavity is chosen as the benchmark problem to see the effect of density change due to temperature gradients. Figure 8.1 represents the schematic diagram of a 2D square cavity where the top and bottom walls are insulated and right and left walls are subjected to hot (T_h) and cold (T_c) temperatures, respectively. An important parameter for natural convection problem is the temperature difference parameter denoted by ϵ , which defined whether the Boussinesq approximation will be valid or not. It is defined as $\epsilon = \frac{T_h - T_c}{T_h + T_c}$ such that $T_h = T_0(1 + \epsilon)$ and $T_c = T_0(1 - \epsilon)$ where T_0 is the mean temperature. If ϵ is large enough, for example $\epsilon = 0.6$, the flow inside the cavity undergoes large density variation due to significant temperature variations. However, with small values of ϵ (< 0.05), the density variation is not significant enough. As such, for this range of problems Boussinesq approximation is also valid which is applicable for incompressible flows only. However, with the present formulation both this limit can be explored without making any change.

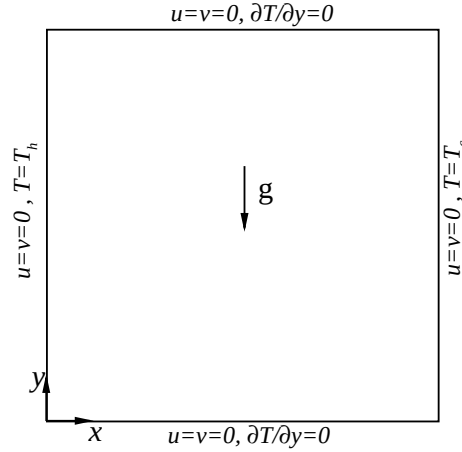


Figure 8.1: Geometry and boundary conditions for square cavity

Considering the Boussinesq and non-Boussinesq limit, numerical simulations are carried out for $\epsilon = 0.01$ and 0.6 with (T_h, T_c) values of $(303 \text{ K}, 297 \text{ K})$ and $(960 \text{ K}, 240 \text{ K})$, respectively. A mesh size of 10,000 hexahedral elements is used for Rayleigh number (Ra) of 10^6 and Prandtl number (Pr) of 0.7 . The values of the properties such as viscosity (μ), thermal conductivity (κ) are assumed to be constant and calculated from the definitions of Ra and Pr , respectively. The time step size (Δt) is taken as 10^{-3} s . The value of acceleration due to gravity in negative y direction is 9.8 m.s^{-2} . The continuity, momentum, energy equations are solved to get the distribution of density, velocity and temperature respectively.

Figure 8.2 displays the comparison of local Nusselt number (Nu) distribution on the hot and cold walls of the cavity for $\epsilon = 0.01$ and 0.6 , respectively. In the Boussinesq limit i.e. $\epsilon = 0.01$ the variation of Nu is symmetric for both the walls whereas in the purely non-Boussinesq limit i.e., $\epsilon = 0.6$, this symmetry in the local Nu distribution is broken down which shows a reasonably good match with the results reported by Darbandi and Hosseinzadeh [152]. Also a comparison of average Nusselt number ($\overline{Nu}$) is shown in Table 8.1 below with the benchmark results of De Vahl Davis [153] and Darbandi and Hosseinzadeh [152].

From the table it can be seen that the % error in the calculation of $\overline{Nu}$ for $\epsilon = 0.01$ and 0.6 are 2.1% and 2.2% respectively, which is under the acceptable limit. This proves the correctness of the present quasi-incompressible model to investigate the flow fields with different magnitude of buoyant forces.

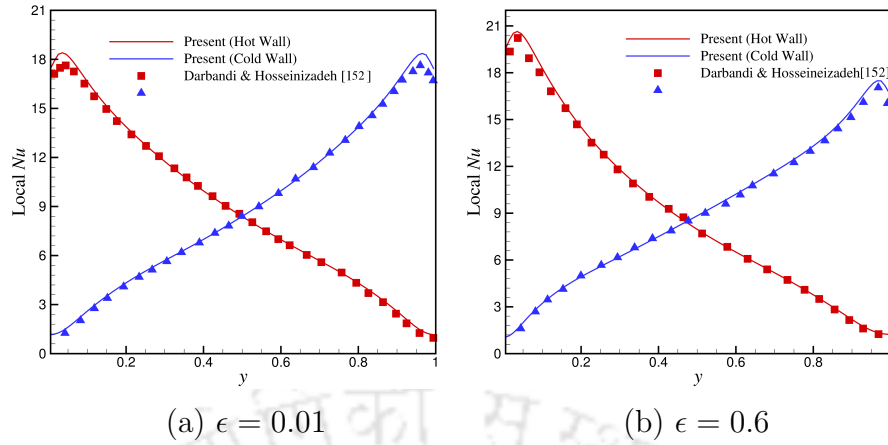


Figure 8.2: Local Nusselt number distribution along the hot and cold walls

Table 8.1: Average Nusselt number comparison

Parameter	$\epsilon=0.01$			$\epsilon=0.6$		
	Present	De Vahl Davis [153]	% Error	Present	Darbandi and Hosseini-zadeh [152]	% Error
$\overline{Nu}_h$	8.99	8.8	2.1	9.08	8.88	2.2
$\overline{Nu}_c$	8.99	8.8	2.1	9.08	8.88	2.2

8.4.2 Two-dimensional natural convection in a square cavity with multiple species

The test problem has been taken from the work of Ebrahimi-Kebria et al. [154] where mixing natural-convection flow in a square cavity with large temperature gradients has been studied. The problem domain is similar to that presented in Section 8.4.1. The cavity is initially filled with two species namely, Nitrogen (N_2) and Oxygen (O_2), which are separated by a diaphragm. The amount of both the species should be such that 79% of total volume will be occupied by N_2 and remaining 21% of volume will be occupied by O_2 . The initial condition and the boundary conditions are schematically shown in Fig. 8.3. The temperature boundary conditions at the right and left walls are such that $\epsilon = 0.6$ with T_h and T_c of 960 K and 240 K, respectively.

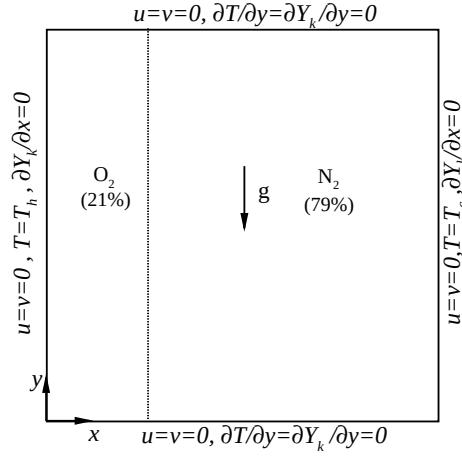
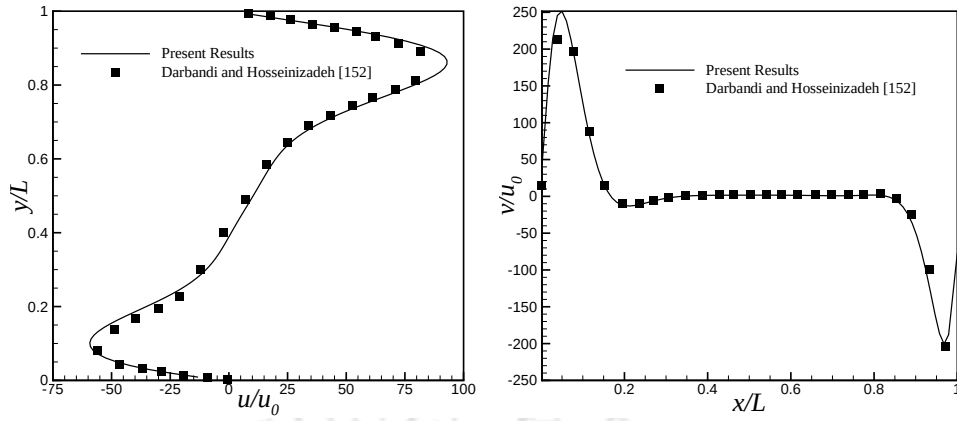


Figure 8.3: Initial and boundary conditions for mixing-thermibuoyant flows

It is expected that as the diaphragm is removed, the convective currents established due to the temperature differences between the two vertical walls lead to the transport of the two species via convection and diffusion. When the steady-state condition will be reached, both the two species will fully mix forming a homogeneous mixture having same composition as that of air. As such, the steady-state results obtained from this test case should match with the available solutions provided for a square cavity filled with air [152]. For this test case, in addition to the continuity, momentum and energy equations, the species conservation equation for O_2 mass-fraction has been solved. For simulations a mesh with 10,000 hexahedral elements has been used with $\Delta t = 10^{-3}$.

Figures 8.4(a) and (b) show a comparison of the longitudinal velocity (u/u_0) and transverse velocity (v/u_0) corresponding to the centerline of the cavity. Here, $u_0 = \frac{\kappa_0}{\rho_0 c_{p0} L}$ where L is the characteristic length and subscript 0 refers to the properties at mean temperature of $T_0 = 600$ K. Both the velocities profiles are in good agreement with the available literature.

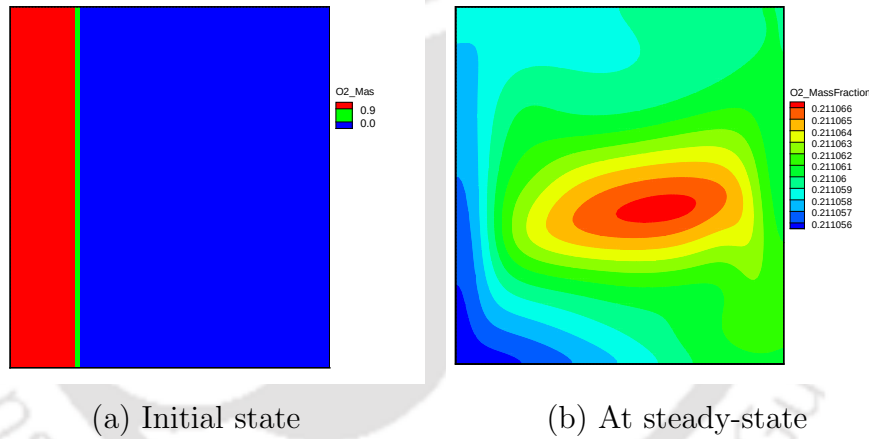
The initial and steady-state mass fractions of O_2 are shown in Figs. 8.5(a) and (b), respectively. From this figure, it has been seen clearly that, at steady state both the two species are uniformly distributed all throughout the domain representing the composition of air. Also the average Nusselt number along the hot and cold walls are 9.08 each which is same as that obtained for the test case of Section 8.4.1. The



(a) u profile along vertical centerline (b) v profile along horizontal centerline

Figure 8.4: Distribution of velocity components along the centerline of the cavity

results justify the correctness of the mass transportation predicted by the current formulation in highly thermobuoyant flow fields.



(a) Initial state

(b) At steady-state

Figure 8.5: O_2 mass-fraction contours

8.4.3 Laminar Diffusion Flames

To validate the reacting flow solver, the two-dimensional laminar diffusion flame test, carried out by Darbandi and Banaeizadeh [155], is considered as a model problem. The burner consists of an upward rectangular burner with dimensions of 40×400 mm. The physical domain is shown schematically in Figure 8.6. The fuel (CH_4) enters from the bottom of the burner with a width of 8 mm whereas dry air with

($Y_{O_2} = 0.232$ and $Y_{N_2} = 0.768$) enters from the rest of bottom through two slots of 16 mm on both sides of the fuel slot. The overall chemical reaction for $CH_4 - Air$ mixture is given as:

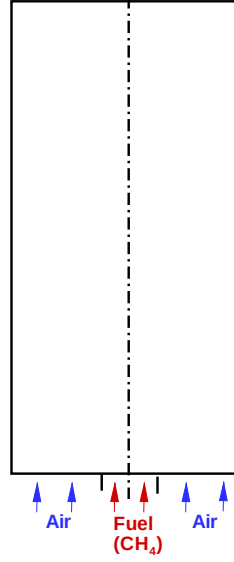
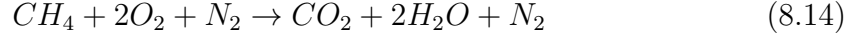


Figure 8.6: Computational domain for laminar diffusion flame test

The flow conditions at the inlet ($y=0$) are as follows:

For fuel inlet

$$u = 0 \text{ cm/s}, \quad v = 11 \text{ cm/s}, \quad T = 298 \text{ K}, \quad Y_{CH_4}=1, \\ Y_{O_2} = \omega_{N_2} = Y_{CO_2} = Y_{H_2O} = 0.0$$

For air inlet

$$u = 0 \text{ cm/s}, \quad v = 21.7 \text{ cm/s}, \quad T = 298 \text{ K}, \quad Y_{O_2} = 0.232, \\ Y_{N_2} = 0.768, \quad Y_{CH_4} = Y_{CO_2} = Y_{H_2O} = 0$$

The pressure at the exit is taken as $p = 1\text{atm}$. The outer tube wall of the burner is assumed to be adiabatic. The flame-sheet concept is used for modelling the chemistry. In this approach, chemistry is modeled by solving only one conserved scalar variable called ‘mixture fraction’ (Z). Temperature and mass fractions of all the five species (Eq. 8.14) are calculated using Eqs. 8.4 - 8.7. The heat release parameter ($\frac{Q}{c_p}$) is taken from the heat of combustion and a representative heat

capacity [151]. In the present case value of $Q = 55.5$ MJ/kg and $c_p = 1598$ J/kg.K are assumed to be constant. The other thermo-physical properties like thermal conductivity (κ), dynamic viscosity (μ) are calculated as a function of temperature (T) by using the relation given as [6]

$$\mu = \mu_0 \left(\frac{T}{T_0} \right)^{0.7} \quad \text{and} \quad \rho D = \frac{\kappa}{c_p} = \frac{\mu}{Pr} \quad (8.15)$$

To start the numerical simulation, first the domain is assumed to be completely filled with air ($Y_{O_2} = 0.232$ and $Y_{N_2} = 0.768$). Then the fuel (CH_4) is injected through the respective inlet. When both fuel and air comes in contact of each other, reaction proceeds to produce the products (CO_2 and H_2O). Figures 8.7(a) - (h) show the contour plots for various variables at steady state. It is evident from the Fig. 8.7(d) that there has been a significant drift of thermodynamic pressure ($\bar{P}$) from the actual value (101325 Pa).

Figure 8.8 shows a comparison of variation of temperature and CH_4 mass-fraction profiles along the width of the channel at different height. A little more deviation has been observed with reference to the results given by Darbandi and Banaeizadeh [155] near the walls. One of the probable reason for this may be the drift of thermodynamic pressure reported above. It has been observed that the drift of $\bar{P}$ can be reduced by increasing the grid resolution as can be seen in Table 8.2.

Table 8.2: Maximum drift in $\bar{P}$

No. of Cells	Max. drift in $\bar{P}$ (Pa)
20,000	3,10,675
84,500	34,147

However, depending on the grid spacing, a significant amount of drift in $\bar{P}$ has also been reported by Day and Bell [7], when they solved an axisymmetric CH_4 -Air diffusion flame with complex chemistry. Thus, it is believed that it is very difficult to completely nullify the drift of $\bar{P}$, but controlling it to the best possible limit can improve the results of the present case.

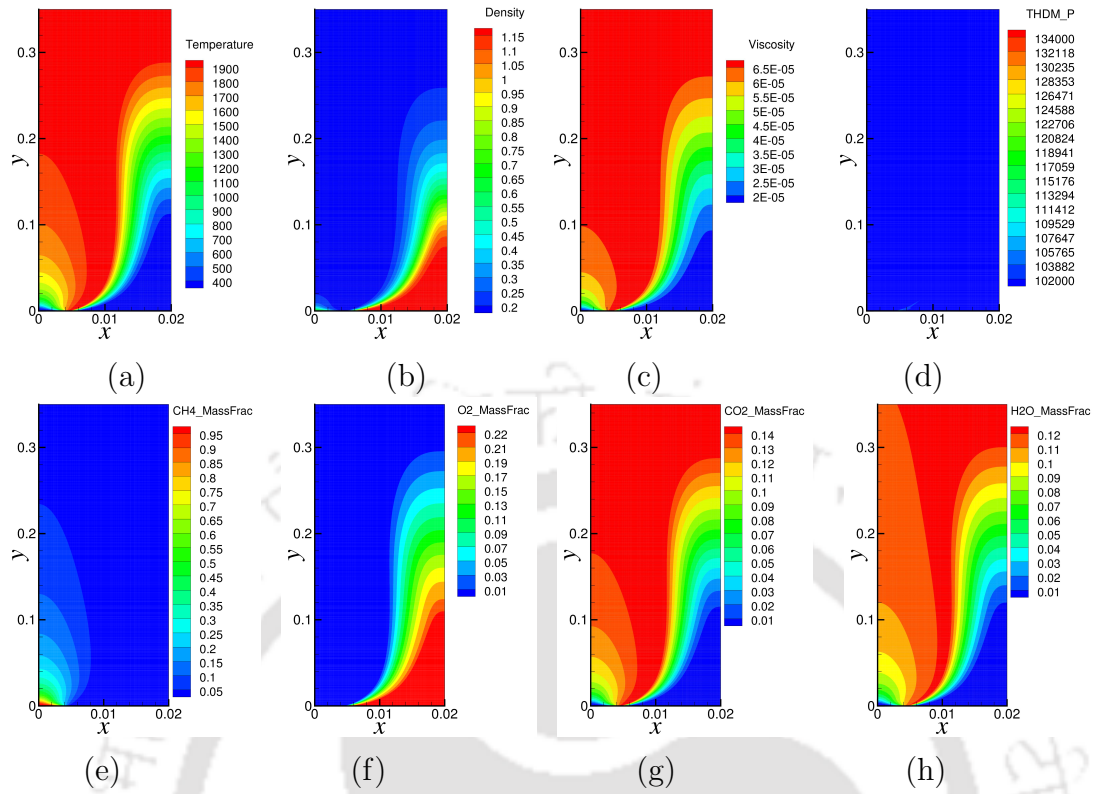


Figure 8.7: Contour plots for laminar diffusion flame test: (a) temperature, (b) density, (c) viscosity, (d) thermodynamic pressure, (e) Y_{CH_4} , (f) Y_{O_2} , (g) Y_{CO_2} , (h) Y_{H_2O}

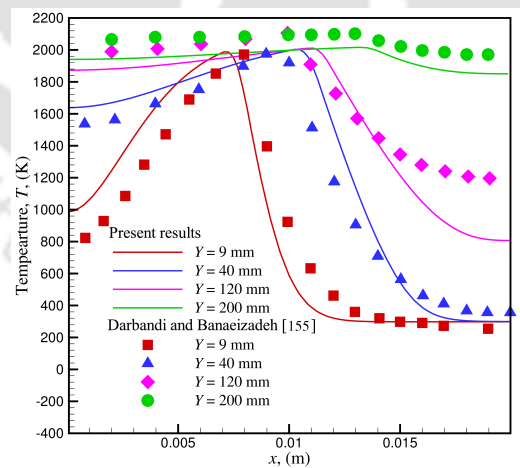


Figure 8.8: Evolution of temperature profiles with height

8.5 Closure

In this section, we have presented an extension of the quasi-incompressible formulation adopted for the simulation of non-reacting mixing flows to study the mixing phenomena in the presence of chemical reaction. We have also discussed about the complexities associated with the numerical modelling of reacting flows. In this first attempt, the simplified chemistry model based on mixture fraction approach, typical of diffusion flame, is implemented for handling the reaction kinetics. The number of chemical species can be found from the single step reaction mechanism. In order to validate the present developed solver with that of reacting flows, the diffusion flame developed by the reaction between methane and air has been analyzed. Results show that the present solver has the capability of studying the laminar diffusion flame with a good amount of accuracy.



Chapter 9

Conclusions and Scope of Future Work

This chapter summarizes the key strategies implemented in the development and application of a single-phase, multi-fluids solver proposed in this thesis. The major contributions of the study highlighting its novel findings are recapitulated. Furthermore, stating about the limitations of the present work, it has also been provided the directions for future work.

9.1 Conclusions

The thesis discusses the development and validation of a generic quasi-incompressible flow solver and its applications to micro and macro mixing as well as combustion. The solver is devised to handle arbitrary polyhedral meshes, both orthogonal and non-orthogonal, both in incompressible and quasi-incompressible flow regimes with no specific constraint on the density ratios of the multiple fluids involved. We studied the relation between local truncation and discretization error on different meshes for convective and diffusive problems. It has been found that truncation and discretization errors are related and method of manufactured solutions can be used to arrive at a quantitative conclusion between the truncation and discretization errors. From this study the salient conclusions are as follows.

1. Convective schemes tested in this work can be arranged in the increasing order of DE as: CUBISTA < Khosla-Rubin < FOU. However, the truncation error also shows the same trend which being apriori can be give a fair indication of the discretization errors which are aposteriori determined.
2. Based on this we conclude that CUBISTA scheme is found to be the better candidate for incurring lesser numerical diffusion.
3. Khosla-Rubin scheme that is obtained as a equi-blend of FOU and CDS schemes, shows an overall first order accuracy, despite the fact that the latter schemes show first and second-order accuracies on smooth flow problems. This indicates that there is no real suppression of the false diffusion that plagues first-order upwind schemes when applied to problems involving mixing of liquids.
4. However, the discretization errors obtained from the Khosla-Rubin scheme is lower than that obtained from FOU scheme as observed from the Taylor-Green vortex problem.

The final developed solver is thoroughly validated for a wide range of problems involving mixing of non-reacting species of both liquids and gases. All the validation studies performed are found to be less than 5% error limit. For e.g., mixing indices obtained for liquid mixing in micromixers are having 2.3% and 3.9% errors compared to numerical and experimental results, respectively. The final developed solver is then applied to solve two pertinent problems related to enhancing the mixing of fluids.

The first study is to explore the fascinating dynamics of mixing of liquids in a novel passive micromixer with thin curved ribs and to access the mixing performances in a two-dimensional cross-T microchannel. The salient conclusions drawn from the two-dimensional study of using curved ribs in microfluidic applications are given below.

1. Mixing efficiencies of the micromixer with curved obstacles is found to be marginally higher than that obtained with the conventional straight obstacles (45% and 43.4%, respectively). However, the key point is that the same can be achieved with a significantly lower pressure drop with the curved obstacles (153.1 Pa) compared to straight obstacles (225.2 Pa).

2. Mixing efficiencies of the channel increase with increasing the number of modules as well as the size of the obstacles.
3. From the angle of inclination study, it has been found that the negative angles lead to much higher pressure drop than compared to that of their positive angle counterparts for the same mixing performance. As such positive angles are more preferred for this type of microchannels.
4. The present obstacle geometry is more preferable for flows with low Re typical for microfluidic applications.

The second study is to exploit the use of curved ribs in a three-dimensional cross-T microfluidic junction to understand the role of three-dimensional effects and obstacle curvature for a wide range of Re flows. We observed a large difference in the mixing performances between the two-dimensional channel as compared to three-dimensional channel. The salient conclusions drawn from the three-dimensional study of using curved ribs as flow obstacles are as follows.

1. The difference in mixing index between curved and straight ribs are much smaller for two-dimensional channel as compared to its three-dimensional counterparts (61.3% and 47.6% for three-dimensional channels with curved and straight ribbed channels, respectively). This leads to an enhancement of 2.5 times with respect to the planner channel by the use of curved ribs whereas the same is around 1.9 times by using conventional straight ribs.
2. The advantage of lower pressure head loss observed in two-dimensional configurations with curved obstacles is also found in three-dimensional configurations.
3. The magnitude of the transversal velocities (v and w) is higher for the channels with curved ribs than that of straight ribs, which however is almost negligible for plane channels. This concludes that superior mixing with curved ribs is due to induced convective transfer.
4. Another difference with respect to 2D study is related to the enhancements with increasing number of modules. The increase in M is dominated by the increase in pressure drop after a certain number of modules which is 4 in this study.

5. Parametric studies conducted in the present work lead to nearly optimum configuration of the channel with $h = 0.75H$, $\theta = -30^\circ$, $l = 0.2 \mu\text{m}$, $N_m = 4$ and $s = 0.135 \mu\text{m}$, which are arrived at considering both mixing index and pressure drop.

The third study is the application of the developed solver in simulating the dynamics of gaseous mixing in a sinusoidally corrugated macrochannel and to evaluate the role of wavelength (λ) and amplitude (a) of the sinusoidal corrugations. We observed that the vortex patterns which arise out of asymmetries in the wavy geometry seem to manifest in mixing compared to that of a plane channel. The salient conclusions drawn from the parametric studies are given below.

1. Asymmetric wavy channels having 0° phase difference (PD) show better mixing capability ($M = 97\%$) than their symmetric counterparts with 180° PD ($M = 74\%$) for otherwise same configuration.
2. Investigations lend support to the fact that generation of higher transverse velocities are responsible for enhanced mixing in asymmetric channels. For a channel with $\lambda = 1.15h$ and $a = 0.1h$, the maximum v -velocity for 0° and 180° PD channels are around 0.16 and 0.08 m/s, respectively.
3. For channel with 0° PD and $a = 0.1h$, the optimum value of wavelength (λ) is found to be $1.15h$ which gives maximum mixing efficiency of 97 %.
4. For the given range of amplitudes studied ($0.05h$ - $0.2h$), mixing efficiency is found to increase with increase in amplitude of the wave.
5. At very high Peclet number, both symmetric and asymmetric channels end up with same mixing efficiency.

Finally, the quasi-incompressible formulation successfully implemented for the simulation of non-reactive mixing is extended to gaseous reacting flows. It has been found that the evaluation of mixture density plays an important role in flows having high density ratio which has not been observed for non-reacting flows. This study is, however, considered as a preliminary work involving demonstration of the capability of the present approach to handle of high density ratio problems. The solver is found to reproduce the benchmark results with a good amount of accuracy. Study of laminar diffusion flames of methane-air mixture can be concluded as follows.

1. Controlling of drift of thermodynamic pressure is very important.
2. Selection of reasonably good mesh resolution reduces the drift of thermodynamic pressure to the acceptable limit and hence on the accuracy of the obtained results.

9.2 Scope of Future Work

The numerical framework described in the thesis is robust, generic and versatile but there are a few lacunae which need to be explored in the future. Some of the possible directions for future research that can further enhance the potential of the numerical framework are listed below.

- Numerical results obtained for mixing of liquids with $Sc \sim O(1000)$ are susceptible to numerical diffusion. Therefore, analysis of different convective schemes, for their numerical errors, needs to be performed for a more realistic problem representative of mixing to select the optimum combination of grid density and schemes.
- Any practical application of mixing of multiple species would demand a configuration that gives as high as mixing efficiency possible with lower pressure drop. Therefore, a better measure/criteria needs to be devised in future studies to compare different configurations for their mixing performances to find the optimal configuration.
- It has been seen from the current study that mixing in liquids is a quite slow process requiring a significant length of the channel to achieve better mixing. As such, it will be good if a study can be conducted to find out a co-relation among the flow properties and the geometric parameters of the mixing channel. It will help in selecting the optimum length of the mixing channel required to carry out the numerical simulations to save computation time.
- Moreover, combination of both the conventional straight obstacles and the newly devised curved obstacles can be analyzed for their mixing capabilities.

- All the cases studied in this work involves smooth flows without any discontinuity in the domain and the developed solver is found to be capable of handling this type of flows with a good amount of accuracy. However, in future, modifications in the solver can be made to account for the discontinuities, if present any, in the problem.
- The reacting flow solver that has been implemented in this thesis is valid only for laminar diffusion flames only. As such, integration of the more generic methodology for simulation of both premixed and non-premixed (diffusion) flames based on the mass-fraction approach is needed.
- Last but not the least, the existing solver runs on a single processor only that demand significantly high computational cost for attempting three-dimensional problems. As such parallelization of the developed solver is highly recommended in order to reduce the computational time for three-dimensional simulations.

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Appendix A

Derivations of Some Basic Equations

A.1 Divergence Constraint of Velocity Field for Liquids

Equation 2.30 of Chapter 2 can be rewritten in a nonconservative form¹ as,

$$\rho \left[\frac{\partial Y_k}{\partial t} + \nabla \cdot (Y_k \mathbf{u}) \right] = \nabla \cdot (\rho D \nabla Y_k) + \rho Y_k \nabla \cdot \mathbf{u} \quad (\text{A.1})$$

$$\Rightarrow \rho \left[\frac{\partial Y_k}{\partial t} + Y_k \nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla Y_k \right] = \nabla \cdot (\rho D \nabla Y_k) + \rho Y_k \nabla \cdot \mathbf{u} \quad (\text{A.2})$$

$$\Rightarrow \rho \left[\frac{\partial Y_k}{\partial t} + \mathbf{u} \cdot \nabla Y_k \right] = \nabla \cdot (\rho D \nabla Y_k) \quad (\text{A.3})$$

Let us consider a mixture of two liquid species with the corresponding mass-fractions and densities of $Y_{1,2}$ and $\rho_{1,2}$. Then the mixture density can be represented as,

$$\rho = \frac{1}{\frac{Y_1}{\rho_1} + \frac{Y_2}{\rho_2}} \quad (\text{A.4})$$

$$\Rightarrow \frac{1}{\rho} - \frac{Y_2}{\rho_2} = \frac{Y_1}{\rho_1} \quad (\text{A.5})$$

¹For simplicity we are using vector forms of the equations

$$\Rightarrow Y_1 = \rho_1 \left(\frac{1}{\rho} - \frac{Y_2}{\rho_2} \right) \quad (\text{A.6})$$

Equation A.3 can be written for the component Y_1 as,

$$\Rightarrow \rho \left[\frac{\partial Y_1}{\partial t} + \mathbf{u} \cdot \nabla Y_1 \right] = \nabla \cdot (\rho D \nabla Y_1) \quad (\text{A.7})$$

Replacing Y_1 of the above equation by Eq. A.6, we get,

$$\Rightarrow \rho \left[\frac{\partial}{\partial t} \left(\frac{\rho_1}{\rho} - \frac{\rho_1 Y_2}{\rho_2} \right) + \mathbf{u} \cdot \nabla \left(\frac{\rho_1}{\rho} - \frac{\rho_1 Y_2}{\rho_2} \right) \right] = \nabla \cdot \left[\rho D \nabla \left(\frac{\rho_1}{\rho} - \frac{\rho_1 Y_2}{\rho_2} \right) \right] \quad (\text{A.8})$$

$$\Rightarrow \rho \left[\rho_1 \frac{\partial}{\partial t} \left(\frac{1}{\rho} \right) - \frac{\rho_1}{\rho_2} \frac{\partial Y_2}{\partial t} + \rho_1 \mathbf{u} \cdot \nabla \left(\frac{1}{\rho} \right) - \frac{\rho_1}{\rho_2} \mathbf{u} \cdot \nabla Y_2 \right] = \nabla \cdot \left[\rho D \left(\rho_1 \nabla \frac{1}{\rho} - \frac{\rho_1}{\rho_2} \nabla Y_2 \right) \right] \quad (\text{A.9})$$

$$\Rightarrow \frac{\rho_1}{\rho} \frac{\partial \rho}{\partial t} - \frac{\rho \rho_1}{\rho_2} \frac{\partial Y_2}{\partial t} + \frac{\rho_1}{\rho} \mathbf{u} \cdot \nabla \rho - \frac{\rho \rho_1}{\rho_2} \mathbf{u} \cdot \nabla Y_2 = \rho_1 \nabla \cdot \left(\frac{D}{\rho} \nabla \rho \right) - \frac{\rho_1}{\rho_2} \nabla \cdot (\rho D \nabla Y_2) \quad (\text{A.10})$$

Cancelling ρ_1 from both sides of the above equation and after rearranging the terms we get,

$$\Rightarrow \frac{1}{\rho} \left(\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho \right) - \frac{\rho}{\rho_2} \left(\frac{\partial Y_2}{\partial t} + \mathbf{u} \cdot \nabla Y_2 \right) = \nabla \cdot \left(\frac{D}{\rho} \nabla \rho \right) - \frac{1}{\rho_2} \nabla \cdot (\rho D \nabla Y_2) \quad (\text{A.11})$$

Rearranging the first term on the L.H.S. of the above equation using continuity equation we get,

$$\Rightarrow -\nabla \cdot \mathbf{u} - \frac{\rho}{\rho_2} \left(\frac{\partial Y_2}{\partial t} + \mathbf{u} \cdot \nabla Y_2 \right) = \nabla \cdot \left(\frac{D}{\rho} \nabla \rho \right) - \frac{1}{\rho_2} \nabla \cdot (\rho D \nabla Y_2) \quad (\text{A.12})$$

$$\Rightarrow \nabla \cdot \mathbf{u} = -\frac{\rho}{\rho_2} \left(\frac{\partial Y_2}{\partial t} + \mathbf{u} \cdot \nabla Y_2 \right) - \nabla \cdot \left(\frac{D}{\rho} \nabla \rho \right) + \frac{1}{\rho_2} \nabla \cdot (\rho D \nabla Y_2) \quad (\text{A.13})$$

Replacing the first term on R.H.S. of the above equation using Eq. A.3 we get,

$$\Rightarrow \nabla \cdot \mathbf{u} = -\frac{1}{\rho_2} \nabla \cdot (\rho D \nabla Y_2) - \nabla \cdot \left(\frac{D}{\rho} \nabla \rho \right) + \frac{1}{\rho_2} \nabla \cdot (\rho D \nabla Y_2) \quad (\text{A.14})$$

$$\Rightarrow \nabla \cdot \mathbf{u} = -\nabla \cdot \left(\frac{D}{\rho} \nabla \rho \right) \quad (\text{A.15})$$

which is the final expression for divergence of the velocity field for quasi-incompressible flows.

A.2 Basic Expression For Diffusive Flux for Momentum Equation

The generalized form of Navier-Stokes equation is given as-

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \vec{\tau} + \mathbf{f} \quad (\text{A.16})$$

where $\vec{\tau}$ is the stress tensor, $\mathbf{f}$ is the body force per unit volume. The expression for $\vec{\tau}$ in vector form is given as

$$\vec{\tau} = \mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T] - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \quad (\text{A.17})$$

where $\mathbf{I}$ is the unit vector. Integrating the diffusive term (the 2nd term on R.H.S. Eq. A.16) over the entire control volume and then using Gauss-divergence theorem, we get

$$\int_v \nabla \cdot \vec{\tau} dv = \int_S \vec{\tau} \cdot d\mathbf{S} \quad (\text{A.18})$$

$$= \int_S \left(\mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T] - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) \cdot d\mathbf{S} \quad (\text{A.19})$$

$$\begin{aligned} &\approx \sum_f \mu \underbrace{\begin{bmatrix} 2\frac{\partial u}{\partial x} & \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) & \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) \\ \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right) & 2\frac{\partial v}{\partial y} & \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) \\ \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}\right) & \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}\right) & 2\frac{\partial w}{\partial z} \end{bmatrix}}_A \begin{bmatrix} S_{fx} \\ S_{fy} \\ S_{fz} \end{bmatrix} \\ &\quad - \underbrace{\sum_f \frac{2}{3} \mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_B \begin{bmatrix} S_{fx} \\ S_{fy} \\ S_{fz} \end{bmatrix} \end{aligned} \quad (\text{A.20})$$

The x - component of Eq. A.20 can be written as

$$\begin{aligned} &= \sum_f \mu \left[2\frac{\partial u}{\partial x} S_{fx} + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) S_{fy} + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) S_{fz} \right] \\ &\quad - \frac{2}{3} \sum_f \mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) S_{fx} \end{aligned} \quad (\text{A.21})$$

$$\begin{aligned}
&= \sum_f \mu \left[\left(\frac{\partial u}{\partial x} S_{fx} + \frac{\partial u}{\partial y} S_{fy} + \frac{\partial u}{\partial z} S_{fz} \right) + \left(\frac{\partial u}{\partial x} S_{fx} + \frac{\partial v}{\partial x} S_{fy} + \frac{\partial w}{\partial x} S_{fz} \right) \right] \\
&\quad - \frac{2}{3} \sum_f \mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) S_{fx} \quad (\text{A.22})
\end{aligned}$$

$$\begin{aligned}
&= \sum_f \mu_f (\nabla u \cdot \mathbf{S}_f) + \sum_f \mu_f \left(\frac{\partial u}{\partial x} S_{fx} + \frac{\partial v}{\partial x} S_{fy} + \frac{\partial w}{\partial x} S_{fz} \right) \\
&\quad - \frac{2}{3} \sum_f \mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) S_{fx} \quad (\text{A.23})
\end{aligned}$$

Similarly, the y, z - components of Eq. A.20 can be written as

$$\begin{aligned}
&= \sum_f \mu_f (\nabla v \cdot \mathbf{S}_f) + \sum_f \mu_f \left(\frac{\partial u}{\partial y} S_{fx} + \frac{\partial v}{\partial y} S_{fy} + \frac{\partial w}{\partial y} S_{fz} \right) \\
&\quad - \frac{2}{3} \sum_f \mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) S_{fy} \quad (\text{A.24})
\end{aligned}$$

$$\begin{aligned}
&= \sum_f \mu_f (\nabla w \cdot \mathbf{S}_f) + \sum_f \mu_f \left(\frac{\partial u}{\partial z} S_{fx} + \frac{\partial v}{\partial z} S_{fy} + \frac{\partial w}{\partial z} S_{fz} \right) \\
&\quad - \frac{2}{3} \sum_f \mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) S_{fz} \quad (\text{A.25})
\end{aligned}$$

Appendix B

Derivations of Reacting Flow Equations

B.1 Divergence Constraint of Velocity Field for Reacting Flows

Equation of state for mixture of gases:

$$\bar{P} = \rho R_u T \sum \frac{Y_k}{W_k} \quad (\text{B.1})$$

Taking the substantial derivative of Eq. B.1

$$\Rightarrow \frac{D\bar{P}}{Dt} = R_u \frac{D}{Dt} \left(\rho T \sum \frac{Y_k}{W_k} \right) \quad (\text{B.2})$$

Applying chain rule we get:

$$\Rightarrow \frac{1}{R_u} \frac{D\bar{P}}{Dt} = \sum \frac{Y_k}{W_k} \frac{D(\rho T)}{Dt} + (\rho T) \frac{D}{Dt} \left(\sum \frac{Y_k}{W_k} \right) \quad (\text{B.3})$$

$$\Rightarrow \frac{1}{R_u} \frac{D\bar{P}}{Dt} = \sum \frac{Y_k}{W_k} \left[\rho \frac{DT}{Dt} + T \frac{D\rho}{Dt} \right] + (\rho T) \frac{D}{Dt} \left(\sum \frac{Y_k}{W_k} \right) \quad (\text{B.4})$$

By writing $\sum \frac{Y_k}{W_k} = \frac{1}{\bar{W}}$, we get:

$$\Rightarrow \frac{1}{R_u} \frac{D\bar{P}}{Dt} = \rho \sum \frac{Y_k}{W_k} \frac{DT}{Dt} + T \sum \frac{Y_k}{W_k} \frac{D\rho}{Dt} + \rho T \frac{D}{Dt} \left(\frac{1}{\bar{W}} \right) \quad (\text{B.5})$$

From continuity equation, we know that $\frac{D\rho}{Dt} = -\rho\nabla \cdot \mathbf{u}$, therefore:

$$\Rightarrow \frac{1}{R_u} \frac{D\bar{P}}{Dt} = \rho \sum \frac{Y_k}{W_k} \frac{DT}{Dt} + T \sum \frac{Y_k}{W_k} (-\rho\nabla \cdot \mathbf{u}) + \rho T \frac{D}{Dt} \left(\frac{1}{\bar{W}} \right) \quad (\text{B.6})$$

$$\Rightarrow T \sum \frac{Y_k}{W_k} \rho\nabla \cdot \mathbf{u} = \rho \sum \frac{Y_k}{W_k} \frac{DT}{Dt} + \rho T \frac{D}{Dt} \left(\frac{1}{\bar{W}} \right) - \frac{1}{R_u} \frac{D\bar{P}}{Dt} \quad (\text{B.7})$$

$$\Rightarrow \nabla \cdot \mathbf{u} = \frac{1}{T} \frac{DT}{Dt} + \rho T \frac{1}{\rho T \sum \frac{Y_k}{W_k}} \frac{D}{Dt} \left(\frac{1}{\bar{W}} \right) - \frac{1}{\rho T \sum \frac{Y_k}{W_k}} \frac{1}{R_u} \frac{D\bar{P}}{Dt} \quad (\text{B.8})$$

$$\Rightarrow \nabla \cdot \mathbf{u} = \frac{1}{T} \frac{DT}{Dt} + \bar{W} \frac{D}{Dt} \left(\frac{1}{\bar{W}} \right) - \frac{\bar{W}}{\rho T R_u} \frac{D\bar{P}}{Dt} \quad (\text{B.9})$$

Also from species conservation equation it can be written as

$$\rho \frac{D}{Dt} \left(\frac{1}{\bar{W}} \right) = \sum_k \nabla \cdot \left[\rho D_k \nabla \left(\frac{Y_k}{M W_k} \right) \right] \quad (\text{B.10})$$

The energy equation for reacting flows can be written as,

$$\Rightarrow \rho c_{p,mix} \frac{DT}{Dt} = \nabla \cdot (\kappa \nabla T) + \sum_k \rho D_k \nabla Y_k \cdot \nabla h_k - \sum_k h_k \omega_k^o + \frac{D\bar{P}}{Dt} \quad (\text{B.11})$$

where ω_k is the reaction source term. Replacing 1st and 2nd term of RHS of Eq. B.9 by Eqs. B.11 and B.10, respectively, we get:

$$\begin{aligned} \Rightarrow \nabla \cdot \mathbf{u} &= \frac{1}{T \rho c_{p,mix}} \left[\nabla \cdot (\kappa \nabla T) + \sum_k \rho D_k \nabla Y_k \cdot \nabla h_k - \sum_k h_k \omega_k^o \right] \\ &+ \frac{\bar{W}}{\rho} \left[\sum_k \nabla \cdot \left\{ \rho D_k \nabla \left(\frac{Y_k}{W_k} \right) \right\} + \sum_k \frac{\omega_k^o}{W_k} \right] - \frac{\bar{W}}{P \bar{W}} \frac{D\bar{P}}{Dt} + \frac{1}{\rho T c_{p,mix}} \frac{D\bar{P}}{Dt} \end{aligned} \quad (\text{B.12})$$

$$\begin{aligned} \Rightarrow \nabla \cdot \mathbf{u} &= \frac{1}{\rho c_{p,mix} T} \left[\nabla \cdot (\kappa \nabla T) + \sum_k \rho D_k \nabla Y_k \cdot \nabla h_k \right] + \frac{\bar{W}}{\rho} \left[\sum_k \nabla \cdot \left\{ \rho D_k \nabla \left(\frac{Y_k}{W_k} \right) \right\} \right] \\ &+ \frac{\bar{W}}{\rho} \sum_k \frac{\omega_k^o}{W_k} - \frac{1}{\rho T c_{p,mix}} \sum_k h_k \omega_k^o + \left(\frac{1}{\rho T c_{p,mix}} - \frac{1}{\bar{P}} \right) \frac{D\bar{P}}{Dt} \end{aligned} \quad (\text{B.13})$$

$$\begin{aligned} \Rightarrow \nabla \cdot \mathbf{u} &= \frac{1}{\rho c_{p,mix} T} \left[\nabla \cdot (\kappa \nabla T) + \sum_k \rho D_k \nabla Y_k \cdot \nabla h_k \right] + \frac{1}{\rho} \sum_k \frac{\bar{W}}{W_k} \nabla \cdot (\rho D_k \nabla Y_k) \\ &+ \frac{1}{\rho} \sum_k \left(\frac{\bar{W}}{W_k} - \frac{h_k}{T c_{p,mix}} \right) \omega_k^o + \left(\frac{1}{\rho T c_{p,mix}} - \frac{1}{\bar{P}} \right) \frac{D\bar{P}}{Dt} \end{aligned} \quad (\text{B.14})$$

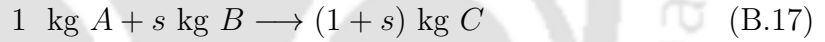
$$\begin{aligned} \nabla \cdot \mathbf{u} = \frac{1}{\rho c_{p,mix} T} & \left[\nabla \cdot (\kappa \nabla T) + \sum_k \rho D_k \nabla Y_k \cdot \nabla h_k \right] + \frac{1}{\rho} \sum_k \frac{\bar{W}}{MW_k} \nabla \cdot (\rho D_k \nabla Y_k) \\ & + \frac{1}{\rho} \sum_k \left(\frac{\bar{W}}{W_k} - \frac{h_k}{T c_{p,mix}} \right) \dot{\omega}_k + \left(\frac{R_u - c_{p,mix}}{\bar{P} c_{p,mix}} \right) \frac{D\bar{P}}{Dt} \end{aligned} \quad (B.15)$$

Eq. B.15 represents the generalized equation for reacting flows. However, for open system $\frac{D\bar{P}}{Dt} = 0$ and for flame sheet concent $\dot{\omega}_k = 0$. Also assuming $c_{p,k} = c_p = \text{constant}$, the second term of RHS of Eq. B.15 becomes zero. As such with these assumptions, the simplified form of the the divergence constraint for reactiong gaseous mixture can be written as,

$$\nabla \cdot \mathbf{u} = \frac{1}{\rho c_{p,mix} T} \nabla \cdot (\kappa \nabla T) + \frac{\bar{W}}{\rho} \nabla \cdot \left[\rho D_k \nabla \left(\sum_k \frac{Y_k}{W_k} \right) \right] \quad (B.16)$$

B.2 Conserved Scalar Equation

Let us consider the single step reaction as



For this single step reaction, we can write the convective, diuiffusive equations for mass fractions of reactants A and B as

$$\frac{\partial(\rho Y_A)}{\partial t} + \nabla \cdot (\rho Y_A \vec{u}) = \nabla \cdot (\rho D_A \nabla Y_A) + R_A \quad (B.18)$$

$$\frac{\partial(\rho Y_B)}{\partial t} + \nabla \cdot (\rho Y_B \vec{u}) = \nabla \cdot (\rho D_B \nabla Y_B) + R_B \quad (B.19)$$

where Y_A and Y_B are not conserved only due to the reaction terms R_A and R_B respectively. Convection and diffusion processes are conservative as they only carry the scalar from one place to another or otherwise spread it.

For the equation (Eq. B.17), every kg of A requires s kg of B . Therefore it is possible to write the reaction rates as

$$R_B = s R_A \quad (B.20)$$

Assuming $D_A = D_B = D_g$, and subtracting $\frac{1}{s}$.Eq. B.19 from Eq. B.18 we get

$$\frac{\partial \rho \left(Y_A - \frac{Y_B}{s} \right)}{\partial t} + \nabla \cdot \left[\rho \left(Y_A - \frac{Y_B}{s} \right) \vec{u} \right] = \nabla \cdot \left[\rho D_g \nabla \left(Y_A - \frac{Y_B}{s} \right) \right] \quad (\text{B.21})$$

Let us define a new scalar $g = Y_A - \frac{Y_B}{s}$

$$\Rightarrow \frac{\partial(\rho g)}{\partial t} + \nabla \cdot (\rho g \vec{u}) = \nabla \cdot (\rho D_g \nabla g) \quad (\text{B.22})$$

The absence of R_A and R_B in the above equation suggests that the scalar s is a conserved quantity with respect to combustion, i.e., its distribution is not affected by combustion, but only by convection and diffusion. The non-dimensional scalar variable, $Z = \frac{g - g_o}{g_f - g_o}$ can now be defined, whose governing equation takes the form as

$$\Rightarrow \frac{\partial(\rho Z)}{\partial t} + \nabla \cdot (\rho Z \vec{u}) = \nabla \cdot (\rho D_Z \nabla Z) \quad (\text{B.23})$$

List of Publications

International Journals:

1. **Borgohain P.**, Dalal A., Natarajan G. and Gadgil H. P. (2018) 'Numerical assessment of mixing performances in cross-T microchannel with curved ribs', *Microsystem Technologies*, vol 24, pp. 1949-1963 (DOI: 10.1007/s00542-017-3591-6).
2. **Borgohain P.**, Choudhary D., Dalal A. and Natarajan G. (2018) 'Numerical investigation of mixing enhancement for multi-species flows in wavy channels', *Chemical Engineering and Processing-Process Intensification*, vol. 127, pp. 191-205 (DOI: 10.1016/j.cep.2018.03.026).
3. **Borgohain P.**, Arumughan J., Dalal A. and Natarajan G. Design and performance of a three-dimensional micromixer with curved ribs, (submitted to *Chemical Engineering Research and Design* after first revision).

International Conferences:

1. Manik J., Parmanand M., Kotoky S., **Borgohain P.**, Dalal A. and Natarajan G. (2017) 'Lessons from AnuPravaha: Towards a general purpose computational framework on hybrid unstructured meshes for multi-physics applications', Paper No. CHT-17-209, ICHMT International Symposium on Advances in Computational Heat Transfer, May 28-June 1, 2017, Napoli, Italy.
2. **Borgohain P.**, Dalal A., Natarajan G. and Gadgil H. P. (2016) 'Numerical modelling of laminar diffusion flames over a hybrid unstructured grid', Sixth International Congress on Computational Mechanics and Simulation (ICCMS2016), IIT Bombay, Mumbai, India.
3. **Borgohain P.**, Dalal A., Natarajan G. and Gadgil H. P. (2015) 'Numerical simulation of laminar nonreacting variable density flows using low Mach number approach on unstructured grids', Paper No. F-FM-072, 68th Annual Session of Indian Institute of Chemical Engineers (CHEMCON 2015), 27-30 December, IIT Guwahati, India.



