The Fluid Dynamics of Mercury Target Delivery and Exhaust for A Muon Collider Particle Production System

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Abstract of the Dissertation

The Fluid Dynamics of Mercury Target Delivery and Exhaust for A Muon Collider Particle Production System

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Liquid mercury has been investigated as a potential high-Z target for the production of Muon particles for the Muon Collider project. This thesis investigates the dynamics of mercury flow in a design of the target delivery system, with the objective of determining pipe configurations that yield weak turbulence intensity at the exit of the pipe. Curved circular pipes with various half-bend angles, with/without nozzles in the exit region, and with/without welds on the pipe inner surface are studied. Theoretical analysis is carried out for steady laminar incompressible flow, whereby the terms representing curvature effects are examined. Subsequent simulations of the turbulent flow regime in the pipes are based on a realizable $k-\varepsilon$ Reynolds-averaged Navier-Stokes (RANS) equations approach. The simulations in this thesis have been based on the FLUENT commercial computational fluid dynamics (CFD) codes. The effects of turning angles, presence of a nozzle, and presence of a weld (on the inner surface of the pipes) on momentum thickness and turbulence intensity at the exit of the curved pipe are discussed, as are the implications for the target delivery pipe designs. It was found that the pressure loss from inlet to outlet is nearly the same for all pipes. Nozzle reduces the turbulence intensity of the flow while a weld increases it.

In order to locate the free surface of the mercury jet exhausting from the pipe into air, a coupled level set (LS) and volume of fluid (VOF) method (CLSVOF) has been applied. When we started this project, FLUENT did not support this approach. Therefore we developed, validated, and employed a coupled VOF and LS method that uses high-order weighted essentially non-oscillatory (WENO) schemes for the re-initialization equation in the LS method. Several successful validations of the developed CLSVOF code are presented in this dissertation. The flow conditions obtained at the pipe outlet have been used as the inlet conditions for the free-jet simulations. The dynamics of mercury jet flow are determined by the combined effects of turning angles and weld.

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List of Abbreviations

LS	Level Set
VOF	Volume of Fluid
MAC	Marker and Cell
CLSVOF	Coupled Level Set Volume of Fluid
RANS	Reynolds-averaged Navier-Stokes
RSM	Reynolds Stress Model
SA	Spalart-Allmaras
SKE	Standard $k - \varepsilon$
RKE	Realizable $k - \varepsilon$
SIMPLE	Semi Implicit Method for Pressure Linked Equations
CSF	Continuum Surface Force
UDS	User Defined Scaler
UDM	User Defined Memory
MUSCL	Monotone Upstream-centered Scheme for Conservation Laws
TVD	Total Variation Diminishing
WENO	Weighted Essentially Non-Oscillatory
RK	Runger-Kutta
RHS	Right Hand Side
CV	convex side
CC	concave side

LES	Large Eddy Simulation
ILES	Implicit Large Eddy Simulation
DNS	Direct Numerical Simulation
NSE	Navier Stokes Equation

List of Symbols

a	pipe radius (m)
R	curvature radius (m)
De	Dean number
Re	Reynolds number
δ	curvature ratio ($\delta \equiv a/R$)
u_τ	mean friction velocity (m/s)
Re_τ	Reynolds number based on u_τ
φ	half-bend angle of the target delivery pipe ($^\circ$)
r	radial direction (m)
θ	azimuthal angle direction ($^\circ$)
z	axial coordinate direction (m)
$\widetilde{z}$	flow direction tangential to the pipe center-line (m)
I	turbulence intensity (%)
k	turbulence kinetic energy (m^2/s^2)
k^*	non-dimensional k
$\overline{k}$	mean turbulence kinetic energy (m^2/s^2)
ε	turbulence kinetic energy dissipation (m^2/s^3)
ε^*	non-dimensional ε
u	instantaneous velocity in the r direction (m/s)

v	instantaneous velocity in the θ direction (m/s)
w	instantaneous velocity in the z direction (m/s)
u^*	non-dimensional u
v^*	non-dimensional v
w^*	non-dimensional w
r^*	normalized r
θ^*	normalized θ
z^*	normalized z
ρ	mass density (kg/m^3)
U_b	bulk velocity (m/s)
∇^{*2}	non-dimensional Laplacian operator
∇^*_n	non-dimensional normal gradient
t	time (s)
p	instantaneous/reduced pressure $(N/m^2, Pa)$
p^*	non-dimensional instantaneous pressure
P^*	non-dimensional mean pressure
$(\hat{p})^*$	non-dimensional fluctuating pressure
$\mathbf{u}^*$	non-dimensional instantaneous velocity vector
$\mathbf{U}^*$	non-dimensional mean velocity vector
$(\hat{\mathbf{u}})^*$	non-dimensional fluctuating velocity vector
τ^*	non-dimensional shear stress tensor
μ^*	non-dimensional dynamic viscosity
μ^*_t	non-dimensional eddy viscosity
C_μ	eddy viscosity coefficient
S^*_{ij}	symmetric part of the deformation tensor
$\overline{\Omega}^*_{ij}$	antisymmetric part of the deformation tensor
A_0	RKE model constant, 4.04

A_s	RKE model constant
σ_k	turbulent Prandtl number for κ
σ_ε	turbulent Prandtl number for ε
G_t	production of turbulence kinetic energy (m^2/s^3)
l^*	non-dimensional turbulent characteristic length
D_h^*	non-dimensional hydraulic diameter
ϕ	level set function (m)
Φ	mean level set function (m)
$\acute{\phi}$	fluctuating level set function (m)
ϕ_0	initial value of ϕ
F_{st}	surface tension term (N/m)
D	rate of deformation tensor
ϵ	half of the interface thickness (m)
H_ϵ	smoothed Heaviside function
σ	surface tension coefficient (N/m)
δ_ϵ	smoothed delta function
$\mathbf{n}$	normal vector of the interface
κ	mean curvature of the interface $(1/m)$
D_T	turbulent diffusivity (m^2/s)
c_1	constant for turbulent diffusivity equation
$S(\phi)$	sign function
d	distance from the local point to the interface (m)
Δ	filter width
J	Jacobian of transformation
F	liquid volume fraction
$\Delta\mathbf{s}$	displacement vector
$\mathbf{A}$	face area vector (m^2)

V	cell volume (m^3)
$\mathbf{r}$	direction vector from cell center to face center
$\sum_\Delta$	points neighbouring of interface
C_{cfl}	CFL number
L_c	continuity equation for flow in a curved pipe
L_{M_1}	r momentum equation for flow in a curved pipe
L_{M_2}	θ momentum equation for flow in a curved pipe
L_{M_3}	z momentum equation for flow in a curved pipe
$\widetilde{L}_c$	continuity equation for flow in a straight pipe
$\widetilde{L}_{M_1}$	r momentum equation for flow in a straight pipe
$\widetilde{L}_{M_2}$	θ momentum equation for flow in a straight pipe
$\widetilde{L}_{M3}$	z momentum equation for flow in a straight pipe
D_c^*	curvature term of continuity equation
D_r^*	curvature term of r momentum equation
D_θ^*	curvature term of θ momentum equation
$D_{\widetilde{z}}^*$	curvature term of $\widetilde{z}$ momentum equation
s	pseudo location coordinate direction
φ	pseudo bend angle coordinate direction
y^+	non-dimensional wall distance
δ_θ	momentum thickness (m)
u'_{rms}	root-mean-squared fluctuating velocity
C_p	static pressure coefficient
We	Weber number
Oh	Ohnesorge numbe
ϱ	ellipticity

List of Superscripts

$*$	non-dimensional parameter
(1)	first time step of RK
(2)	second time step of RK
n	time step of n
$n+1$	time step of n+1

List of Subscripts

l	liquid phase
g	gas phase
i	i index
j	j index
k	k index
ξ	curvilinear coordinates ξ
η	curvilinear coordinates η
ζ	curvilinear coordinates ξ
CD	central differencing
SOU	second-order up-winding
f	value on the face
0	cell 0
1	cell 1
c	continuity equation
M_1	r momentum equation
M_2	θ momentum equation
M_3	z momentum equation

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Chapter 1

Introduction

In this chapter, we present the background of the study, motivations, review of flow in curved pipes, and objectives of the thesis work.

1.1 Mercury Target Issues in the Muon Collider Project

The MERIT experiment at CERN [1, 2] is a proof-of-principle test for a target system that converts a 4-MW proton beam into a high-intensity muon beam for either a neutrino factory complex or a Muon Collider (Fig. 1.1). The mercury jet issues from the nozzle at the end of a delivery pipe to form a target that intercepts an intense proton beam inside a 15-T solenoid magnet. The use of liquid targets overcomes problematic effects of solid targets, such as melting/vaporization of components, damage by beam-induced pressure waves for pulsed beams, and extensive radiation damage. Also, liquid target systems offer the advantage of continuous regeneration of the target volume. However, the design of the mercury delivery pipe introduces new challenges.

The MERIT experiment uses a 180° bend, which has half-bend angles of 90° in the shape of a "U", for the delivery of the mercury. This geometry complicates the flow relative to that in a straight pipe, and affects the quality of the jet. Since the quality of the jet greatly influences the production of muon particles, it is pertinent to investigate the dynamics of

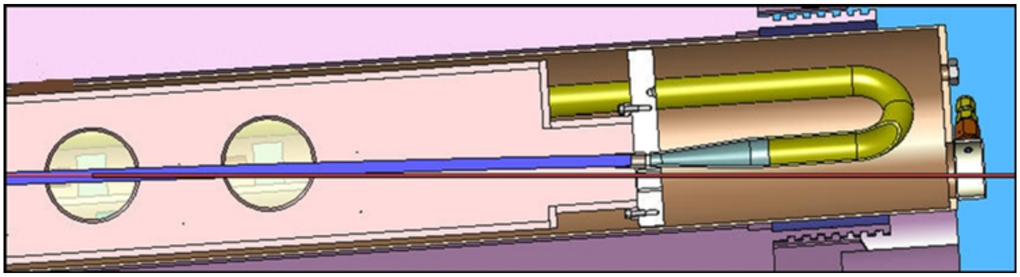

Figure 1.1: Sectional view of the target supple pipe of the MERIT experiment. The mercury jet generated at the end of the nozzle is on top of the nominal beam trajectory. Both mercury jet and proton beam move from right to left

the flow of mercury in the 180° bend, with a focus on exit-flow properties. Furthermore, for optimum muon particles production, the mercury jet flow should be near laminar.

1.2 Motivations of the Study

In the MERIT experiment, the coupling between pipe geometry, magnetic field, energy deposition results in very complex flow conditions. In this thesis, investigation of mercury internal flow and jet flow is carried out without magnetic field or high energy deposition. This clarifies the pure geometry effects of delivery pipe on dynamics of mercury flow and it is the baseline to understand the effects of magnetic field as well as the high energy deposition.

Due to the difficulties of experimental investigation to optimize the target delivery pipe, computational fluid dynamics (CFD) is a valuable tool and provides access to various hydrodynamical characteristics in the entire geometry. The commercial code, ANSYS FLUENT, is a general purpose CFD code, which is very stable in simulating incompressible low speed flow. Also FLUENT has a VOF method for modeling of two phase flows. A CLSVOF method developed in this thesis couples LS method and VOF method via UDFs in FLUENT to achieve a better free interface capturing capability. This thesis investigates mercury flow in curved pipes and mercury jet flow taking advantage of UDFs in the FLUENT code.

1.3 Review of Flow in Curved Pipes

Eustice [3, 4] is among the first to demonstrate the existence of a secondary flow in a curved pipe, an observation he made from injecting ink into water flowing through a pipe. Dean [5, 6] introduced a parameter which bears his name (Dean number, $De \equiv Re\delta^{1/2}$, where Re is the Reynolds number based on the area-averaged mean velocity through a pipe of diameter of $2a$, and δ is curvature radio ($\delta \equiv a/R$, where R is radius of curvature and a is the pipe radius)) to characterize the magnitude and shape of the secondary motion inside a loosely coiled pipe ($\delta << 1$). Subsequent work by others have investigated curved pipes with different values of R. Adler [7] presents experimental results of laminar and turbulent flows in three pipes with different R values. Rowe [8] investigates turbulent water flows for a curvature ratio $\delta = 1/24$ in a circular 180° bend. Total pressure and yaw angle relative to the bend axis are measured for Reynolds number $Re = 236,000$. Enayat *et al.* [9] reports on the axial components of the mean and fluctuating velocities for the turbulent water flow in a circular 90° bend for a δ value of 1/5.6 and for a wide range of Reynolds numbers. Azzola *et al.* [10] compute and measure the developed turbulent flow in a 180° bend for $\delta = 1/6.75$ and Reynolds number values of 57,400 and 110,000. The standard $k - \varepsilon$ model is used. Answer *et al.* [11] measures the Reynolds stresses and mean velocity components in vertical and horizontal planes containing the pipe axis, for air flow in a 180° bend, with $\delta = 1/13$ and $Re = 50,000$. Sudo *et al.* [12] reports on the measurements of turbulent flow through a circular 90° bend for $\delta = 1/4$. Sudo and his co-workers [13] also measure turbulent air flow in a 180° circular bend for the same δ value, but with $Re = 60,000$. The axial, radial, and circumferential components of the mean velocity and the corresponding components of the Reynolds stress tensor are reported. Hüttl *et al.* [14] investigate the influence of curvature and torsion on turbulent flow in helically-coiled pipes for a Reynolds number $Re_\tau = 230$, where Re_τ is based on the mean friction velocity, u_τ. The pipe curvature was found to induce a secondary flow, which has a strong effect on the dynamics. Rudolf *et al.* [15] study the flow characteristics in several curved ducts: single elbow to coupled elbows in shapes of "U,"

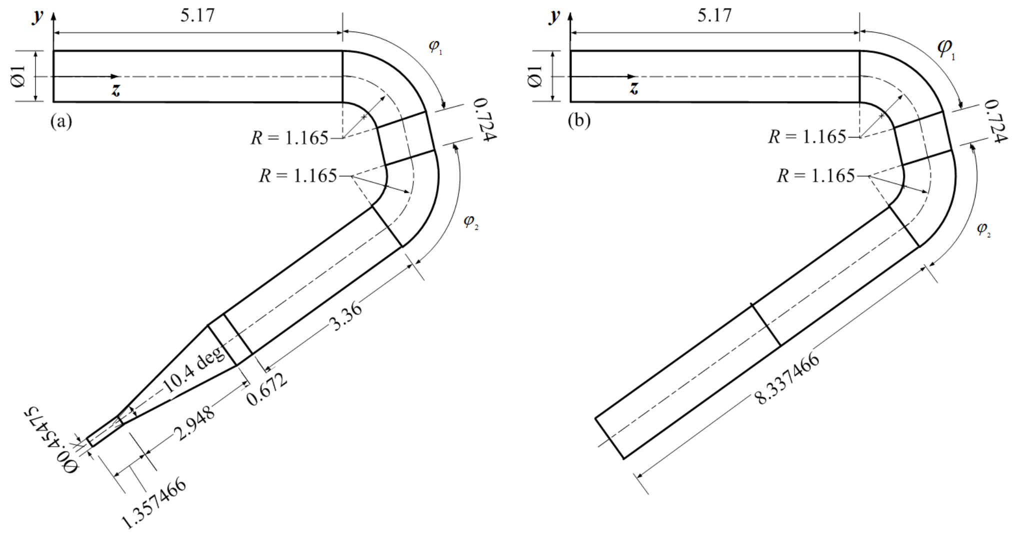

Figure 1.2: Coordinates along a curved pipe

"S," and noncoplanar right angle, for a fixed value of $\delta = 1/4$ and $Re = 60,000$.

The uniqueness of the present study can be found in the effects of the half-bend angle, φ (as shown in Figure 1.2), and that of the presence of a nozzle in the exit region of eight pipe configurations on the momentum thickness and turbulence intensity at the pipe exit. The curvature ratios match those of the pipes that are tested in the MERIT experiment. The pipe geometries investigated are shown in Figure 1.3.

1.4 Review of Turbulent Flows through Pipes with Rough Inner Surfaces

Turbulent flows in pipes has always been a major source of inspiring practical problems in the study of fluid dynamics. Among the numerous investigations in the field, noticeable efforts have been devoted to the cases in which the pipe had inner-surface roughness, e.g., grooves, fins, and other constrictions. These types of problems attracted special attentions for their wide applications in the fields of heat transfer [17, 18, 19], cardiac-vascular blood flow studies [20, 21, 22], and the design of unsteady flow meters [23, 24].

Two categories of roughness on the inner surfaces of pipes are usually considered in the

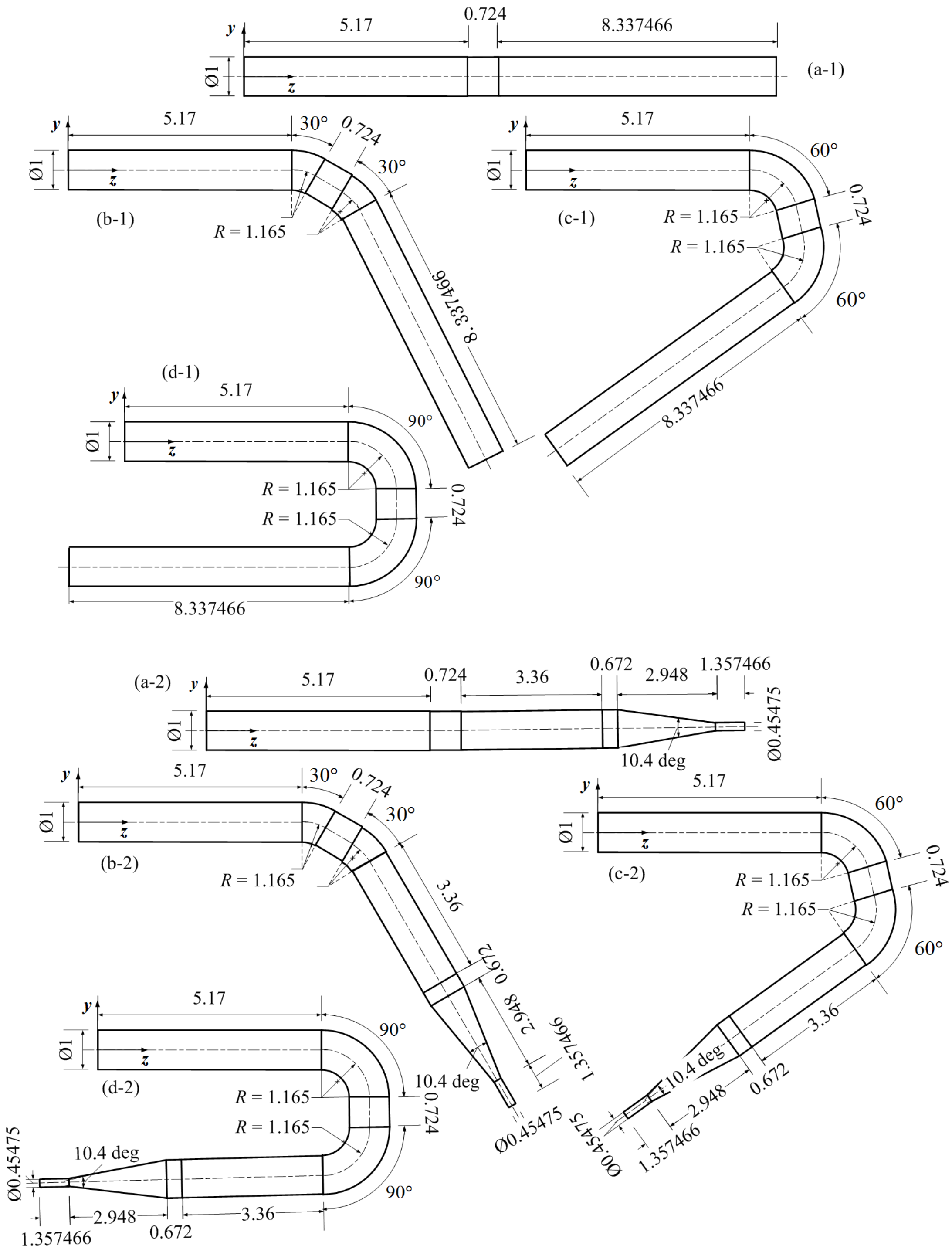

Figure 1.3: Configurations of pipes investigated: without nozzles for φ_1/φ_2 of (a-1) 0°/0° (b-1) 30°/30° (c-1) 60°/60° (d-1) 90°/90°; with nozzles for φ_1/φ_2 of (a-2) 0°/0° (b-2) 30°/30° (c-3) 60°/60° (d-2) 90°/90°

literature. The first category includes corrugations and grooves, in which case the main research interests lie in the interactions between vorticity occupying cavities and core flows along the axial direction of pipes [25, 26, 28, 29]. The other category is related to various types of constrictions, such as valves in blood vessels [30, 31], welded pipe-flange joints [32, 33], and turbulators in heat exchangers [16, 19]. For both categories, several physical quantities are used to describe the properties of the flows, including pressure gradient, pressure loss, vorticity, maximum velocity, shear stress, turbulence kinetic energy, and turbulence viscosity. In the following sections, we will review the effects of the two types of inner-surface roughness on turbulent pipe flows in detail.

1.4.1 Turbulent Flows through Pipes with Corrugations

Corrugations are discrete grooves placed at periodic intervals along the inner surfaces of pipes. A lot of efforts have been devoted to the investigation of the interactions between recirculating fluid inside the grooves and the main flows in the pipe. Previous works tried to find out the isolating conditions of the main flow from the recirculating flow, the circumstances of a momentum transfer phenomenon, and the extent to which Reynolds stress is affected in the vicinity of cavities.

One of the earliest contributions to the study of the effects of corrugations on turbulent flows through pipes was carried out by Perry and collaborators [25]. In their work, the "d-type" and "k-type" corrugations were introduced, based on their different effects on the interactions between flows in grooves and main flows along the axial direction of pipes. Cavities with a length-to-height ratio less than 4 are referred to as "d-type" corrugations, which are able to largely isolate the recirculating flows in the grooves from the main flow. In this case, the equivalent surface roughness length scale depends only on the boundary layer thickness. On the other hand, the "k-type" corrugations are those with larger than 4 length-to-height ratios, which allow prominent momentum transfers between cavity flows and the main flow.

Later experimental studies by Djenidi *et al.* [26, 27] illustrate that the isolation of the recirculating fluid in cavities from outer flows is not a general property of all the d-type corrugations. They find out significant increases in turbulent intensities in the vicinities of downstream corners of the cavities. The existence of interactions between main and groove flows in pipes with "d-type" corrugations is furthered supported by the numerical study of Chang and his collaborators [34]. It is shown that both normal and shear stresses increased noticeably at the opening of cavities. They also observe that the most significant enhancement occurred near the downstream corners of the cavities, which is consistent with the aforementioned results from Djenidi *et al.* [27].

Sutardi *et al.* [35] perform experiments on the turbulent flows through pipes with three different types of transverse grooves and two different Reynolds numbers. For all the six tests, the friction factors measured are all larger than those of smooth inner-surface pipe flows. Moreover, they show that the square groove results in a 50% higher drag force than the semi-circular and triangular grooves. They explain by comparing structures of vorticities in the three types of grooves, and find that only the square cavity could sustain the existence of two smaller eddies above the main vortex, which is capable to result in more fluid ejections and momentum transfers from the groove into the core flow.

Increased friction factors in pipes with corrugations compared with those with smooth inner-surfaces is reported by Eiamsa-ard *et al.* [28] through simulations. Turbulent forced convection through channels with "k-type", "d-type", and intermediate cavities are simulated. Their main conclusion is consistent with that by Sutardi's group [35]: grooved channels provides considerable increase in the friction factor over smooth channels. This kind of increase in drag force is also reported by Luo *et al.* [36] in their simulations for a horizontal parallel-plate channel with periodic transverse ribs. Recirculating flow patterns are formed in the cavity between two adjacent ribs, and their interaction with the core flow is inferred to be the cause of the increasing of the friction factor. The interaction between vortex flows in grooves and the main flow in the axial direction is further corroborated by Yang[37], Vijiapurapu and Cui [38], and experiments by Promvonge and Thianpong [39] and Dong *et al.* [40].

1.4.2 Turbulent Flows in Pipes with Constrictions

Turbulent flows through constrictions have attracted much attention recently for their increasing relevance in many engineering applications. Both experimental studies and numerical simulations have revealed the ability of constrictions to cause significant resistance to flow and pressure loss [41, 42, 43]. Independent studies [44, 45] showed that vortical structures occurred in the vicinity of the constrictions when the main flow is in the deceleration phase. Besides, several authors reported that the increases in shear stress and loss of pressure resulting from the existence of restrictions are larger in the deceleration phase than in the acceleration phase [46, 47, 48]. Here we don't make detail descriptions for these applications in the physiological sciences and bioengineering, since they are not our interest.

In this dissertation, a case for the study of a constriction/weld is analyzed in the field of mechanical engineering, which has not been stated by other people as we know.

1.5 Review of Multiphase Models

There are generally two approaches for modelling two-phase flow: one-fluid model and two-fluid model. The main difference between these two models is the number of conservation equations solved. The one-fluid model solves a single set of conservation equations and is more widely used than the two-fluid model for two-phase flow. In the one-fluid model, the interfacial motion can be computed using Lagrangian tracking methods or Eulerian capturing methods. Lagrangian tracking techniques [49] are very accurate and efficient for flexible moving boundaries with small deformations, such as MAC (marker and cell) methods [50], arbitrary Lagrangian-Eulerian methods, [51, 53, 54] or front tracking methods. [55, 56] However, it is difficult to use in the cases where the interface breaks up or coalesces with another interface. Also, additional remeshing is needed when a large deformation of the interface occurs. Eulerian capturing methods use an auxiliary function for the motion of the interface and have a wide range of applicability. The LS and VOF methods are two examples of one-fluid model using the Eulerian capturing methods. They are very robust but require a higher mesh resolution. In this work, both of these two methods are used.

The LS method [57, 58, 59, 60] uses a zero contour of a continuous signed distance function, known as the level set function, to represent the interface. The distance function is positive on one side and negative on the other side of the interface. The motion of interface is governed by the level set transport equation and a re-initialization equation is applied to keep the level set function as a signed distance function. The LS method has better accuracy in computing curvature and normal to the interface, however, it is not conservative, leading to a significant, physically incorrect loss/gain of mass for incompressible two-phase flow.

The VOF method [61, 62, 63, 71] describes the interface with a volume of fluid function, F, which is defined as the volume fraction of one of the fluids in each cell. F is zero or unity in pure fluid cells and has a value of $0 < F < 1$ in multi-fluid cells. The interface is explicitly described in each multi-fluid cell based on F. The distribution of F is solved through an advection equation using the reconstructed interface and the underlying velocity field. In an incompressible continuity equation, the conservation of mass equals to the conservation of volume. Therefore, the volume-of-fluid advection to advance an interface conserves the volume. The conservation of volume of each fluid is an important property of the VOF method. However, VOF method lacks an accurate method for calculation of surface tension in the problems with high density ratios. Moreover, a higher-order of accuracy is hard to achieve for VOF method because of the discontinuity in the volume fraction.

In order to obtain better performance in capturing an interface, a combination of LS and VOF, abbreviated as CLSVOF, has been used by many researchers [72, 73, 74, 75, 76, 77, 78]. The CLSVOF method retains the advantages of each method: LS, to compute curvature and normal to the interface, and VOF, to capture the interface. Normally, the CLSVOF method is superior to both the standalone LS and VOF methods. [72, 79, 80]

1.6 Objectives of the Research

The objectives of this study are as follows: (i) Theoretical studies of the secondary flow in a curved pipe; (ii) Numerical simulation of turbulent mercury flow in a curved pipe with/without a weld, with the purposes of studying the effects of pipe geometry and weld on the turbulence intensity of flow at the pipe exit; (iii) Numerical simulation of mercury jet flow using the exit conditions of pipe flow as the inlet conditions.

Rather than proposing a new numerical code, this study works with the user-defined functions (UDFs) in commercial code FLUENT to carry out the various simulations in this study.

In this dissertation, we describe mathematical models, numerical algorithms, numerical verification and validation, numerical simulations for the internal flow and jet flow. In chapter 2, the governing equations for internal laminar and turbulent flow, LS method, VOF method, the coupling between LS and VOF, and the continuum surface model will be introduced. In chapter 3, the numerical procedure of solving the governing equations will be described. In Chapter 4, numerical verification and validations to understand the secondary flow, to choose the realizable $k-\varepsilon$ model, and to test the developed CLSVOF method will be given. The results of internal mercury flow and mercury jet flow will be shown in chapter 5. The dissertation will conclude with future work in chapter 6.

Chapter 2

Governing Equations and Boundary Conditions

2.1 Governing Equations for Laminar Flow in Curved Pipes

To better understand the global resulting flow in the target delivery pipe, a first preliminary study is restricted to the modeling of laminar flow through standard bends, without magnetic field or energy deposition.

The motion of a fluid particle in a pipe segment, assuming isothermal conditions, is governed by the conservation of mass and momentum in the flow. The cylindrical polar coordinate system (r, θ, z) is used for the baseline straight pipe of circular cross-section, where r is the radial distance, θ is the azimuthal angle, and z is the axial coordinate direction. The vector (u,v,w), in dimensional form, denotes the components of the instantaneous velocity in the r, θ, and z coordinate directions, respectively. Steady state and incompressible flow conditions are assumed. The non-dimensional continuity equation in the straight pipe can be written as

$$L_c(u^*, v^*, w^*) = 0, \tag{2.1}$$

where (u^*, v^*, w^*) are the non-dimensional components of the instantaneous velocity.

The non-dimensional momentum equations in the normalized r^*, θ^*, and z^* coordinate directions of the straight circular pipe can be written as

$$L_{M_i}(u^*, v^*, w^*) = 0, \tag{2.2}$$

where $i = 1$, 2, and 3 refer to the r^*, θ^*, and z^* components, respectively. Thus, [84]

$$L_c(u^*, v^*, w^*) \equiv \frac{\partial u^*}{\partial r^*} + \frac{u^*}{r^*} + \frac{1}{r^*}\frac{\partial v^*}{\partial \theta^*} + \frac{\partial w^*}{\partial z^*}, \tag{2.3}$$

$$\begin{aligned} L_{M_1}(u^*, v^*, w^*) \equiv \frac{\partial u^*}{\partial t^*} + u^*\frac{\partial u^*}{\partial r^*} + \frac{v^*}{r^*}\frac{\partial u^*}{\partial \theta^*} + w^*\frac{\partial u^*}{\partial z^*} - \frac{v^{*2}}{r^*} + \frac{\partial p^*}{\partial r^*} \\ -\frac{1}{Re}(\nabla^{*2}u^* - \frac{u^*}{r^{*2}} - \frac{2}{r^{*2}}\frac{\partial v^*}{\partial \theta^*}), \end{aligned} \tag{2.4}$$

$$\begin{aligned} L_{M_2}(u^*, v^*, w^*) \equiv \frac{\partial v^*}{\partial t^*} + u^*\frac{\partial v^*}{\partial r^*} + \frac{v^*}{r^*}\frac{\partial v^*}{\partial \theta^*} + w^*\frac{\partial v^*}{\partial z^*} + \frac{u^* v^*}{r^*} + \frac{1}{r^*}\frac{\partial p^*}{\partial \theta^*} \\ -\frac{1}{Re}(\nabla^{*2}v^* + \frac{2}{r^{*2}}\frac{\partial u^*}{\partial \theta^*} - \frac{v^*}{r^{*2}}), \end{aligned} \tag{2.5}$$

$$L_{M_3}(u^*, v^*, w^*) \equiv \frac{\partial w^*}{\partial t^*} + u^*\frac{\partial w^*}{\partial r^*} + \frac{v^*}{r^*}\frac{\partial w^*}{\partial \theta^*} + w^*\frac{\partial w^*}{\partial z^*} + \frac{\partial p^*}{\partial z^*} - \frac{1}{Re}\nabla^{*2}w^*. \tag{2.6}$$

The scales for dimensionalization are as follows:

$$\begin{aligned} u^* = u/U_b, v^* = v/U_b, w^* = w/U_b, r^* = r/a, z^* = z/a, \\ p^* = p/\rho U_b^2, Re \equiv \frac{2aU_b\rho}{\mu}, \end{aligned} \tag{2.7}$$

where p is the reduced pressure, ρ is the mass density of fluid, a is the radius of the circular pipe, and U_b is the bulk velocity:

$$U_b = \frac{\int u(r,\theta) r dr d\theta}{\int r dr d\theta}, \tag{2.8}$$

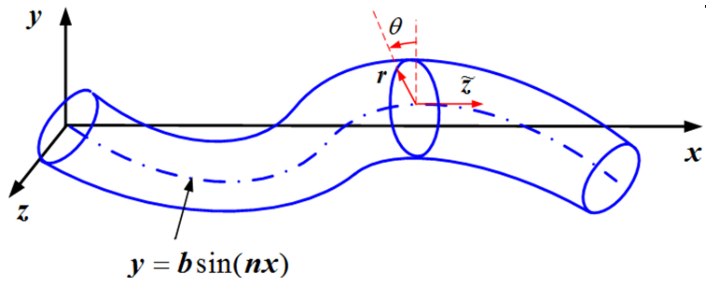

Figure 2.1: Curvilinear coordinates for the periodically-curved pipe $y = b\sin(nx)$

where $u(r, \theta)$ is the instantaneous axial velocity component.

The Laplacian operator, ∇^{*2}, is

$$\nabla^{*2} \equiv \frac{1}{r^*}\frac{\partial}{\partial r^*}(r^*\frac{\partial}{\partial r^*}) + \frac{1}{r^{*2}}\frac{\partial^2}{\partial \theta^{*2}} + \frac{\partial^2}{\partial z^{*2}}. \tag{2.9}$$

The motion of a fluid in a curved pipe whose center-line varies locally in a two-dimensional plane will be described in the curvilinear coordinates $(r, \theta, \tilde{z})$, as shown in Fig. 2.1.

The coordinates r and θ are the same as those defined for a straight pipe, while $\tilde{z}$ is a coordinate direction which is positive along the flow direction and is tangential to the pipe center-line. The coordinates $(r, \theta, \tilde{z})$ are a right-handed system and are always mutually orthogonal when the pipe center-line is a two-dimensional curve. [85] The vector (u,v,w) represents the instantaneous velocity components in the r, θ, and $\tilde{z}$ coordinate directions, respectively.

Murata [85] has analyzed the steady laminar motion of a fluid through pipes of circular cross-section, assuming small center-line curvatures. We will use his model as the starting point for identifying the sources of secondary flows and compare the velocity distributions associated with such sources to one obtained from a CFD analysis of the same physical problem. For this purpose, we consider a pipe profile of the form $y = b\sin(nx)$ (Figure 2.1), where $b = 0.1, \cdots, 1, 2, 3, \cdots$ and $n = 0.05, 0.1, \cdots, 1, \cdots$. We illustrate with the results for $b = 3.0$ and $n = 0.1$. The results will be examined at the arbitrary point at $x = 60$, where the flow is already fully-developed. The following relations are defined:

$$x = \tilde{z} - \frac{nbr\cos\theta}{L}\cos(nx), y = b\sin(nx) + \frac{r\cos\theta}{L}, z = r\sin\theta,$$
$$\Gamma^1_{33} = -L\kappa_c\sqrt{g_{33}}\cos\theta, \Gamma^2_{33} = \frac{L}{r}\kappa_c\sqrt{g_{33}}\sin\theta, \Gamma^3_{13} = \Gamma^3_{31} = \frac{L}{\sqrt{g_{33}}}\kappa_c\cos\theta,$$
$$\Gamma^3_{23} = \Gamma^3_{32} = -\frac{L}{\sqrt{g_{33}}}\kappa_c r\sin\theta, \Gamma^3_{33} = \frac{1}{\sqrt{g_{33}}}\frac{\partial}{\partial\tilde{z}}\sqrt{g_{33}}, \tag{2.10}$$

where

$$L = [1 + n^2b^2\cos^2(nx)]^{1/2}, \tag{2.11}$$
$$\sqrt{g_{33}} = L(1 + r\kappa_c\cos\theta), \tag{2.12}$$
$$\kappa_c = \frac{n^2b\sin(nx)}{L^3}. \tag{2.13}$$

Compared to Eqn. (2.3) through (2.6), the additional terms can be non-dimensionalized using the following scales:

$$g^*_{33} = g_{33},\ \Gamma^{1*}_{33} = a\Gamma^1_{33}, \Gamma^{2*}_{33} = \Gamma^2_{33}a^2,\ \Gamma^{3*}_{13} = a\Gamma^3_{13},\ \Gamma^{3*}_{31} = a\Gamma^3_{31},\ \Gamma^{3*}_{23} = \Gamma^3_{23},$$
$$\Gamma^{3*}_{32} = \Gamma^3_{32},\ \Gamma^{3*}_{33} = a\Gamma^3_{33}. \tag{2.14}$$

The non-dimensional continuity and momentum equations can then be written as follows:

Continuity

$$\widetilde{L}_c(u^*, v^*, w^*) = 0, \tag{2.15}$$

where

$$\widetilde{L}_c(u^*, v^*, w^*) = \frac{1}{r^*}\frac{\partial(r^*u^*)}{\partial r^*} + \frac{1}{r^*}\frac{\partial v^*}{\partial\theta} + \frac{1}{\sqrt{g_{33}}}\frac{\partial w^*}{\partial\tilde{z}^*} + \Gamma^{3*}_{31}u^* + \Gamma^{3*}_{32}\frac{v^*}{r^*}. \tag{2.16}$$

Momentum

$$\widetilde{L}_{M_i}(u^*, v^*, w^*) = 0, \tag{2.17}$$

where

$$\begin{aligned}
\widetilde{L}_{M_1}(u,v,w) &= u^*\frac{\partial u^*}{\partial r^*}+\frac{v^*}{r^*}\frac{\partial u^*}{\partial \theta^*}-\frac{v^{*2}}{r^*}+\frac{w^*}{\sqrt{g_{33}}}\frac{\partial u^*}{\partial \widetilde{z}^*}+\Gamma^{1*}_{33}\frac{w^{*2}}{g_{33}}+\frac{\partial p^*}{\partial r^*}\\
&\quad -\frac{1}{Re}[\frac{\partial^2 u^*}{\partial r^{*2}}+\frac{1}{r^*}\frac{\partial u^*}{\partial r^*}-\frac{u^*}{r^{*2}}+\frac{1}{r^{*2}}\frac{\partial^2 u^*}{\partial \theta^{*2}}+\frac{1}{g_{33}}\frac{\partial^2 u^*}{\partial \widetilde{z}^{*2}}\\
&\quad -\frac{2}{r^{*2}}\frac{\partial v^*}{\partial \theta^*}+\frac{\Gamma^{1^*}_{33}}{g_{33}}(\Gamma^{3*}_{13}u^*+\Gamma^{3*}_{23}\frac{v^*}{r^*}-\frac{\partial u^*}{\partial r^*})+\frac{\Gamma^{2*}_{33}}{g_{33}}(v^*-\frac{\partial u^*}{\partial \theta^*})\\
&\quad +\frac{\Gamma^{3*}_{33}}{g_{33}}\frac{\partial u^*}{\partial \widetilde{z}^*}+\frac{1}{g_{33}}\{\frac{w^*}{\sqrt{g_{33}}}\frac{\partial}{\partial \widetilde{z}^*}(\Gamma^{1*}_{33})+2\Gamma^{1*}_{33}\frac{\partial}{\partial \widetilde{z}^*}(\frac{w^*}{\sqrt{g_{33}}})\}],
\end{aligned} \tag{2.18}$$

$$\begin{aligned}
\widetilde{L}_{M_2}(u^*,v^*,w^*) &= u^*\frac{\partial v^*}{\partial r^*}+\frac{v^*}{r^*}\frac{\partial v^*}{\partial \theta^*}+\frac{u^*v^*}{r^*}+\frac{w^*}{\sqrt{g_{33}}}\frac{\partial v^*}{\partial \widetilde{z}^*}+\Gamma^{2*}_{33}\frac{r^*w^{*2}}{g_{33}}\\
&\quad +\frac{1}{r^*}\frac{\partial p^*}{\partial \theta^*}-\frac{1}{Re}[\frac{\partial^2 v^*}{\partial r^{*2}}+\frac{1}{r^*}\frac{\partial v^*}{\partial r^*}-\frac{v^*}{r^{*2}}+\frac{1}{r^{*2}}\frac{\partial^2 v^*}{\partial \theta^{*2}}\\
&\quad +\frac{1}{g_{33}}\frac{\partial^2 v^*}{\partial \widetilde{z}^{*2}}+\frac{2}{r^{*2}}\frac{\partial u^*}{\partial \theta^*}+\frac{\Gamma^{2*}_{33}}{g_{33}}(\Gamma^{3*}_{13}r^*u^*-u^*+\Gamma^{3*}_{23}v^*-\frac{\partial v^*}{\partial \theta^*})\\
&\quad -\frac{\Gamma^{1*}_{33}}{g_{33}}\frac{\partial v^*}{\partial r^*}-\frac{\Gamma^{3*}_{33}}{g_{33}}\frac{\partial v^*}{\partial \widetilde{z}^*}+\frac{r^*}{g_{33}}\{\frac{w^*}{\sqrt{g_{33}}}\frac{\partial}{\partial \widetilde{z}^*}(\Gamma^{2*}_{33})+2\Gamma^{2*}_{33}\frac{\partial}{\partial \widetilde{z}^*}(\frac{w^*}{\sqrt{g_{33}}})\}],
\end{aligned} \tag{2.19}$$

$$\begin{aligned}
\widetilde{L}_{M_3}(u^*,v^*,w^*) &= u^*\frac{\partial}{\partial r^*}(\frac{w^*}{\sqrt{g_{33}}})+\frac{v^*}{r^*}\frac{\partial}{\partial \theta^*}(\frac{w^*}{\sqrt{g_{33}}})+\frac{w^*}{g_{33}}\frac{\partial w^*}{\partial \widetilde{z}^*}\\
&\quad +\frac{2w^*}{\sqrt{g_{33}}}(\Gamma^{3*}_{31}u^*+\Gamma^{3*}_{32}\frac{v^*}{r^*})+\frac{1}{g_{33}}\frac{\partial p^*}{\partial \widetilde{z}^*}\\
&\quad -\frac{1}{Re}[\frac{\partial^2}{\partial r^{*2}}(\frac{w^*}{\sqrt{g_{33}}})+\frac{1}{r^*}\frac{\partial}{\partial r^*}(\frac{w^*}{\sqrt{g_{33}}})+\frac{1}{r^{*2}}\frac{\partial^2}{\partial \theta^2}(\frac{w^*}{\sqrt{g_{33}}})\\
&\quad +\frac{1}{g_{33}}\frac{\partial}{\partial \widetilde{z}^*}(\frac{1}{\sqrt{g_{33}}}\frac{\partial w^*}{\partial \widetilde{z}^*})+\frac{1}{g_{33}}\{u^*\frac{\partial}{\partial \widetilde{z}^*}(\Gamma^{3*}_{13})+\frac{v^*}{r^*}\frac{\partial}{\partial \widetilde{z}^*}(\Gamma^{3*}_{23})\}\\
&\quad +\frac{w^*}{\sqrt{g_{33}}}\{\frac{\partial}{\partial r^*}(\Gamma^{3*}_{13})+\frac{1}{r^{*2}}\frac{\partial}{\partial \theta}(\Gamma^{3*}_{23})\}\\
&\quad +\Gamma^{3*}_{13}\{\frac{2}{g_{33}}\frac{\partial u^*}{\partial \widetilde{z}^*}+2\frac{\partial}{\partial r^*}(\frac{w^*}{\sqrt{g_{33}}})+\frac{1}{r^*}\frac{w^*}{\sqrt{g_{33}}}\}\\
&\quad +\frac{2\Gamma^{3*}_{23}}{r^{*2}}\{\frac{r^*}{g_{33}}\frac{\partial v^*}{\partial \widetilde{z}^*}+\frac{\partial}{\partial \theta^*}(\frac{w^*}{\sqrt{g_{33}}})\}+\frac{w^*}{\sqrt{g_{33}}}\{(\Gamma^{3*}_{13})^2+(\frac{\Gamma^{3*}_{32}}{r^*})^2\}\\
&\quad -\frac{1}{g_{33}}\{\Gamma^{1*}_{33}\frac{\partial}{\partial r^*}(\frac{w^*}{\sqrt{g_{33}}})+\Gamma^{2*}_{33}\frac{\partial}{\partial \theta^*}(\frac{w^*}{\sqrt{g_{33}}})\}].
\end{aligned} \tag{2.20}$$

2.2 Governing Equations for Turbulent Flow

2.2.1 Continuity and Momentum Equations

As stated earlier, the mean flow ($\mathbf{U}^*, P^*$) is calculated with RANS, where the mean flow is related to the instantaneous ($\mathbf{u}^*, p^*$) and fluctuating ($(\mathbf{u}')^*, (p')^*$) components as follows:

$$\mathbf{u}^* = \mathbf{U}^* + (\mathbf{u}')^* \tag{2.21}$$

$$p^* = P^* + (p')^* \tag{2.22}$$

The governing equations for the mean flow can be expressed in terms of mass conservation (continuity),

$$\frac{\partial \mathbf{U}^*}{\partial t} + \nabla^* \cdot \mathbf{U}^* = 0, \tag{2.23}$$

and the momentum conservation,

$$\frac{\partial \mathbf{U}^*}{\partial t} + \mathbf{U}^* \cdot \nabla^* \mathbf{U}^* = -\frac{1}{\rho^*} \nabla^* P^* + \frac{1}{Re} \nabla^* \cdot \tau^* + \mathbf{F}. \tag{2.24}$$

The internal mercury pipe flow is assumed to be steady state without gravity force, thus the continuity and momentum equations can be simplified to be

$$\nabla^* \cdot \mathbf{U}^* = 0, \tag{2.25}$$

and the momentum conservation,

$$\mathbf{U}^* \cdot \nabla^* \mathbf{U}^* = -\frac{1}{\rho^*} \nabla^* P^* + \frac{1}{Re} \nabla^* \cdot \tau^*. \tag{2.26}$$

The shear stress tensor, τ^*, is modeled as

$$\tau^*_{ij} = (\mu^* + \mu^*_t)\left(\frac{\partial U^*_i}{\partial x^*_j} + \frac{\partial U^*_j}{\partial x^*_i}\right) \tag{2.27}$$

and the eddy viscosity is computed from

$$\mu_t^* = \rho^* C_\mu \frac{k^{*2}}{\varepsilon^*}, \tag{2.28}$$

where k^* is the kinetic energy of turbulence, $k^* \equiv \frac{1}{2}(\overline{(u')^*} + \overline{(v')^*} + \overline{(w')^*})$, and ε^* is its dissipation rate. C_μ is modeled as [89]

$$C_\mu = \frac{1}{A_0 + A_s \frac{k^* U^{(*)}}{\varepsilon^*}}, \tag{2.29}$$

where

$$U^{(*)} \equiv \sqrt{S_{ij}^* S_{ij}^* + \overline{\Omega}_{ij}^* \overline{\Omega}_{ij}^*}, \tag{2.30}$$

$$S_{ij}^* = \frac{1}{2}(U_{i,j}^* + U_{j,i}^*), \tag{2.31}$$

$$\overline{\Omega}_{ij}^* = \frac{1}{2}(U_{i,j}^* - U_{j,i}^*). \tag{2.32}$$

S_{ij}^* is the symmetric part of the rate-of-strain (deformation) tensor, with $\overline{\Omega}_{ij}^*$ the antisymmetric part.

The model constants A_0 and A_s are given as [89]

$$A_0 = 4.04, A_s = \sqrt{6}\cos\phi, \tag{2.33}$$

where

$$\phi = \frac{1}{3}\cos^{-1}(\sqrt{6}W), W = \frac{S_{ij}^* S_{jk}^* S_{ki}^*}{\widetilde{S}^{*3}}, \widetilde{S}^* = \sqrt{S_{ij}^* S_{ij}^*}. \tag{2.34}$$

2.2.2 Realizable $k - \varepsilon$ model

A Reynolds-averaged Navier-Stokes (RANS) equation approach will suffice for the current problem in which the fluid is bounded by a circular, no-slip wall, and the interest is mainly on the mean flow. The Reynolds stress model (RSM) [86] has been judged to be the most accurate RANS model for turbulent flow in curved pipes, as it includes memory effects and the effects of streamline curvature. However, RSM is a six-equation model that is computationally expensive for practical engineering problems. Several options exist for the simpler one- or two-equation RANS approaches, including the Spalart-Allmaras (SA), [87] Standard $k-\varepsilon$ (SKE), [88] and Realizable $k-\varepsilon$ (RKE) [89] models. In this work, the RKE model is selected for the curved-pipe internal flow problem.

The $k-\varepsilon$ turbulent model is found to be a useful engineering approach to predict the mean velocity profiles of turbulent flows. In general, the stand $k-\varepsilon$ model qualitatively predicts most turbulent flows, while it fails to give consistent prediction for the plane jet and round jet problems [90, 91]. The RKE model is also used for the turbulent jet flow simulation.

The non-dimensional equations for RKE model can then be written as [89]

$$\mathbf{U}^{*}\cdot\nabla^{*}k^{*} = \nabla^{*}\cdot[(\frac{1}{Re}+\frac{1}{\sigma_k Re_t})\nabla^{*}k^{*}] + G_t^{*} - \varepsilon^{*}, \tag{2.35}$$

$$\mathbf{U}^{*}\cdot\nabla^{*}\varepsilon^{*} = \nabla^{*}\cdot[(\frac{1}{Re}+\frac{1}{\sigma_\varepsilon Re_t})\nabla^{*}\varepsilon^{*}] + C_1 S^{*}\varepsilon^{*} - C_2\frac{1}{a}\frac{\varepsilon^{*2}}{k^{*}+\sqrt{\nu^{*}\varepsilon^{*}}}, \tag{2.36}$$

where σ_k and σ_ε are the turbulent Prandtl numbers for k and ε, respectively. Re_t is the Reynolds number based on the eddy viscosity (Eqn. (2.28)).

The production of turbulence kinetic energy, G_t^{*}, is evaluated in a manner consistent with the Boussinesq hypothesis:

$$G_t^{*} = (2\frac{1}{Re_t}S_{ij}^{*} - \frac{2}{3}k^{*}\delta_{ij})U_{i,j}^{*}. \tag{2.37}$$

The constants for the realizable $k-\varepsilon$ model are

$$\sigma_k = 1.0, \sigma_\varepsilon = 1.2, C_1 = \max[0.43, \frac{\Gamma}{\Gamma+5}], C_2 = 1.9, \tag{2.38}$$

where

$$\Gamma = S\frac{k}{\varepsilon}, S = \sqrt{2S_{ij}S_{ij}}. \tag{2.39}$$

2.2.3 Boundary conditions

The inlet velocity for all pipes is that of a fully developed flow for a straight pipe aligned with the x-direction:

$$U^* = V^* = 0, W^* = W^*(r^*). \tag{2.40}$$

The discrete form of $W^*(r^*)$ is taken as the solution at the exit of a straight pipe obtained from an auxiliary simulation, with the axial velocity profile shown in Fig. 2.2. At the inlet, the mean pressure is $P = 30$ bar (or $P^* = 30$), while the turbulence conditions are

$$k^* = \frac{3}{2}(U^* I)^2, \varepsilon^* = \frac{C_\mu^{3/4} k^{*3/2}}{l^*}, \tag{2.41}$$

where I is the turbulence intensity, $I = 0.16Re^{-1/8}$. The values of C_μ and l^* are:

$$C_\mu = 0.09, l^* = 0.07D_h^*, \tag{2.42}$$

and $D_h^* = 2$. No-slip conditions are specified at the wall,

$$U^* = V^* = W^* = 0, \tag{2.43}$$

while zero-gradient conditions are assumed at the pipe outlet:

$$\nabla_n^* U^* = \nabla_n^* V^* = \nabla_n^* W^* = \nabla_n^* P^* = \cdots = 0, \tag{2.44}$$

where $\nabla_n^* \equiv \partial^*/\partial n^*$ and "n^*" is the outward-pointing normal at the outlet.

2.3 Level Set Method

In the level set (LS) [57, 60, 92, 93, 94], the level set function, ϕ, is used to represent and propagate the free surface. The interface, where the points have the ϕ value of 0, divides the

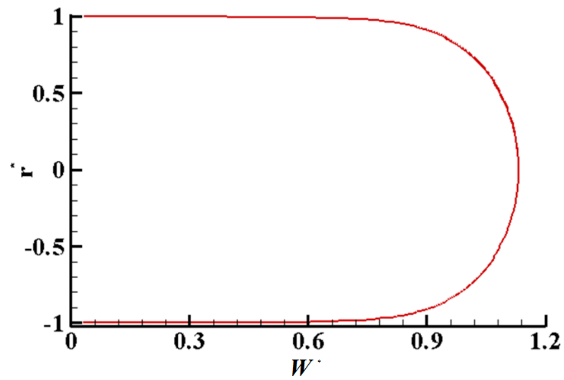

Figure 2.2: Fully developed normalized velocity profile $W^*(r^*)$ at pipe inlet

liquid region ($\phi > 0$) from the gas region ($\phi < 0$). The interface is transported by the level set equation,

$$\phi_t + \mathbf{u} \cdot \nabla \phi = 0. \tag{2.45}$$

Note that the dimensional form of the equations are presented and used for the description of the two-phase problem.

2.3.1 Reynolds-averaged level set equation

In an incompressible flow, $\nabla \cdot \mathbf{u} = 0$, and the LS equation is equivalent to the conservation law:

$$\phi_t + \nabla \cdot (\mathbf{u}\phi) = 0. \tag{2.46}$$

In a turbulent flow field, ϕ and $\mathbf{u}$ may be decomposed into mean and fluctuation components:

$$\phi = \Phi + \phi', \tag{2.47}$$

$$\mathbf{u} = \mathbf{U} + \mathbf{u}'. \tag{2.48}$$

Applying Reynolds averaging procedure to the instantaneous equation yields

$$\overline{\phi}_t + \nabla \cdot (\mathbf{U}\overline{\phi} + \overline{\mathbf{u}'\phi}) = 0. \tag{2.49}$$

The scalar flux term is modeled via the gradient-flux approximation [96]:

$$-\overline{\mathbf{u}'\phi'} = D_T \nabla \overline{\phi}, \tag{2.50}$$

where the turbulent diffusivity is

$$D_T = c_1 \overline{k}^2 / \varepsilon \tag{2.51}$$

and c_1 is a constant. Nilsson and Bai used $c_1 = 0.129$ [97], a value that will also be used in this thesis. Thus, the averaged equation, omitting the averaging symbols, can be written as

$$\phi_t + \nabla \cdot (\mathbf{U}\phi - D_T \nabla \phi) = 0. \tag{2.52}$$

In the LS method, the density and the dynamic viscosity are described as

$$\rho(\mathbf{x}, t) = \rho_l [1 - H_\epsilon(\phi(\mathbf{x}, t))] + \rho_g H_\epsilon(\phi(\mathbf{x}, t)), \tag{2.53}$$

$$\mu(\mathbf{x}, t) = \mu_l [1 - H_\epsilon(\phi(\mathbf{x}, t))] + \mu_g H_\epsilon(\phi(\mathbf{x}, t)), \tag{2.54}$$

where the subscripts l and g denote liquid and gas phases, respectively[98]. H_ϵ is the smoothed Heaviside function[58]

$$H_\epsilon(\phi) = \begin{cases} 0 & if\ \phi < -\epsilon, \\ (\phi + \epsilon)/2\epsilon + \sin(\pi\phi/\epsilon)/2\pi & if\ |\phi| < \epsilon, \\ 1 & if\ \phi > \epsilon, \end{cases} \tag{2.55}$$

where ϵ is a parameter whose value ranges from one to two times the local mesh size close to the interface. Physically, ϵ represents half of the interface thickness.

2.3.2 Re-initialization equation

In order to keep ϕ as the signed normal distance and interface as the zero level set function, a re-initialization equation is required [58]:

$$\phi_\tau + S(\phi^0)(|\nabla\phi| - 1) = 0, \tag{2.56}$$

where ϕ^0 is the initial condition of ϕ and S is the sign function, which can be defined as

$$S(\phi_0) = \frac{\phi_0}{\sqrt{\phi_0^2 + \delta_\epsilon}}, \tag{2.57}$$

where the parameter, $\delta_\epsilon = 10^{-16}$, in order to avoid division by zero.

Equation (2.56) is written in the form

$$\phi_\tau + \mathbf{w} \cdot \nabla\phi = S(\phi^0), \tag{2.58}$$

for the purpose of spatial discretization, where $\mathbf{w}$ is the unit velocity vector pointing away from the interface $\phi^0 = 0$. ϕ^0 is the initial condition to Eqn. (2.58).

$$\mathbf{w} = S(\phi_0)\frac{\nabla\phi}{|\nabla\phi|}, \tag{2.59}$$

2.4 Volume of Fluid Method

The volume of fluid (VOF) method uses the volume fraction of one of the fluids within each cell to determine the interface. The volume fraction is one if the cell is filled with the liquid phase, zero if the cell is filled with the gas phase, and between zero and one in the cells where there is an interface. The liquid volume fraction is advected with the velocity field:

$$\frac{\partial F}{\partial t} + \mathbf{U} \cdot \nabla F = 0. \tag{2.60}$$

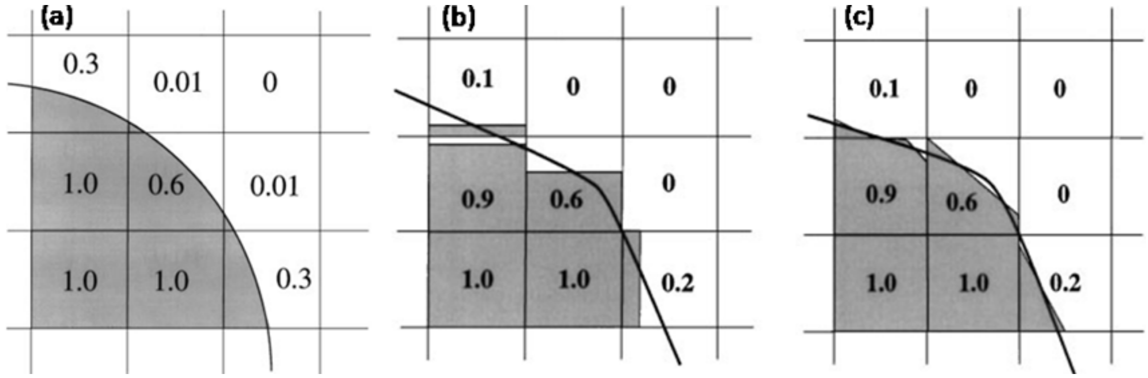

Figure 2.3: (a) the exact interface for a circular arc over a square grid; Interface reconstructed by the scheme of (b) Simple Line Interface Calculation (SLIC) (c) Piecewise Linear Interface Calculation (PLIC)

Given the fixed grid, the velocity field $\mathbf{U}$, and the field F at the previous step, the liquid volume fraction field F can be updated in general. The 2D interface is considered to be a continuous, piecewise smooth line. In order to reconstruct the interface, first we need to determine which cells contain the interface, and then decide the location in these cell by considering the volume fraction, F, in the cells bounding the interface. The simplest reconstruction of the interface are the Simple Line Interface Calculation (SLIC) [100], which is first order accurate. More accurate VOF techniques attempt to fit the interface through piecewise linear segments, like Piecewise Linear Interface Calculation (PLIC) [63]. Figure 2.3 (a) shows a exact volume of fraction for a smooth circular arc over a square grid. An interface that has been reconstructed using SLIC method is shown in Fig. 2.3(b), while the one constructed by the PLIC method is given in Fig. 2.3(c).

In the VOF method, the density and the dynamic viscosity are approximated by the following formulas:

$$\rho(x,t) = \rho_g + (\rho_l - \rho_g)F, \tag{2.61}$$

$$\mu(x,t) = \mu_g + (\mu_l - \mu_g)F, \tag{2.62}$$

where l and g denote “liquid” and “gas” phases, respectively, and F is the liquid volume fraction.

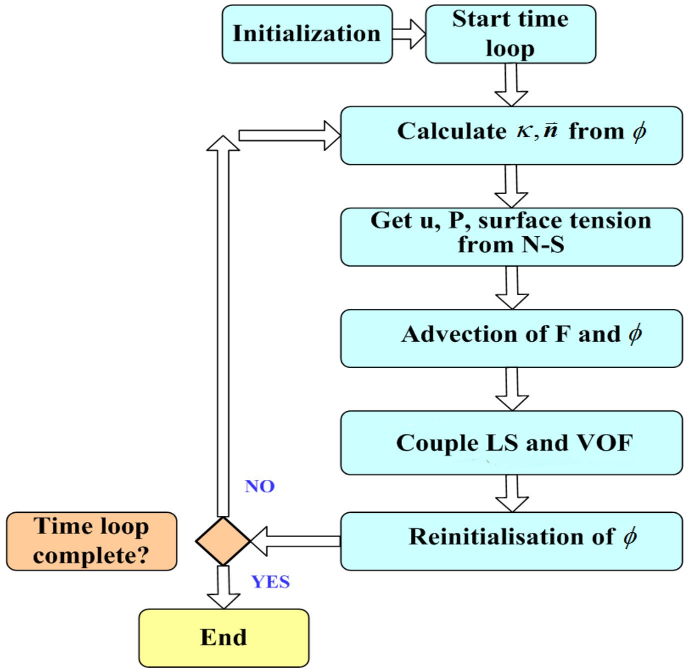

Figure 2.4: Algorithm of CLSVOF method used in this thesis

2.5 Coupling Level Set and Volume of Fluid

The LS method tends to lose/gain mass [79]. The VOF method encounters numerical difficulties at the interface and it is difficult to calculate the interface curvature. CLSVOF method overcomes these problems by mitigating the disadvantages of these two methods.

To couple the VOF method and the LS method, the volume fraction F, in a given cell of the domain, at time t, is defined as a function of the level set ϕ[64]:

$$F(\Omega, t) = \frac{1}{|\Omega|} \int_{\Omega} H_{\epsilon}(\phi(x, y, t)) dx dy, \tag{2.63}$$

where H_{ϵ} is the smoothed Heaviside function defined in Eqn. (2.55).

When starting the project, FLUENT doesn't have the function of CLSVOF method but only implements the VOF method. Therefore we only need to solve the LS method and couple it to the VOF method inside FLUENT. In Nichita's Ph.D. thesis [49] , a detailed algorithm for the CLSVOF method in FLUENT is presented (Fig. 2.4), which is also used in this thesis.

However, his code is implemented only for structured (Cartesian) grids for laminar flow. Based on Nichita's CLSVOF algorithm, this work develops a CLSVOF module that is applicable to unstructured meshes, by solving the level set and re-initialization equations in a transformed coordinate system.

2.6 Continuum Surface Model

For multiphase flow, the surface tension force is considered in the momentum equation. The CSF (Continuum Surface Force) model of Brackbill *et al.* [67], is used to approximate the surface tension force:

$$\mathbf{F}_{st} = \sigma \kappa(\phi) \mathbf{n} \delta_\epsilon(\phi), \tag{2.64}$$

where σ is the surface tension coefficient. For mercury-air, its value is 0.4855 N/m at room temperature. $\delta_\epsilon(\phi)$ is the smoothed delta function, which is defined as the derivative of the smoothed Heaviside function, $H_\epsilon(\phi)$, with respect to ϕ:

$$\delta_\epsilon(\phi) = \begin{cases} 0 & if \ \ |\phi| > \epsilon, \\ 1/2\epsilon + \cos(\pi\phi/\epsilon)/2\epsilon & if \ \ |\phi| < \epsilon. \end{cases} \tag{2.65}$$

κ is the mean curvature of the interface, and $\mathbf{n}$ is the normal vector of the interface. In the LS method, they are defined by

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|}, \kappa = \nabla \cdot \frac{\nabla\phi}{|\nabla\phi|}. \tag{2.66}$$

Chapter 3

Numerical Procedure

3.1 Discretization of The Continuity Equation

Control-volume-based technique is used in the commercial FLUENT code, which requires integrating the governing equations about each control volume. Eqn. (2.23) is a non-dimensional continuity equation in differential form. The integral form of a dimensional continuity equation for an arbitrary control volume Ω can be written as

$$\frac{\partial}{\partial t}\int_{\Omega}\mathbf{U}d\Omega + \int_{S}(\mathbf{U}\cdot\mathbf{n}_S)dS = 0, \tag{3.1}$$

where $\mathbf{n}_S$ is the local, outward-pointing unit normal to the S.

Equation (3.1) can be discretized on a given control volume in the computational domain to yield the discretized equation

$$\frac{\partial \mathbf{U}}{\partial t}\triangle V + \sum_{f}^{N_{faces}}\mathbf{U}_f\mathbf{A}_f = 0 \tag{3.2}$$

where N_{faces} is the number of faces enclosing the control volume, U_f is the velocity normal to the face f, and A_f is the area of face f (note that the normal vector $\mathbf{n}_S$ has been dotted with the velocity vector along $\mathbf{n}_S$).

3.1.1 Temporal Discretization

The first-order explicit discretization is used for temporal term:

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^{n}}{\Delta t}\Delta V = \Gamma(\mathbf{U}^{n}), \tag{3.3}$$

where Γ incorporates any spatial discretization.

3.1.2 Spatial Discretization

The spatial discretization in Eq. (3.2) in the integral form is

$$\Gamma(\mathbf{U}) = \int_{S}(\mathbf{U} \cdot \mathbf{n}_S)dS. \tag{3.4}$$

And its discretized form can be written as

$$\Gamma(\mathbf{U}) = -\sum_{f}^{N_{faces}} \mathbf{U}_f \mathbf{A}_f. \tag{3.5}$$

The FLUENT saves all fluid information at the cell centers. Taking the 2D control volume shown in Fig. 3.1 (uniform Δx and Δy) as an example, the discretized form of the continuity equation is

$$\Gamma(\mathbf{U}) = -(U_{i+1/2,j} - U_{i-1/2,j}) \triangle y - (V_{i,j+1/2} - V_{i,j-1/2}) \triangle x, \tag{3.6}$$

where $U_{i+1/2,j}, U_{i-1/2,j}, V_{i,j+1/2}$, and $V_{i,j-1/2}$ are the velocities on the faces surrounding the control volume (i, j).

The values of the velocities at the cell surfaces $(U_{i+1/2,j}, U_{i-1/2,j}, V_{i,j+1/2}, V_{i,j-1/2})$, can be calculated from the values of velocity at the cell centers. Linear interpolation of cell-centered velocities to the face results in unphysical checker-boarding of pressure [68]. Instead, a procedure similar to that by Rhie and Chow [69] is used to prevent checkerboarding. The

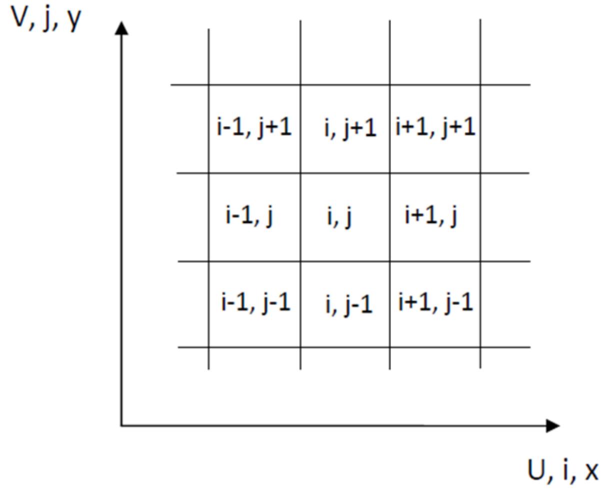

Figure 3.1: Two dimensional control volume for continuity equation

values of the velocities at the cell surfaces are momentum-weighted averaging instead of using the linear average.

$$
\begin{aligned}
U_f &= \frac{U_{c_0}/a_{p,c_0} + U_{c_1}/a_{p,c1}}{1/a_{p,c_0} + 1/a_{p,c1}} + \frac{d_f}{\rho_f}[(P_{c_0} + (\nabla P)_{c_0} \cdot \mathbf{r}_0) - (P_{c_1} + (\nabla P)_{c_1} \cdot \mathbf{r}_1)] \\
&= \widehat{J}_f + \frac{d_f}{\rho_f}(P_{c_0} - P_{c_1}), \qquad (3.7)
\end{aligned}
$$

where U_{c_0}, U_{c1} and P_{c_0}, P_{c_1} are the normal velocities and pressures within the two cells on either side of the face f , a_{p,c_0} and $a_{p,c1}$ are the under-relaxation factors for velocity. The under-relaxation factors are used in the pressure-based solver in FLUENT to stabilize the convergence behavior of the outer nonlinear iterations [68]. $\widehat{J}_f$ contains the influence of velocities in these cells. The term d_f is a function of $\overline{a}_P$, the average of the momentum equation coefficients a_P for the cells on either side of face f [68]. ρ_f is value of density at the cell surfaces.

This procedure works well as long as the velocity variation between cell centers is smooth. However when there are jumps or large gradients of velocity, the value velocities cannot be interpolated using this momentum-weighted averaging [68]. Instead, other alternate interpolation methods should be used:

(1) The linear scheme computes the face velocities as the average of the velocity values in the adjacent cells.

$$U_f = \frac{U_{c_0} + U_{c_1}}{2}. \tag{3.8}$$

(2) The second-order upwind scheme

$$U_f = U + \nabla U \cdot \mathbf{r}, \tag{3.9}$$

where U and ∇U are the cell-centered value and its gradient in the upstream cell, and $\mathbf{r}$ is the displacement vector from the upstream cell centroid to the face centroid. The determination of ∇U is required in this scheme, which can be computed by Green-Gauss cell-based method or least squares cell-based method. When a polyhedral mesh is used, the cell-based least square gradients are recommended for use over the Green-Gauss cell-based method. The details of the evaluation of gradients can also be found in the FLUENT theory guide [68]. It is described in the FLUENT theory guide that the second-order scheme is not applicable for the VOF model [68].

(3) The central-differencing scheme

The central-differencing scheme provides improved accuracy for LES (Large Eddy Simulation) calculations.

$$U_f = \frac{1}{2}(U_{c_0} + U_{c_1}) + \frac{1}{2}(\nabla U_{c_0} \cdot \mathbf{r}_{c_0} + \nabla U_{c_1} \cdot \mathbf{r}_{c_1}), \tag{3.10}$$

where ∇U_{c_0} and ∇U_{c1} are the normal velocities within the two cells on either side of the face f respectively, and $\mathbf{r}$ is the vector directed from the cell centroid toward the face centroid.

3.2 Discretization of The Momentum Equation

The non-dimensional differential form of momentum equation is given in Eq. (2.24. The dimensional integral form of the momentum equation is

$$\rho[\frac{\partial}{\partial t}\int_{\Omega}\mathbf{U}d\Omega+\int_{S}(\mathbf{U}\mathbf{U}\cdot\mathbf{n}_S)dS]=-\int_{S}P\mathbf{n}_S dS+\int_{S}(\tau\cdot\mathbf{n}_S)dS+\int_{\Omega}\mathbf{F}d\Omega. \tag{3.11}$$

The discretization of above equation on a given control volume, or cell yields

$$\rho\frac{\partial\mathbf{U}}{\partial t}\Delta V+\rho\sum_{f}^{N_{faces}}(\mathbf{U}_f\mathbf{U}_f\cdot\mathbf{A}_f)=-\sum_{f}^{N_{faces}}P\mathbf{A}_f+\sum_{f}^{N_{faces}}\tau\cdot\mathbf{A}_f+\mathbf{F}\Delta V, \tag{3.12}$$

where N_{faces} is the number of faces enclosing the control volume, $\mathbf{U}_f$ is the velocity normal to the face f, $\mathbf{U}_f\cdot\mathbf{A}_f$ is the volume flux through the face, $\mathbf{A}_f$ is the face area vector, ΔV is the volume of the cell.

3.2.1 Temporal Discretization

The generic expression for the above equation is given by

$$\rho\frac{d}{dt}\int_{\Omega}\mathbf{U}d\Omega=\Gamma(\mathbf{U}), \tag{3.13}$$

where Γ incorporates any spatial discretization. The first-order explicit discretization is

$$\rho\frac{\mathbf{U}^{n+1}-\mathbf{U}^{n}}{\Delta t}\Delta V=\Gamma(\mathbf{U}^{n}). \tag{3.14}$$

3.2.2 Spatial Discretization

The spatial discretization in momentum equation in integral form is

$$\Gamma(\mathbf{U})=-\int_{S}(\mathbf{U}\mathbf{U}\cdot\mathbf{n}_S)dS-\int_{S}P\mathbf{n}_S dS+\int_{S}(\tau\cdot\mathbf{n}_S)dS+\int_{\Omega}\mathbf{F}d\Omega. \tag{3.15}$$

Thus its discretized form is.

$$\Gamma(\mathbf{U}) = -\rho \sum_{f}^{N_{faces}} (\mathbf{U}_f \mathbf{U}_f \cdot \mathbf{A}_f) - \sum_{f}^{N_{faces}} P\mathbf{A}_f + \sum_{f}^{N_{faces}} \overline{\overline{\tau}} \cdot \mathbf{A}_f + \mathbf{F}\Delta V. \tag{3.16}$$

Applied to the same 2D control volume shown in Fig. 3.1,the corresponding discretizations are as follows:

$$\begin{aligned} \Gamma(U) &= -(E^{(1)}_{i+1/2,j} - E^{(1)}_{i-1/2,j}) \triangle y - (K^{(1)}_{i,j+1/2} - K^{(1)}_{i,j-1/2}) \triangle x \\ &\quad -(P_{i+1,j} - P_{i,j})\Delta y + F^{(1)}_{i,j} \Delta x \Delta y \end{aligned} \tag{3.17}$$

$$\begin{aligned} \Gamma(V) &= -(E^{(2)}_{i+1/2,j} - E^{(2)}_{i-1/2,j}) \triangle y - (K^{(2)}_{i,j+1/2} - K^{(2)}_{i,j-1/2}) \triangle x \\ &\quad -(P_{i,j+1} - P_{i,j})\Delta x + F^{(2)}_{i,j} \Delta x \Delta y, \end{aligned} \tag{3.18}$$

where $E^{(1)}$, $E^{(2)}$, $K^{(1)}$, and $K^{(2)}$ are defined as follows

$$E^{(1)} = \rho U^2 - (\mu + \mu_t)\frac{\partial U}{\partial x}, \tag{3.19}$$

$$E^{(2)} = \rho UV - (\mu + \mu_t)\frac{\partial V}{\partial x}, \tag{3.20}$$

$$K^{(1)} = \rho UV - (\mu + \mu_t)\frac{\partial U}{\partial y}, \tag{3.21}$$

$$K^{(2)} = \rho V^2 - (\mu + \mu_t)\frac{\partial V}{\partial y}. \tag{3.22}$$

Thus

$$E^{(1)}_{i+1/2,j} = \rho U^2_{i+1/2,j} - (\mu + \mu_t) \left.\frac{\partial U}{\partial x}\right|_{i+1/2,j}, \tag{3.23}$$

$$E^{(1)}_{i-1/2,j} = \rho U^2_{i-1/2,j} - (\mu + \mu_t) \left.\frac{\partial U}{\partial x}\right|_{i-1/2,j}, \tag{3.24}$$

$$E^{(2)}_{i+1/2,j} = \rho (UV)_{i+1/2,j} - (\mu + \mu_t) \left.\frac{\partial V}{\partial x}\right|_{i+1/2,j}, \tag{3.25}$$

$$E^{(2)}_{i-1/2,j} = \rho (UV)_{i-1/2,j} - (\mu + \mu_t) \left.\frac{\partial V}{\partial x}\right|_{i-1/2,j}, \tag{3.26}$$

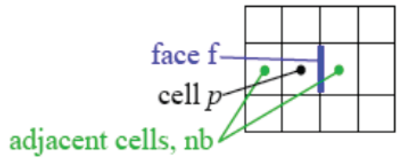

Figure 3.2: cell p and its adjacent cells nb, neighboring the cell p

$$K^{(1)}_{i,j+1/2} = \rho(UV)_{i,j+1/2} - (\mu+\mu_t)\left.\frac{\partial U}{\partial y}\right|_{i,j+1/2}, \tag{3.27}$$

$$K^{(1)}_{i,j-1/2} = \rho(UV)_{i,j-1/2} - (\mu+\mu_t)\left.\frac{\partial U}{\partial y}\right|_{i,j-1/2}, \tag{3.28}$$

$$K^{(2)}_{i,j+1/2} = \rho V^2{}_{i,j+1/2} - (\mu+\mu_t)\left.\frac{\partial V}{\partial y}\right|_{i,j+1/2}, \tag{3.29}$$

$$K^{(2)}_{i,j-1/2} = \rho V^2{}_{i,j-1/2} - (\mu+\mu_t)\left.\frac{\partial V}{\partial y}\right|_{i,j-1/2}. \tag{3.30}$$

The face velocities and face gradients can be interpolated through the values at the cell centers by the schemes described in the context of the discretization of the continuity equation. Consequently, Eqns. (3.17) and (3.18) can be written as

$$\Gamma(U) = -a_{i,j}U_{i,j} - \sum_{nb} a_{nb}U_{nb} - \Delta y(P_{i+1,j} - P_{i,j}) - F^1_{i,j}\Delta x\Delta y, \tag{3.31}$$

$$\Gamma(V) = -b_{i,j}V_{i,j} - \sum_{nb} b_{nb}V_{nb} - \Delta x(P_{i,j+1} - P_{i,j}) - F^2_{i,j}\Delta x\Delta y, \tag{3.32}$$

where a, a_{nb} b, and b_{nb} are linearized coefficients for U, U_{nb}, V, and V_{nb} respectively. $\sum_{nb} a_{nb}U_{nb}$ and $\sum_{nb} b_{nb}V_{nb}$ signify all the convective and diffusive contributions from the neighboring nodes. The subscript nb refers to the neighbor cells as the locations between the cell center p and the adjacent cells nb shown in Fig. 3.2.

3.2.3 Pressure-Velocity Coupling SIMPLE (Semi Implicit Method for Pressure Linked Equations) Scheme

The SIMPLE algorithm uses the relationship between velocity and pressure corrections to enforce mass conservation and to obtain the pressure field [68]. First, guess a pressure

P^*. Then a velocity U_f^* can be computed by P^* through Eqn.(3.7)

$$U_f^* = \widehat{J}_f^* + \frac{d_f}{\rho_f}(P_{c_0}^* - P_{c_1}^*). \tag{3.33}$$

However, U_f^* does not satisfy the continuity equation. A correction U_f' is considered for a corrected U_f

$$U_f = U_f^* + U_f', \tag{3.34}$$

which satisfies the continuity equation. The SIMPLE scheme postulates that U_f' be written as

$$U_f' = \frac{d_f}{\rho_f}(P_{c_0}' - P_{c_1}'), \tag{3.35}$$

where P' is the cell pressure correction.

Substitute the correction equations (3.34) and (3.35) into the discrete continuity equation (3.2) to obtain a discrete equation for the pressure correction P' in the cell:

$$a_P P' = \sum_{nb} a_{nb} P_{nb}' + c, \tag{3.36}$$

where the source term c is the net flow rate into the cell:

$$c = \sum_{f}^{N_{faces}} U_f^* A_f. \tag{3.37}$$

Once a solution for the Eqn. (3.36) has been obtained, the cell pressure and face velocity are corrected by

$$P = P^* + a_P P', \tag{3.38}$$

$$U_f = J_f^* + \frac{d_f}{\rho_f}(P_{c_0}' - P_{c_1}'), \tag{3.39}$$

where a_p is the under-relaxation factor for pressure. The corrected U_f satisfies the discrete continuity equation identically during each iteration.

3.3 Discretization of k and ε Equations

The integral form of the k and ε equations are

$$\rho[\frac{\partial}{\partial t}\int_{\Omega} k d\Omega + \int_{S}(k\mathbf{U}\cdot\mathbf{n}_S)dS] = \int_{S}[(\mu + \frac{\mu_t}{\sigma_k})\nabla k \cdot \mathbf{n}_S]dS + \int_{\Omega}(G_k - \rho\varepsilon)d\Omega, \quad (3.40)$$

$$\rho[\frac{\partial}{\partial t}\int_{\Omega} \varepsilon d\Omega + \int_{S}(\varepsilon\mathbf{U}\cdot\mathbf{n}_S)dS] = \int_{S}[(\mu + \frac{\mu_t}{\sigma_\varepsilon})\nabla \varepsilon \cdot \mathbf{n}_S]dS + \int_{\Omega}(\rho C_1 S\varepsilon - \rho C_2\frac{\varepsilon^2}{k + \sqrt{\nu\varepsilon}})d\Omega. \quad (3.41)$$

Appling the above equations to each control volume, or cell, in the computational domain, yields the discretized k and ε equations on a given cell:

$$\rho\frac{\partial k}{\partial t}\Delta V + \rho\sum_{f}^{N_{faces}} k_f\mathbf{U}_f\cdot\mathbf{A}_f = \sum_{f}^{N_{faces}}(\mu + \frac{\mu_t}{\sigma_k})\nabla k_f \cdot \mathbf{A}_f + (G_k - \rho\varepsilon)\Delta V, \quad (3.42)$$

$$\rho\frac{\partial \varepsilon}{\partial t}\Delta V + \rho\sum_{f}^{N_{faces}} \varepsilon_f\mathbf{U}_f\cdot\mathbf{A}_f = \sum_{f}^{N_{faces}}(\mu + \frac{\mu_t}{\sigma_\varepsilon})\nabla k_f \cdot \mathbf{A}_f + (\rho C_1 S\varepsilon - \rho C_2\frac{\varepsilon^2}{k + \sqrt{\nu\varepsilon}})\Delta V. \quad (3.43)$$

3.3.1 Temporal Distretization

The temporal discretization uses the first-order explicit integration as the temporal discretization of the continuity and momentum equations:

$$\frac{k^{n+1} - k^n}{\Delta t}\Delta V = \Gamma(k^n), \quad (3.44)$$

$$\frac{\varepsilon^{n+1} - \varepsilon^n}{\Delta t}\Delta V = \Gamma(\varepsilon^n), \quad (3.45)$$

where Γ equation incorporates the spatial discretization of the k or ε equation.

3.3.2 Spatial Discretization

The spatial discretization in k and ε equations in integral form are

$$\Gamma(k) = -\int_S (k\mathbf{U}\cdot\mathbf{n}_S)dS] + \int_S [(\mu + \frac{\mu_t}{\sigma_k})\nabla k \cdot \mathbf{n}_S]dS + \int_\Omega (G_k - \rho\varepsilon)d\Omega, \quad (3.46)$$

$$\Gamma(\varepsilon) = -\int_S (\varepsilon\mathbf{U}\cdot\mathbf{n}_S)dS] + \int_S [(\mu + \frac{\mu_t}{\sigma_\varepsilon})\nabla \varepsilon \cdot \mathbf{n}_S]dS + \int_\Omega (\rho C_1 S\varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu\varepsilon}})d\Omega. \quad (3.47)$$

Their corresponding discretized equations can be written as

$$\Gamma(k) = -\rho \sum_f^{N_{faces}} k_f \mathbf{U}_f\cdot\mathbf{A}_f + \sum_f^{N_{faces}} (\mu + \frac{\mu_t}{\sigma_k})\nabla k_f \cdot \mathbf{A}_f + (G_k - \rho\varepsilon)\Delta V, \quad (3.48)$$

$$\Gamma(\varepsilon) = -\rho \sum_f^{N_{faces}} \varepsilon_f \mathbf{U}_f\cdot\mathbf{A}_f + \sum_f^{N_{faces}} (\mu + \frac{\mu_t}{\sigma_\varepsilon})\nabla k_f \cdot \mathbf{A}_f + (\rho C_1 S\varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu\varepsilon}})\Delta V. \quad (3.49)$$

Applied to the same 2D control volume shown in Fig. 3.1,the corresponding discretizations are as follows:

$$\Gamma(k) = -(M^{(1)}_{i+1/2,j} - M^{(1)}_{i-1/2,j}) \triangle y - (N^{(1)}_{i,j+1/2} - N^{(1)}_{i,j-1/2}) \triangle x + (G_k - \rho\varepsilon)_{i,j}\Delta x \Delta y \quad (3.50)$$

$$\Gamma(\varepsilon) = -(E^{(2)}_{i+1/2,j} - E^{(2)}_{i-1/2,j}) \triangle y - (K^{(2)}_{i,j+1/2} - K^{(2)}_{i,j-1/2}) \triangle x + (\rho C_1 S\varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu\varepsilon}})_{i,j}\Delta x \Delta y, \quad (3.51)$$

where $M^{(1)}$, $M^{(2)}$, $N^{(1)}$, and $N^{(2)}$ are defined as follows

$$M^{(1)} = \rho k U - (\mu + \frac{\mu_t}{\sigma_k})\frac{\partial k}{\partial x}, \quad (3.52)$$

$$M^{(2)} = \rho \varepsilon U - (\mu + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial \varepsilon}{\partial x}, \quad (3.53)$$

$$N^{(1)} = \rho k V - (\mu + \frac{\mu_t}{\sigma_k})\frac{\partial k}{\partial y}, \tag{3.54}$$

$$N^{(2)} = \rho \varepsilon V - (\mu + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial \varepsilon}{\partial y}. \tag{3.55}$$

Thus

$$M^{(1)}_{i+1/2,j} = \rho(kU)_{i+1/2,j} - (\mu + \frac{\mu_t}{\sigma_k}) \left.\frac{\partial k}{\partial x}\right|_{i+1/2,j}, \tag{3.56}$$

$$M^{(1)}_{i-1/2,j} = \rho(kU)_{i-1/2,j} - (\mu + \frac{\mu_t}{\sigma_k}) \left.\frac{\partial k}{\partial x}\right|_{i-1/2,j}, \tag{3.57}$$

$$M^{(2)}_{i+1/2,j} = \rho(\varepsilon U)_{i+1/2,j} - (\mu + \frac{\mu_t}{\sigma_\varepsilon}) \left.\frac{\partial \varepsilon}{\partial x}\right|_{i+1/2,j}, \tag{3.58}$$

$$M^{(2)}_{i-1/2,j} = \rho(\varepsilon U)_{i-1/2,j} - (\mu + \frac{\mu_t}{\sigma_\varepsilon}) \left.\frac{\partial \varepsilon}{\partial x}\right|_{i-1/2,j}, \tag{3.59}$$

$$N^{(1)}_{i,j+1/2} = \rho(kV)_{i,j+1/2} - (\mu + \frac{\mu_t}{\sigma_k}) \left.\frac{\partial k}{\partial y}\right|_{i,j+1/2}, \tag{3.60}$$

$$N^{(1)}_{i,j-1/2} = \rho(kV)_{i,j-1/2} - (\mu + \frac{\mu_t}{\sigma_k}) \left.\frac{\partial k}{\partial y}\right|_{i,j-1/2}, \tag{3.61}$$

$$N^{(2)}_{i,j+1/2} = \rho(\varepsilon V)_{i,j+1/2} - (\mu + \frac{\mu_t}{\sigma_\varepsilon}) \left.\frac{\partial \varepsilon}{\partial y}\right|_{i,j+1/2}, \tag{3.62}$$

$$N^{(2)}_{i,j-1/2} = \rho(\varepsilon V)_{i,j-1/2} - (\mu + \frac{\mu_t}{\sigma_\varepsilon}) \left.\frac{\partial \varepsilon}{\partial y}\right|_{i,j-1/2}. \tag{3.63}$$

The values of k and ε at the cell surface ($k_{i+1/2,j}, k_{i,j+1/2}, k_{i-1/2,j}, k_{i,j-1/2}, \varepsilon_{i+1/2,j}, \varepsilon_{i,j+1/2}, \varepsilon_{i-1/2,j}, \varepsilon_{i,j-1/2},$) is accomplished using upwind schemes and the diffusion terms in k and ε equations always use second-order central-differenced schemes. The first-order upwind and second-order upwind schemes are described in the context of discretization of continuity equation. The third-order MUSCL (Monotone Upstream-centered Scheme for Conservation Laws) scheme is used for the discretization of the k and ε equations when a high order scheme is required. The third-order MUSCL scheme blends a central differencing scheme and second-order upwind scheme as [68]

$$\gamma_f = \theta\gamma_{f,CD} + (1-\theta)\gamma_{f,SOU}, \tag{3.64}$$

where γ represents a general scalar, $\gamma_{f,CD}$ is a face value obtained with a central differencing scheme and $\gamma_{f,SOU}$ is a face value obtained with a second-order upwind scheme. The first term is written as follows:

$$\gamma_{f,CD} = \frac{1}{2}(\gamma_0 + \gamma_1) + \frac{1}{2}(\nabla\gamma_0 \cdot \mathbf{n}_0 + \nabla\gamma_1 \cdot \mathbf{n}_1), \tag{3.65}$$

where γ_0 and γ_1 are the values at the centroids of two neighboring control volumes sharing the same face, $\nabla\gamma_0$ and $\nabla\gamma_1$ are the gradients of the scalar computed at cell centroids and $\mathbf{n}_0$ and $\mathbf{n}_1$ are the direction vectors pointing from cell centroid to the face centroid.

The second term, $\gamma_{f,SOU}$, is computed as

$$\gamma_{f,SOU} = \gamma + \nabla\gamma \cdot \triangle\mathbf{s}, \tag{3.66}$$

where γ and $\nabla\gamma$ are the value at the cell center and its gradients in the upstream cell, respectively. $\triangle\mathbf{s}$ is the displacement vector from the upstream cell centroid to the face centroid. The gradient $\nabla\gamma$ is computed using the divergence theorem,

$$\nabla\gamma = \frac{1}{\Delta V} \sum_{f}^{N_{face}} \widetilde{\gamma}_f \mathbf{A}_f \tag{3.67}$$

Here the face value $\widetilde{\gamma}_f$ are computed by averaging γ from the two cells adjacent to the face.

3.4 Numerical Procedure for the Level Set Method

3.4.1 UDFs in ANSYS FLUENT

Figure 3.4 illustrates the solution process for the pressure-based solvers, which is used in this study. It begins with a two-step initialization sequence that is executed outside the solution iteration loop. This sequence begins by initializing equations to user-specified (or default) values taken from the ANSY FLUENT user interface. Next, PROFILE UDFs are called, followed by a call to INIT UDFs. Initialization UDFs overwrite initialization values that were previously set. The solution iteration loop begins with the execution of ADJUST UDFs. Next ANSYS FLUENT solves the governing equations of continuity and momentum sequentially or in a coupled fashion. Subsequently, the energy and species equations are solved, followed by turbulence and other scalar transport equations, as required. Note that PROFILE and SOURCE UDFs are called by each "Solve" routine for the variable currently under consideration (e.g., species, velocity).

After the conservation equations, properties are updated, including PROPERTY UDFs. For CLSVOF method, the re-initialization equation and the couple between LS and VOF method are carried at the end of each iteration. A check for either convergence or additional requested iterations is done, and the loop either continues or stops.

Since FLUENT already contains a VOF method, only the LS method needs to be implemented in the code via UDFs. The level set equation is solved by enabling the User Defined Scalar (UDS) equation in FLUENT. The use of macros DEFINE_UDS_UNSTEADY, DEFINE_UDS_FLUX, and DEFINE_DIFFUSIVITY set up the scalar equation for level set function in FLUENT. The unsteady and advection terms are hooked to FLUENT in the User-Defined Scalars panel. The scalar diffusivity is assigned in the Materials panel. The boundary condition for the scalar equation is assigned in the Boundary Condition panel. Especially note that the boundary condition for the LS function at inlet must be fixed to zero, due to that hyperbolic nature of Eq. (2.56). The characteristics propagate outward from the zero level set, $\phi = 0$.

3.4.2 UDF's for the unsteady term in level set equation

The unsteady term of the level set function Eq.(2.52) is moved to the right hand side and discretized as follows:

$$\begin{aligned} unsteady\,term &= -\int \frac{\partial \phi}{\partial t} dV = -[\frac{\phi^{n+1} - \phi^n}{\Delta t}] \cdot \Delta V \\ &= -\frac{\triangle V}{\triangle t}\phi^{n+1} + \frac{\triangle V}{\triangle t}\phi^n. \end{aligned} \tag{3.68}$$

The macro DEFINE_UDS_UNSTEADY is used for the user-defined scalar time derivatives. The temporal discretization uses the first-order explicit time integration as

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \Gamma(\phi^n). \tag{3.69}$$

3.4.3 UDF's for the flux term in level set equation

The advection term in the level set equation has the following form:

$$flux\,term = \nabla \cdot (\mathbf{U}\phi). \tag{3.70}$$

The integral and discretization of the flux term on a given cell are

$$flux\,term\,in\,the\,integral\,form = \int_S (\phi \mathbf{U} \cdot \mathbf{n}_S) dS \tag{3.71}$$

$$flux\,term\,in\,the\,disrectized\,form = \sum_f^{N_{faces}} (\phi_f \mathbf{U_f} \cdot \mathbf{A}_f). \tag{3.72}$$

The third-order MUSCL scheme is used to calculate the face value ϕ_f,

$$\phi_f = \theta \phi_{f,CD} + (1 - \theta)\phi_{f,SOU}, \tag{3.73}$$

where the factor θ is set to 0.125 for the problem being studied, and,

$$\phi_{f,CD} = \frac{1}{2}(\phi_0 + \phi_1) + \frac{1}{2}(\nabla\phi_0 \cdot \mathbf{r}_0 + \nabla\phi_1 \cdot \mathbf{r}_1), \tag{3.74}$$

$$\phi_{f,SOU} = \phi + \nabla\phi \cdot \triangle\mathbf{s}, \tag{3.75}$$

where ϕ_0 and ϕ_1 are the cell centroid values of the two neighboring control volumes sharing the same face, $\nabla\phi_0$ and $\nabla\phi_1$ are the gradients of the scalar computed at cell centroids and $\mathbf{r}_0$ and $\mathbf{r}_1$ are the direction vectors pointing from cell centroid to the face centroid, ϕ and $\nabla\phi$ are the cell-centered value and its gradients in the upstream cell, and $\triangle\mathbf{s}$ is the displacement vector from the upstream cell centroid to the face centroid. The gradient is computed using the divergence theorem,

$$\nabla\phi = \frac{1}{\Delta V}\sum_{f}^{N_{face}} \widetilde{\phi}_f \mathbf{A}_f. \tag{3.76}$$

Here the face value $\widetilde{\phi}_f$ are computed by averaging ϕ from the two cells adjacent to the face.

The macro DEFINE_UDS_FLUX is used for the flux term and it needs to return the scalar value $\mathbf{U} \cdot \mathbf{A}$ to FLUENT, where $\mathbf{A}$ is the face normal vector. Since Eqn. (3.70) is without the fluid density, it's just simple to include "return F_FLUX(f,t)/ρ" in the DEFINE_UDS_FLUX UDF. The denominator ρ can be determined by averaging the adjacent cell's density values C_R (F_C0(f,t), THREAD_T0(t)) and C_R (F_C1(f,t), THREAD_T1(t)), where C_R is flow variable macro in UDF for density, t is a pointer to the thread on which the user-defined scalar flux is to be applied, and f is an index that identifies a face within the given thread. F_C0, F_C1, THREAD_T0 and THREAD_T1 are neighboring cells of the face f, and their corresponding threads (35).

3.4.4 UDF's for the diffusion term in level set equation

The diffusion term in the Reynolds-averaged LS equation is

$$diffusion\,term = \nabla \cdot (-D_T \nabla \phi). \tag{3.77}$$

The integral and discretized forms of the diffusion term are

$$flux\,term\,in\,the\,integral\,form = -\int_S (D_T \nabla \phi \cdot \mathbf{n}_S) dS, \tag{3.78}$$

$$flux\,term\,in\,the\,discretized\,form = -\sum_f^{N_{faces}} (D_T \nabla \phi_f \cdot \mathbf{A}_f). \tag{3.79}$$

The face value ϕ_f uses the same MUSCL scheme as described in Eq.(3.73), and the gradient of ϕ on the face is computed using the divergence theorem,

$$\nabla \phi_f = \frac{1}{\Delta V} \sum_f^{N_{face}} \phi_f \mathbf{A}_f. \tag{3.80}$$

The diffusion coefficient, D_T, used in the macro "DEFINE_DIFFUSIVITY " is defined as

$$D_T = c_1 k^2 / \varepsilon, \tag{3.81}$$

and $c_1 = 0.129$ is a constant.

3.4.5 Discretization of Re-initialization Equation

The re-initialization equation is implemented and solved at every time step and a DEFINE_EXECUTE_AT_END UDF is used. The temporal term is discretized by means of TVD Runge-Kutta (RK) methods. The third-order time integration schemes can be written as

$$\phi^{(1)} = \phi^n + \Delta t \cdot L(\phi^n), \tag{3.82}$$

$$\phi^{(2)} = \frac{1}{4}[3\phi^n + \phi^{(1)} + \Delta t \cdot L(\phi^{(1)})], \tag{3.83}$$

$$\phi^{n+1} = \frac{1}{3}[\phi^n + 2\phi^{(2)} + 2\Delta t \cdot L(\phi^{(2)})], \tag{3.84}$$

where $L(\phi)$ is (Eqn.(2.58))

$$L(\phi) = S(\phi_0) - \mathbf{w} \cdot \nabla\phi. \tag{3.85}$$

The procedure of flux evaluation must be carried out during each stage of the Runge-Kutta method. The explicit scheme considered above requires the computation of a time step Δt to be used in Eqn. (3.84), such that the stability of the numerical method is ensured. One way of choosing Δt is

$$\Delta t = \frac{C_{cfl}}{U_0} \times \min(\Delta x, \Delta y, \Delta z), \tag{3.86}$$

where U_0 is initial bulk velocity, C_{cfl} is the CFL number and is chosen as

$$0 < C_{cfl} \leq 1/3. \tag{3.87}$$

in three space dimensions.

The convection term in Eqn. (2.58) can be expanded as

$$\mathbf{w} \cdot \nabla\phi = W_\xi \phi_\xi + W_\eta \phi_\eta + W_\zeta \phi_\zeta, \tag{3.88}$$

where W_i are the contravariant velocities, defined by

$$W_\xi = w_x \xi_x + w_y \xi_y + w_z \xi_z, \tag{3.89}$$

$$W_\eta = w_x \eta_x + w_y \eta_y + w_z \eta_z, \tag{3.90}$$

$$W_\zeta = w_x \zeta_x + w_y \zeta_y + w_z \zeta_z, \tag{3.91}$$

where

$$w_x = S(\phi_0)\frac{\phi_x}{|\nabla\phi|}, \quad (3.92)$$

$$w_y = S(\phi_0)\frac{\phi_y}{|\nabla\phi|}, \quad (3.93)$$

$$w_z = S(\phi_0)\frac{\phi_z}{|\nabla\phi|}. \quad (3.94)$$

Two sets of codes are made to evaluate the partial derivatives $\phi_x, \phi_y, \phi_z, \phi_\xi, \phi_\eta$, and ϕ_ζ in the spatial discretization using two different finite different methods. The partial derivatives of ϕ in the coordinate system (x, y, z) is computed as

$$\frac{\partial\phi}{\partial x} = J[(\frac{\xi_x}{J}\phi)_\xi + (\frac{\eta_x}{J}\phi)_\eta + (\frac{\zeta_x}{J}\phi)_\zeta], \quad (3.95)$$

$$\frac{\partial\phi}{\partial y} = J[(\frac{\xi_y}{J}\phi)_\xi + (\frac{\eta_y}{J}\phi)_\eta + (\frac{\zeta_y}{J}\phi)_\zeta], \quad (3.96)$$

$$\frac{\partial\phi}{\partial z} = J[(\frac{\xi_z}{J}\phi)_\xi + (\frac{\eta_z}{J}\phi)_\eta + (\frac{\zeta_z}{J}\phi)_\zeta], \quad (3.97)$$

where $\xi_x, \eta_x, \zeta_x, \xi_y, \eta_y, \zeta_y, \xi_z, \eta_z$, and ζ_z are metrics.

(1) Second-order finite difference scheme

For derivatives of ϕ with respect to (x, y, z), the central finite difference is used as described in Eqn. (3.98). Here, the examples are given for the term $(\frac{\xi_x}{J}\phi)_\xi$, similarly for other components $()_\eta$ and $()_\zeta$. The central second-order finite differences is evaluated as

$$(\frac{\xi_x}{J}\phi)_\xi = \frac{1}{2}[(\frac{\xi_x}{J}\phi)_{i+1,j,k} - (\frac{\xi_x}{J}\phi)_{i-1,j,k}], \quad (3.98)$$

when both cell $(i-1, j, k)$ and $(i+1, j, k)$ are available. Otherwise, one-sided second-order finite differences is used. The form of right-sided second-order finite differences is

$$(\frac{\xi_x}{J}\phi)_\xi = \frac{1}{2}[-3 * (\frac{\xi_x}{J}\phi)_{i,j,k} + 4 * (\frac{\xi_x}{J}\phi)_{i+1,j,k} - (\frac{\xi_x}{J}\phi)_{i+2,j,k}], \quad (3.99)$$

and the left-sided second-order finite difference is

$$(\frac{\xi_x}{J}\phi)_\xi = \frac{1}{2}[3 * (\frac{\xi_x}{J}\phi)_{i,j,k} - 4 * (\frac{\xi_x}{J}\phi)_{i-1,j,k} + (\frac{\xi_x}{J}\phi)_{i-2,j,k}]. \tag{3.100}$$

For the calculation of ϕ_ξ,ϕ_η, and ϕ_ζ in Eqn. (3.88), first-order upwind scheme is used. The values of the contravariant velocities are used to decide the upwind stencil.

$$\phi_\xi = \phi_{i+1/2,j,k} - \phi_{i-1/2,j,k}, \tag{3.101}$$

$$\phi_\eta = \phi_{i,j+1/2,k} - \phi_{i,j-1/2,k}, \tag{3.102}$$

$$\phi_\zeta = \phi_{i,j,k+1/2} - \phi_{i,j,k-1/2}. \tag{3.103}$$

The midpoint values are calculated using the first-order upwind scheme,

$$\phi_{i+1/2,j,k} = \begin{cases} \phi_i & W_\xi 0 \\ \phi_{i+1} & W_\xi < 0 \end{cases}, \tag{3.104}$$

$$\phi_{i-1/2,j,k} = \begin{cases} \phi_{i-1} & W_\xi 0 \\ \phi_i & W_\xi < 0 \end{cases}. \tag{3.105}$$

Similarly for $\phi_{i,j\pm1/2,k}$ and $\phi_{i,j,k\pm1/2}$.

(2) Fifth-order Hamilton-Jacobi WENO scheme

To evaluate the gradient terms using a fifth-order WENO scheme, a point (i, j, k) needs three points behind and three points after it in every direction. This poses no difficulties for a point inside the domain, but when the point is within 3 points from the boundary, the scheme doesn't work anymore due to the lack of points. The stencil structure for the fifth-order WENO scheme is shown in Fig. 3.3.

The definitions of ϕ_x, ϕ_y, and ϕ_z are given in Eqns.(3.95), (3.96), and (3.97). The partial derivative terms $(\frac{\xi_x}{J}\phi)_\xi$, $(\frac{\eta_x}{J}\phi)_\eta$, $(\frac{\zeta_x}{J}\phi)_\zeta$, $(\frac{\xi_y}{J}\phi)_\xi$, $(\frac{\eta_y}{J}\phi)_\eta$, $(\frac{\zeta_y}{J}\phi)_\zeta$, $(\frac{\xi_z}{J}\phi)_\xi$, $(\frac{\eta_z}{J}\phi)_\eta$, and $(\frac{\zeta_z}{J}\phi)_\zeta$ are evaluated using WENO scheme, as are ϕ_ξ, ϕ_η, and ϕ_ζ. Here, the details are only given for the partial derivatives of ϕ with respect to (ξ, η, ζ).

To solve ϕ_ξ, ϕ_η, and ϕ_ζ using Sussman's method [64], the following equations are introduced:

$$a = \phi_\xi^-,\ b = \phi_\xi^+,\ c = \phi_\eta^-,\ d = \phi_\eta^+,\ e = \phi_\zeta^-,\ f = \phi_\zeta^+, \tag{3.106}$$

where a, b, c, d, e, and f are computed with a fifth-order Hamilton-Jacobi WENO approximation. First the derivative of ϕ in 1D is described and then its formulations in 3D are given. To approximate ϕ_ξ on a left biased stencil $\{i-3, i-2, i-1, i, i+1, i+2\}$, we introduce $\phi_i = \phi(i)$, $\Delta^+\phi_i = \phi_{i+1} - \phi_i$, and $\Delta^-\phi_i = \phi_i - \phi_{i-1}$. The WENO approximation of ϕ_ξ is a combination of the weighted average of ϕ_ξ, computed by ENO schemes. The 3rd order accurate ENO scheme will choose one from the following

$$\phi_{\xi,i}^{-,0} = \frac{1}{3}\Delta^+\phi_{i-3} - \frac{7}{6}\Delta^+\phi_{i-2} + \frac{11}{6}\Delta^+\phi_{i-1} \tag{3.107}$$

$$\phi_{\xi,i}^{-,1} = -\frac{1}{6}\Delta^+\phi_{i-2} + \frac{5}{6}\Delta^+\phi_{i-1} + \frac{1}{3}\Delta^+\phi_i \tag{3.108}$$

$$\phi_{\xi,i}^{-,2} = \frac{1}{3}\Delta^+\phi_{i-1} + \frac{5}{6}\Delta^+\phi_i - \frac{1}{6}\Delta^+\phi_{i+1}, \tag{3.109}$$

where $\phi_{\xi,i}^{-,s}$ is the third-order approximation to ϕ_ξ based on the sth substencil $\{i+s-3, i+s-2, i+s-1, i+s\}$ for $s = 0, 1, 2$.

The WENO approximation of ϕ_ξ is a weighted average of $\phi_{\xi,i}^{-,s}$ $(s = 0, 1, 2)$:

$$\phi_{\xi,i}^- = \omega_0\phi_{\xi,i}^{-,0} + \omega_1\phi_{\xi,i}^{-,1} + \omega_2\phi_{\xi,i}^{-,2}. \tag{3.110}$$

Here ω_s is the weight associated with the sth substencil and the weights satisfy the consistency equality: $\omega_0 + \omega_1 + \omega_2 = 1$. The definitions of the weights will be given shortly. Substituting $\phi_{\xi,i}^{-,s}$ into $\phi_{\xi,i}^-$, we obtain

$$\begin{aligned}\phi_{\xi,i}^- = {} & \frac{1}{12}(-\Delta^+\phi_{i-2} + 7\Delta^+\phi_{i-1} + 7\Delta^+\phi_i - \Delta^+\phi_{i+1}) \\ & -\phi^{WENO}(\Delta^-\Delta^+\phi_{i-2}, \Delta^-\Delta^+\phi_{i-1}, \Delta^-\Delta^+\phi_i, \Delta^-\Delta^+\phi_{i+1}),\end{aligned} \tag{3.111}$$

where[49]

$$\phi^{WENO}(a,b,c,d) = \frac{1}{3}\omega_0(a-2b+c) + \frac{1}{6}(\omega_2 - \frac{1}{2})(b-2c+d) \quad (3.112)$$

and the weights ω_0 and ω_2 are defined as

$$\omega_0 = \frac{\alpha_0}{\alpha_0+\alpha_1+\alpha_2}, \quad (3.113)$$

$$\omega_2 = \frac{\alpha_2}{\alpha_0+\alpha_1+\alpha_2}, \quad (3.114)$$

where

$$\begin{aligned} \alpha_0 &= \frac{1}{(\delta_\epsilon + IS_0)^2}, \\ \alpha_1 &= \frac{6}{(\delta_\epsilon + IS_1)^2}, \alpha_2 = \frac{3}{(\delta_\epsilon + IS_2)^2}, \\ IS_0 &= 13(a-b)^2 + 3(a-3b)^2, \\ IS_1 &= 13(b-c)^2 + 3(b+c)^2, \\ IS_2 &= 13(c-d)^2 + 3(3c-d)^2. \end{aligned} \quad (3.115)$$

Here, δ_ϵ is used to prevent the denominators from becoming zero. We set $\delta_\epsilon = 10^{-16}$.

By symmetry, the fifth-order WENO for $\phi^+_{\xi,i}$ on the right-biased stencil $\{i+s-2, i+s-1, i+s, i+s+1\}$ for $s = 0, 1$, and 2, can be written as

$$\begin{aligned} \phi^+_{\xi,i} &= \frac{1}{12}(-\Delta^+\phi_{i-2} + 7\Delta^+\phi_{i-1} + 7\Delta^+\phi_i - \Delta^+\phi_{i+1}) \\ &+\phi^{WENO}(\Delta^-\Delta^+\phi_{i+2}, \Delta^-\Delta^+\phi_{i+1}, \Delta^-\Delta^+\phi_i, \Delta^-\Delta^+\phi_{i-1}). \end{aligned} \quad (3.116)$$

For the general 3D case, the fifth-order Hamilton-Jacobi WENO approximations for the first derivative of ϕ with respect to ξ, η, and ζ are:

$$\begin{aligned} \phi^\pm_{\xi,i,j,k} &= \frac{1}{12}(-\Delta^+_\xi\phi_{i-2,j,k} + 7\Delta^+_\xi\phi_{i-1,j,k} + 7\Delta^+_\xi\phi_{i,j,k} - \Delta^+_\xi\phi_{i+1,j,k}) \\ &\pm\phi^{WENO}(\Delta^-_\xi\Delta^+_\xi\phi_{i\pm2,j,k}, \Delta^-_\xi\Delta^+_\xi\phi_{i\pm1,j,k}, \Delta^-_\xi\Delta^+_\xi\phi_{i,j,k}, \Delta^-_\xi\Delta^+_\xi\phi_{i\mp1,j,k}), \end{aligned} \quad (3.117)$$

$$
\begin{aligned}
\phi^{\pm}_{\eta,i,j,k} &= \frac{1}{12}(-\Delta^{+}_{\eta}\phi_{i,j-2,k} + 7\Delta^{+}_{\eta}\phi_{i,j-1,k} + 7\Delta^{+}_{\eta}\phi_{i,j,k} - \Delta^{+}_{\eta}\phi_{i,j+1,k}) \\
&\pm\phi^{WENO}(\Delta^{-}_{\eta}\Delta^{+}_{\eta}\phi_{i\pm 2,j,k}, \Delta^{-}_{\eta}\Delta^{+}_{\eta}\phi_{i\pm 1,j,k}, \Delta^{-}_{\eta}\Delta^{+}_{\eta}\phi_{i,j,k}, \Delta^{-}_{\eta}\Delta^{+}_{\eta}\phi_{i\mp 1,j,k}), \quad (3.118) \\
\phi^{\pm}_{\zeta,i,j,k} &= \frac{1}{12}(-\Delta^{+}_{\zeta}\phi_{i,j,k-2} + 7\Delta^{+}_{\zeta}\phi_{i,j,k-1} + 7\Delta^{+}_{\zeta}\phi_{i,j,k} - \Delta^{+}_{\zeta}\phi_{i,j,k+1}) \\
&\pm\phi^{WENO}(\Delta^{-}_{\zeta}\Delta^{+}_{\zeta}\phi_{i,j,k\pm 2}, \Delta^{-}_{\zeta}\Delta^{+}_{\zeta}\phi_{i,j,k\pm 1}, \Delta^{-}_{\zeta}\Delta^{+}_{\zeta}\phi_{i,j,k}, \Delta^{-}_{\zeta}\Delta^{+}_{\zeta}\phi_{i,j,k\mp 1}). \quad (3.119)
\end{aligned}
$$

If we define a^+, b^-, c^+, d^-, e^+, and f^+ as follows:

$$
\begin{aligned}
a^+ &\equiv \max(a,0),\ b^- \equiv \min(b,0), \\
c^+ &\equiv \max(c,0),\ d^- \equiv \min(d,0), \\
e^+ &\equiv \max(e,0),\ f^- \equiv \min(f,0). \qquad (3.120)
\end{aligned}
$$

Then ϕ_ξ , ϕ_η , and ϕ_ζ can be calculated as follows:

$$
\begin{aligned}
\phi_\xi &\equiv f_s(a^+,b^-)\sqrt{\max[(a^+)^2,(b^-)^2]}, \\
\phi_\eta &\equiv f_s(c^+,d^-)\sqrt{\max[(c^+)^2,(d^-)^2]}, \\
\phi_\zeta &\equiv f_s(e^+,f^-)\sqrt{\max[(e^+)^2,(f^-)^2]}, \qquad (3.121)
\end{aligned}
$$

where f_s is given by

$$
f_s(a^+,b^-) = \begin{cases} sign(a) & if\ \max[(a^+)^2,(b^-)^2 = (a^+)^2, \\ sign(b) & if\ \max[(a^+)^2,(b^-)^2 = (b^-)^2. \end{cases} \qquad (3.122)
$$

For points that don't have a complete WENO stencil, second-order schemes are used to get the gradient of ϕ: one-sided second-order scheme for points on the boundary and central second-order scheme for the rest. The formulations are shown in Eqns. (3.98), (3.99), and (3.100).

3.5 Discretization of Volume of Fluid Equation

The integral form for the volume of fluid equation is

$$\int_\Omega \frac{\partial F}{\partial t} dV + \int F\mathbf{U} \cdot \mathbf{n}_S dA = 0. \tag{3.123}$$

Its discretization on a given cell volume ΔV is

$$\frac{\partial F}{\partial t}\Delta V + \sum_f^{N_{faces}} F_f \mathbf{U}_f \cdot \mathbf{A}_f = 0. \tag{3.124}$$

The first-order explicit temporal discretization is used,

$$\frac{F^{n+1} - F^n}{\Delta t}\Delta V + \sum_f^{N_{faces}} F_f^n \mathbf{U}_f^n \cdot \mathbf{A}_f = 0. \tag{3.125}$$

The face value of F is achieved by the second-order upwind scheme.

$$F_f = F + \nabla F \cdot \mathbf{r}, \tag{3.126}$$

where F and ∇F are the cell-centered value and its gradient in the upstream cell, and $\mathbf{r}$ is the displacement vector from the centroid of the upstream cell to that of the face.

3.6 Coupling Method

3.6.1 Reconstruction of level set values with planes in partial cells

After solving the convection equations of the level set function ϕ and the volume fraction value F, we need to use F to correct ϕ before solving the reinitialization equation of ϕ. This is exactly where the coupling between LS and VOF methods happens, which is necessary to overcome the volume loss problem of the original LS method. To make this correction feasible, we first need to define the interface in the cell Ω_{ijk} as a plane (a straight line in

2D). As in Sussman and Puckett [64] , the following reconstructed level set ϕ^R_{ijk} is defined:

$$\phi^R_{ijk}(x,y,z) = a_{ijk}(x-x_i) + b_{ijk}(y-y_j) + c_{ijk}(z-z_k) + d_{ijk}. \tag{3.127}$$

When the equation is normalized such that $a^2_{ijk} + b^2_{ijk} + c^2_{ijk} = 1$, as pointed out by Menard et al [65], the unit vector $\mathbf{n}_{ijk} = (a_{ijk}, b_{ijk}, c_{ijk})$ represents the normal to the interface. Correspondingly, d_{ijk} denotes the normal distance from the cell center $(x_{ijk}, y_{ijk}, z_{ijk})$ to the interface.

To make ϕ^R_{ijk} an accurate approximation to the original level set function ϕ, as in Sussman and Puckett [64], we minimize the following L_2 error:

$$E_{ijk} = \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{z_{k-1/2}}^{z_{k+1/2}} \delta(\phi)\left(\phi - \phi^R_{ijk}(x,y,z)\right) \mathrm{dxdydz}. \tag{3.128}$$

We choose a 27-point stencil and the discrete form of the above error function reads[65]:

$$E_{ijk} = \sum_{i'=i-1}^{i'=i+1} \sum_{j'=j-1}^{j'=j+1} \sum_{k'=k-1}^{k'=k+1} w_{i'-i,j'-j,k'-k}\delta_\epsilon(\phi_{i'j'k'})\left(\phi_{i'j'k'} - \phi^R_{ijk}(x,y,z)\right), \tag{3.129}$$

where $\delta_\epsilon(\phi)$ is the smoothed Dirac function with the thickness $\epsilon = \sqrt{2}min(dx, dy, dz$, where dx, dy, and dz are space step size. $W_{\alpha,\beta,\gamma}$ are weights that are larger on the central cell (i,j,k) and smaller on the surrounding cells (i',j',k'). In particular, we choose a ratio of 16 between central cell weight and those of the surrounding cells as in Menard *et al.*[65]:

$$w_{l,m,n} = \begin{cases} 16 & (l,m,n) = (0,0,0) \\ 1 & (l,m,n) \neq (0,0,0) \end{cases}. \tag{3.130}$$

To minimize E_{ijk}, its first order derivatives with respect to a_{ijk}, b_{iijk}, c_{ijk}, and d_{ijk} should all vanish:

$$\frac{\partial E_{ijk}}{\partial a_{ijk}} = \frac{\partial E_{ijk}}{\partial b_{ijk}} = \frac{\partial E_{ijk}}{\partial c_{ijk}} = \frac{\partial E_{ijk}}{\partial d_{ijk}} = 0, \tag{3.131}$$

which leads to the following linear system:

$$\begin{bmatrix} \sum\sum\sum whX^2 & \sum\sum\sum whXY & \sum\sum\sum whXZ & \sum\sum\sum whX \\ \sum\sum\sum whXY & \sum\sum\sum whY^2 & \sum\sum\sum whYZ & \sum\sum\sum whY \\ \sum\sum\sum whXZ & \sum\sum\sum whYZ & \sum\sum\sum whZ^2 & \sum\sum\sum whZ \\ \sum\sum\sum whX & \sum\sum\sum whY & \sum\sum\sum whZ & \sum\sum\sum wh \end{bmatrix} \cdot \begin{bmatrix} a_{ijk} \\ b_{ijk} \\ c_{ijk} \\ d_{ijk} \end{bmatrix} = \begin{bmatrix} \sum\sum\sum whX\phi \\ \sum\sum\sum whY\phi \\ \sum\sum\sum whZ\phi \\ \sum\sum\sum wh\phi \end{bmatrix}, \tag{3.132}$$

where the following abbreviations are adopted:

$$\sum\sum\sum = \sum_{i'=i-1}^{i'=i+1} \sum_{j'=j-1}^{j'=j+1} \sum_{k'=k-1}^{k'=k+1},\ wh = w_{i'-i,j'-j,k'-k}\delta_\epsilon\left(\phi_{i'j'k'}\right),$$
$$X = \left(x_{i'} - x_i\right),\ Y = \left(y_{j'} - y_j\right),\ Z = \left(z_{k'} - z_k\right),\ \phi = \phi_{i'j'k'}. \tag{3.133}$$

To solve the above linear system, we use the Gaussian elimination method with pivoting as illustrated in Press *et al.* [66].

3.6.2 Correct level set values with volume fractions

With the plane reconstruction of level set values, we are ready to correct them with the knowledge of volume fractions, in order to avoid mass loss. The essence of this correction is based on the idea that the volume of liquid in a given partial cell must be the same, no matter what method is used to calculate it. More specifically, the liquid volumes calculated from the level set plane and from the result of the convection equation of the liquid volume fraction should agree with each other. If we use F_{ijk} to denote the volume fraction of liquid, we obtain [65]:

$$\frac{1}{\mathrm{dxdydz}} \int_{z_{k-1/2}}^{z_{k+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} H\left(\phi_{ijk}^R\left(x,y,z\right)\right) \mathrm{dxdydz} = F_{ijk}. \tag{3.134}$$

Practically, the above equality will not be satisfied after we solve the advection equations of ϕ_{ijk} and F_{ijk} by using FLUENT, as a result, the Newton iterative method is adopted to modify the parameter d_{ijk} until a given precision is satisfied for the above equation:

$$d_{ijk}^{\text{new}} = d_{ijk} - \frac{\frac{1}{\text{dxdydz}} \int_{z_{k-1/2}}^{z_{k+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} H\left(\phi_{ijk}^{R}(x,y,z)\right) \text{dxdydz} - F_{ijk}}{\frac{1}{\text{dxdydz}} \int_{z_{k-1/2}}^{z_{k+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} \delta\left(\phi_{ijk}^{R}(x,y,z)\right) \text{dxdydz}}. \tag{3.135}$$

It is important to note that the Newton iterations are only performed for the cells around the interface between air and liquid.

3.7 Surface Tension Force for Multiphase Flow

The momentum equations have surface tension terms in two-phase flow. The surface tension term is approximated using the CSF (Continuum Surface Force) model, as in Eqn. (2.64). The DEFINE_SOURCE UDF specifies custom source term for momentum equations in FLUENT,

$$source \;\; term = \sigma\kappa(\phi)\mathbf{n}\delta_{\epsilon}(\phi). \tag{3.136}$$

We need to determine the interface curvature, κ, and the normal to the interface, $\mathbf{n}$. Utilizing level set function, ϕ, curvature and normal to the interface are computed through DEFINE_ADJUST function and are then stored in the User Defined Memory (UDM) for each cell center.

By definition of the normal vector to a level surface, the unit normal $\vec{n}$ is achieved by normalizing $\nabla\phi$ with $|\nabla\phi|$:

$$n_x = \frac{\partial\phi}{\partial x}/[(\frac{\partial\phi}{\partial x})^2 + (\frac{\partial\phi}{\partial y})^2 + (\frac{\partial\phi}{\partial z})^2]^{1/2}, \tag{3.137}$$

$$n_y = \frac{\partial\phi}{\partial y}/[(\frac{\partial\phi}{\partial x})^2 + (\frac{\partial\phi}{\partial y})^2 + (\frac{\partial\phi}{\partial z})^2]^{1/2}, \tag{3.138}$$

$$n_z = \frac{\partial\phi}{\partial z}/[(\frac{\partial\phi}{\partial x})^2 + (\frac{\partial\phi}{\partial y})^2 + (\frac{\partial\phi}{\partial z})^2]^{1/2}. \tag{3.139}$$

The mean surface curvature is computed by taking the partial derivatives of the unit normal components in the manner consistent with the partial derivatives of ϕ:

$$\frac{\partial n_x}{\partial x} = J[(\frac{\xi_x}{J}n_x)_\xi + (\frac{\eta_x}{J}n_x)_\eta + (\frac{\zeta_x}{J}n_x)_\zeta)], \tag{3.140}$$

$$\frac{\partial n_y}{\partial y} = J[(\frac{\xi_y}{J}n_y)_\xi + (\frac{\eta_y}{J}n_y)_\eta + (\frac{\zeta_y}{J}n_y)_\zeta)], \tag{3.141}$$

$$\frac{\partial n_z}{\partial z} = J[(\frac{\xi_z}{J}n_z)_\xi + (\frac{\eta_z}{J}n_z)_\eta + (\frac{\zeta_z}{J}n_z)_\zeta], \tag{3.142}$$

$$\Longrightarrow \kappa = \frac{\partial n_x}{\partial x} + \frac{\partial n_y}{\partial y} + \frac{\partial n_z}{\partial z}. \tag{3.143}$$

Each component of the partial derivatives is evaluated using second-order finite differences as Eqs. (3.98), (3.99), and (3.100).

We now discuss the computation of the metrics. Metrics are solved numerically through the expressions by x_ξ, x_η, x_z, etc., which can be computed by finite difference approximations. To obtain the relations, the differential expressions are considered:

$$\begin{aligned} dx &= \frac{\partial x}{\partial \xi}d\xi + \frac{\partial x}{\partial \eta}d\eta + \frac{\partial x}{\partial \zeta}d\zeta, \\ dy &= \frac{\partial y}{\partial \xi}d\xi + \frac{\partial y}{\partial \eta}d\eta + \frac{\partial y}{\partial \zeta}d\zeta, \\ dz &= \frac{\partial z}{\partial \xi}d\xi + \frac{\partial z}{\partial \eta}d\eta + \frac{\partial z}{\partial \zeta}d\zeta. \end{aligned} \tag{3.144}$$

The above equations can be cast in a matrix form:

$$\begin{bmatrix} dx \\ dy \\ dz \end{bmatrix} = \begin{bmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ y_\xi & y_\eta & y_\zeta \end{bmatrix} \begin{bmatrix} d\xi \\ d\eta \\ d\zeta. \end{bmatrix} \tag{3.145}$$

Inverting, we have

$$\begin{aligned} d\xi &= \frac{\partial \xi}{\partial x}dx + \frac{\partial \eta}{\partial y}dy + \frac{\partial \zeta}{\partial z}dz, \\ d\eta &= \frac{\partial \eta}{\partial x}dx + \frac{\partial \eta}{\partial y}dy + \frac{\partial \eta}{\partial z}dz, \end{aligned}$$

$$d\zeta = \frac{\partial \zeta}{\partial x}dx + \frac{\partial \zeta}{\partial y}dy + \frac{\partial \zeta}{\partial z}dz, \tag{3.146}$$

or

$$\begin{bmatrix} d\xi \\ d\eta \\ d\zeta \end{bmatrix} = \begin{bmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{bmatrix} \begin{bmatrix} dx \\ dy \\ dz. \end{bmatrix} \tag{3.147}$$

Comparing the two matrices, we see that

$$\begin{bmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{bmatrix} = \begin{bmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ y_\xi & y_\eta & y_\zeta \end{bmatrix}^{-1}, \tag{3.148}$$

from which

$$\xi_x = J(y_\eta z_\zeta - y_\zeta z_\eta), \xi_y = J(x_\zeta z_\eta - x_\eta z_\zeta), \xi_z = J(x_\eta y_\zeta - x_\zeta y_\eta), \tag{3.149}$$

$$\eta_x = J(y_\zeta z_\xi - y_\xi z_\zeta), \eta_y = J(x_\xi z_\zeta - x_\zeta z_\xi), \eta_z = J(x_\zeta y_\xi - x_\xi y_\zeta), \tag{3.150}$$

$$\zeta_x = J(y_\xi z_\eta - y_\eta z_\xi), \zeta_y = J(x_\eta z_\xi - x_\xi z_\eta), \zeta_z = J(x_\xi y_\eta - x_\eta y_\xi), \tag{3.151}$$

where J is the Jacobian of transformation defined by

$$J = \frac{\partial(\xi, \eta, \zeta)}{\partial(x, y, z)} = \frac{1}{x_\xi(y_\eta z_\zeta - y_\zeta z_\eta) + x_\eta(y_\zeta z_\xi - y_\xi z_\zeta) + x_\zeta(y_\xi z_\eta - y_\eta z_\xi)}. \tag{3.152}$$

In 2D problem, the expression for J is

$$J = [\frac{\partial(x, y)}{\partial(\xi, \eta)}]^{-1} = (x_\xi y_\eta - x_\eta y_\xi)^{-1}, \tag{3.153}$$

so that

$$\xi_x = J * y_\eta,\ \xi_y = -J * x_\eta,\ \eta_x = -J * y_\xi,\ \eta_y = J * x_\xi. \tag{3.154}$$

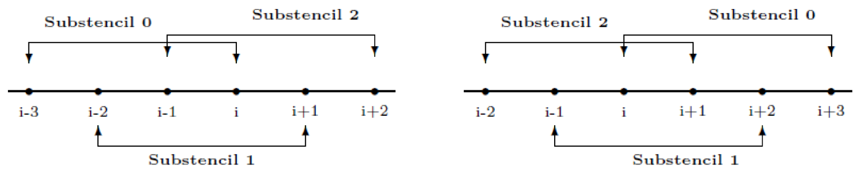

Figure 3.3: The three substencils: (a) the left-biased stencil; (b) the right-biased stencil

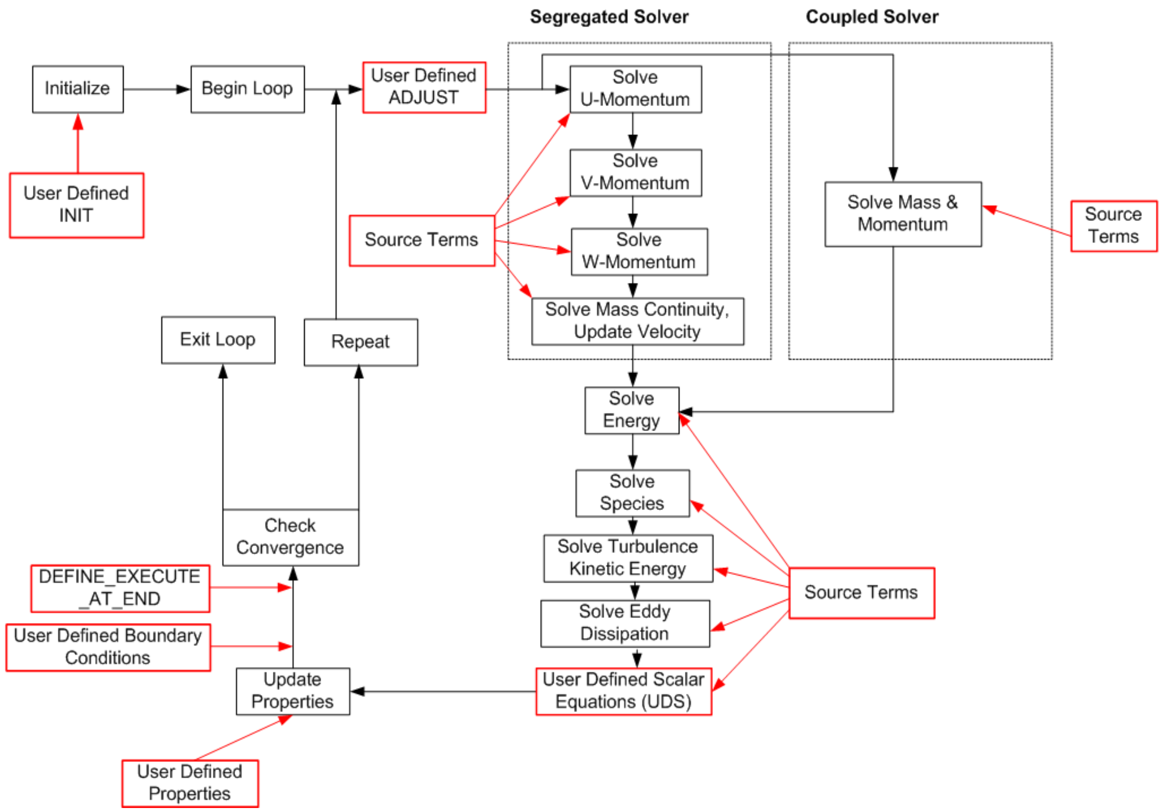

Figure 3.4: Solution procedure for the pressure-based segregated/coupled solver

Second-order finite differences are used to discretize the derivatives $x_\xi, x_\eta, x_\zeta, y_\xi, y_\eta, y_\zeta, z_\xi, z_\eta$, and z_ζ. The procedure is the same as those shown in Eqs. (3.98), (3.99), and (3.100).

Chapter 4

Numerical Verification and Validation

4.1 Understanding the Secondary Flows in Curved Pipes

For better understanding of the secondary flows in a curved pipe, we compare the governing equations for a curved pipe with those for a straight pipe and study the terms that represent the differences between two sets of equations. We decompose the equations for a curved pipe as follows

$$\widetilde{L}_c(u^*, v^*, w^*) = L_c(u^*, v^*, w^*) + D_c^*, \tag{4.1}$$

$$\widetilde{L}_{M_1}(u^*, v^*, w^*) = L_{M_1}(u^*, v^*, w^*) + D_r^*, \tag{4.2}$$

$$\widetilde{L}_{M_2}(u^*, v^*, w^*) = L_{M_2}(u^*, v^*, w^*) + D_\theta^*, \tag{4.3}$$

$$\widetilde{L}_{M_3}(u^*, v^*, w^*) = L_{M_3}(u^*, v^*, w^*) + D_{\widetilde{z}}^*, \tag{4.4}$$

where the first terms on the right-hand side of the equations represent the contribution of a straight pipe and the remaining terms are due to curvature. The latter can easily be written as follows:

$$D_c^* \equiv \frac{\partial w^*}{\partial \widetilde{z}^*}\left(\frac{1}{\sqrt{g_{33}}} - 1\right) + \Gamma_{31}^{3*} u^* + \Gamma_{32}^{3*} \frac{v^*}{r^*}, \tag{4.5}$$

$$D_r^* \equiv w^* \frac{\partial u^*}{\partial \tilde{z}^*}(\frac{1}{\sqrt{g_{33}}} - 1) + \Gamma_{33}^{1*} \frac{w^{*2}}{g_{33}} - \frac{1}{Re}[\frac{\partial^2 u^*}{\partial \tilde{z}^{*2}}(\frac{1}{g_{33}} - 1) + \frac{\Gamma_{33}^{1*}}{g_{33}}(\Gamma_{13}^{3*} u^* + \Gamma_{23}^{3*} \frac{v^*}{r^*} - \frac{\partial u^*}{\partial r^*})$$
$$+ \frac{\Gamma_{33}^{2*}}{g_{33}}(v^* - \frac{\partial u^*}{\partial \theta^*}) - \frac{\Gamma_{33}^{3*}}{g_{33}} \frac{\partial u^*}{\partial \tilde{z}^*} + \frac{1}{g_{33}}\{\frac{w^*}{\sqrt{g_{33}}} \frac{\partial}{\partial \tilde{z}^*}(\Gamma_{33}^{1*}) + 2\Gamma_{33}^{1*} \frac{\partial}{\partial \tilde{z}^*}(\frac{w^*}{\sqrt{g_{33}}})\}], \tag{4.6}$$

$$D_\theta^* \equiv w^* \frac{\partial v^*}{\partial \tilde{z}^*}(\frac{1}{\sqrt{g_{33}}} - 1) + \Gamma_{33}^{2*} \frac{r^* w^{*2}}{g_{33}} - \frac{1}{Re}[\frac{\partial^2 v^*}{\partial \tilde{z}^{*2}}(\frac{1}{g_{33}} - 1) + \frac{\Gamma_{33}^{2*}}{g_{33}}(\Gamma_{13}^{3*} r^* u^* - u^* + \Gamma_{23}^{3*} v^*$$
$$- \frac{\partial v^*}{\partial \theta^*}) - \frac{\Gamma_{33}^{1*}}{g_{33}} \frac{\partial v^*}{\partial r^*} - \frac{\Gamma_{33}^{3*}}{g_{33}} \frac{\partial v^*}{\partial \tilde{z}^*} + \frac{r^*}{g_{33}}\{\frac{w^*}{\sqrt{g_{33}}} \frac{\partial}{\partial \tilde{z}^*}(\Gamma_{33}^{2*}) + 2\Gamma_{33}^{2*} \frac{\partial}{\partial \tilde{z}^*}(\frac{w^*}{\sqrt{g_{33}}})\}], \tag{4.7}$$

$$D_{\tilde{z}}^* \equiv (u^* \frac{\partial w^*}{\partial r^*} + \frac{v^*}{r^*} \frac{\partial w^*}{\partial \theta^*})(\frac{1}{\sqrt{g_{33}}} - 1) - \frac{w^*}{g_{33}}(u^* \frac{\partial \sqrt{g_{33}}}{\partial r^*} - \frac{v^*}{r^*} \frac{\partial \sqrt{g_{33}}}{\partial \theta^*})$$
$$+ (w^* \frac{\partial w^*}{\partial \tilde{z}^*} + \frac{\partial p^*}{\partial \tilde{z}^*})(\frac{1}{g_{33}} - 1) + \frac{2w^*}{\sqrt{g_{33}}}(\Gamma_{31}^{3*} u^* + \Gamma_{32}^{3*} \frac{v^*}{r^*})$$
$$- \frac{1}{Re}[(\frac{1}{\sqrt{g_{33}}} - 1)(\frac{\partial^2 w^*}{\partial r^{*2}} + \frac{1}{r^*} \frac{\partial w^*}{\partial r^*} + \frac{1}{r^{*2}} \frac{\partial^2 w^*}{\partial \theta^{*2}}) + (\frac{1}{(\sqrt{g_{33}})^3} - 1) \frac{\partial^2 w^*}{\partial \tilde{z}^{*2}}$$
$$- (\frac{2}{g_{33}} \frac{\partial w^*}{\partial r^*} - \frac{w^*}{g_{33}^2} \frac{\partial g_{33}}{\partial r^*} + \frac{w^*}{r^* g_{33}}) \frac{\partial \sqrt{g_{33}}}{\partial r^*} - (\frac{2}{g_{33}} \frac{\partial w^*}{\partial \theta^*} - \frac{w^*}{g_{33}^2} \frac{\partial g_{33}}{\partial \theta^*}) \frac{1}{r^{*2}} \frac{\partial \sqrt{g_{33}}}{\partial \theta^*}$$
$$- \frac{1}{g_{33}^2} \frac{\partial w^*}{\partial \tilde{z}^*} \frac{\partial \sqrt{g_{33}}}{\partial \tilde{z}^*} - \frac{w^*}{g_{33}}(\frac{\partial^2 \sqrt{g_{33}}}{\partial r^{*2}} + \frac{1}{r^{*2}} \frac{\partial^2 g_{33}}{\partial \theta^{*2}}) + \frac{w^*}{\sqrt{g_{33}}}\{\frac{\partial}{\partial r^*}(\Gamma_{13}^{2*}) + \frac{1}{r^{*2}} \frac{\partial}{\partial \theta^*}(\Gamma_{23}^{3*})\}$$
$$+ \frac{1}{g_{33}}\{u^* \frac{\partial}{\partial \tilde{z}^*}(\Gamma_{13}^{3*}) + \frac{v^*}{r^*} \frac{\partial}{\partial \tilde{z}^*}(\Gamma_{23}^{3*})\} + \Gamma_{13}^{3*}\{\frac{2}{g_{33}} \frac{\partial u^*}{\partial \tilde{z}^*} + 2\frac{\partial}{\partial r^*}(\frac{w^*}{\sqrt{g_{33}}}) + \frac{1}{r^*} \frac{w^*}{\sqrt{g_{33}}}\}$$
$$+ \frac{w^*}{\sqrt{g_{33}}}\{(\Gamma_{12}^{3*})^2 + (\frac{\Gamma_{33}^{3*}}{r^*})^2\} + \frac{\Gamma_{23}^{3*}}{r^{*2}}\{\frac{2r^*}{g_{33}} \frac{\partial v^*}{\partial \tilde{z}^*} + 2\frac{\partial}{\partial \theta^*}(\frac{w^*}{\sqrt{g_{33}}})\}$$
$$- \frac{1}{g_{33}}\{\Gamma_{33}^{1*} \frac{\partial}{\partial r^*}(\frac{w^*}{\sqrt{g_{33}}}) + \Gamma_{33}^{2*} \frac{\partial}{\partial \theta^*}(\frac{w^*}{\sqrt{g_{33}}})\}]. \tag{4.8}$$

For fully-developed laminar flow in a straight pipe, $D_c^* = D_r^* = D_\theta^* = D_{\tilde{z}}^* = 0$ when $g_{33} = 0$, $\kappa_c = 0$, $L = 0$, $\Gamma_{ij}^{k*} = 0$, $u^* = v^* = 0$, and $w^* = w^*(r^*)$. For fully-developed laminar flow in the sinusoidal pipe configuration, Eqs. (2.10) to (2.13), and the conditions $u^* = u^*(r^*, \theta^*)$, $v^* = v^*(r^*, \theta^*)$, and $w^* = w^*(r^*, \theta^*)$ lead to the following simplification of the curvature terms:

$$D_c^*(u^*, v^*, w^*) \equiv \Gamma_{31}^{3*} u^* + \Gamma_{32}^{3*} \frac{v^*}{r^*} = \frac{\kappa_c \cos\theta^*}{1 + r^* \kappa_c \cos\theta^*} u^* - \frac{\kappa_c \sin\theta^*}{1 + r^* \kappa_c \cos\theta^*} v^*, \tag{4.9}$$
$$D_r^*(u^*, v^*, w^*) \equiv \Gamma_{33}^{1*} \frac{w^{*2}}{g_{33}} = -\frac{w^{*2} \kappa_c \cos\theta^*}{1 + r^* \kappa_c \cos\theta^*}, \tag{4.10}$$
$$D_\theta^*(u^*, v^*, w^*) \equiv \Gamma_{33}^{2*} \frac{r^* w^{*2}}{g_{33}} = \frac{w^{*2} \kappa_c \sin\theta^*}{1 + r^* \kappa_c \cos\theta^*}, \tag{4.11}$$

$$
\begin{aligned}
&D^*_{\tilde{z}}(u^*, v^*, w^*) \equiv (u^*\frac{\partial w^*}{\partial r^*} + \frac{v^*}{r^*}\frac{\partial w^*}{\partial \theta^*})(\frac{1}{\sqrt{g_{33}}} - 1) - \frac{w^*}{g_{33}}(u^*\frac{\partial \sqrt{g_{33}}}{\partial r^*} - \frac{v^*}{r^*}\frac{\partial \sqrt{g_{33}}}{\partial \theta^*}) \\
&+\frac{\partial p^*}{\partial \tilde{z}^*}(\frac{1}{g_{33}} - 1) + \frac{2w^*}{\sqrt{g_{33}}}(\Gamma^{3*}_{31}u^* + \Gamma^{3*}_{32}\frac{v^*}{r^*}) \\
&= (u^*\frac{\partial w^*}{\partial r^*} + \frac{v^*}{r^*}\frac{\partial w^*}{\partial \theta^*})[\frac{1}{L(1 + r\kappa_c \cos\theta^*)} - 1] - \frac{w^*}{g_{33}}(u^*\frac{\partial \sqrt{g_{33}}}{\partial r^*} \\
&-\frac{v^*}{r^*}\frac{\partial \sqrt{g_{33}}}{\partial \theta^*}) + \frac{\partial p^*}{\partial \tilde{z}^*}(\frac{1}{L^2(1 + r\kappa_c \cos\theta^*)^2} - 1) \\
&+\frac{2w^*}{\sqrt{g_{33}}}\kappa_c\frac{\cos\theta^* u^* - \sin\theta^* v^*}{1 + r^*\kappa_c \cos\theta^*}.
\end{aligned}
\tag{4.12}
$$

We propose that Eqns. (4.10) and (4.11) describe the secondary flows in a curved pipe. To test this hypothesis, we evaluate these terms (D^*_r and D^*_θ) using velocities obtained from a straight pipe, and compare the results to the velocities (u^* and v^*) obtained directly from a numerical simulation of the flow in a curved pipe. Physically, D^*_r and D^*_θ represent inertial forces caused by the presence of the curvature, with units in Newtons when expressed in dimensional form. The profiles of u^* and v^* are plotted in Fig. 4.1(a) and Fig. 4.1(b), respectively. The iso-contours of D^*_r and D^*_θ are obtained by substituting the straight-pipe velocity solutions into the expression for these terms. The results are shown in Fig. 4.1(c) and Fig. 4.1(d). The qualitative similarity between Fig. 4.1(a) (Fig. 4.1(b)) and Fig. 4.1 (c) (Fig. 4.1(d)) support the suggestion that the inertial terms identified above contribute to the secondary flow in curved pipes. The inertial terms identified in this paper are consistent with the centrifugal force terms discussed in Berger *et al.* [106]. It is also important to note that D^*_r and D^*_θ do not include the terms v^{*2}/r^* and u^*v^*/r^*, respectively. Although these other terms were referred to as centrifugal force terms in Webster and Humphrey [107], it seems as if their significance is found in their ability to promote instability, even in a straight pipe.

The authors acknowledge that the procedure just described for identifying the secondary flow terms in the equations is ad hoc. A more rigorous approach could try to isolate explicit, physically-meaningful terms in the momentum equations, in the same manner that the Navier-Stokes equations in a rotating frame of reference involve the additional terms

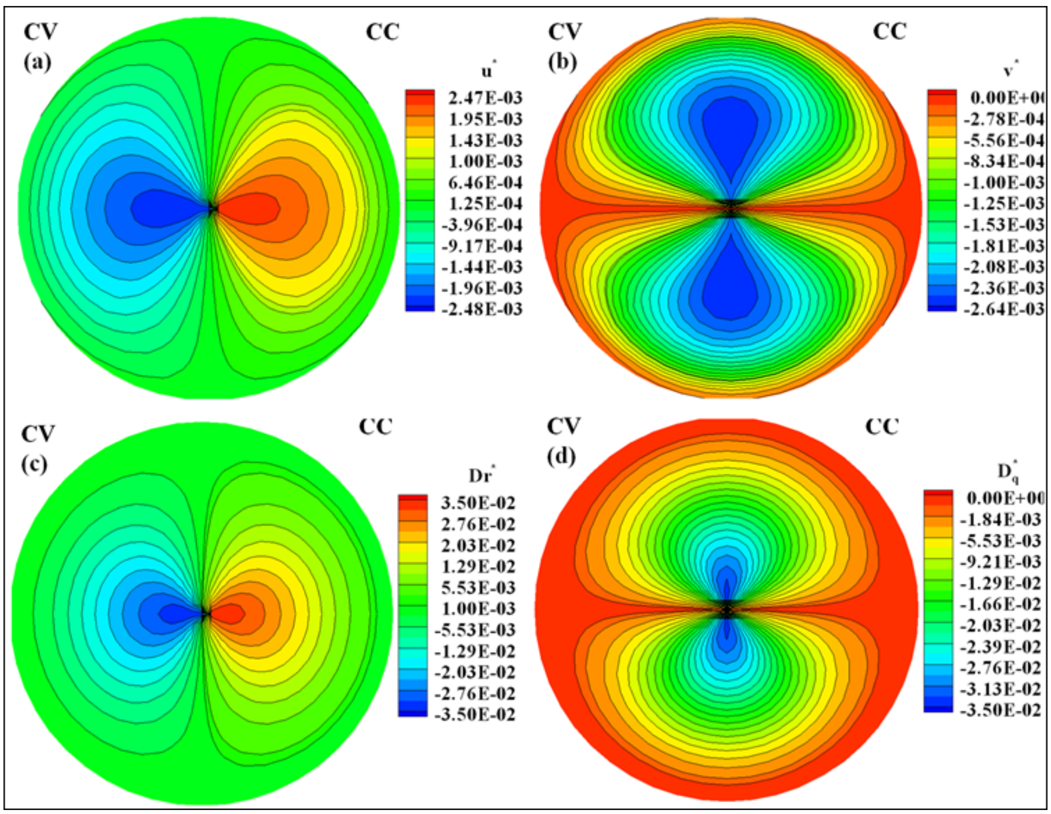

Figure 4.1: Contour plots of (a) u^*, (b) v^*, (c) D_r^*, and (d) D_θ^* at $x = 60$ of the periodically-curved pipe ($Re = 1000$)

$\rho[\mathbf{\Omega} \times \mathbf{\Omega} \times \mathbf{r} + 2\mathbf{\Omega} \times \mathbf{u}]$ [108], which, respectively, consist of the centrifugal and Coriolis force fields. ($\mathbf{\Omega}$, $\mathbf{r}$ and $\mathbf{u}$ are the vectors of angular velocity, position, and instantaneous rotating frame velocity, respectively.) The present problem appears to be more complicated and the foregoing analysis has been carried out only for insight.

4.2 Realizable $k - \varepsilon$ Model For Flow in Curved Pipes

SA, SKE, and RKE models are applied to simulate turbulence flow in a 90° bend curved pipe. The results show that RKE model has a better performance than the other two. The test conditions are taken from Sudo [12] and consist of a 90° bend (Fig. 4.2) with $\delta = 1/4$. The pipe has a 100-diameter upstream tangent section and a 40-diameter downstream tangent section. The results are compared in Fig. 4.3 for the static pressure coefficient, C_p, at 17.6 diameters upstream of the bend. The variable s is a pseudo coordinate direction, introduced in this section for the purpose of describing the locations on the straight (tangent) portions of the pipe. This consists of the upstream tangent ($-1 \leq s \leq 0^-$) and the region after the bend ($0^+ \leq s \leq 5$). Note that $\theta = -90°$ is the convex side of the bend, while $\theta = 90°$ is the concave side, which is consistent with the use in Sudo's experiment. Fairly close agreement between the methods is apparent. However, the RKE results match the experimental data better than the results from SA and SKE for the three locations plotted in Figure 4.3. Thus, the RKE model is used for subsequent pipe calculations in this paper.

4.3 Numerical Validations of the Developed CLSVOF Model

Numerical tests are presented in this section to verify and validate the accuracy and stability of the CLSVOF method. The ϵ in Eq. (2.55) is set to $1.5\Delta x$, where Δx is the mesh size in the x direction. The CLSVOF method is validated with two forms of convection velocities: constant velocity and vortex velocity. Pure movements of interface are expected without any deformation under constant velocity with the goal to validate the CLSVOF

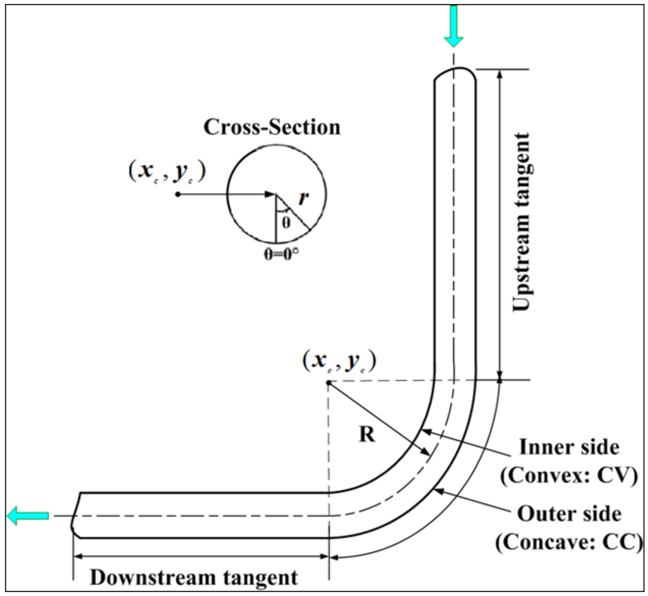

Figure 4.2: The sketch of a curved pipe with a 90° bend. CV implies "convex (inner) side", CC is "concave (outer) side", (x_c, y_c) denotes the curvature center and R is the radius of curvature

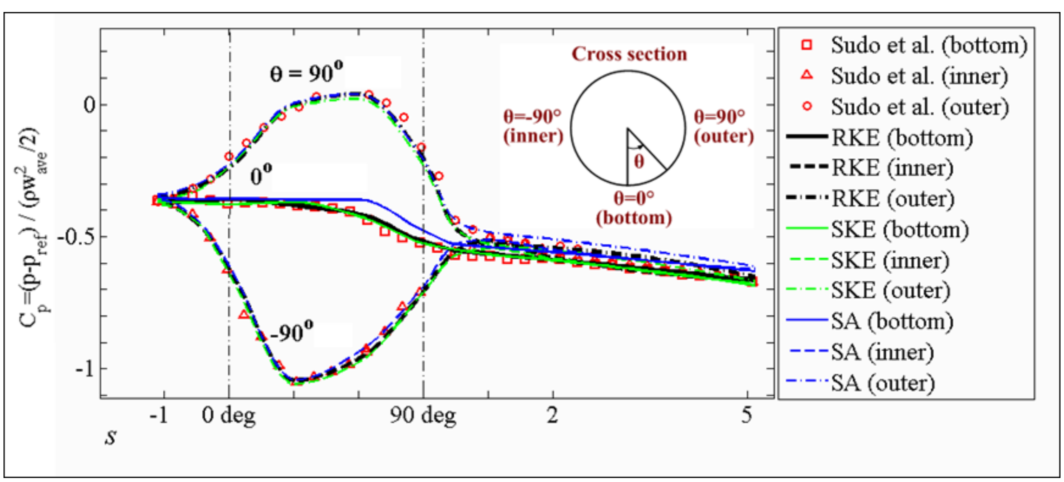

Figure 4.3: Longitudinal distribution of static pressure at the convex ($\theta = -90°$), concave ($\theta = 90°$) and bottom ($\theta = 0°$) sides of the 90° bend ($Re = 60,000$)

code doesn't have any artificial velocities on the momentum equations. The deformation of interface happens under the vortex velocity. The results of the CLSVOF method developed in this paper is compared with the CLSVOF method built in ANSYS FLUENT as well as with some results in the literature.

4.3.1 Droplet movement due to a constant velocity field

A circle of fluid with a radius of 0.15 mm, initially centered at (−0.25, 0.25) in a unit square domain. Wall boundary condition was set to all sides. Three types of constant velocities are tested: $(U = 1, V = 0)$, $(U = 0, V = -1)$, and $(U = 1, V = -1)$.The results are shown in Figs. 4.4, 4.5, and 4.6. No deformation of droplet but only pure movement is observed in all cases, which excludes the artificial movements when the velocity field is constant.

4.3.2 Droplet deformation due to a vortex velocity field

Using the same conditions as in Rider's work [52], the simulation of the time reversed single vortex flow are presented. A circle of fluid with a radius of 0.15 mm, initially centered at (0.5, 0.75) in a unit square domain, is deformed by a vortex velocity field defined by the following stream function:

$$\psi(x, y) = \frac{1}{\pi} \sin^2[\pi x] \sin^2[\pi y] \cos(\pi t/T), \tag{4.13}$$

where T is the period and the velocity components are defined by

$$U = -\frac{\partial \psi}{\partial y}, V = \frac{\partial \psi}{\partial x}. \tag{4.14}$$

Water is filled within the circle and air is outside the circle. A surface tension coefficient of $0.1N/m$ was used for air-water. A no slip wall boundary condition was used for all

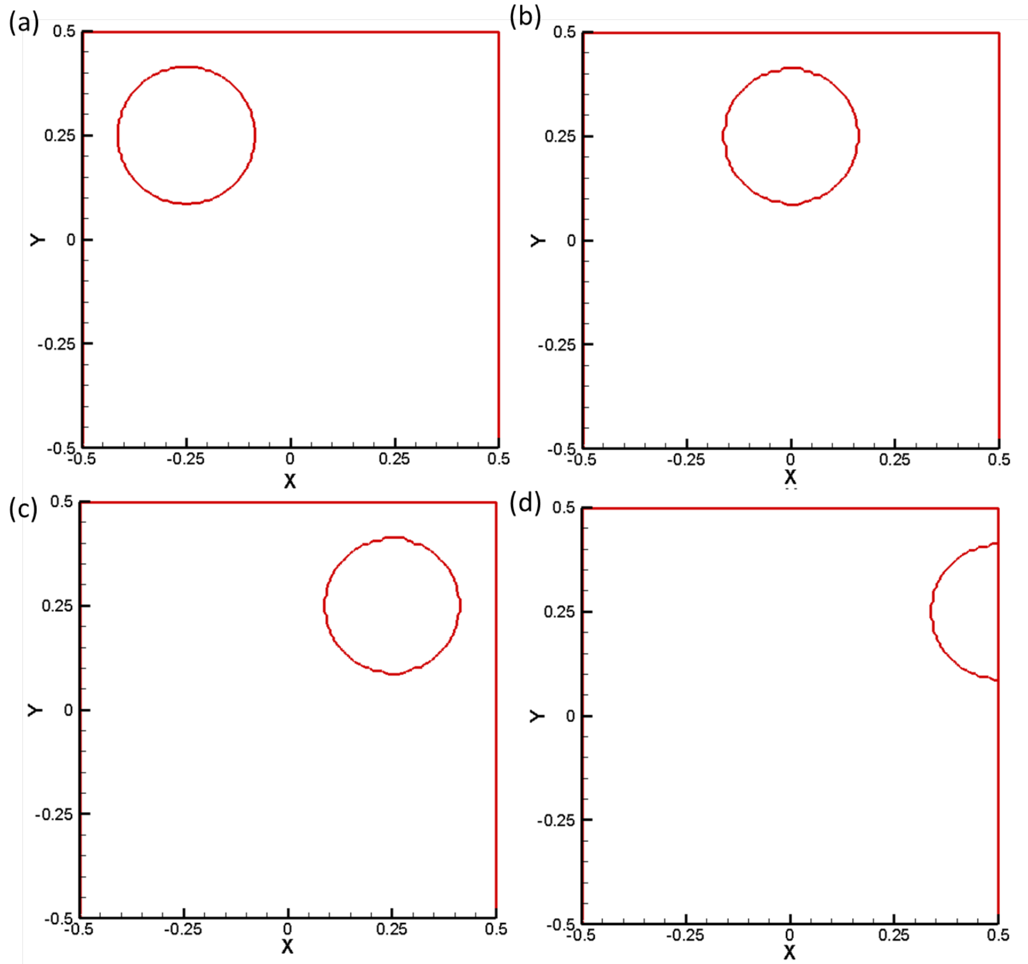

Figure 4.4: Movement of circle of fluid under the velocity ($U = 1$,$V = 0$) in the developed CLSVOF method and a grid of $128 * 128$ at (a) $t = 0s$, (b) $t = 0.25s$, (c) $t = 0.5s$, and (d)$t = 0.75s$

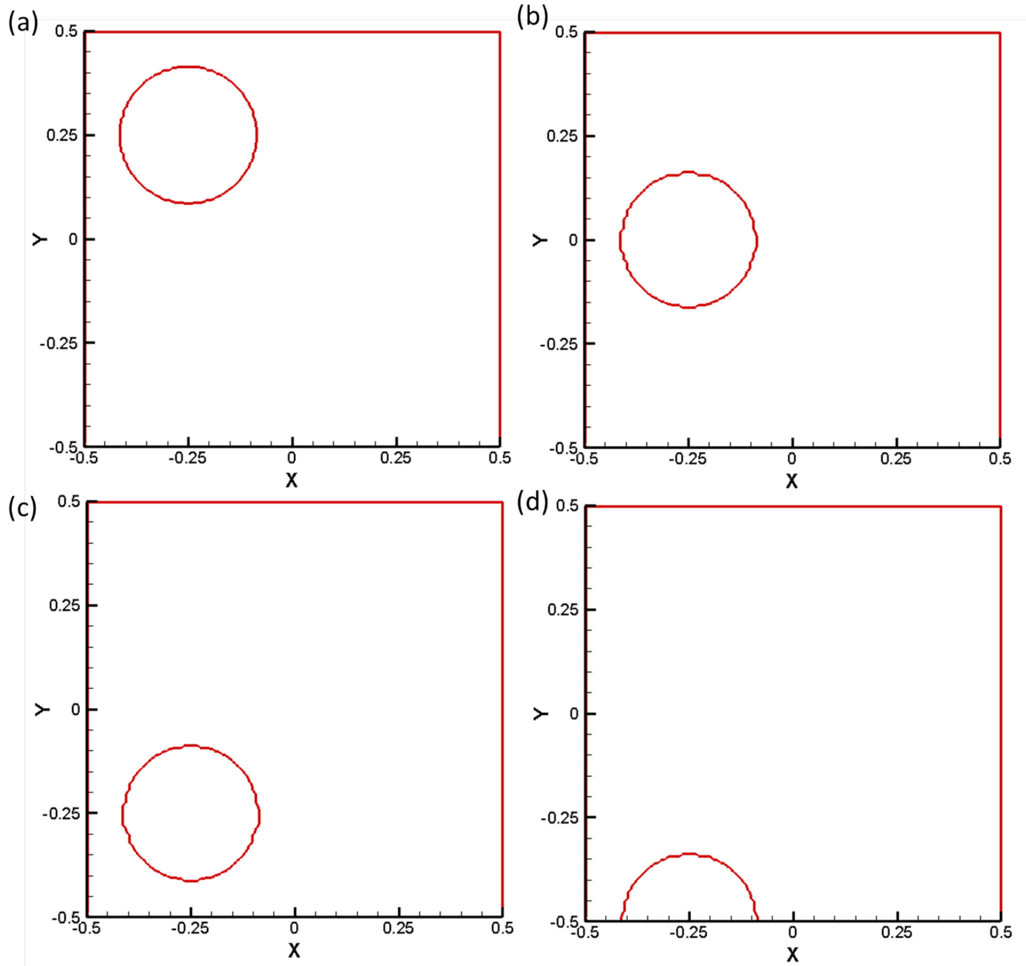

Figure 4.5: Movement of circle of fluid under the velocity ($U = 0$,$V = -1$) in the developed CLSVOF method and a grid of $128 * 128$ at (a) $t = 0s$, (b) $t = 0.25s$, (c) $t = 0.5s$, and (d)$t = 0.75s$

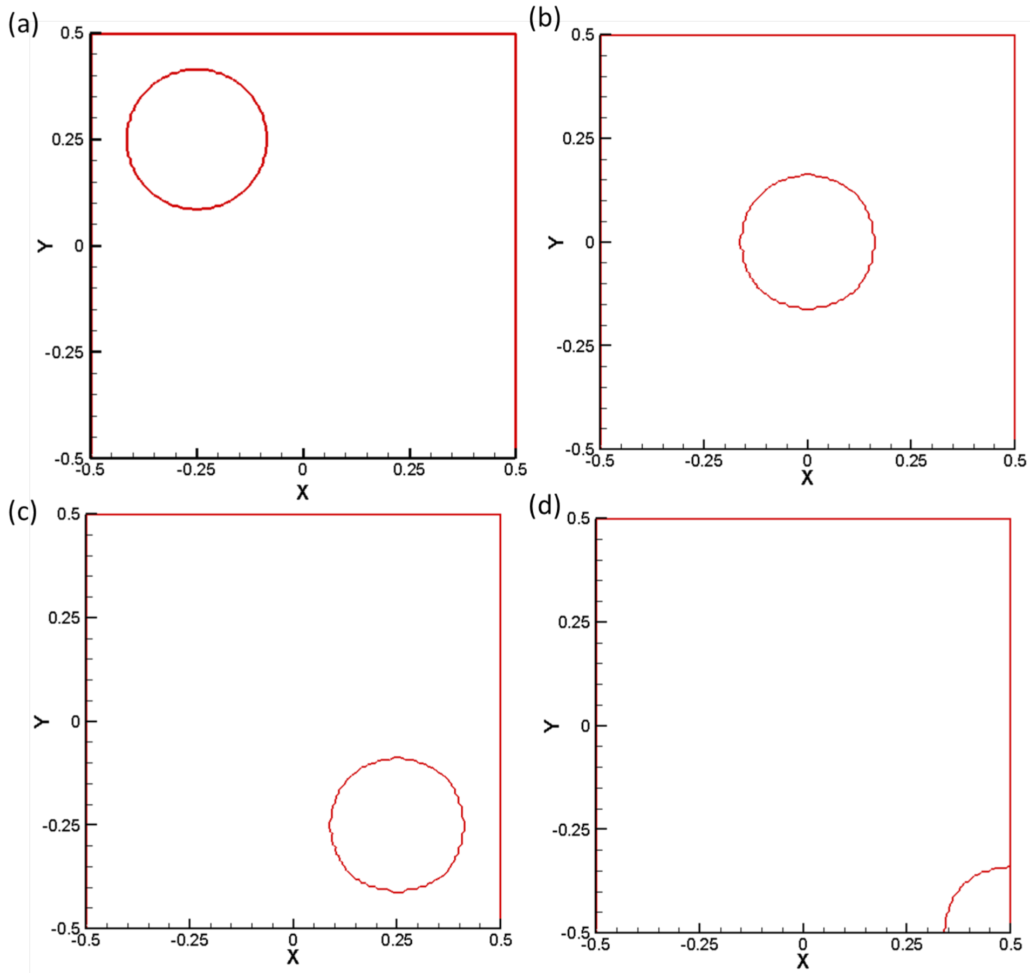

Figure 4.6: Movement of circle of fluid under the velocity ($U = 1$,$V = -1$) in the developed CLSVOF method and a grid of $128 * 128$ at (a) $t = 0s$, (b) $t = 0.25s$, (c) $t = 0.5s$, and (d)$t = 0.75s$

boundaries. Under the formation of the time periodic vortex velocity field, the largest deformation of the circle of fluid happens at $t = T/2$ and it goes back to its initial shape at $t = T$. This test can be used to access the code's capacity to resolve the thin fluid filaments formed by the interface stretching. The deformation reaches different levels when the time period is different. Three different time periods were tested for the developed CLSVOF method: $T = 2.0s$, $T = 6.0$, and $T = 12.0s$, using three different mesh densities: $128 * 128$, $256 * 256$, and $512 * 512$. Since detail simulation results of $T = 6.0s$ is available in Nichita's developed CLSVOF method [49], here we compare the results of $T = 6.0$ among the developed CLSVOF method in this paper, CLSVOF method in FLUENT and available data in Nichita's paper [49].

Figs. (4.7), (4.8), and (4.9) present the interface deformation with a time period of $T = 2$ on a grid of $128*128$, and $256*256$, and $512*512$ mesh points, respectively. Figs. (4.10) and (4.12) present the interface deformation with a time period of $T = 6$ on a grid of $128 * 128$, and $256 * 256$, and $512 * 512$ mesh points, respectively. Figs. (4.19) and (4.21) present the interface deformation with a time period of $T = 12$ on a grid of $128 * 128$, and $256 * 256$, and $512 * 512$ mesh points, respectively. All these results point out that the deformation of droplet increases as the time period increases and breakup happens at large time period, e.g. $T = 12$. The tip of the filament becomes sharper and the difference of enlarged comparison between (a) and (c) smaller when mesh is finer. When mesh points is $512 * 512$, the droplet goes back perfectly to its initial shape. Also, for the simulations with a time period of $T = 6$, the results of ANSYS FLUENT are shown in Fig. (4.13) on a grid of $128 * 128$ mesh points, and the results from Nichita's simulations [49] are shown in Figs. (4.16), (4.17), and (4.18). We can clearly see that the results of developed CLSVOF method are consistent to those in ANSYSN FLUENT and Nichita's simulations.

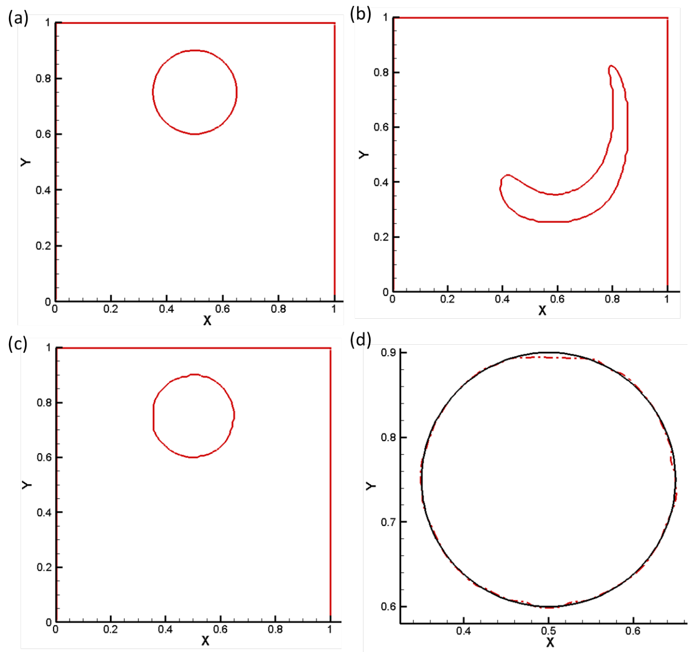

Figure 4.7: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/2)$ in the developed CLSVOF method and a grid of $128*128$ at (a) $t=0s$ (b) $t=1s$ (c) $t=2s$ (d) enlarged comparison between (a) and (c)

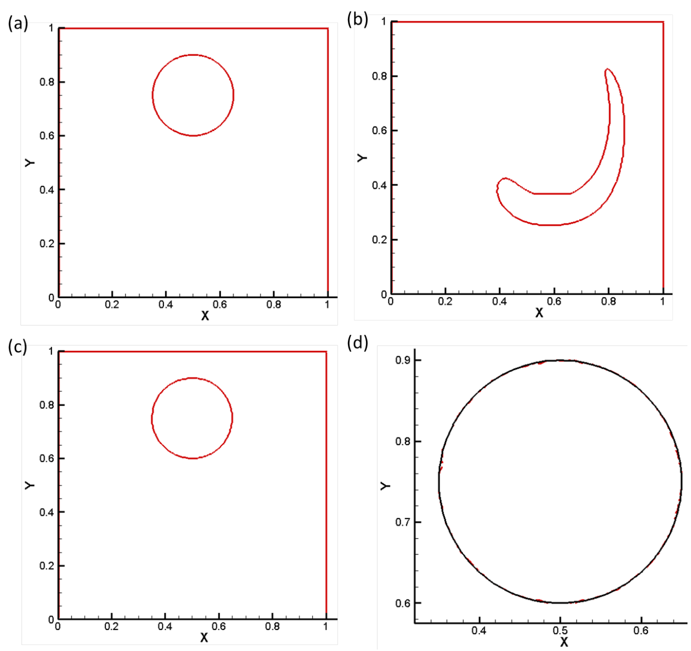

Figure 4.8: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/2)$ in the developed CLSVOF method and a grid of $256*256$ at (a) $t=0s$ (b) $t=1s$ (c) $t=2s$ (d) enlarged comparison between (a) and (c)

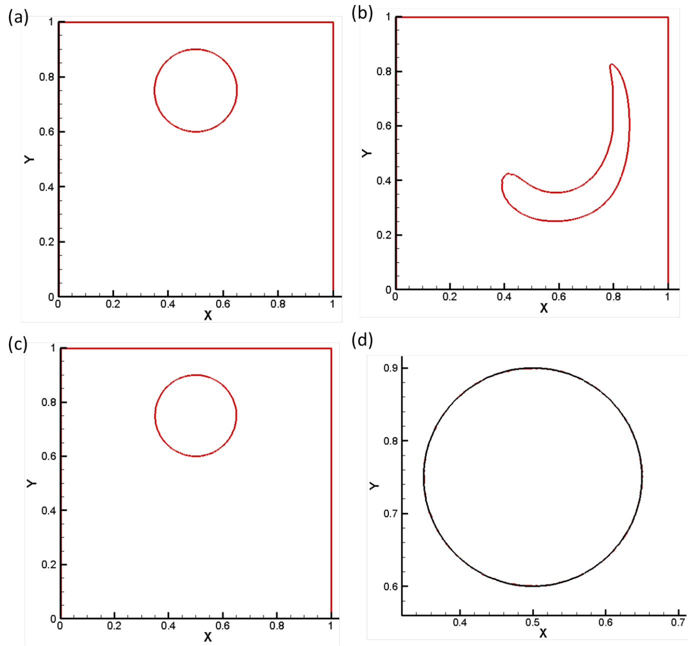

Figure 4.9: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/2)$ in the developed CLSVOF method and a grid of $512*512$ at (a) $t=0s$ (b) $t=1s$ (c) $t=2s$ (d) enlarged comparison between (a) and (c)

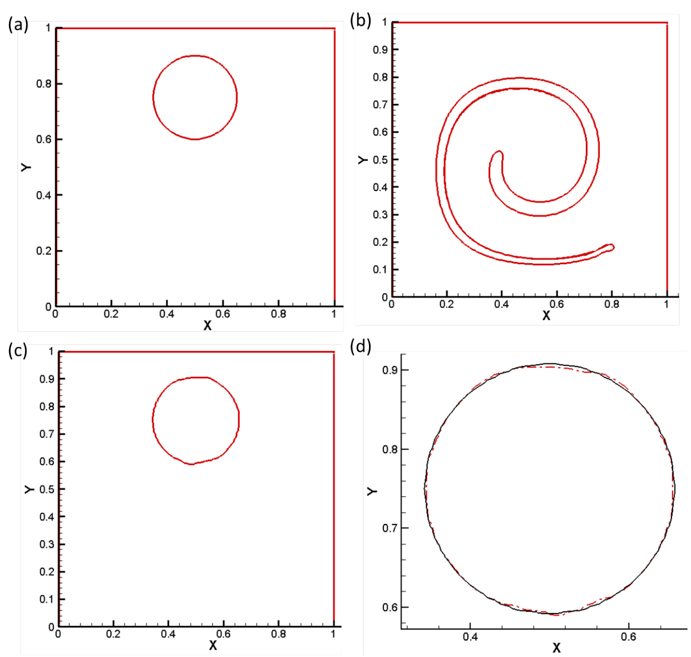

Figure 4.10: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/6)$ in the developed CLSVOF method and a grid of $128*128$ at (a) $t=0s$ (b) $t=3s$ (c) $t=6s$ (d) enlarged comparison between (a) and (c)

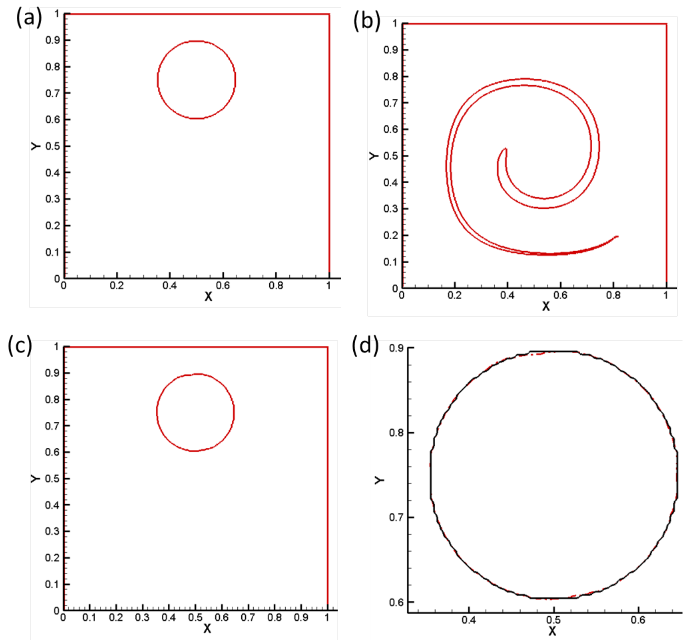

Figure 4.11: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/6)$ in the developed CLSVOF method and a grid of $256*256$ at (a) $t=0s$ (b) $t=3s$ (c) $t=6s$ (d) enlarged comparison between (a) and (c)

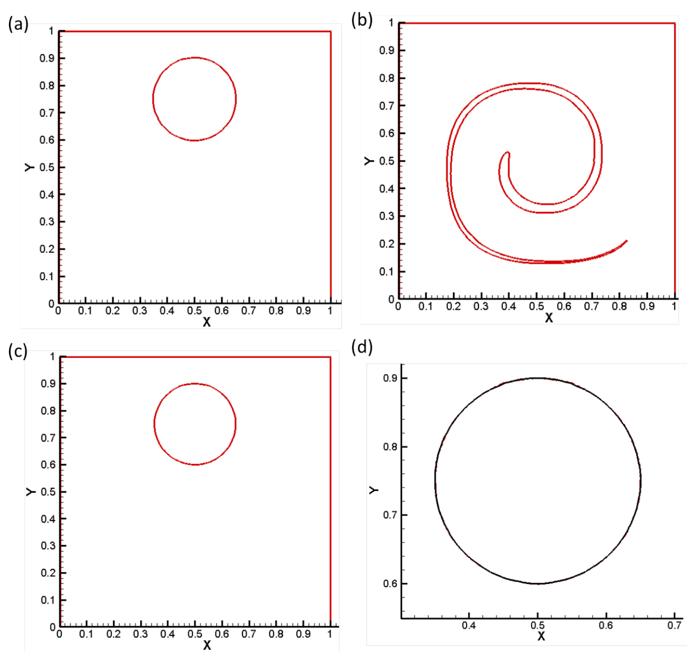

Figure 4.12: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/6)$ in the developed CLSVOF method and a grid of $512*512$ at (a) $t=0s$ (b) $t=3s$ (c) $t=6s$ (d) enlarged comparison between (a) and (c)

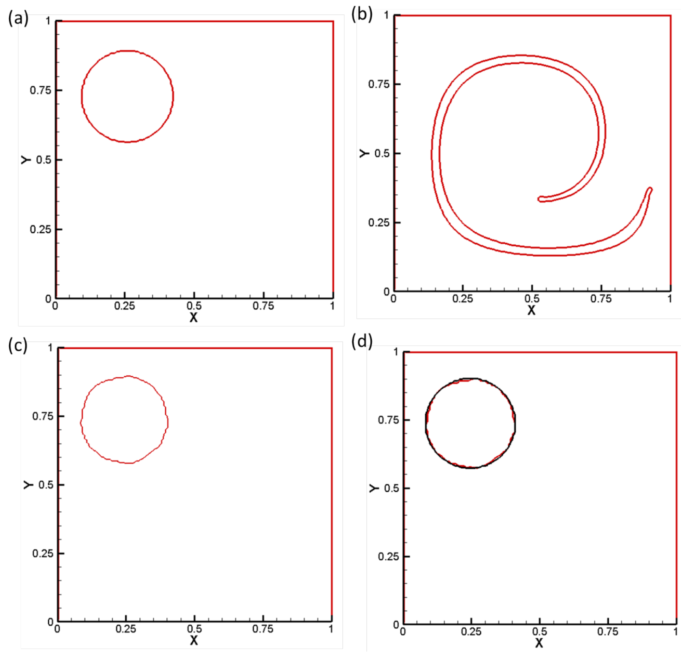

Figure 4.13: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/6)$ in the CLSVOF method in ANSYS FLUENT and a grid of $128 * 128$ at (a) $t = 0s$ (b) $t = 3s$ (c) $t = 6s$ (d) enlarged comparison between (a) and (c)

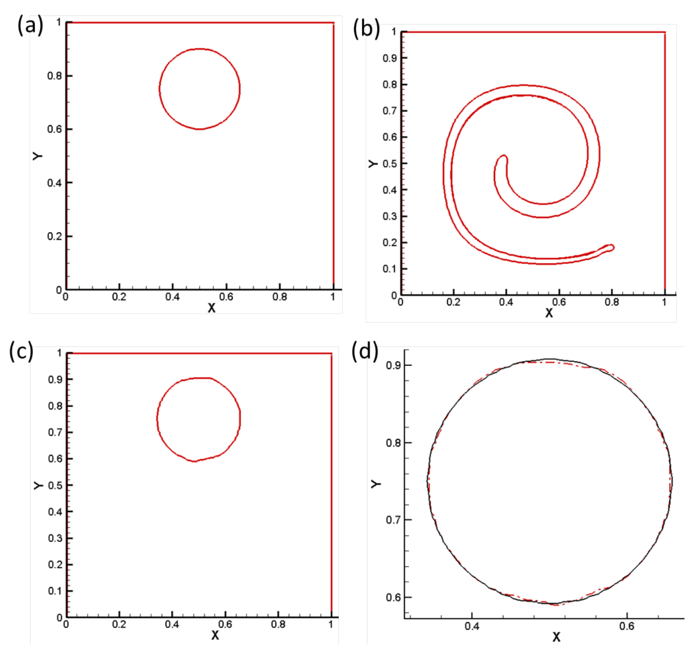

Figure 4.14: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/6)$ in the CLSVOF method in ANSYS FLUENT and a grid of $256 * 256$ at (a) $t = 0s$ (b) $t = 3s$ (c) $t = 6s$ (d) enlarged comparison between (a) and (c)

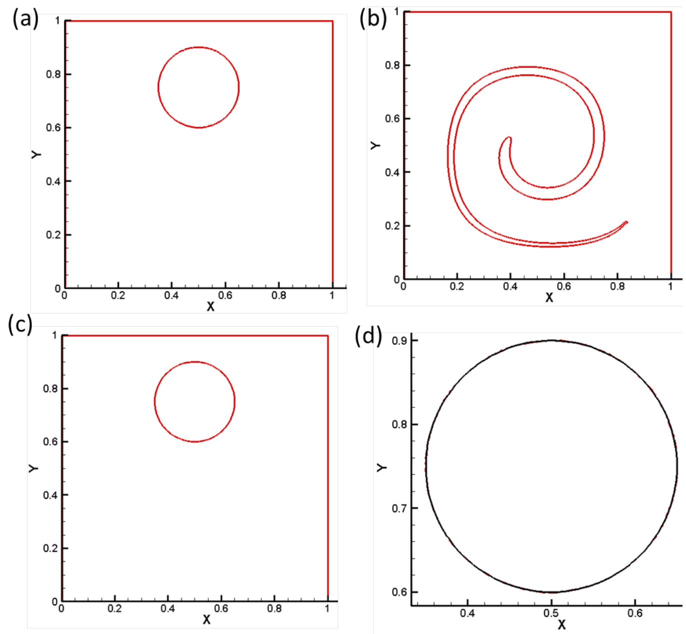

Figure 4.15: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/6)$ in the CLSVOF method in ANSYS FLUENT and a grid of $512 * 512$ at (a) $t = 0s$ (b) $t = 3s$ (c) $t = 6s$ (d) enlarged comparison between (a) and (c)

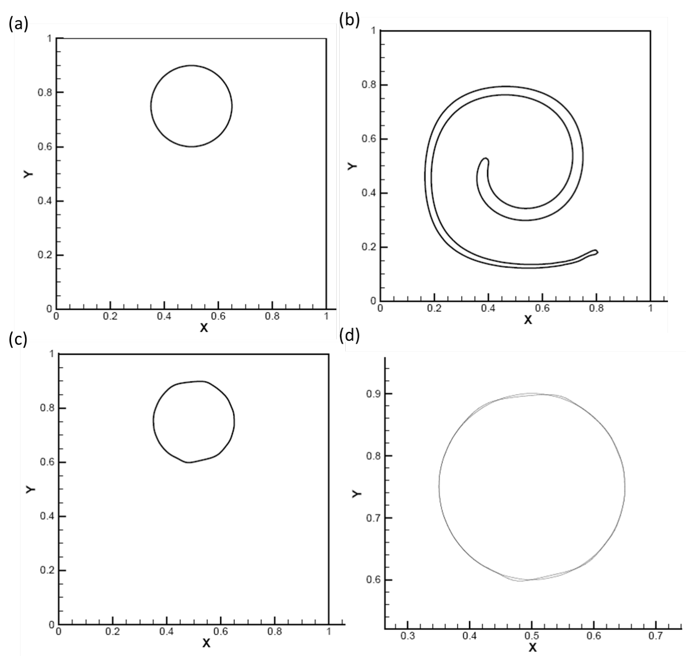

Figure 4.16: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/6)$ from the Nichita's simulation and a grid of $128 * 128$ at (a) $t = 0s$ (b) $t = 3s$ (c) $t = 6s$ (d) enlarged comparison between (a) and (c)

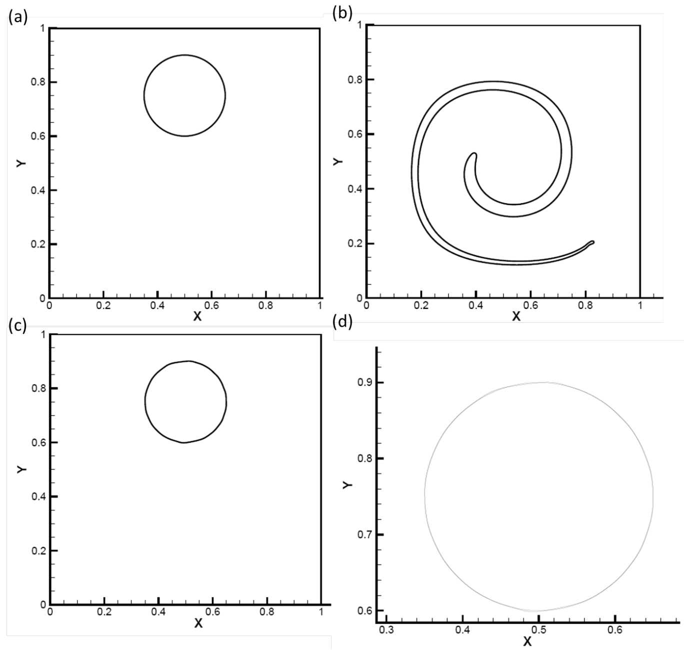

Figure 4.17: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/6)$ from the Nichita's simulation and a grid of $256 * 256$ at (a) $t = 0s$ (b) $t = 3s$ (c) $t = 6s$ (d) enlarged comparison between (a) and (c)

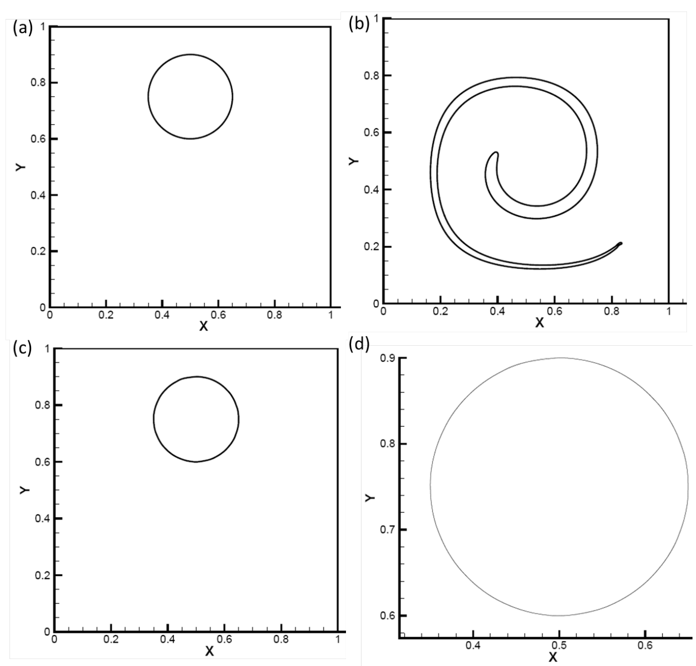

Figure 4.18: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/6)$ from the Nichita's simulation and a grid of $512 * 512$ at (a) $t = 0s$ (b) $t = 3s$ (c) $t = 6s$ (d) enlarged comparison between (a) and (c)

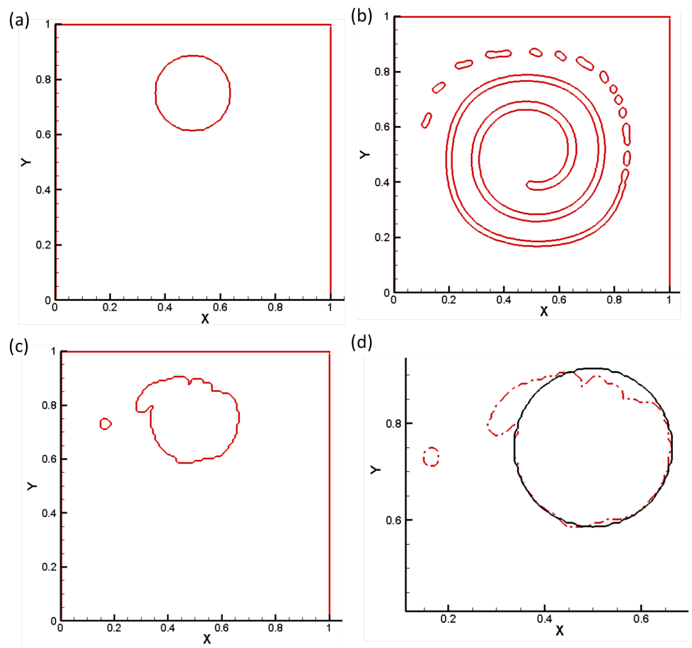

Figure 4.19: Deformation of circle of fluid under the vortex field of $\psi(x,y)=\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/12)$ in the developed CLSVOF method and a grid of $128 * 128$ at (a) $t = 0s$ (b) $t = 6s$ (c) $t = 12s$ (d) enlarged comparison between (a) and (c)

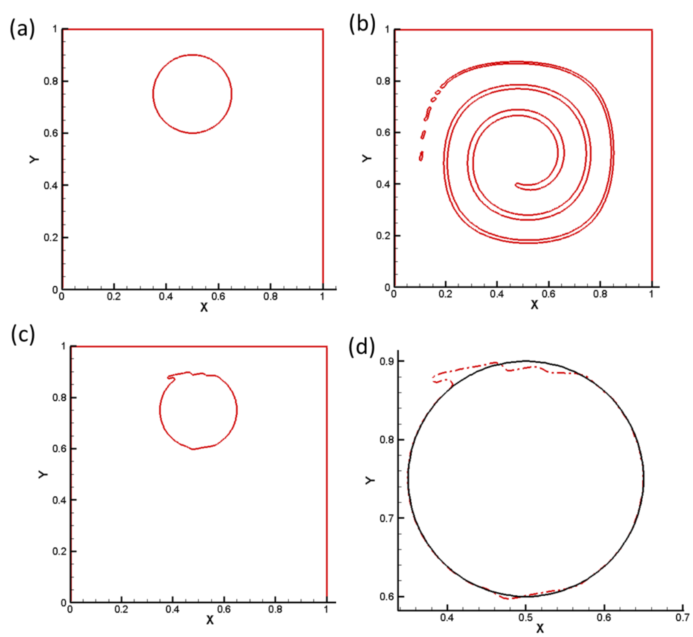

Figure 4.20: Deformation of circle of fluid under the vortex field of $\psi(x,y)=\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/12)$ in the developed CLSVOF method and a grid of $256 * 256$ at (a) $t = 0s$ (b) $t = 6s$ (c) $t = 12s$ (d) enlarged comparison between (a) and (c)

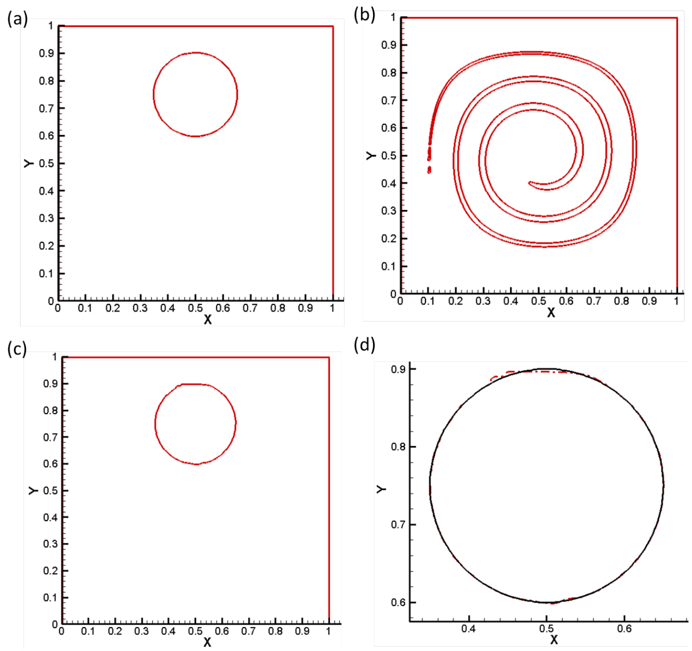

Figure 4.21: Deformation of circle of fluid under the vortex field of ψ(x,y)=$\frac{1}{\pi}\sin^2[\pi x]\sin^2[\pi y]\cos(\pi t/12)$ in the developed CLSVOF method and a grid of $512 * 512$ at (a) $t = 0s$ (b) $t = 6s$ (c) $t = 12s$ (d) enlarged comparison between (a) and (c)

4.4 Two Dimensional Jet Simulations Based on FLUENT Code

Before starting the simulation of mercury jet for the Muon Collider project, two dimensional jet is studied first to verify the FLUENT code, which will be applied for the mercury jet simulation.

4.4.1 Two Dimensional Laminar Round Jet Flow

The two dimensional jet simulation studied in this part is a laminar round jet with the advantage of analytical solution given by Schlichting[109]. The solved problem is shown in Fig. 4.22. Air emerges into a still air from a circular orifice at $x = 0$. At any cross section, the momentum flux is constant. Air jet spreads at constant pressure, which is 1 bar. Temperature is constant 300 K. The Reynolds number based on the inlet velocity (0.64 m/s)

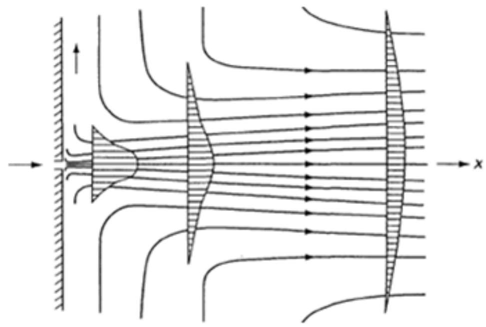

Figure 4.22: Typical free 2D laminar round jet streamline pattern

is 400. The density of air is $1.16 kg/m^3$ and kinematic viscosity is $1.610-5 m^2/s$.

The governing equations for the 2D laminar round jet flow are

$$\frac{\partial \overline{u}}{\partial x} + \frac{1}{r}\frac{\partial (r\overline{v})}{\partial r} = 0 \quad (4.15)$$

$$\overline{u}\frac{\partial \overline{u}}{\partial x} + \overline{v}\frac{\partial \overline{u}}{\partial r}\frac{1}{r}\frac{\partial (r\overline{v})}{\partial r} \approx \frac{\nu}{r}\frac{\partial}{\partial r}(r\frac{\partial \overline{u}}{\partial r}) \quad (4.16)$$

The analytical solution is

$$\overline{u} = \frac{3J}{8\pi\mu x}(1+\frac{C^2\eta^2}{4})^{-2}, \quad (4.17)$$

where $C \equiv (\frac{3J}{16\pi\rho\nu^2})^{1/2}$, $J = \rho\int_{-\infty}^{\infty} u^2 2\pi r dr$, and $\eta = \frac{r}{x}$.

The boundary conditions for the 2D laminar round jet are shown in Fig. 4.23. Constant axial velocity is assumed at the velocity inlet. The side edges on the inlet side are set as non-slip wall. Considering the round jet, axis boundary condition is used for the center line and only halved model for the simulation. The results of the 2D laminar round jet simulation are analyzed as below. Figure 4.24 shows the center line velocity ($\overline{u}_c$) changes with the distance (x) away from the jet nozzle. $\overline{u}_c$ drops as x increases, roughly following the order of $1/x$. The radial distribution of mean stream velocity ($\overline{u}$) at locations $x = 10d$,$x = 30d$, $x = 50d$, $x = 70d$, and $x = 90d$ are shown in Fig. 4.25. The numerical $\overline{u}$ is very close to theoretical $\overline{u}$ at $x = 30d$, but the difference becomes bigger at more downstream locations. Jet half width is defined as the radial distance from the axis to the position at the which the absolute value of the axial velocity drops to half its value on the axis. The relationship between jet

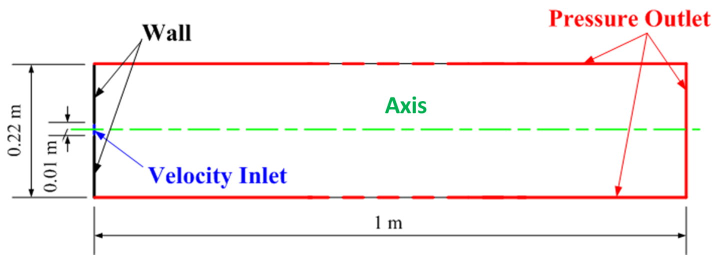

Figure 4.23: Boundary conditions settings for 2D laminar round jet

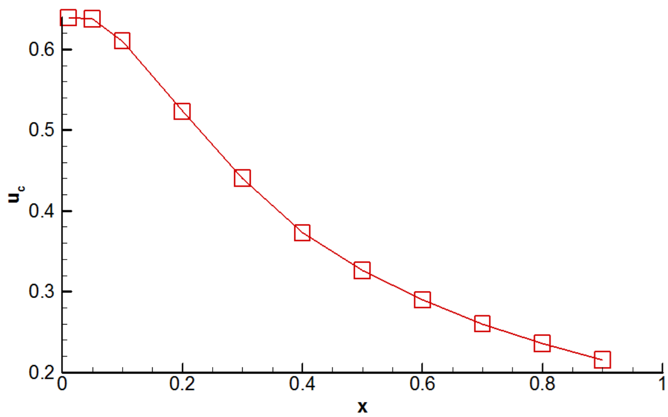

Figure 4.24: Center line velocity of the 2D round jet changes with the distance

half width and distance from the jet nozzle is mostly linear, which can be seen in Fig. 4.26. Good jet self-similarity is observed in Fig.4.27 by plotting the flow profile along the radial direction. Last, Fig. 4.28 shows the changes in momentum thickness at different locations downstream of the jet. It is obvious can seen that the changing rate of momentum thickness slows down at downstream of the jet.

4.4.2 Two Dimensional Laminar Plane Jet Flow

Schlichting also solved out the analytical solutions for a 2D laminar plane jet [109]. The solved problem is shown in Fig. 4.29. Air emerges into a still air from a 2D slot at $x = 0$. At any cross section, the momentum flux is constant. Air jet spreads at constant pressure, which is 1 bar. Temperature is constant 300 K. The Reynolds number based on the inlet velocity (0.64 m/s) is 400. The density of air is 1.225 kg/m$^3 andkinematicviscosityis$1.46073Ã10-5$m^2/s$.

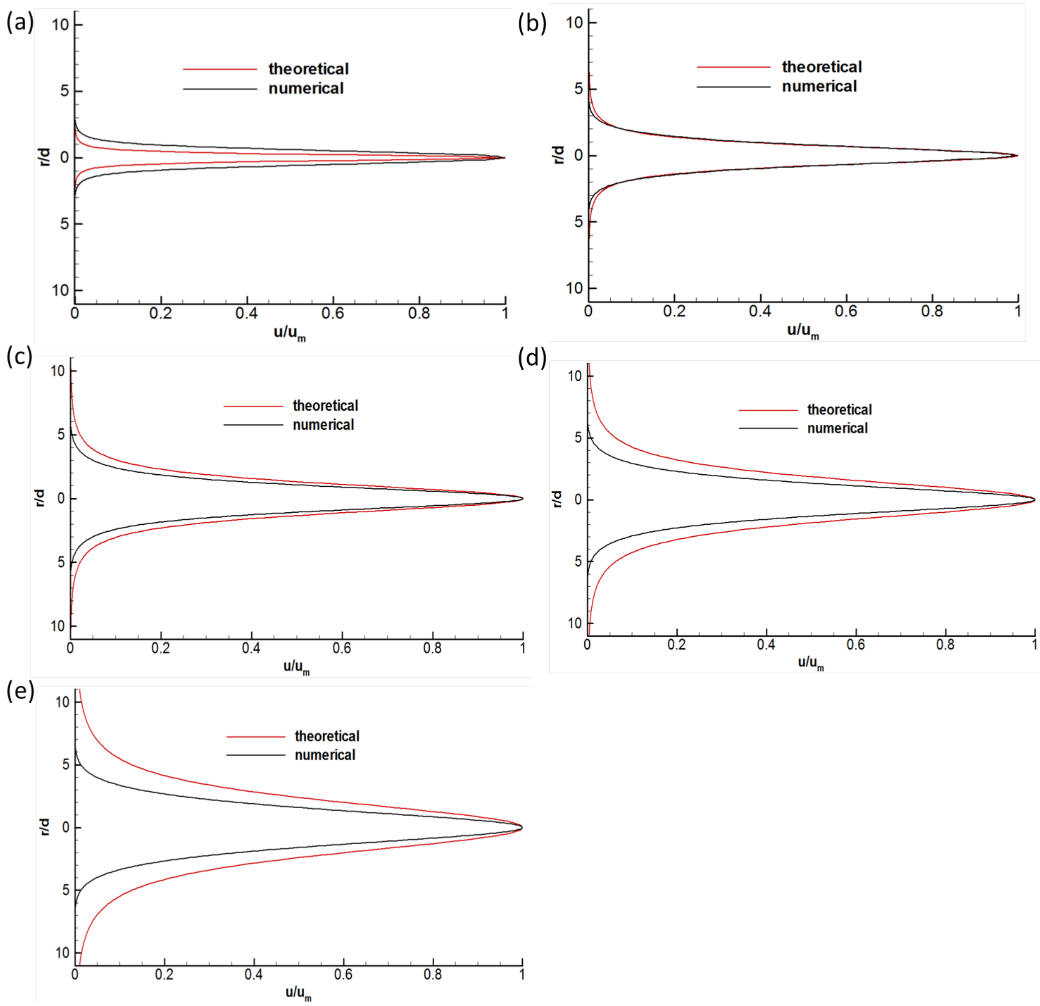

Figure 4.25: Radial distribution of the mean stream velocity of the 2D round jet at (a) $x/d = 10$, (b)$x/d = 30$, (c) $x/d = 50$, (d) $x/d = 70$, and (e) $x/d = 90$. Note that $\overline{u}$ is normalized by $\overline{u}_{\max}$ ($\overline{u}_{\max}$ =max($\overline{u}$)) and radius r by jet inlet diameter d.

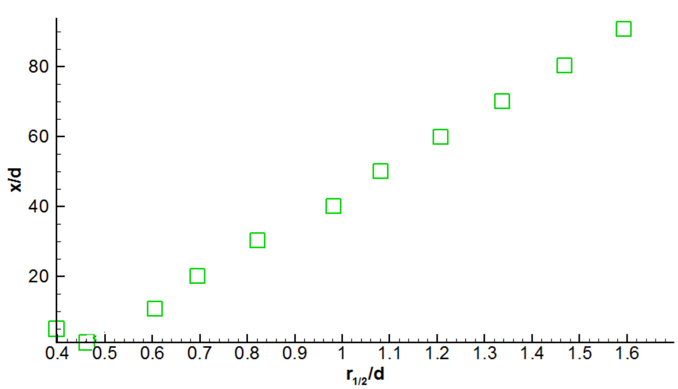

Figure 4.26: Half width of the 2D round jet changes with the distance. Note that $r_{1/2}$ and distance x are normalized by jet inlet diameter d.

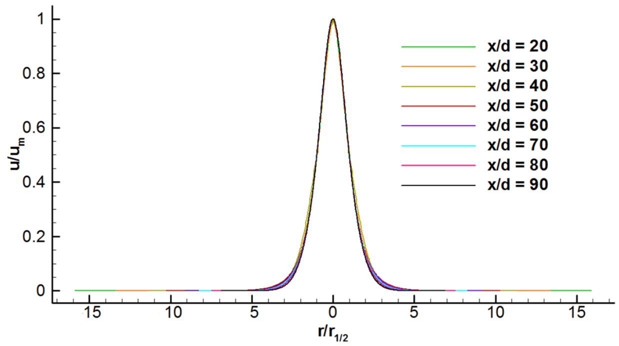

Figure 4.27: 2D round jet self-similarity

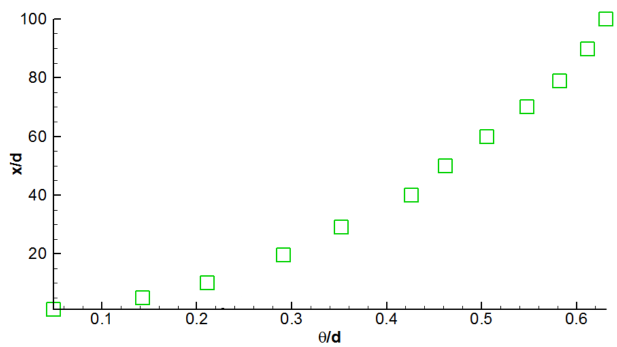

Figure 4.28: Momentum thickness of 2D round jet changes with distance. Note that θ and distance x are normalized by jet inlet diameter d.

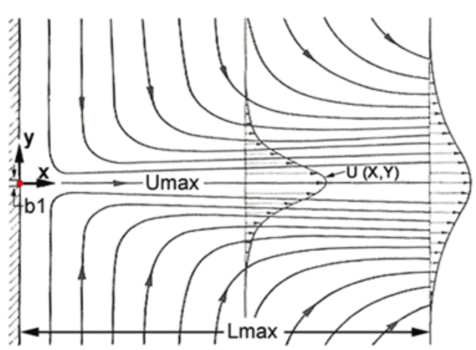

Figure 4.29: Typical free 2D laminar plane jet streamline pattern

The governing equations for the 2D laminar plane jet are

$$\frac{\partial \overline{u}_x}{\partial x} + \frac{\partial \overline{u}_y}{\partial y} = 0 \tag{4.18}$$

$$\overline{u}_x \frac{\partial \overline{u}_x}{\partial x} + \overline{u}_y \frac{\partial \overline{u}_y}{\partial r} \approx \nu \frac{\partial^2 \overline{u}_y}{\partial y^2} \tag{4.19}$$

The analytical solution is

$$\overline{u}_x = (\frac{3J^2}{32\nu x})^{1/3} \sec h^2(\gamma), \tag{4.20}$$

$$\overline{u}_y = (\frac{J\nu}{6x^2})^{1/3} [2\gamma \sec h^2(\gamma) - \tanh(\gamma)], \tag{4.21}$$

where $\gamma \equiv (\frac{J}{48\nu^2})^{1/3} \frac{y}{x^{2/3}}$, and $J = \int_{-\infty}^{\infty} u^2 dy$.

The boundary conditions for the 2D laminar round jet are shown in Fig. 4.30. Constant axial velocity is assumed at the velocity inlet. The side edges on the inlet side are set as non-slip wall. Considering the symmetry of the jet, symmetry boundary condition is used for the center line and only halved model for the simulation. The results of the 2D laminar plane jet simulation are analyzed the same as the 2D laminar round jet. Figure 4.31 shows the center line velocity ($\overline{u}_c$) changes with the distance (x) away from the jet nozzle. $\overline{u}_c$ drops with x roughly following the order $x^{1/3}$. The radial distribution of mean stream velocity ($\overline{u}$) at locations $x = 10d$,$x = 30d$, $x = 50d$, $x = 70d$, and $x = 90d$ are shown in Fig. 4.32. The numerical $\overline{u}$ is very close to theoretical $\overline{u}$ at $x = 30d$, but diverges from the analytical solution as flow is more downstream. The relationship between jet half width and distance from the jet nozzle is mostly linear, which can be seen in Fig. 4.33. Good jet self-similarity is observed in Fig.4.34 by plotting the flow profile along the radial direction. Last, Fig. 4.35 shows the changes in momentum thickness at different locations downstream of the jet. It is obvious can seen that the changing rate of momentum thickness slows down at downstream of the jet.

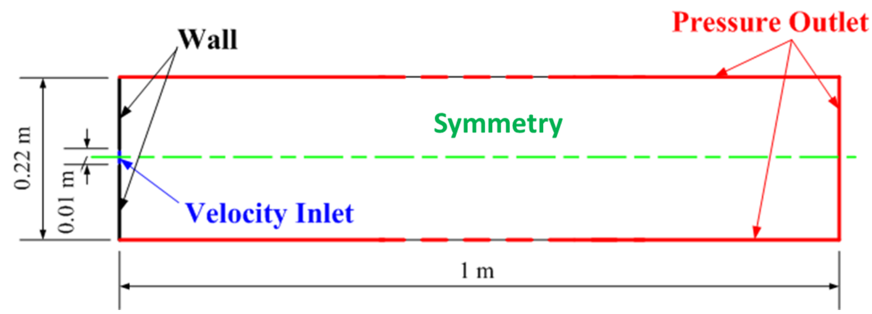

Figure 4.30: Boundary conditions settings for 2D laminar plane jet

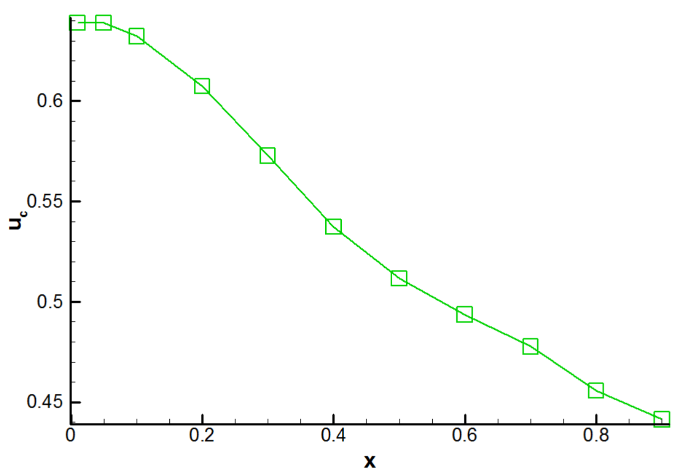

Figure 4.31: Center line velocity of the 2D plane jet changes with the distance

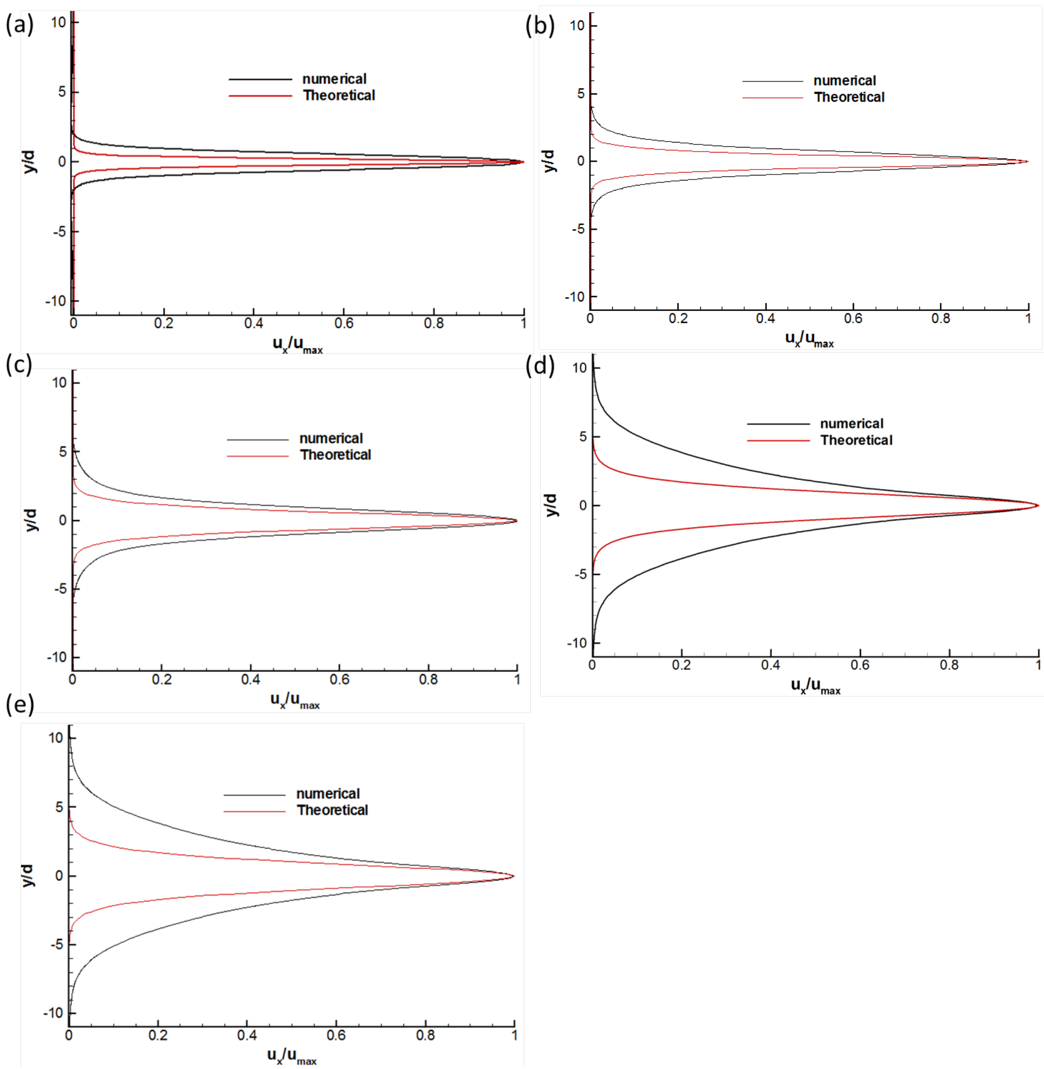

Figure 4.32: Radial distribution of the mean stream velocity of the 2D plane jet at (a) $x/d = 10$, (b)$x/d = 30$, (c) $x/d = 50$, (d) $x/d = 70$, and (e) $x/d = 90$. Note that $\overline{u}$ is normalized by $\overline{u}_{\max}$ ($\overline{u}_{\max}$ =max($\overline{u}$)) and radius r by jet inlet diameter d.

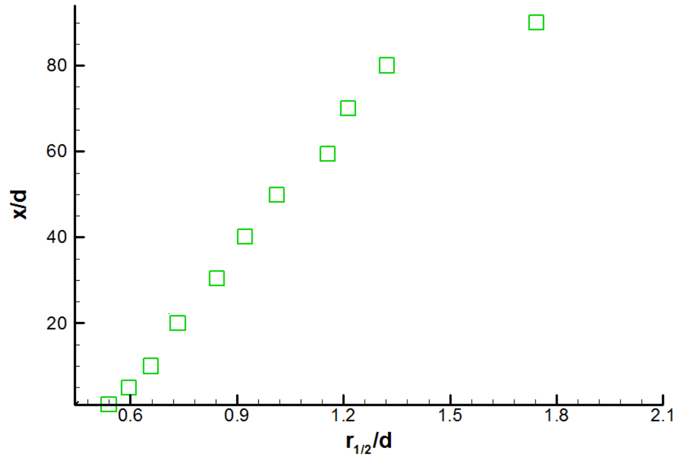

Figure 4.33: Half width of the 2D plane jet changes with the distance. Note that $r_{1/2}$ and distance x are normalized by jet inlet diameter d.

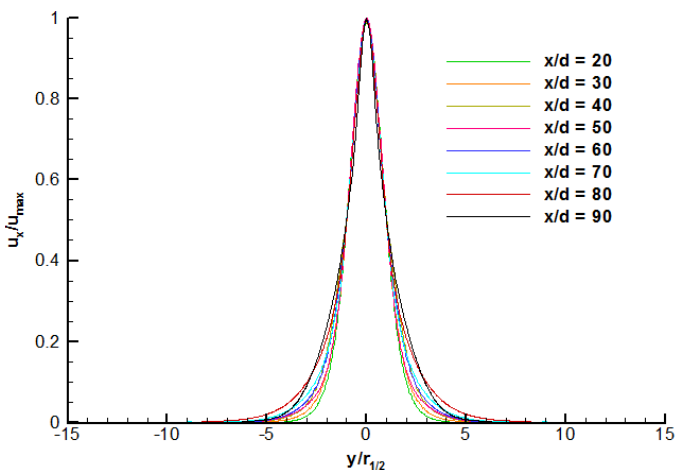

Figure 4.34: 2D plane jet self-similarity

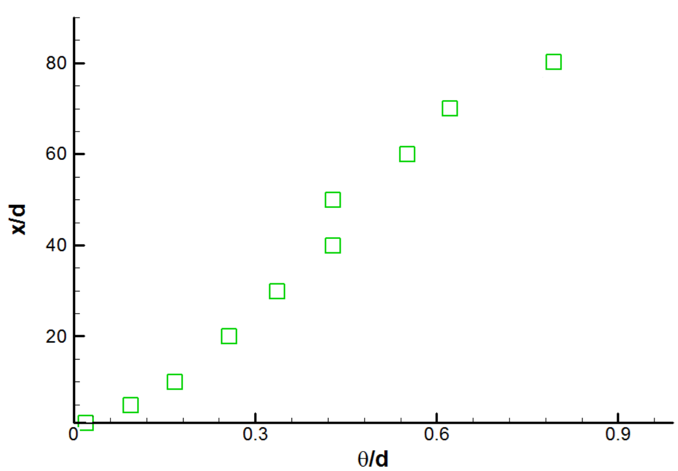

Figure 4.35: Momentum thickness of 2D round jet changes with distance. Note that /*theta* and distance x are normalized by jet inlet diameter d.

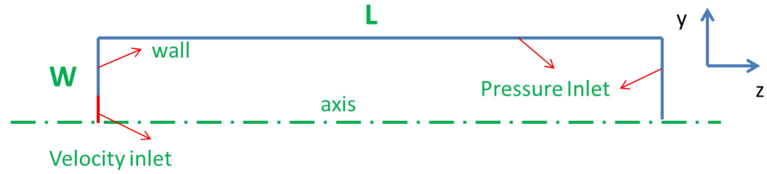

Figure 4.36: The boundary conditions for the 2D turbulent jet simulations

4.4.3 Two Dimensional Turbulent Jet Flow

In this part, the ability of FLUENT code in capturing the jet breakup is tested. An axis-symmetric liquid jet flows into still gas with a mean bulk velocity of 100 m/s. The inlet jet diameter is $100\mu m$, thus the Reynolds number UD/ν_{liquid} is equal to 5800. Figure 4.36 shows the boundary conditions of the problem. The jet inlet uses constant velocity of 100 m/s. The width of the computational domain is chosen $3D$ or $5D$, where D is the jet inlet diameter. The length is $50D$. The properties of the two phases are in table 4.1. To define the mesh size, we assume that only primary break up occurs for the smallest droplet. This implies that the Weber number is at least smaller that 10 [65], which gives to the minimum mesh size of $2.36\mu m$.

$$We \equiv \frac{\rho u^2 \triangle x}{\sigma} = 10 \Rightarrow \triangle x = \frac{we\sigma}{\rho u^2} = \frac{10 * 0.06}{696 * 100 * 100} = 2.36\mu m \quad (4.22)$$

With the grid spacing of $2.36\mu m$, the uniform grid size is 127×2120 for $3D$ width case and 212×2120 for $5D$ width case.

Table 4.1: The properties of two phases in 2D turbulent jet simulation

phase	Density	Viscosity	Surface Tension
Gas	$25kg/m^3$	$4 \times 10^{-7}m^2/s$	$0.06N/m$
Liquid	$696kg/m^3$	$1.724 \times 10^{-6}m^2/s$	

VOF method is the built-in two-phase method in FLUENT code. Further, the current ANSYS FLUENT 14.5 version has the CLSVOF method. Here, we apply both VOF and CLSVOF method in FLUENT to simulate the 2D two-phase jet flow. Large-eddy simulations

Table 4.2: The locations of the onset of turbulent breakup for 2D jet simulations in FLUENT codes

Case	Location of onset of turbulent breakup
3 Jet-Diameter in VOF	$14D$
3 Jet-Diameter in CLSVOF	$1.6D$
5 Jet-Diameter in VOF	$11.6D$
5 Jet-Diameter in VOF	$0.4D$

(LES) has been widely used to simulate turbulent jet flow and it seems to be a feasible candidate to obtain the necessary unsteady date for jet [110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121]. In LES, the scales of turbulent eddies larger than the computational mesh spacing are computed directly. Eddies smaller than the grid spacing (subgrid scale eddies) are modeled with an appropriate turbulence model. Therefore, more scales of turbulent eddies can be modeled directly when mesh is finer, eg. direct numerical simulation (DNS) solves all eddy scales. Here implicit large eddy simulation (ILES) is applied. Navier-Stokes equations (NSE) are discretized through finite volumes on a fine mesh of the problem, which is finer than that of LES but coarser than that of DNS. Discretization error appears in the division term. There is no explicit filtering in ILES but the discretization provides top-hat-shaped-kernel implicit filtering [122] ($\frac{1}{\delta V_p}\int_{\Omega_P} f dV$, where δV_p is volume of the mesh unit, Ω_P is the domain of the mesh unit). The resolved and subgrid scales are decoupled through the numerics. ILES resolves large eddies and uses physics-capturing numerics.

Figures 4.37, 4.38, and 4.39 are results of $3D$ jet case using VOF method, while Figs. 4.40, 4.41 and 4.42 are results using CLSVOF method. The CLSVOF results have more jet breakups and the onset location of breakup is closer to the jet inlet. So is the $5D$ jet CLSVOF simulation, as shown in Figs. 4.43, 4.44,4.45, 4.46, 4.47, and 4.48. Table 4.2 gives the locations of onset of turbulent breakup for 2D turbulent jet simulation in FLUENT codes.

When $100 < We_l < 1.1 \times 10^6$, $3400 < Re_l < 8.5 \times 10^5$, and $0.001 < OH_l < 0.017$, P.K Wu worked out a surface breakup regime map for turbulent liquid jets in still gases, seen in Fig. 4.49 [123], where We is Weber numbers, $We = \frac{\rho D U^2}{\sigma}$ and OH is Ohnesorge numbers,

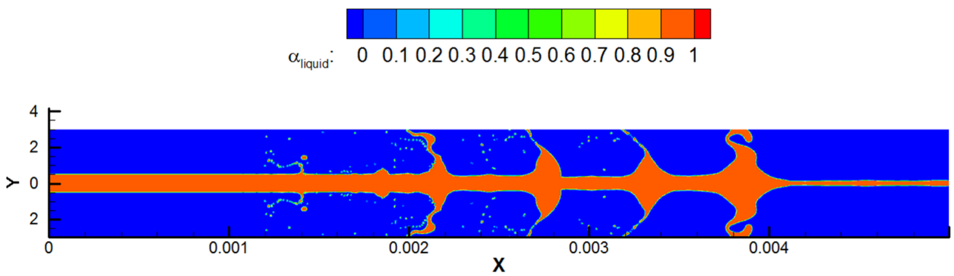

Figure 4.37: The contour of volume of fraction of liquid for the 3-jet-diameter simulation in VOF method of FLUENT code. Note 3-jet-diameter simulation means the width of the computational domain is 3 times the jet inlet diameter.

$OH = \frac{\mu}{\sqrt{\rho D \sigma}}$. Also the equations for location of onset/end of turbulent breakup are given in Fig. 4.49. The We_l, Re_l, and OH_l for the studied jet problem are

$$We_l = \frac{\rho_l D U^2}{\sigma} = \frac{696 \times 0.0001 \times 100^2}{0.06} = 11600, \tag{4.23}$$

$$OH_l = \frac{\mu_l}{\sqrt{\rho D \sigma}} = \frac{\sqrt{We_l}}{Re_l} = \frac{\sqrt{11600}}{5800} = 0.01857, \tag{4.24}$$

which are within the considered range of Wu's work. Therefore, the location of onset/end of turbulent breakup for the studied problem is

$$x_i = 2000 We_l^{-0.67} D = 3.783D \tag{4.25}$$

$$x_e = 1.58 \times 10^{-5} We_l^{1.68} D = 106.4D, \tag{4.26}$$

where x_i is the onset location and x_e is the end location of breakup. Since the computational domain only has a length of $50D$, the calculated end location of breakup reaches as far as $106.4D$ (Eq. (4.26)). Therefore, only the onset location of breakup can be compared between the calculation (Eq. (4.26)) and the simulation (4.2). Although both the VOF and CLSVOF results of onset location are not $3.783D$ as in Eq. (4.26), the CLSVOF results leads to a smaller value of $x - i$, which is much better than those of VOF results. In later jet simulations, the CLSVOF model will be used for the two-phase flow model.

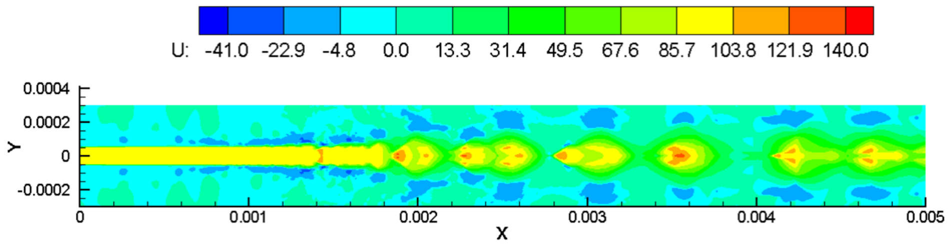

Figure 4.38: The contour of axial velocity for the 3-jet-diameter simulation in VOF method of FLUENT code. Note 3-jet-diameter simulation means the width of the computational domain is 3 times the jet inlet diameter.

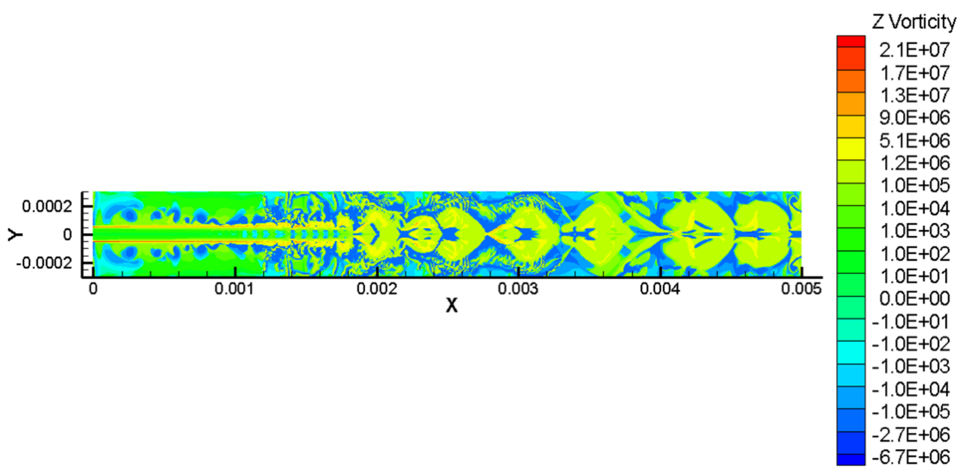

Figure 4.39: The contour of Z vorticity for the implicit LES 3-jet-diameter simulation using VOF multiphase model. Note 3-jet-diameter simulation means the half width of the computational domain is 3 times the jet inlet diameter.

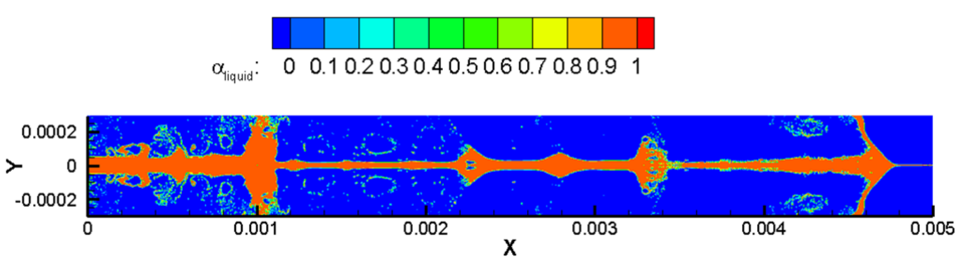

Figure 4.40: The contour of volume of fraction of liquid for the implicit LES 3-jet-diameter simulation using CLSVOF multiphase model. Note 3-jet-diameter simulation means the half width of the computational domain is 3 times the jet inlet diameter.

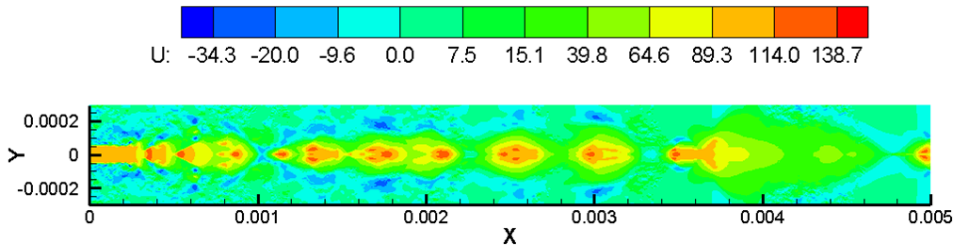

Figure 4.41: The contour of axial velocity for the implicit LES 3-jet-diameter simulation using CLSVOF multiphase model. Note 3-jet-diameter simulation means the half width of the computational domain is 3 times the jet inlet diameter.

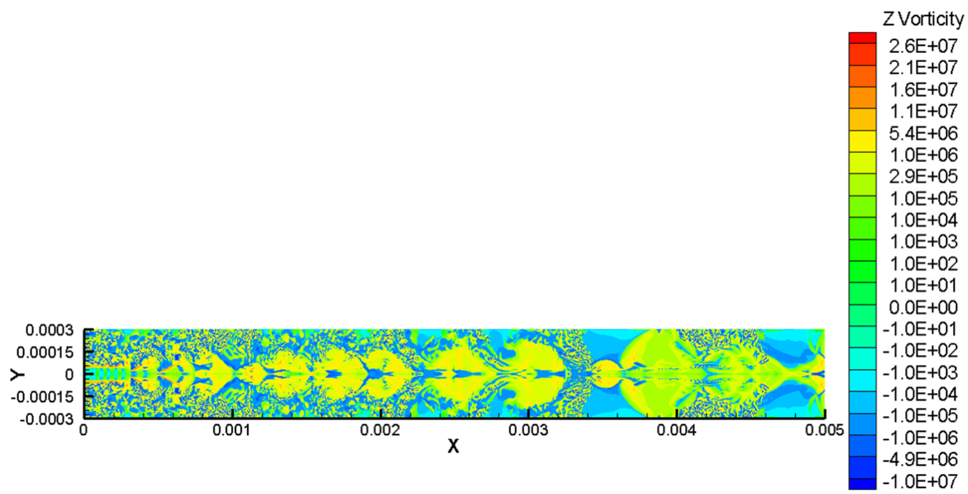

Figure 4.42: The contour of Z vorticity for the implicit LES 3-jet-diameter simulation using CLSVOF multiphase model. Note 3-jet-diameter simulation means the half width of the computational domain is 3 times the jet inlet diameter.

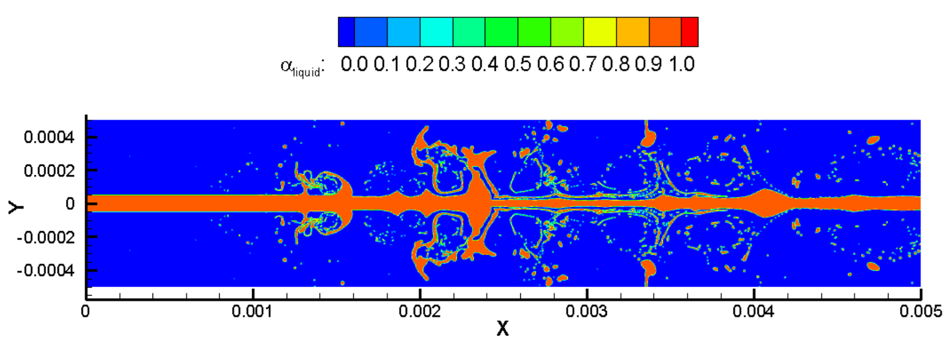

Figure 4.43: The contour of volume of fraction of liquid for the implicit LES 5-jet-diameter simulation using VOF multiphase model. Note 5-jet-diameter simulation means the half width of the computational domain is 5 times the jet inlet diameter.

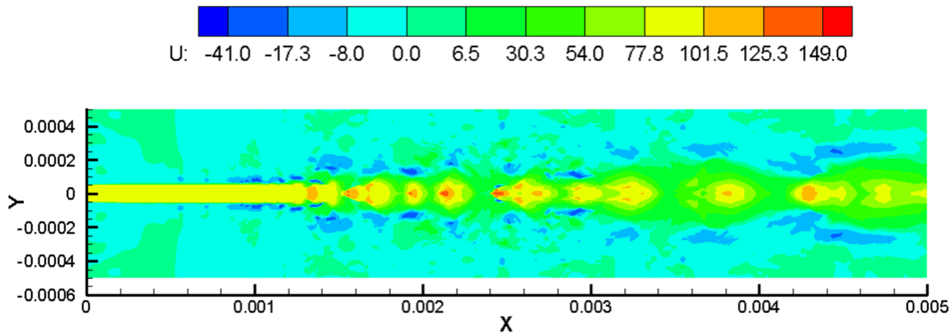

Figure 4.44: The contour of axial velocity for implicit LES 5-jet-diameter simulation using VOF multiphase model. Note 5-jet-diameter simulation means the half width of the computational domain is 3 times the jet inlet diameter.

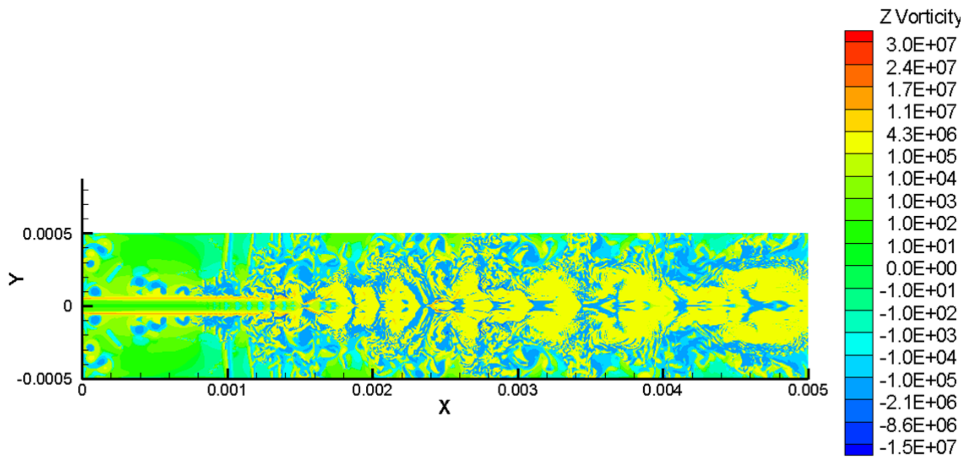

Figure 4.45: The contour of Z vorticity for the implicit LES 5-jet-diameter simulation using VOF multiphase model. Note 5-jet-diameter simulation means the half width of the computational domain is 5 times the jet inlet diameter.

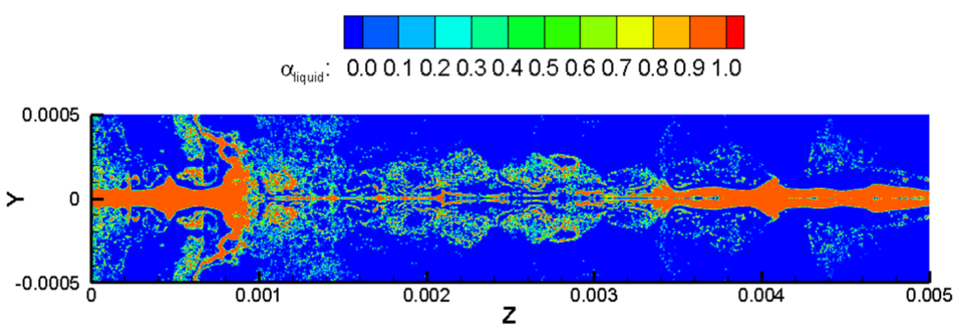

Figure 4.46: The contour of volume of fraction of liquid for the implicit LES 5-jet-diameter simulation using CLSVOF multiphase model. Note 5-jet-diameter simulation means the half width of the computational domain is 5 times the jet inlet diameter.

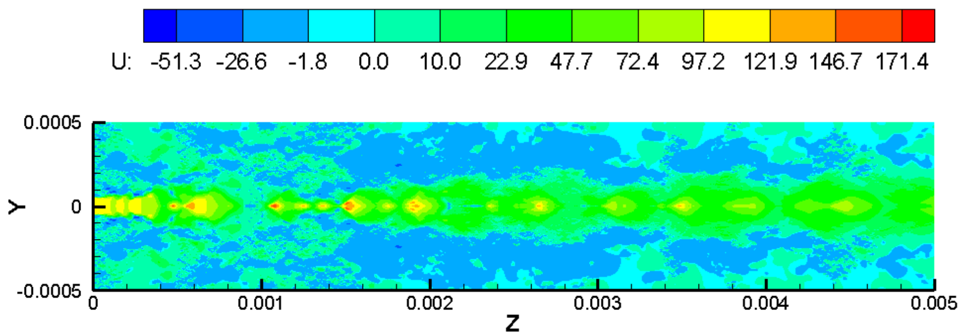

Figure 4.47: The contour of axial velocity for the implicit LES 5-jet-diameter simulation using CLSVOF multiphase model. Note 5-jet-diameter simulation means the half width of the computational domain is 5 times the jet inlet diameter.

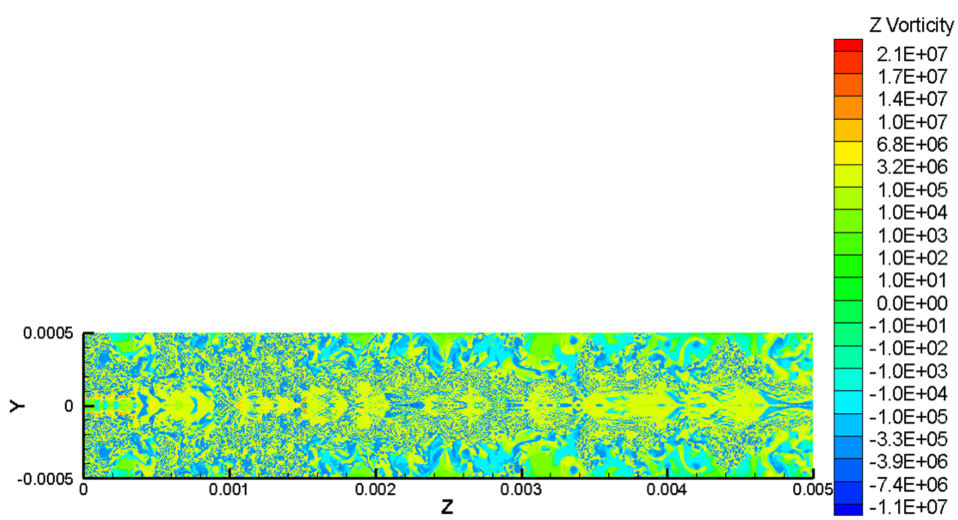

Figure 4.48: The contour of Z vorticity for the implicit LES 5-jet-diameter simulation using CLSVOF multiphase model. Note 5-jet-diameter simulation means the half width of the computational domain is 5 times the jet inlet diameter.

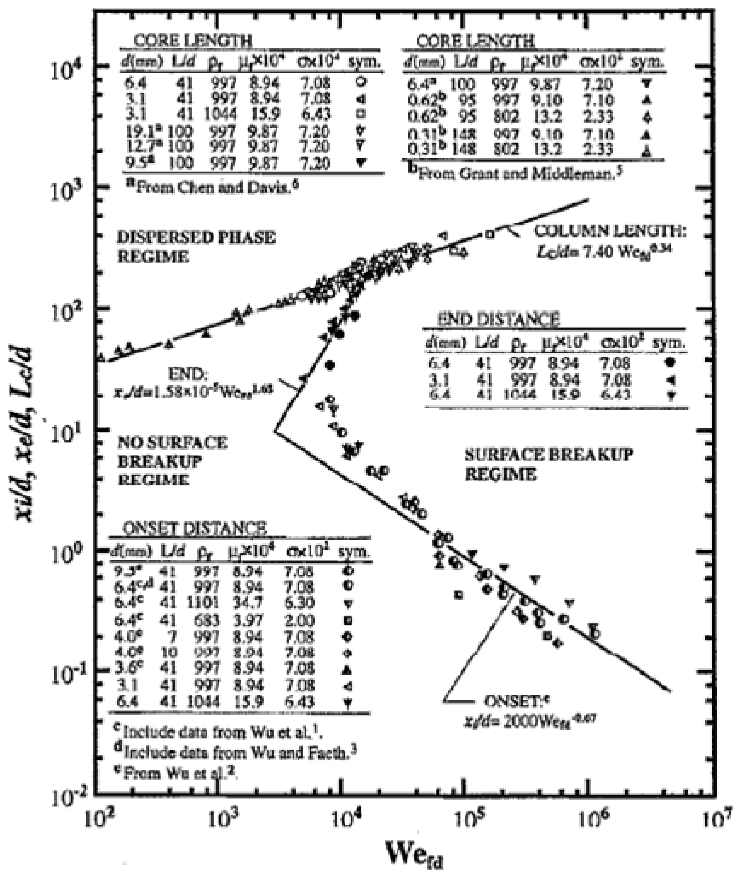

Figure 4.49: Surface breakup regime map for turbulent liquid jets in still gases when aerodynamic effects are small (liquid/gas density ratios are larger than 500)

Chapter 5

Results

5.1 Mercury Internal Flow in A Curved Pipe Without A Weld

5.1.1 Problem description

Since mercury flow becomes fully-developed long before approaching the first 90° half-bend angle, this geometry has been simplified by shortening the inflow section. The eight geometries investigated (Fig. 1.3) have length dimensions that are the same as in the MERIT experiment: the pipe radius is a, curvature radius $R = 2.33a$, and the inflow and outflow lengths of straight pipe are matched, with or without a nozzle at the exit region. The half-bend angles φ_1/φ_2 investigated are $0°/0°$, $30°/30°$, $60°/60°$, and $90°/90°$. The Reynolds number based on the bulk velocity and pipe diameter is approximately equal to 8.244×10^5 and the Dean number is 5.401×10^5.

A full model is tested for the pipe without a weld, whereas symmetry conditions are used for the pipe without or with a nozzle, allowing the use of half of the model, to save on computational cost. The computational grid points are $3.7 \times 10^6 \sim 5 \times 10^6$ and $3.9 \times 10^6 \sim 6 \times 10^6$ for pipes of various turning angles without and with nozzles, respectively. There are

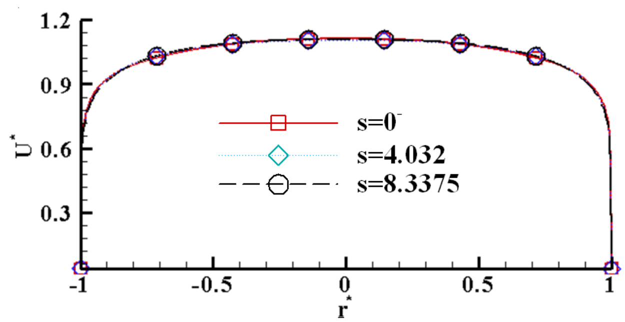

Figure 5.1: Radial distribution of the U^* as a function of location along the 0°/0° pipe

48 grid points in the circumferential direction and the grid density is 1.8°/ node for the half-bend angle. The distance of the first grid point adjacent to the wall is decided by $y^+ \approx 1$, where $y^+ \equiv u_\tau y/\nu$, u_τ is the friction velocity at the wall, y is the distance to the wall and ν is the local kinematic viscosity of the fluid. Approximately 15 grid points are within the inner layer. The boundary conditions have been described in the Chapter 2 of this paper.

5.1.2 Axial velocity distribution

As studied earlier, the pseudo coordinate distance, s, is used to describe the locations of points in the straight portions of the pipe, while the bend angles, φ_1 and φ_2, are used for the curved portions. These coordinates are depicted in Figure 1.2. The upstream tangents of all the curved pipes investigated in this paper are of the same length ($-5.17 \le s \le 0^-$). So are the downstream tangents ($0^+ \le s \le 8.3375$). Figure 5.1 - Figure 5.4 show the radial (r^*) axial-velocity (U^*) distribution for pipes without a nozzle. The effects of the bend angle on flow in the curved pipes are presented only for the cases without nozzles in order to isolate the complication of the nozzles.

In Fig. 5.1, the velocity distribution is identical for the three values of distance s examined, since there is no bend and the flow has already reached the fully developed profile by the inlet of the pipe. The 30°/30°, 60°/60°, and 90°/90° pipes are also imposed the fully developed flow at the inlet, which is a similar, symmetrical, radial distribution of U^*, shown in Fig. 5.1. At the start of the first half-bend ("Bend Starts" for 30°/30° (Fig. 5.2), "Bend Starts" for

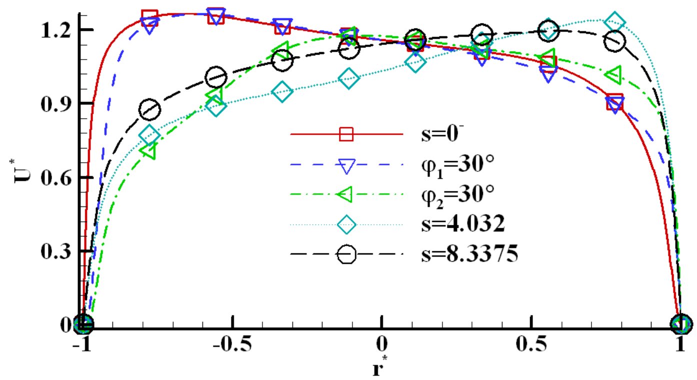

Figure 5.2: Radial distribution of U^* as a function of location along the 30°/30° pipe

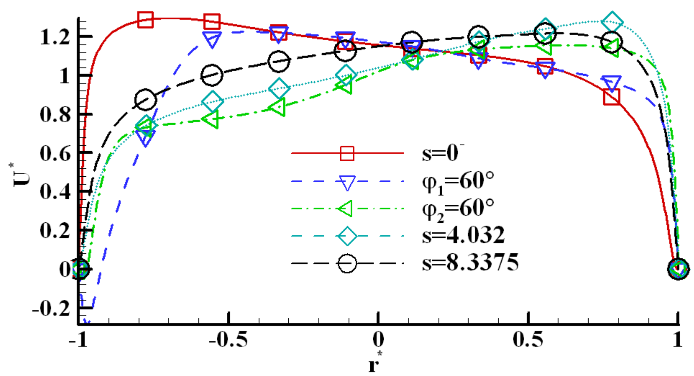

Figure 5.3: Radial distribution of U^* as a function of location along the 60°/60° pipe

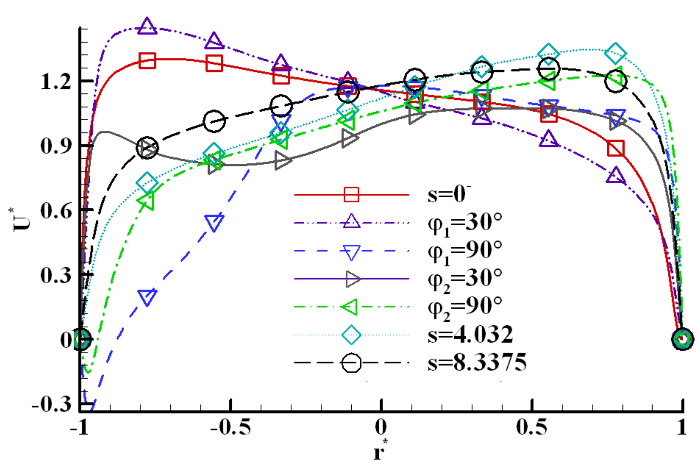

Figure 5.4: Radial distribution of U^* as a function of location along the 90°/90° pipe

60°/60°(Fig. 5.3), and "Bend Starts" for 90°/90° (Fig. 5.4)), the convex (inner) side of the pipe (near $r^* = -1$) shows higher magnitudes of U^*. At the end of the first half-bend ($\varphi_1 = 30°$ for 30°/30° (Fig. 5.2), $\varphi_1 = 60°$ for 60°/60°(Fig. 5.3) maintains its direction at the start of the bend, but with reduced magnitude. That is, at "Bend Starts" and at $\varphi_1 = 30°$ for the 30°/30° pipe (Fig. 5.2), $\partial U^*/\partial r^*$ is negative with a magnitude that is smaller for $\varphi_1 = 30°$ relative to "Bend Starts". Similarly, for the 60°/60° (Fig. 5.3) pipe, $\partial U^*/\partial r^*$ is negative with a reduced magnitude at $\varphi_1 = 60°$. However, for the 90°/90° (Fig. 5.4) pipe, $\partial U^*/\partial r^*$ changes its direction at $\varphi_1 = 90°$. That is $\partial U^*/\partial r^*$ is positive with high velocity region at the center of pipe. For all curved pipes, $\partial U^*/\partial r^*$ is negative, and the high velocity region is located near the concave side ($r^* = 1$) as the flow leaves the second half bend. Actually, for the 90°/90° pipe, the high velocity region moves to the concave side ($r^* = 1$) before the flow leaves out of the second half bend (Fig. 5.4)).

In Fig. 5.5 - Fig. 5.9, the effects of having a nozzle at the exit are shown. For the straight pipe, the nozzle causes a symmetric velocity profile respect to the radial direction, as we move downstream through the pipe (Fig. 5.5). The flow develops complicated patterns (back flow) near the inner side of the half-bend, with one turning point in the velocity profile for both curved pipe with and without a nozzle. The back flow is stronger in the pipe of larger half bend angle. However, the existence of the second half-bend recovers the oscillation (in $r^* = -1$) for all curved pipes. That is to say back flow is weaker at the same relative locations after the second half-bend as those after the first half-bend. Take the 90°/90° pipe as an example, the back flow near the convex side ($r^* = -1$) is stronger in $\varphi_1 = 90°$ (Fig. 5.8(d)) than in $\varphi_2 = 90°$ (Fig. 5.9(g)). At the exit plane ($s = 8.3375$), the flow in the pipes with nozzles tend to have higher velocities in the $-0.9 < r^* < 1$ region, the velocity profile is uniform radially, and the wall boundary layer is much thinner, when compared with those without a nozzle (Fig. 5.5(c), Fig. 5.6(e), Fig. 5.7(e), and Fig. 5.9(g)). The results show that the effect of the nozzle on the upstream flow is extremely weak. The nozzle only comes into effect on the flow at the beginning of the nozzle ($s = 4.032$). The decreasing cross-

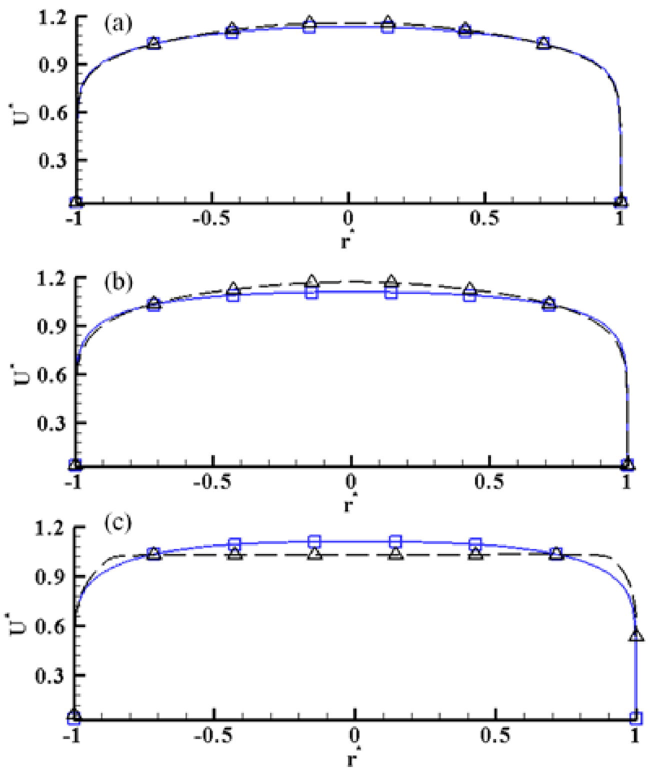

Figure 5.5: Comparison of radial distribution of U^* at the same location along the 0°/0° pipe without (square symbols) and with (delta symbols) a nozzle: (a)$s = 0^-$ (b)$s = 4.032$ (c)$s = 8.3375$

sectional area of the nozzle along the flow path leads to a decrease in the static pressure. The flow being subsonic, the velocity profile becomes sloper at the beginning of the nozzle ($s = 4.032$). The 90°/90° pipes are further investigated in Fig. 5.10 and 5.11 because of the current application in the MERIT experiment (90°/90°). The velocity distribution is similar for these two cases until the nozzle appears ($s = 4.032$). At the end of the first bend, the axial velocity magnitude increases near the concave side while decreasing near the convex side. This pattern is caused by the cross-stream pressure gradient. Once the high velocity fluid encounters the adverse pressure gradient on the convex side, it starts to move towards the concave side (The abbreviations "CC" and "CV" are used in these figures to denote the concave and convex sides, respectively.) . The flow becomes more and more stratified toward the exit ($s = 8.3375$) when the effect of the bend becomes insignificant.

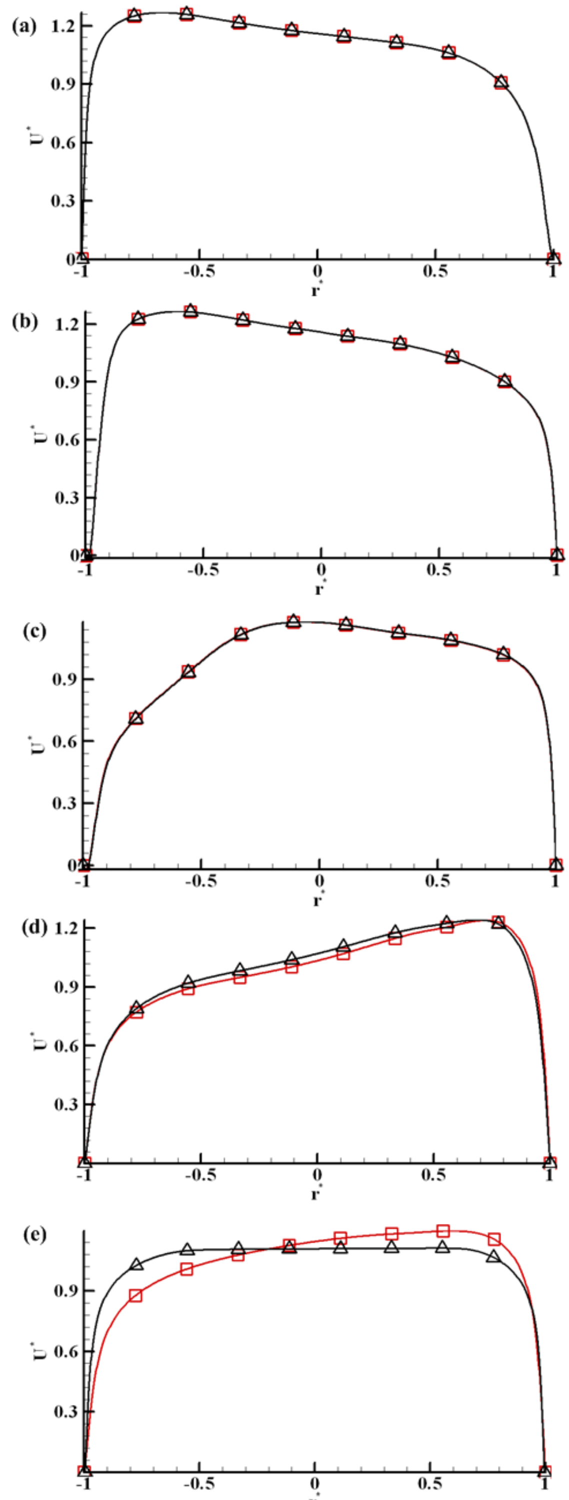

Figure 5.6: Comparison of radial distribution of U^* at the same location along the 30°/30° pipe without (square symbols) and with (delta symbols) a nozzle: (a)$s = 0^-$ (b)$\varphi_1 = 30°$ (c)$\varphi_2 = 30°$ (d)$s = 4.032$ (e)$s = 8.3375$

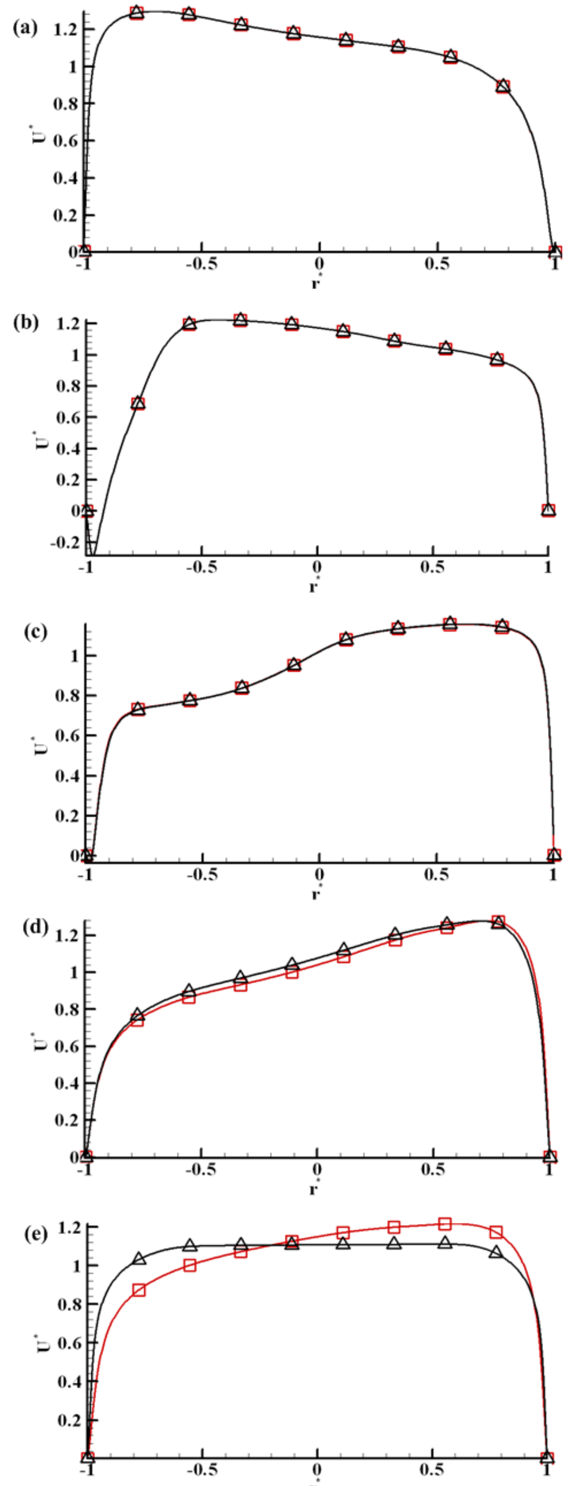

Figure 5.7: Comparison of radial distribution of U^* at the same location along the 60°/60° pipe without (square symbols) and with (delta symbols) a nozzle: (a)$s = 0^-$ (b)$\varphi_1 = 60°$ (c)$\varphi_2 = 60°$ (d)$s = 4.032$ (e)$s = 8.3375$

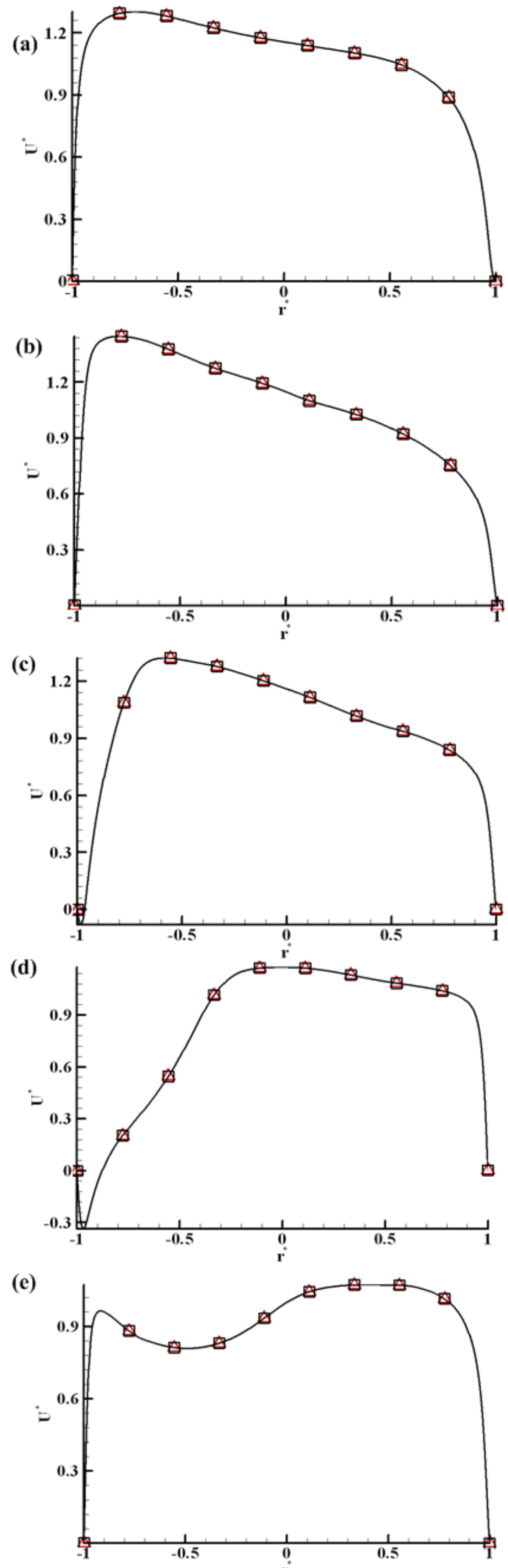

Figure 5.8: Comparison of radial distribution of U^* at the same location along the 90°/90° pipe without (square symbols) and with (delta symbols) a nozzle: (a)$s = 0^-$ (b)$\varphi_1 = 30°$ (c)$\varphi_1 = 60°$ (d)$\varphi_1 = 90°$ (e)$\varphi_2 = 0°$

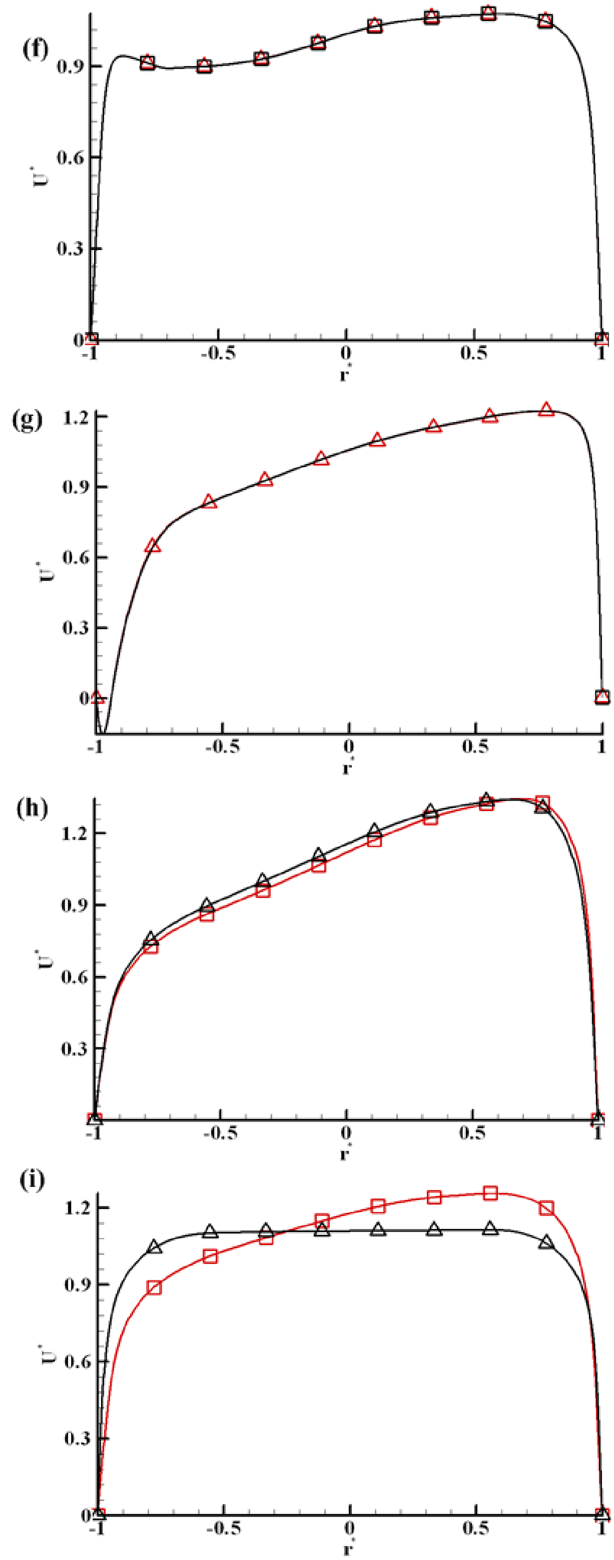

Figure 5.9: Comparison of radial distribution of U^* at the same location along the $90°/90°$ pipe without (rectangular symbols) and with (triangular symbols) a nozzle: (f)$\varphi_2 = 90°$ (f)$s = 4.032$ (g)$s = 8.3375$

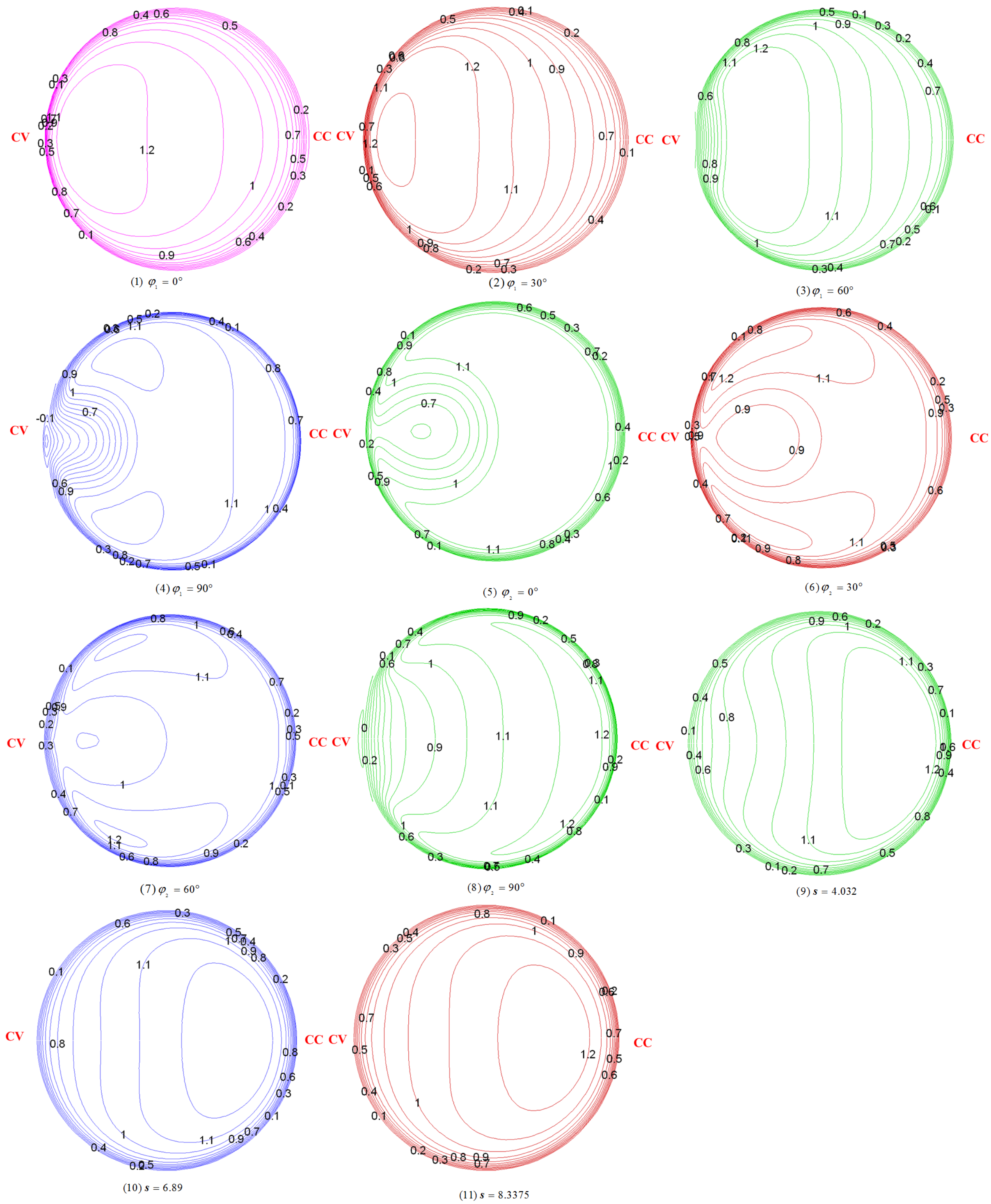

Figure 5.10: The contour of U^* as function of location along the 90°/90° without a nozzle

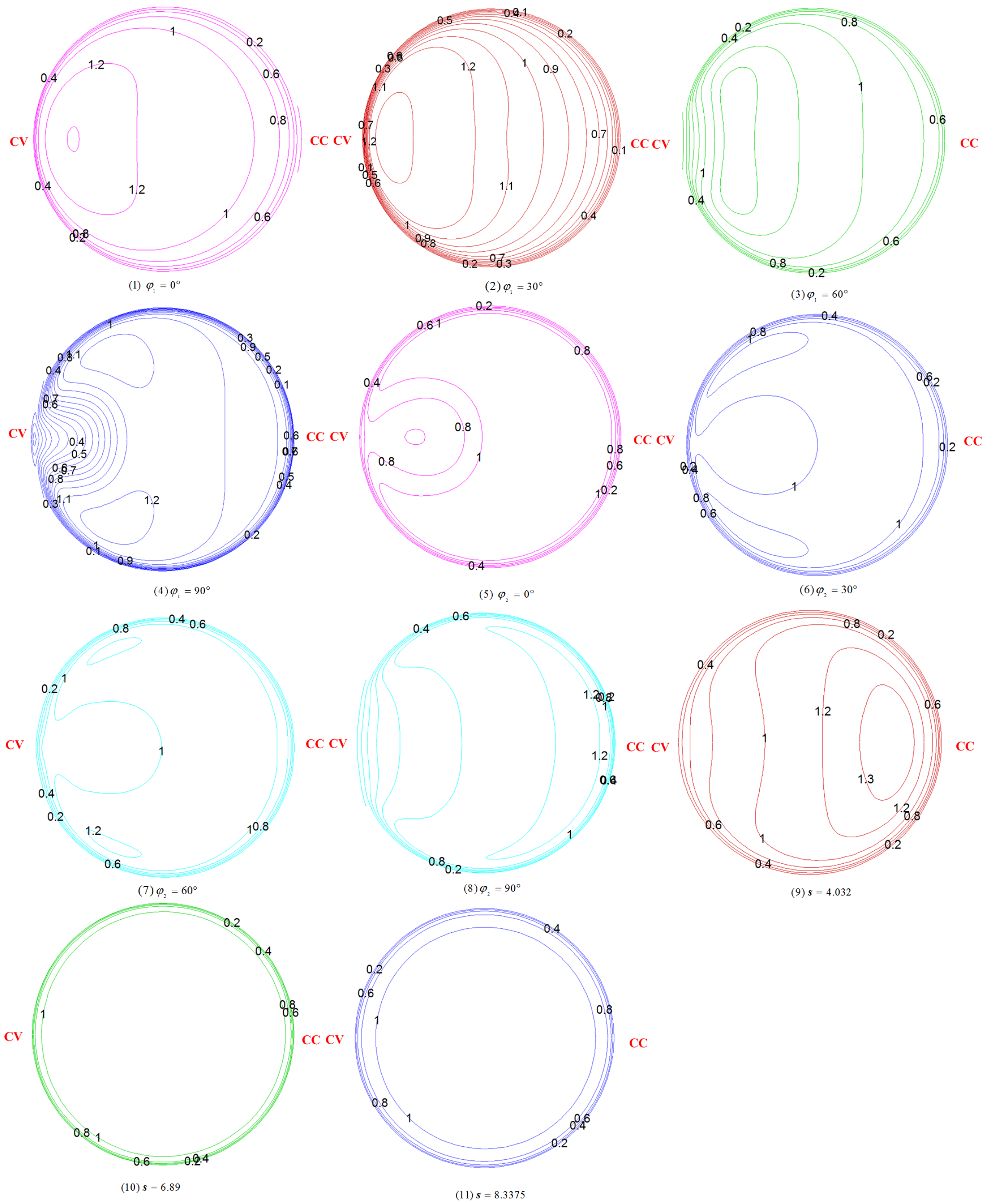

Figure 5.11: The contour of U^* as function of location along the 90°/90° with a nozzle

5.1.3 Momentum thickness

One goal of the present study is to determine the pipe configuration that has the potential to give the least disturbance in the circular jet shear layer that eventually issues from the nozzle. Therefore, some knowledge of the distribution of the momentum thickness δ_θ at the nozzle exit becomes important. For example, linear stability analysis of Michalke [126] and Plaschko [127] and the experimental work of Cohen and Wygnanski, [128] Corke *et al.*, [129] and Corke and Kusek [130] showed that for large $2a/\delta_\theta$ ($2a/\delta_\theta \gg 1$), both axisymmetric ($m = 0$) and the first spinning or helical instability modes ($m = \pm 1$ or -1) are unstable in the initial jet shear layer.

The polar distribution of δ_θ is shown in Fig. 5.12 and Fig. 5.13 for pipes without and with a nozzle, respectively. The number "0" in the polar plots refers to the wall, while the numbers "1", "2", and "3" respectively refer to the distances $0.1a$, $0.2a$, and $0.3a$ measured from the wall. Momentum thickness decreases with decreasing radius. For pipes without a nozzle (Fig. 5.12), the distribution of δ_θ is nonuniform at the exit but similar. The azimuthal variation of δ_θ becomes stronger as the half-bend angle increases. Thus 90°/90° shows the strongest azimuthal variation of δ_θ compared to other pipes. At the exit plane, δ_θ attains its minimum value at $\theta = 0°$ and its maximum value at $\theta = 180°$. Note that the straight pipe does not show an azimuthal variation of δ_θ. Figure 5.13 shows a fairly uniform δ_θ distribution for all pipes, when nozzles are present at the exit.

The differences in the azimuthal variation of δ_θ can be explained by the relationship between momentum thickness and axial velocity, where the latter, at pipe exit, is shown in Figs. 5.2-5.4 for the various pipe configurations. Note that the 90°/90° pipe shows the most asymmetry in the distribution of the axial velocity (Fig. 5.4), and hence in the azimuthal distribution of δ_θ. For pipes with nozzles, the axial velocity profile is fairly uniform in the azimuth, which explains the uniform azimuthal distribution of δ_θ.

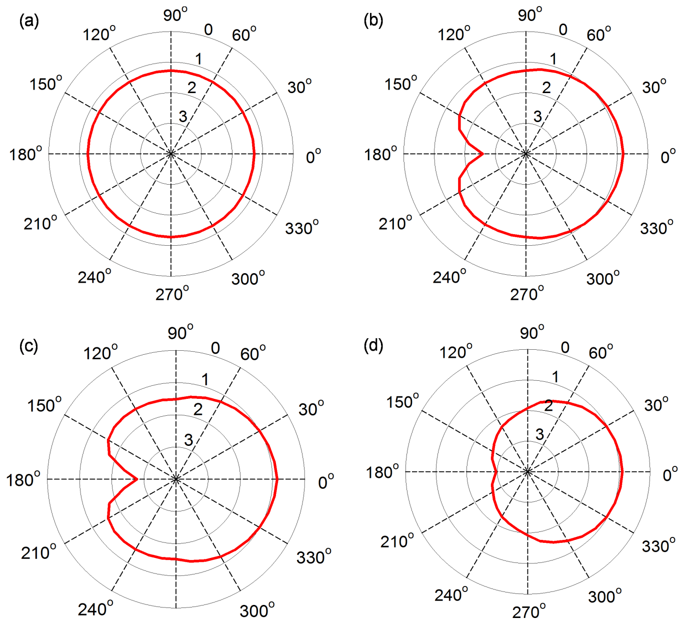

Figure 5.12: Momentum thickness distribution at the exit plane of pipes for turning angles of: (a)0°/0° (b)30°/30° (c)60°/60° (d)90°/90°. These pipes do not have nozzles and $\theta = 180°$, 0° correspond to the convex and concave sides of the pipes, respectively

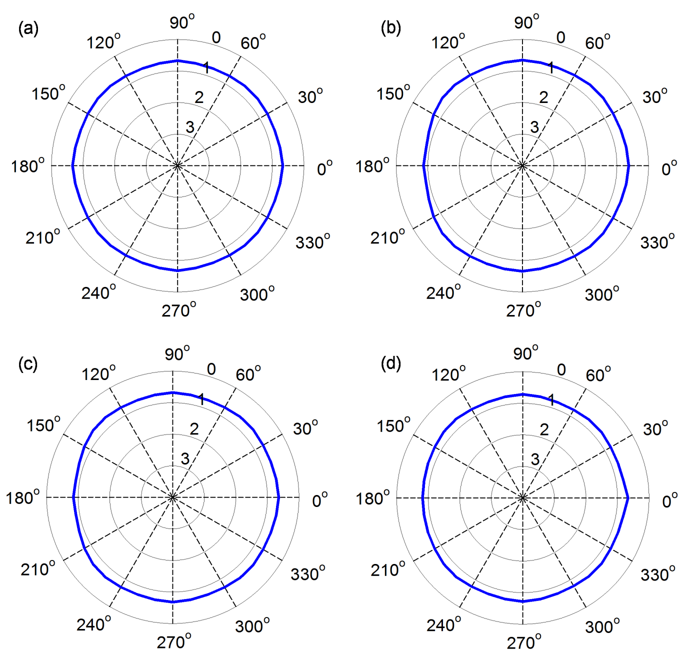

Figure 5.13: Momentum thickness distribution at the exit plane of pipes for turning angles of: (a)0°/0° (b)30°/30° (c)60°/60° (d)90°/90°. These pipes have nozzles and $\theta = 180°$, 0° correspond to the convex and concave sides of the pipes, respectively

5.1.4 Turbulence intensity

The turbulence intensity at the exit of pipe is of interest, as it determines the turbulence level in the jet. This quantity is defined in this paper as

$$I = \sqrt{\frac{2}{3}(\frac{k}{U_b^2})}, \tag{5.1}$$

where k is the turbulence kinetic energy per unit mass and U_b has been used as a scale for $\acute{u}_{rms}$, the root-mean-squared fluctuating velocity. The radial distribution of I at the exit plane along the horizontal direction is presented in Fig. 5.14. I is found to have high values near the walls, with a large gradient for all pipes. It is clear to see that I is reduced when having a nozzle. For the pipe without a nozzle, I increases as the half-bend angle increases. For example, the 90°/90° pipe has the strongest turbulence intensity. The radial distribution of I is symmetrical for the straight pipe (0°/0°), with a flat interior, as expected. The profile of I with r^* along the horizontal direction for the 30°/30°, 60°/60°, and the 90°/90° pipes without nozzles, shows higher values near $r^* = -1$ (concave side) compared to $r^* = 1$ (convex side). The higher values of I on the convex side for the 60°/60° pipe without a nozzle are related to the instabilities associated with adverse pressure gradient. With nozzles, there is a steeper radial gradient of I near wall in the 0°/0°, 30°/30°, 60°/60°, and 90°/90° pipes compared to those without nozzles. I is nearly flat in the interior region ($-0.6 < r^* < 0.6$). In the region of $-1 < r^* < -0.6$, I has relatively higher values as the half-bend angle decreases from nonzero value. Generally speaking, the straight pipe with a nozzle is the pipe with least turbulence intensity among all eight pipes.

5.1.5 Discussions

The objective of this study is to comparatively evaluate various pipe configurations that have been proposed for liquid target delivery in the Muon Collider project. The desirable configurations are those that lead to the weakest turbulence intensity levels and the smallest

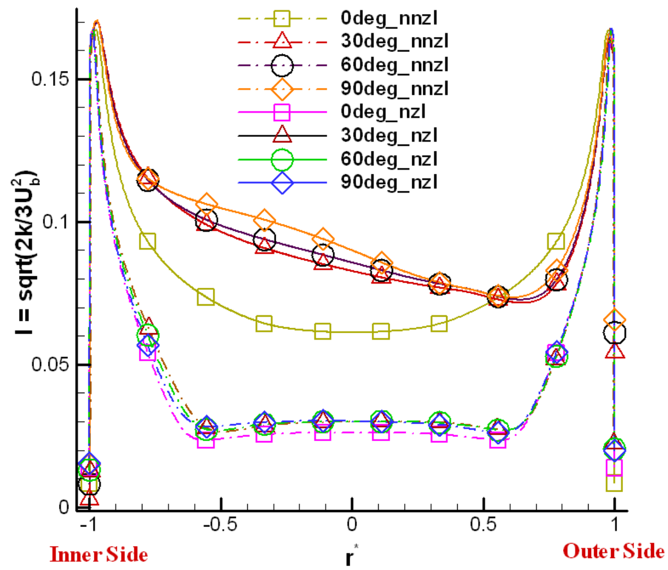

Figure 5.14: The horizontal distribution of turbulence intensity at the exit plane. Subscripts "with" and "without" denote presence or absence of a nozzle at pipe exit

momentum thickness at the exit plane. Eight pipe configurations with different turning angles are studied, without and with a nozzle at the exit region of the pipe. A simple analytical study is performed to describe the laminar flow in curved pipes, in relation to the terms representing curvature effects. The realizable $k - \varepsilon$ (RKE) RANS model has been applied to simulate turbulent flows in the pipes. At the exit plane of the pipe without a nozzle, δ_θ is smaller at $\theta = 0°$ relative to the value at $\theta = 180°$ (Figure 5.12), where a lower level of turbulence intensity occurs. The effects of nozzle include the azimuthal homogenization of the flow, and hence a uniform velocity, as well as a uniform azimuthal distribution of δ_θ. The nozzle also significantly reduces the turbulence intensity at the pipe exit. However, the straight pipe has the least turbulence intensity, because of the absence of secondary flows. From the effects of bend and nozzle shown in this study, a straight pipe with a convergent nozzle was found to have the weakest turbulence intensity level at the exit plane.

5.2 Mercury Internal Flow in A Curved Pipe With A Weld

5.2.1 Problem Description

From the borescope video of the interior of the titanium nozzle for the Muon Collider project, ominous weld beads are visible. It seems like these "turbulators" are responsible for much of the poor performance of the jet. The key issue is the azimuthal symmetry of the bead. As a start, an azimuthally symmetric bead is modeled for the 90°/90° pipe. Then nozzle with beads more closer to reality are modeled, which is azimuthally asymmetric, for example a 30° azimuthal bead with its center transverse to the bend plane. Both the azimuthally symmetric and asymmetric beads locate close to the beginning of the nozzle taper and have a semicircle cross-section, as illustrated in Figure 5.15 (a) and (b) respectively. We can see that the inner radius of the semicircle bead is 1/16 inches.

5.2.2 Computation of the pipe simulation with an azimuthal complete weld

In order to find proper mesh for the pipe simulation with a weld, a mesh independence check has been carried out to the 90°/90° pipe with an azimuthally symmetric bead, as shown in Fig. 5.16. The results of turbulent intensity, I, at the pipe exit are very consistent when the grid number is 2.5 million and 3.2 million.The information of a proper mesh density in the directions of r^*, θ , and $\tilde{z}^*$ for a bend pipe simulation with weld is achieved and the pipe simulation is independent of mesh when grid number is 2.5 million.

The effects of the azimuthal symmetry semicircle bead/weld are studied by comparing the I (turbulence intensity) at the exits of the pipe with/without a weld. The comparison can be found in Fig. 5.17. It is clear to see that the turbulence level is higher at the center region of the pipe in the case of the pipe with a weld, which implies the weld disturbs the

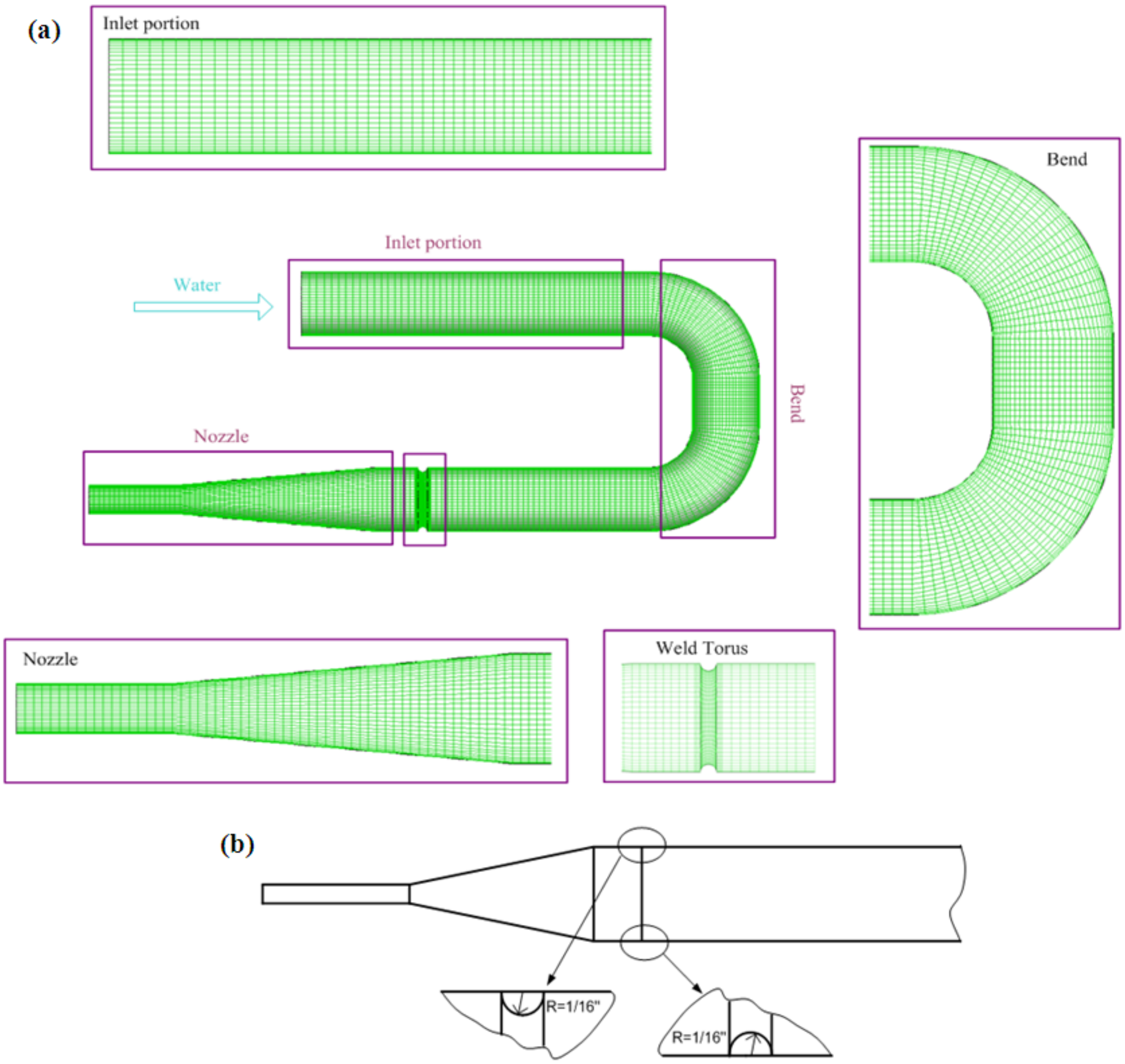

Figure 5.15: (a) Location of the studied bead in the 90°/90° pipe (b) Dimension of the semicircle bead

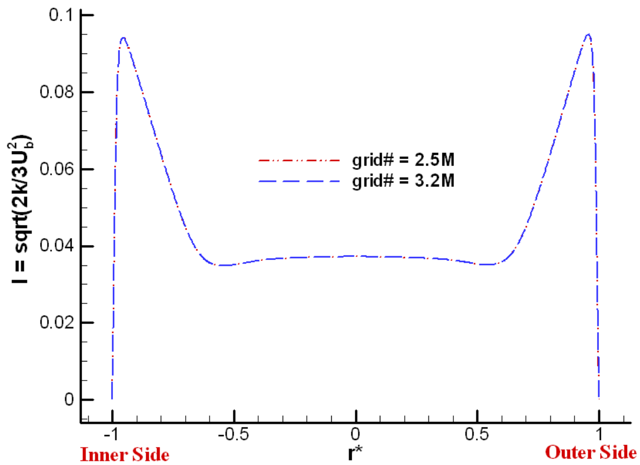

Figure 5.16: Mesh independence check for the pipe with an azimuthally symmetric bead

flow resulting in a more turbulent flow. The large gradient of velocity near the wall of the pipe makes flow really turbulent, which is same for the pipe with or without a weld. The effects of bend do not retain at the pipe exit no matter the existence of the weld, which can tell by the less asymmetric distribution of I in the direction of r^*.

5.2.3 Computation of the pipe simulation with an azimuthal incomplete weld

The geometry of 90°/90° pipe with an azimuthally asymmetric 30° weld is shown in figure 5.18. The 30° bead locates at the same location along the flow direction as the 360° bead does. The inner diameter as well as the geometry of the bead are consistent with these of the 360° bead but just have a azimuthal length of 30° instead of 360°.

Four different meshes are applied to the simulation when the pipe has a 30° weld. The total mesh grids go from very coarse 0.7 million to very fine 16 million. The later simulations are carried out for all four different mesh grids. It turns out a mesh independence for the pipe with a 30° weld when grid number reaches 5 million. The analyses of asymmetric weld

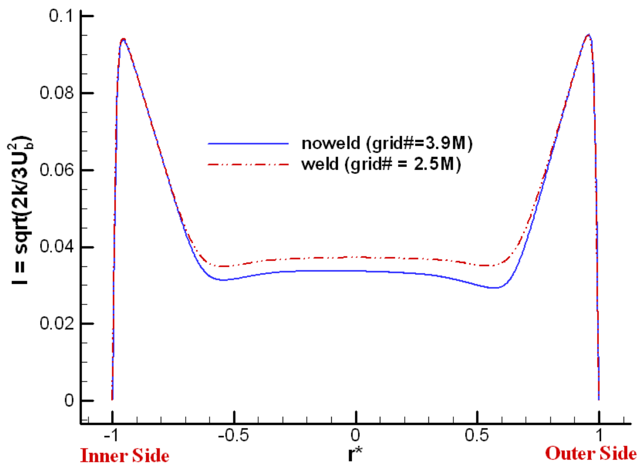

Figure 5.17: Comparison of turbulence intensity between the pipe without a weld and the pipe with an azimuthally symmetric weld

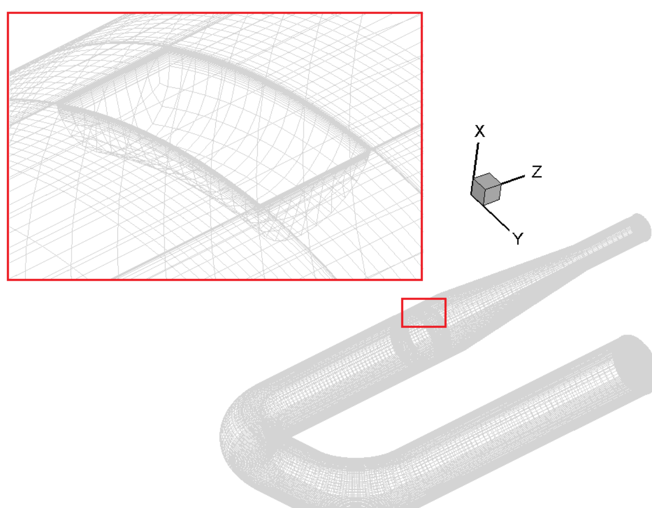

Figure 5.18: The 90°/90° pipe with an azimuthally asymmetric 30° bead/weld

calculations are carried on for the following parameters:

(1) Wall shear stress, τ_w, is calculated by

$$\tau_w = \mu \frac{\partial U}{\partial n}|_w, \tag{5.2}$$

where $\frac{\partial U}{\partial n}|_w$ is velocity gradient at the wall. From the wall shear stress, a velocity scale, U_w (friction velocity or called shear velocity), is introduced

$$U_w = \sqrt{\frac{\tau_w}{\rho}}. \tag{5.3}$$

The shear velocity characterizes the turbulence strength, u_{rms}, and laminar sub-layer thickness at the boundary, δ_S

$$u_{rms} \sim U_* \tag{5.4}$$

$$\delta_S = 5\nu/U_*. \tag{5.5}$$

(2) Turbulence kinetic energy (TKE), k, is the mean kinetic energy per unit mass associated with eddies in turbulent flow. Generally, the turbulent kinetic energy is calculated by the mean of the turbulence normal stresses:

$$k = \frac{1}{2}(\overline{u^2} + \overline{v^2} + \overline{w^2}). \tag{5.6}$$

(3) Momentum thickness, δ_θ, is the distance by which a surface would have to be moved parallel to itself towards the reference plane in an inviscid fluid stream of velocity $U_{\max}$ to give the same total momentum as exists between the surface and the reference plane in a real fluid.

$$\delta_\theta = \int_0^a \frac{U}{U_{\max}}(1 - \frac{U}{U_{\max}})dr. \tag{5.7}$$

The distribution of the wall shear stress (τ_w), kinetic energy of turbulence (k), kinetic energy dissipation rate (ϵ), the mean velocity (U), and the friction velocity (U_w) from the beginning to the end of pipe is shown in Figs. 5.19 and 5.20 for the top line distribution and bottom line distribution respectively. The top line is defined on the pipe surface passing through the middle of the weld, while the bottom line is on the pipe surface far away from the top line, as shown in Fig. 5.21. The "S" on the x-axis of these figures is defined as the normalized arc length by the pipe diameter at the inlet. The results are compared among four different mesh densities: 0.7 million, 3 million, 5 million, and 16 million. The results of 5 million case and 16 million case show good agreements for the variable distributions, indicating the mesh independence is achieved when the grid number reaches 5 million. The top line distribution of τ_w, k, ϵ, U, and U_w (Fig. 5.19) presents a local drop at roughly $S = 13$, where exactly the 30° weld centers. However there is no changes to the distribution of k and ϵ at $S = 13$ on the bottom line, as shown on Fig. 5.20, which implicates the effects of the 30° weld are too week to influence the flow on the other side far away from the weld. Downstream the 30° weld, τ_w, k, ϵ, and U_w except U keep increasing fast along both top and bottom lines until $S = 16.62$, where the narrowest straight part of the nozzle starts.

Figs. 5.22 and 5.23 give the detail distribution of τ_w, k, ϵ, U, and U_w along two orthogonal lines passing through the middle of the weld. The locations of the two orthogonal lines on the weld surface are shown in Fig. 5.24. The mesh independence is supported again by the agreements between the 5 million case and 16 million case in the two figures. The distribution of τ_w, k, ϵ, U, and U_w along the line of constant Z (Fig. 5.22) is almost symmetry with the exception that near wall the magnitude of τ_w, k, ϵ, U, and U_w is smaller on the outer side ($Y = -0.0716$) than the inner side ($Y = -0.0664$) of the pipe. However, this difference is very small seen from the Fig. 5.22. Also for the distribution of τ_w and U_w, the lowest value at the pipe center region ($-0.0706 < Y < -0.0666$) locates slightly to the outer side ($Y = -0.0716$) of the pipe. These implies that the downstream effects of the bends still remain upto the location of the 30° weld but are not significant any more. Along the line of constant Y in the weld region, the magnitude of τ_w, k, ϵ, U, and U_w is much larger in

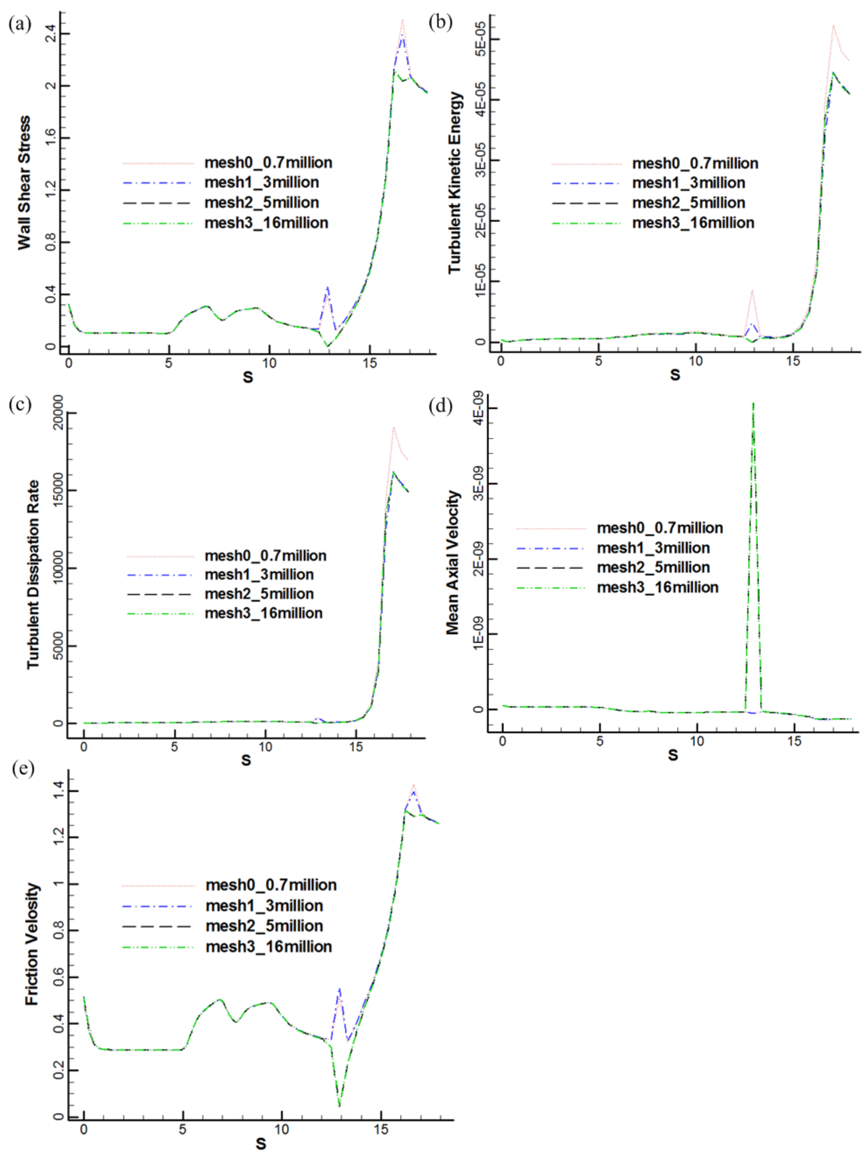

Figure 5.19: The distribution of wall shear stress, turbulent kinetic energy, turbulent dissipation rate, mean axial velocity, and friction velocity along the top line on the pipe wall

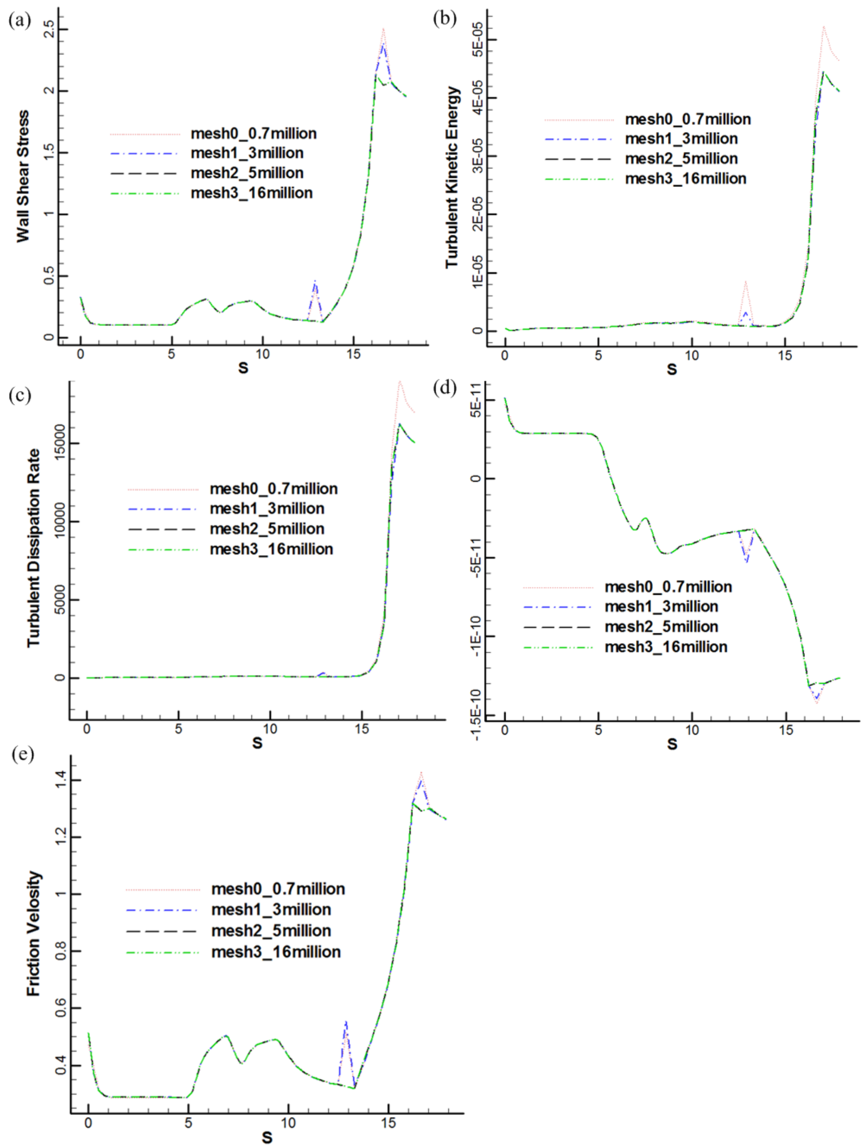

Figure 5.20: The distribution of wall shear stress, turbulent kinetic energy, turbulent dissipation rate, mean axial velocity, and friction velocity along the bottom line on the pipe wall

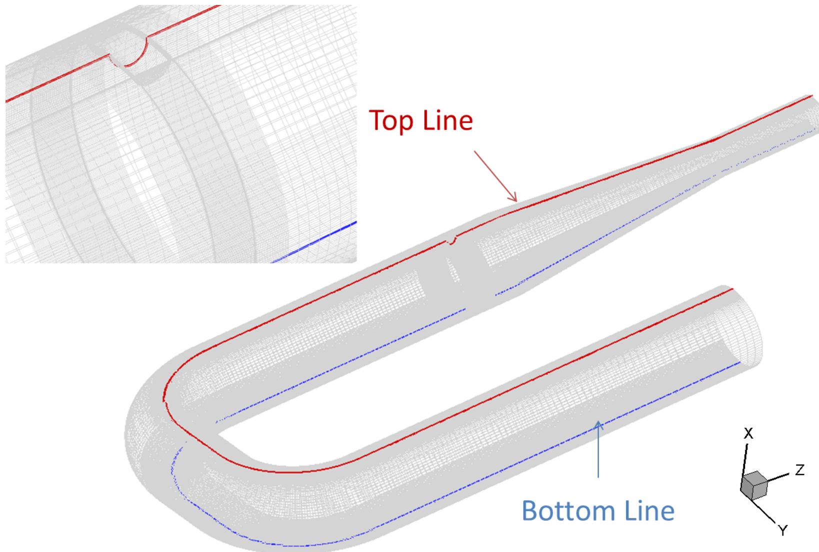

Figure 5.21: The locations of top and bottom lines on the pipe wall

the upstream than in the downstream of the weld. This can be well explained by the flow separation. When pressure in the direction of flow increases, known as an adverse pressure gradient, the boundary layers tend to separate from a surface. As a result of the increasing fluid pressure, the potential energy of the fluid increases, leading to a decreased kinetic energy. When boundary layer separation happens, the boundary layer thickens, resulting in a reduced wall shear stress.

The exit of the nozzle is akin to the start of the jet flow, therefore the distribution of k and δ_θ at the pipe exit is close to subsequent jet flow study as shown in Figs. 5.25 and 5.26 respectively. After the convergent nozzle, both the distribution of k and δ_θ are very uniform, although the magnitude of k and δ_θ differs among different meshes. Also two planes normal to the pipe axis in the vicinity of the weld, as shown in Figs. 5.27 are chosen to check the distribution of k and δ_θ in the vicinity of the weld. The plane of $z = 0.0430405$ is upstream compared to the plane of $z = 0.0380405$. Compared with the high magnitude region of k at the weld location on the plane of $z = 0.0430405$ (Fig. 5.28), the magnitude of k increases by 200% on the plane of $z = 0.00380405$ (Fig. 5.29) at the same weld location. k at the pipe center doesn't changes neither magnitude nor the position of its biggest magnitude. δ_θ

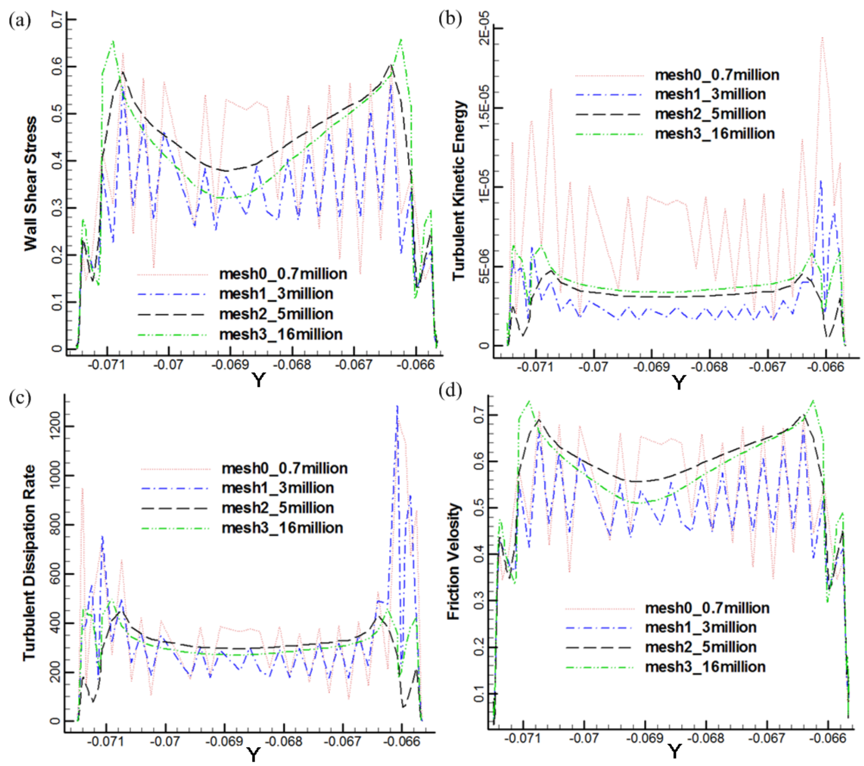

Figure 5.22: The distribution of wall shear stress, turbulent kinetic energy, turbulent dissipation rate, and friction velocity along the constant Z line across the weld center

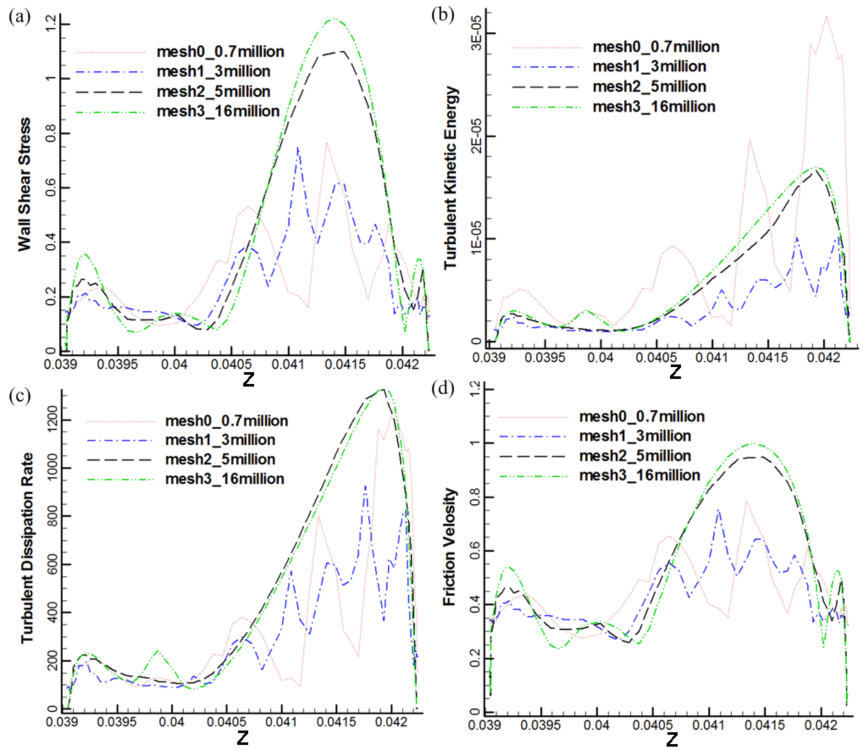

Figure 5.23: The distribution of wall shear stress, turbulent kinetic energy, turbulent dissipation rate, and friction velocity along the constant Y line across the weld center

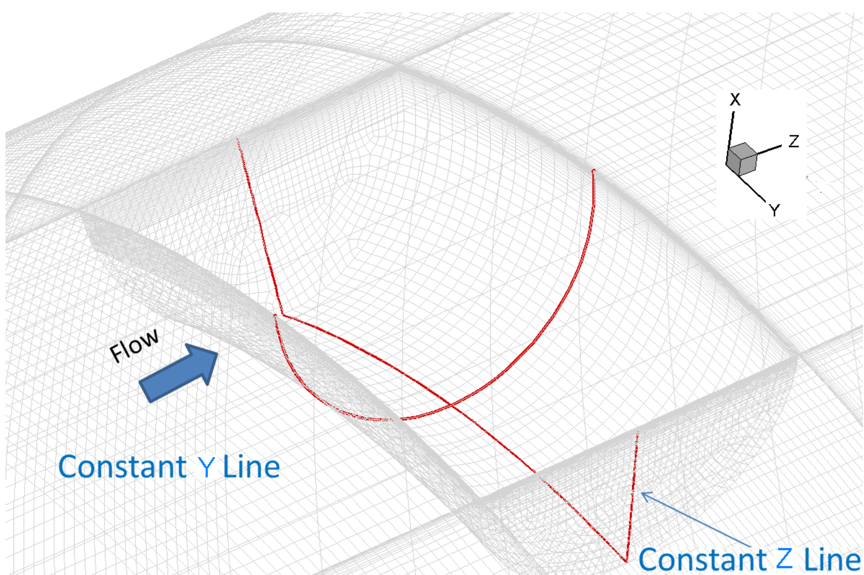

Figure 5.24: The locations of top and bottom lines on the pipe wall crossing the weld center

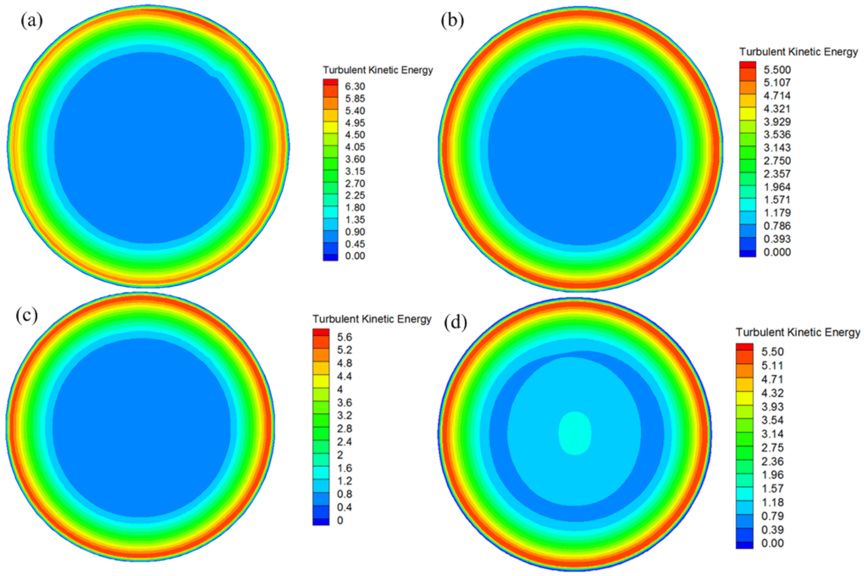

Figure 5.25: Distribution of k at the pipe exit when grid number is (a) 0.7 million (b) 3 million (c) 5 million (d)16 million

increase locally in the vicinity of the 30° weld (90° location in Fig. 5.30), which is caused by the thicken boundary layer when flow separation happens. Also δ_θ increases smoothly and is locally symmetry in the nearby region of 180° location (Fig. 5.31). Other than these locations, δ_θ keeps the same values before and after the weld.

5.2.4 Study On the Effects of Bend And Weld

In order to study the effects of bend and weld on the internal pipe flow, three types of pipe flows are chosen for the discussions: straight pipe without a weld, 90°/90° pipe without a weld, and 90°/90° pipe with a 30° weld. Static pressure, wall shear stress, axial velocity, momentum thickness, turbulence intensity, and turbulent kinetic energy dissipation rate are analyzed for the flows in these three pipes.

Static Pressure Develops From the Inlet to the Outlet of the Pipe

The static pressure difference between the inlet and the outlet of the pipe is almost the same for all three cases. The pressure loss is 297 Pa for the straight pipe without a weld,

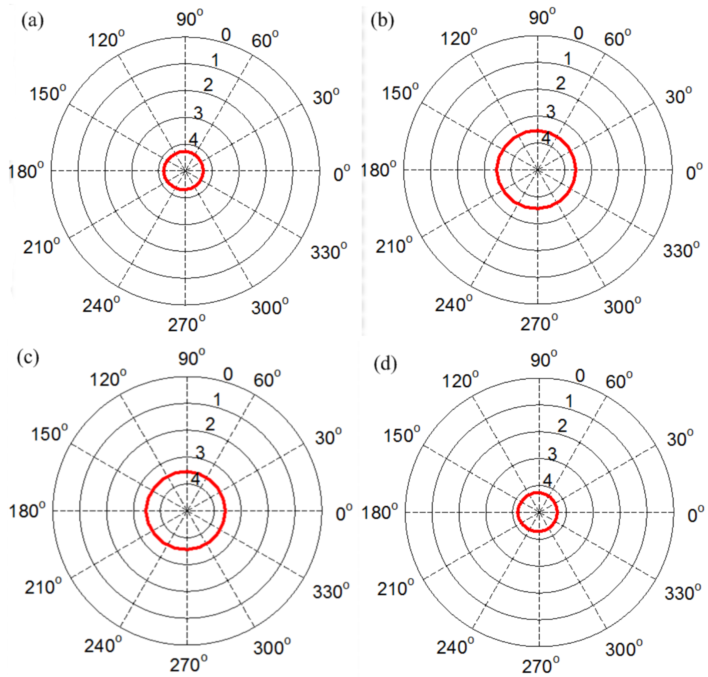

Figure 5.26: Distribution of δ_θ at the pipe exit when grid number is (a) 0.7 million (b) 3 million (c) 5 million (d)16 million

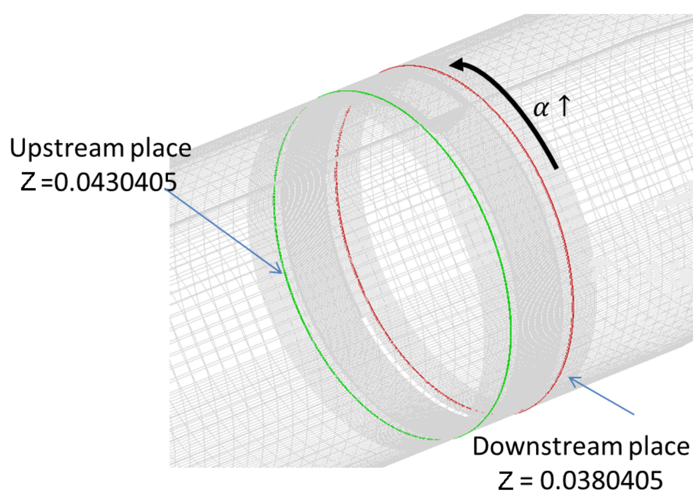

Figure 5.27: Locations of two constant Z planes in the vicinity of the 30° weld

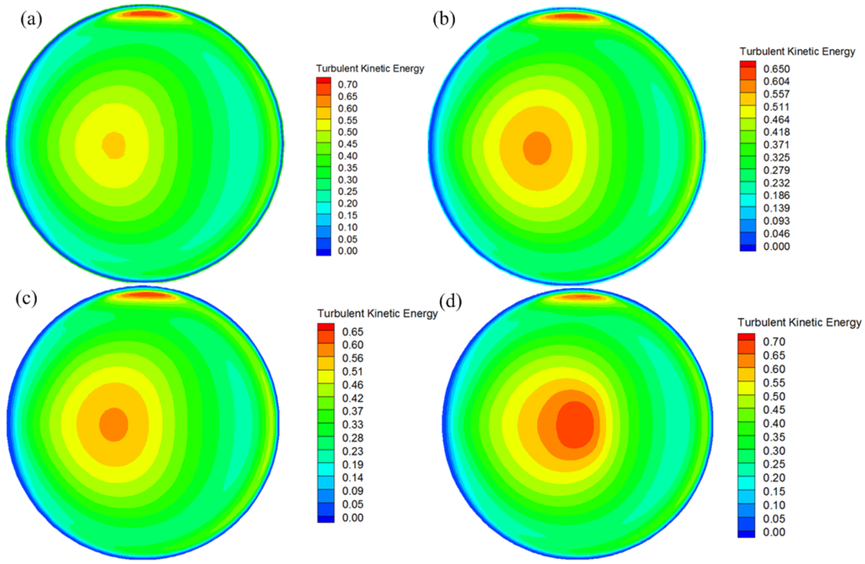

Figure 5.28: Distribution of k on the plane of $z = 0.0430405$ when grid number is (a) 0.7 million (b) 3 million (c) 5 million (d)16 million

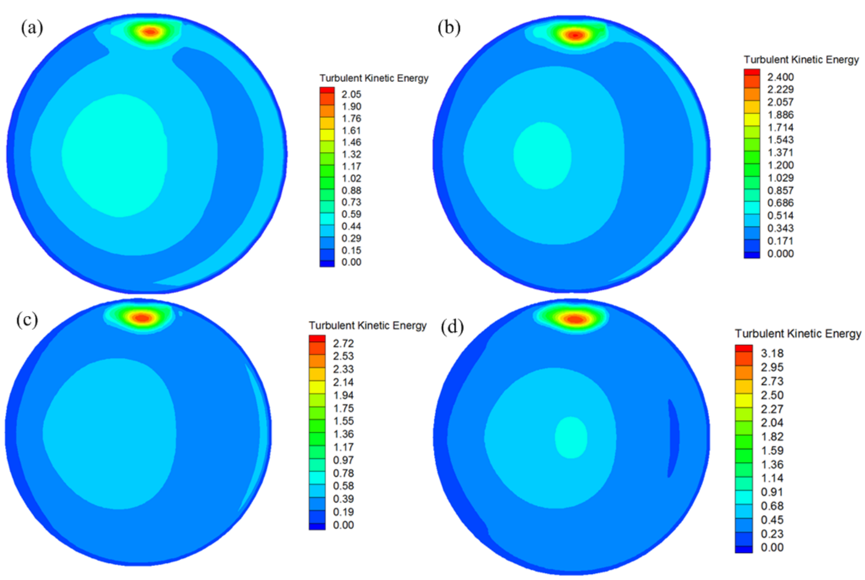

Figure 5.29: Distribution of k on the plane of $z = 0.0380405$ when grid number is (a) 0.7 million (b) 3 million (c) 5 million (d)16 million

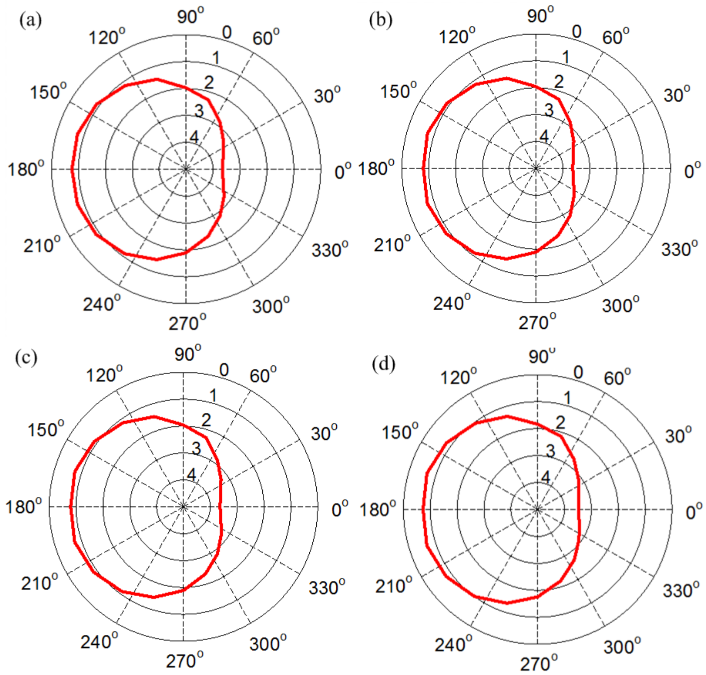

Figure 5.30: Distribution of δ_θ on the plane of $z = 0.0430405$ when grid number is (a) 0.7 million (b) 3 million (c) 5 million (d)16 million

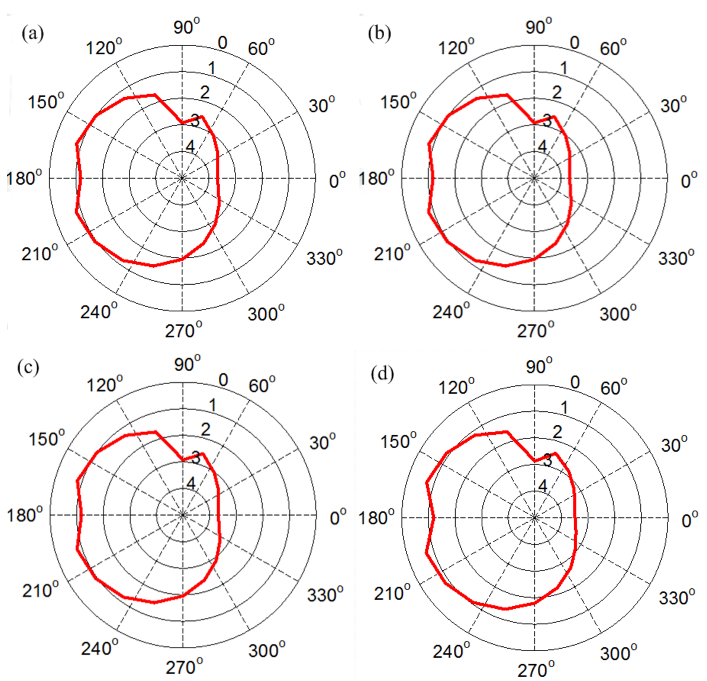

Figure 5.31: Distribution of δ_θ on the plane of $z = 0.0380405$ when grid number is (a) 0.7 million (b) 3 million (c) 5 million (d)16 million

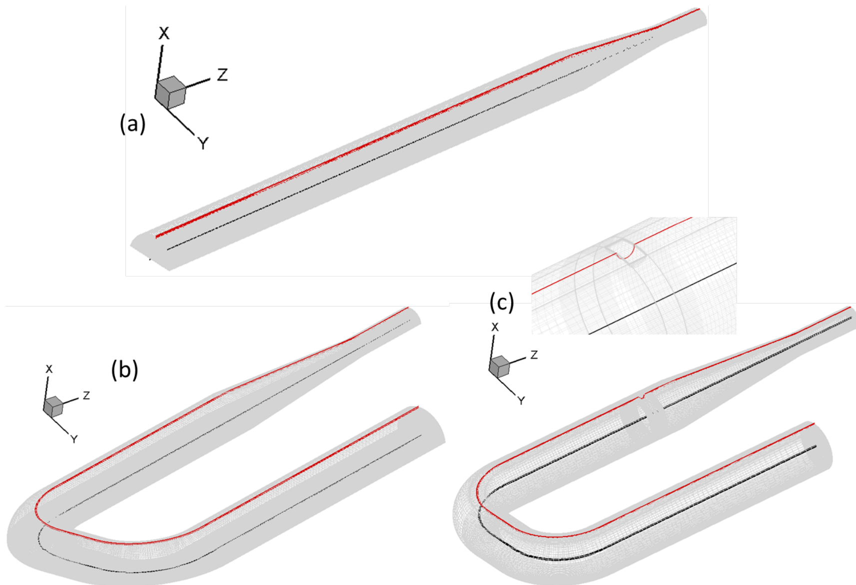

Figure 5.32: Center line and line along the wall (over the weld) of the pipe (a) straight pipe without a weld, (b) 90°/90° pipe without a weld, and (c) 90°/90° pipe with a 30° weld

301 pa for the 90°/90° pipe without a weld, and 301 pa for the 90°/90° pipe with a 30° weld. This tells little effects of bend and weld on the change of static pressure.

In more detail, static pressure from inlet to outlet of the pipe are analyzed along the center line of the pipe as well as the line along the wall (over the weld), whose locations are shown in Fig. 5.32. Fig. 5.33 is the static pressure change along the center line as well as the enlarged plot near the weld location. And Fig. 5.34 is the plot along the line on the wall over the weld and the near-weld enlarged plot. In general, the distribution of static pressure doesn't have too much difference for the three pipes but only differs a little near the weld location: for the bend pipe with/without a weld, the static pressure only differs along the wall, while the static pressure of a straight pipe differs from that of bend pipes along both the center line and the line on the wall.

Wall Shear Stress Changes From the Inlet to the Outlet of the Pipe

Figure 5.35 shows the wall shear stress change from the inlet to the outlet of the pipe along the wall. The wall shear stress of the straight pipe without a weld behaves differently

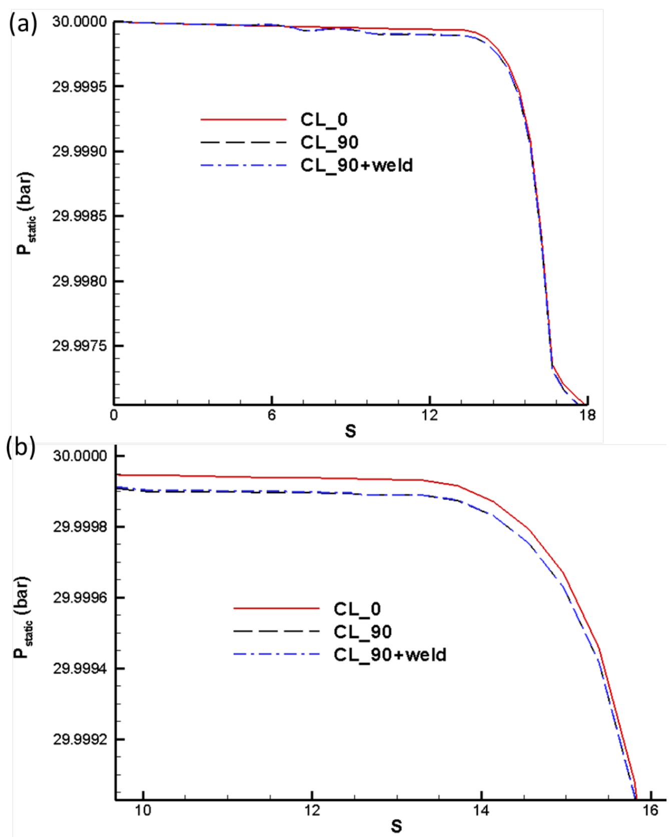

Figure 5.33: Static pressure changes along the center line (a) from inlet to outlet of of the three studied pipes and (b) enlarged plot near the weld location (weld centers at $s = 12.482$). "CL_ 0" is the center line along the straight pipe without a weld, "CL_ 90" is the center line along the 90°/90° pipe without a weld, and "CL_ 90+weld" is the center line along the 90°/90° pipe with a 30° weld

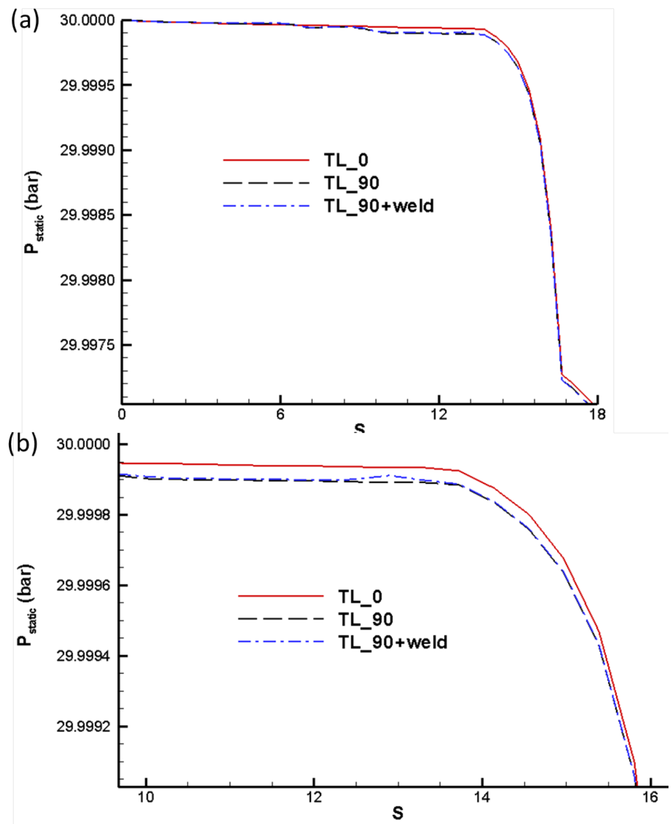

Figure 5.34: Static pressure changes along the line on the wall (a) from inlet to outlet of of the three studied pipes and (b) enlarged plot near the weld location (weld centers at $s = 12.482$). "TL_ 0" is the line along the wall of the straight pipe without a weld, "TL_ 90" is the line along the wall of the 90°/90° pipe without a weld, and "TL_ 90+weld" is the line along wall of the 90°/90° pipe with a 30° weld

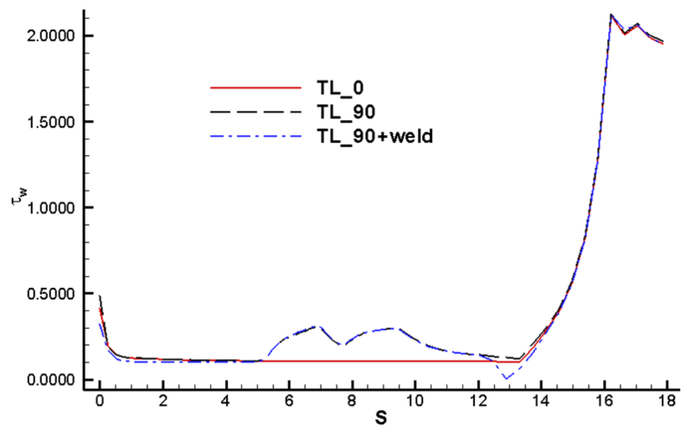

Figure 5.35: Wall shear stress changes along the line on the wall from inlet to outlet of of the three studied pipes. "TL_ 0" is the line along the wall of the straight pipe without a weld, "TL_ 90" is the line along the wall of the 90°/90° pipe without a weld, and "TL_9 0+weld" is the line along wall of the 90°/90° pipe with a 30° weld

from that of other two bend pipes starting from $s = 5.17$ (the location of the first bend) to $s = 15$ (after the weld). The difference of wall shear stress only exists near the location of weld for the two bend pipes.

Plots Near the Vicinity of the Weld Location

The axial velocity, momentum thickness, turbulence intensity, and turbulent kinetic energy dissipation rate are plotted at four s locations for the studied three pipes. Figure 5.36 gives the locations of the four s planes: $s = 12.478$ (before the weld), $s = 12.482$ (middle of the weld), $s = 12.601$ (after the weld), and $s = 17.892$ (the exit). Figures 5.37, 5.38, and 5.39 are the axial velocity plots of straight pipe without a weld, the 90°/90° pipe without a weld, and the 90°/90° pipe with a 30° weld, respectively. The bend pipes have asymmetry distributions of axial velocity when flow passes through the bends. Further, back flow happens before the weld and even enhances after the weld for the bend pipe with a weld. Flow becomes uniform distributed after the nozzle for all the three pipes. Figures 5.40, 5.41, and 5.42 are plots of the momentum thickness of the three pipes. It shows a consistent uniform distribution of momentum thickness at all four s locations for the three pipes. The plots of turbulence intensity for the three pipes are shown in Figs. 5.43, 5.44, and 5.45. The

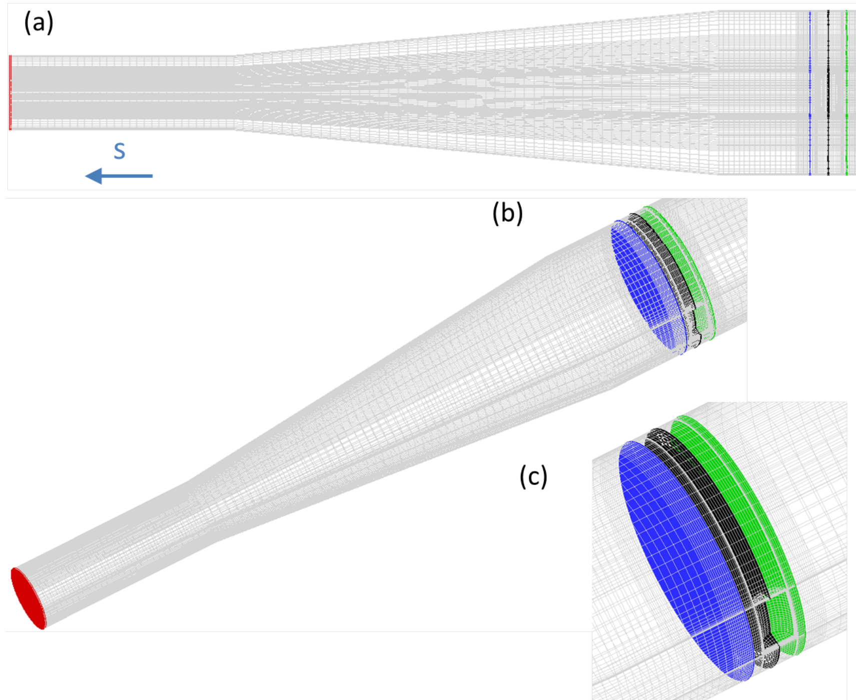

Figure 5.36: Planes at $s = 12.478$, $s = 12.482$, $s = 12.601$, and the exit ($s = 17.892$). (a) $y - z$ view of the plane locations, (b) default view of the plane locations, and (c) enlarged view of the plane locations in the vicinity of a weld

turbulence intensity at exits of pipes without welds reduces compared to other s locations. However, the turbulence intensity increases at the exit of the pipe with a weld. In common, all three pipes have nozzles. It seems that nozzle reduces the turbulence intensity of the flow, while the weld makes the flow more turbulent. Turbulent kinetic energy dissipation rate increases at the exits of all three pipes, as shown in Figs. 5.46, 5.47, and 5.48.

5.3 Mercury Turbulent Jet Flow

Mercury flow comes out of the target delivery pipe and forms a free jet. The sketch of the mercury free jet with MHD (magnetohydrodynamic) and energy deposition for the MERIT experiment is shown in Fig. 5.49. The mercury jet study in this paper doesn't consider MHD and energy deposition but only mercury-air two-phase jet flow, which is the base line of the complicated real jet problem in MERIT experiment.

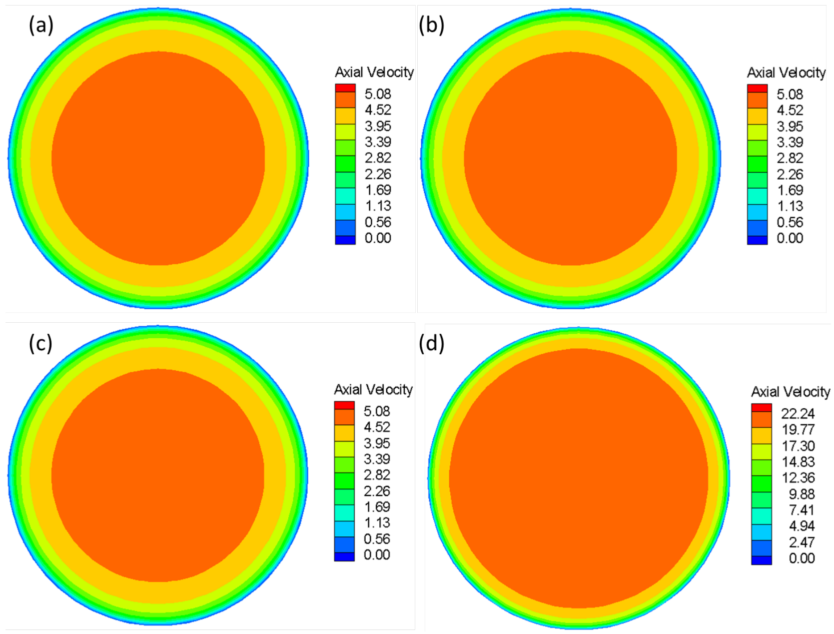

Figure 5.37: Contour of axial velocity for the straight pipe without a weld at (a)$s = 12.478$, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

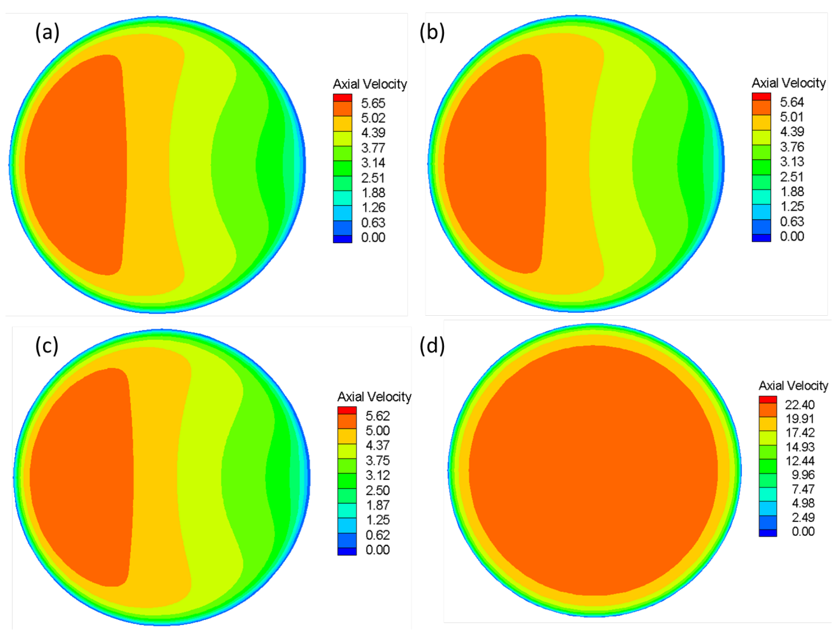

Figure 5.38: Contour of axial velocity for the 90°/90° pipe without a weld at (a)$s = 12.478$, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

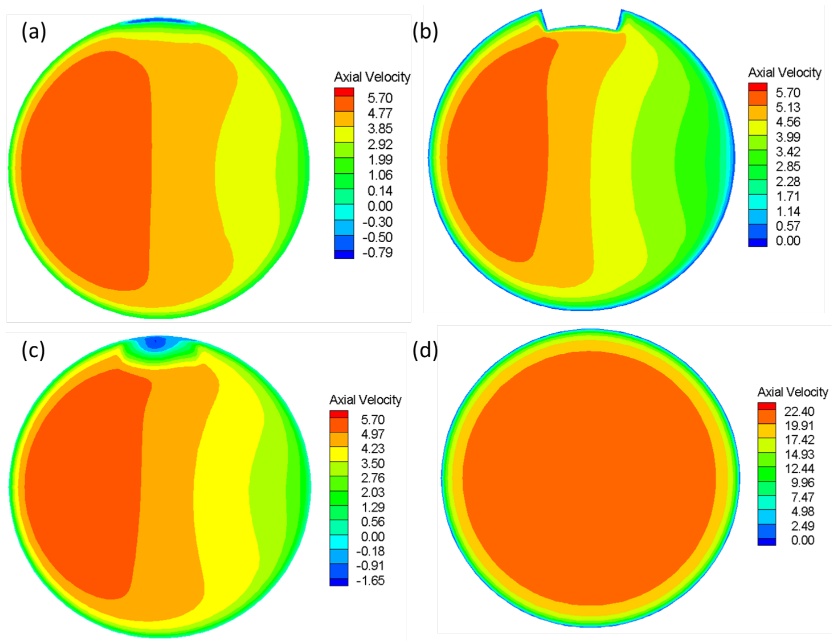

Figure 5.39: Contour of axial velocity for the 90°/90° pipe with a 30° weld at (a)$s = 12.478$, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

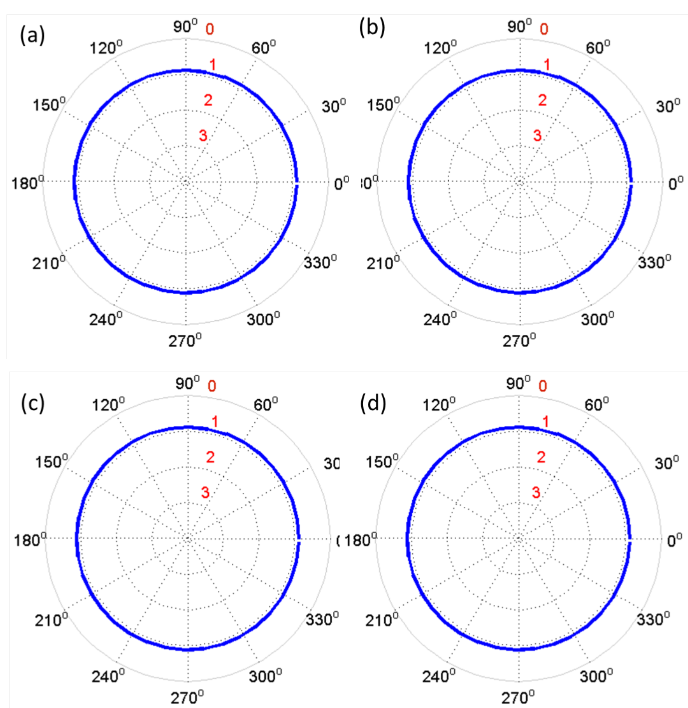

Figure 5.40: Plot of momentum thickness for the straight pipe without a weld at (a)$s = 12.478$, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

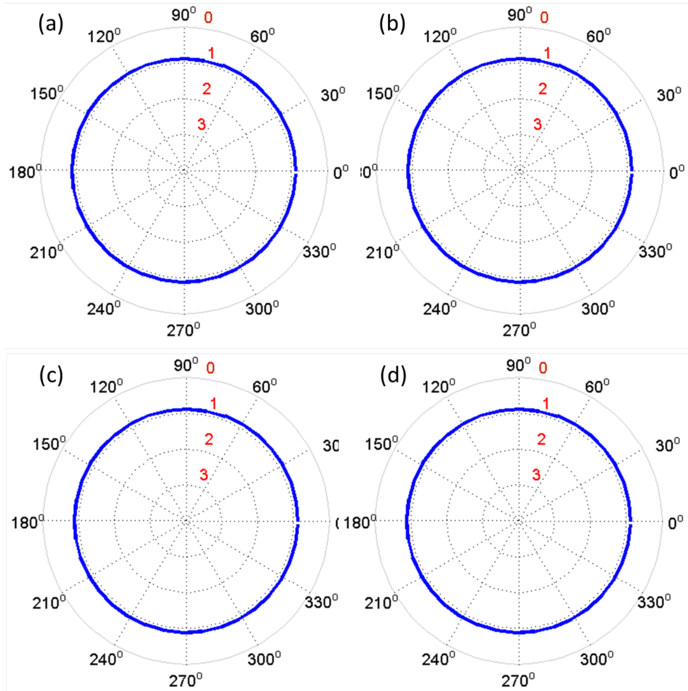

Figure 5.41: Plot of momentum thickness for the 90°/90° pipe without a weld at (a)s = 12.478, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

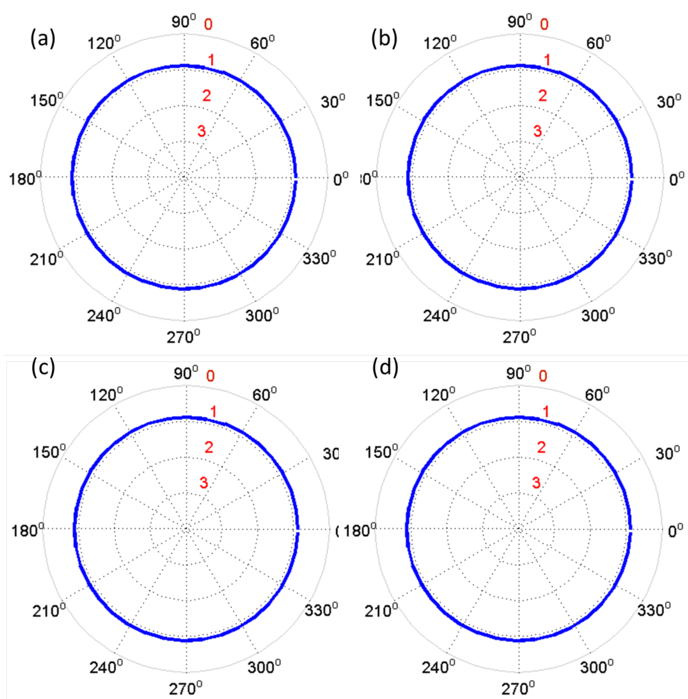

Figure 5.42: Plot of momentum thickness for the 90°/90° pipe with a 30° weld at (a)s = 12.478, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

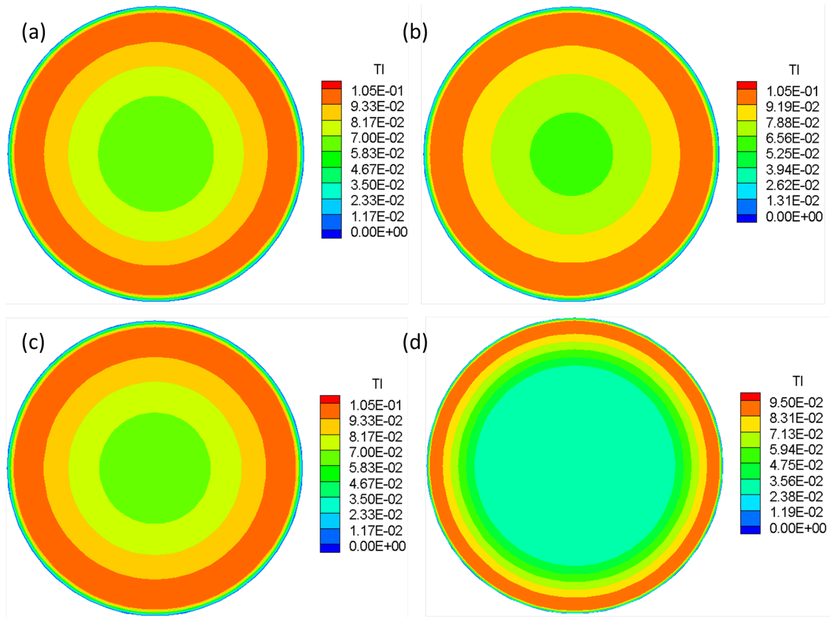

Figure 5.43: Contour of turbulent intensity for the straight pipe without a weld at (a)$s = 12.478$, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

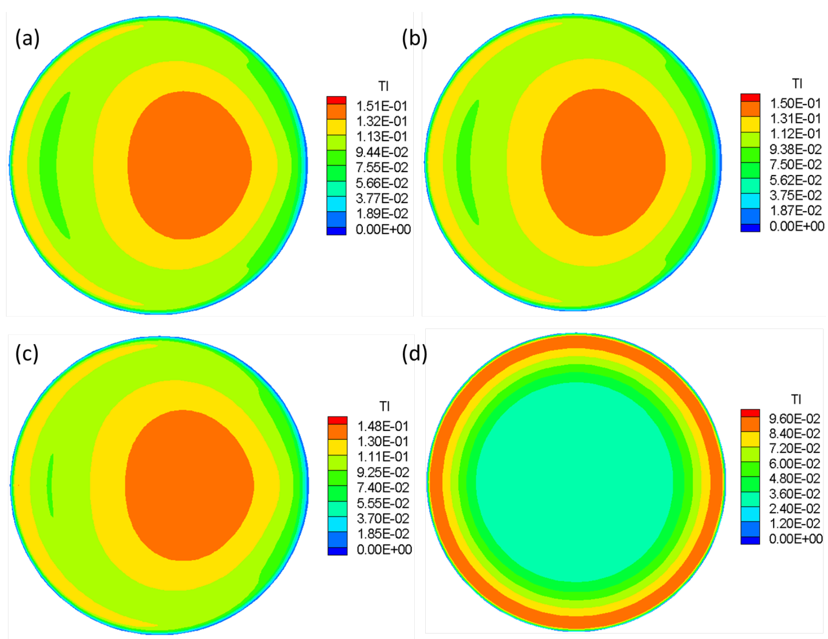

Figure 5.44: Contour of turbulent intensity for the 90°/90° pipe without a weld at (a)$s = 12.478$, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

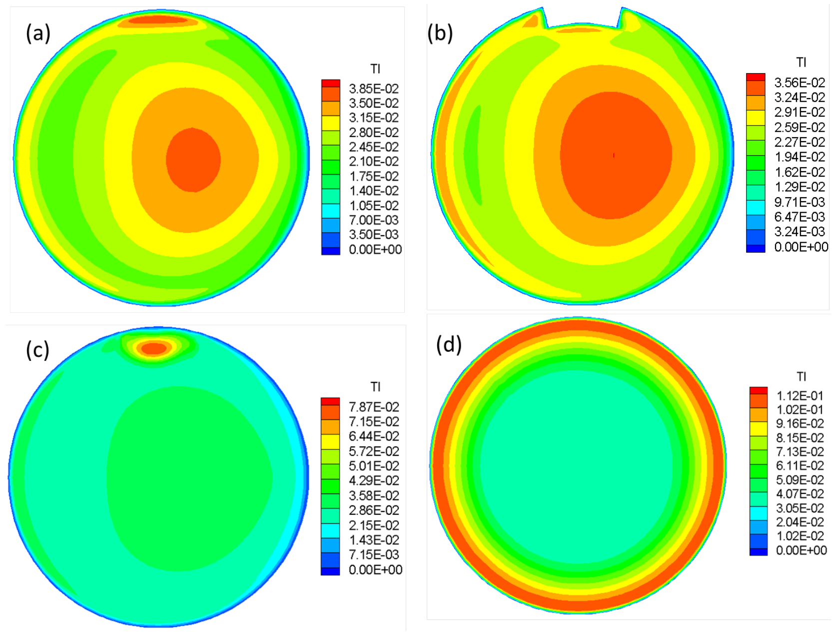

Figure 5.45: Contour of turbulent intensity for the 90°/90° pipe with a 30° weld at (a)$s = 12.478$, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

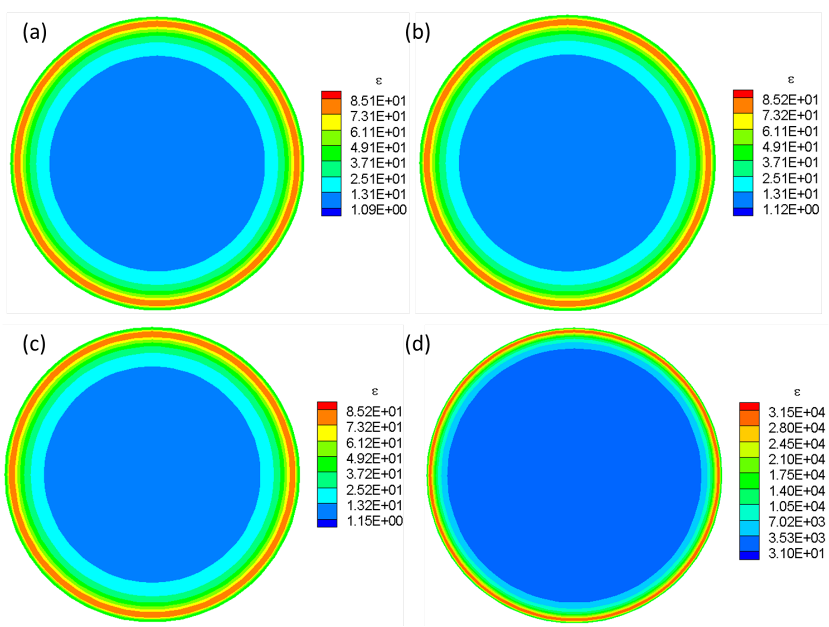

Figure 5.46: Contour of turbulent kinetic energy dissipation rate for the straight pipe without a weld at (a)$s = 12.478$, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

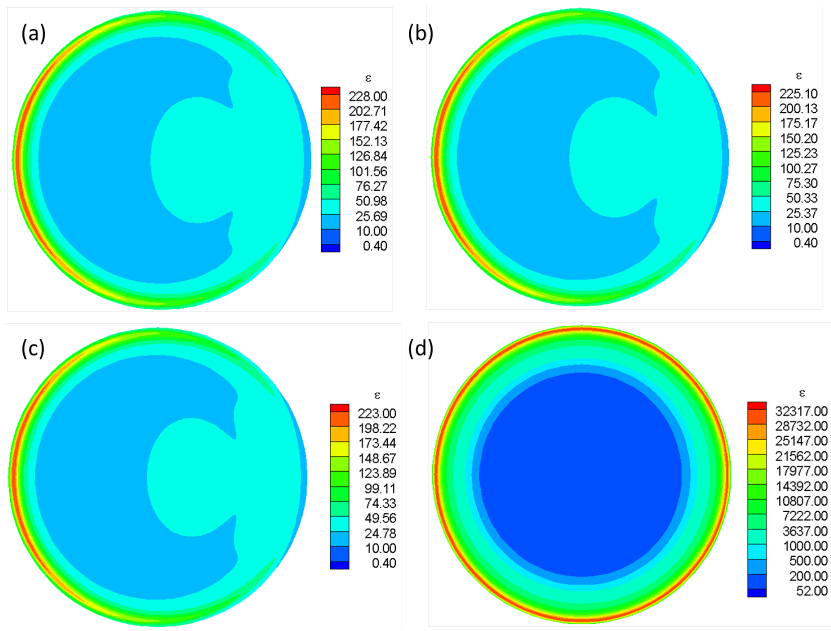

Figure 5.47: Contour of turbulent kinetic energy dissipation rate for the 90°/90° pipe without a weld at (a)$s = 12.478$, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

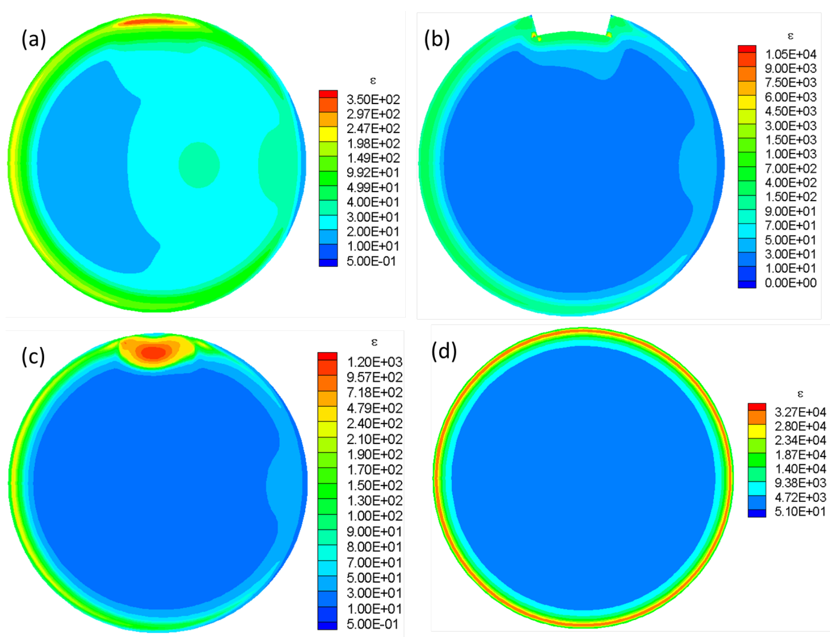

Figure 5.48: Contour of turbulent kinetic energy dissipation rate for the 90°/90° pipe with a 30° weld at (a)$s = 12.478$, (b) $s = 12.482$, (c) $s = 12.601$, and (d) exit

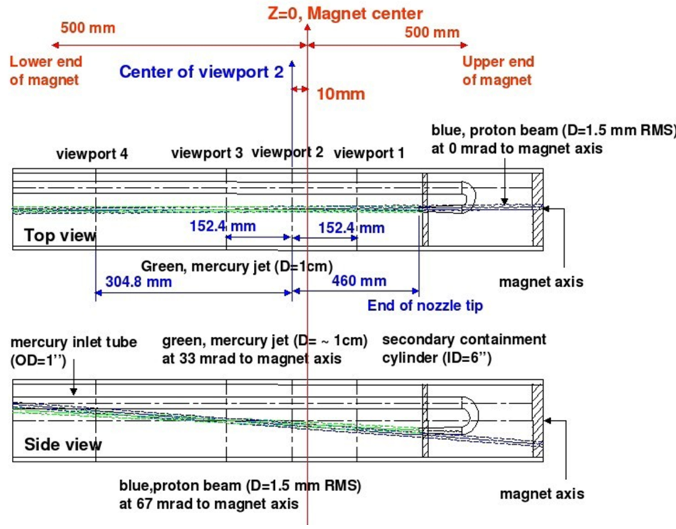

Figure 5.49: Sketch of the mercury free jet with MHD and energy deposition for the MERIT experiment

5.3.1 Two Dimensional Mercury Turbulent Jet Flow

A 2D mercury jet into air is studied first. When only assume the primary breakup, the critical liquid Weber number is less than 10 [65]. Therefore, we can know the smallest mesh size required for capturing jet break up is $0.9\mu m$:

$$We \equiv \frac{\rho u^2 \triangle x}{\sigma} = 10 \Rightarrow \triangle x = \frac{we\sigma}{\rho u^2} = \frac{10 * 0.4855}{13456 * 20 * 20} = 0.9\mu m \approx 8.86 * 10^{-5} D, \qquad (5.8)$$

where D is the jet diameter.

From the mercury jet sketch in the MERIT experiment (Fig. 5.49), we can get the side view of mercury jet flow on the $y-z$ plane in both dimension (Fig. 5.50(a)) and non-dimension (Fig. 5.50(b)). The real mercury jet problem has a computational domain with a width of $15D$ and a length of $124.4D$. With the mesh size requirement (Eq. 5.8), it would need a mesh grid number of $2.44 * 10^{11}$ when mesh is uniform. Therefore, we reduced the lengths of the computational domain with the least influences on the jet flow. Also, a halved model is applied when considering a axis boundary condition for the center line. Also the computational domain is reduced in length, width, and height, seen in Fig. 5.51. Figure. 5.52

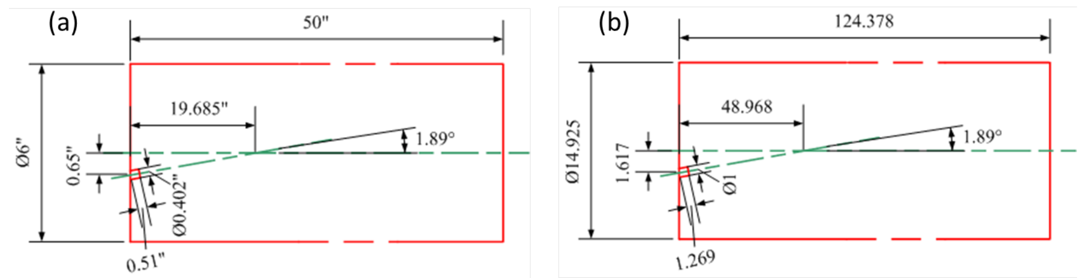

Figure 5.50: The Side view of mercury jet flow (a)in dimension (b)normalized by jet inlet diameter

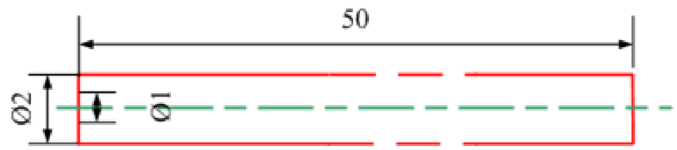

Figure 5.51: Simplified two dimensional mercury jet model with reduced length, width, and height

shows the boundary conditions for the 2D mercury jet simulation. The velocity profile at the outlet of a straight nozzle pipe is assumed (Fig. 5.53) at the inlet of the jet flow. The result of α_{Hg} is shown in Fig. 5.54, which has very rich jet breakups.

5.3.2 Three Dimensional Mercury Turbulent Jet Flow

Figure 5.55 is the schematics of target delivery system in MERIT experiment. The simulation of a three dimensional mercury jet using the length, width, and height in Fig. 5.55 would lead to a total mesh grid number of 6.8×10^{15} with the uniform mesh spacing $0.9\mu m$ (Eq. (5.8)). Therefore, it has to reduce the lengths of the computational model. Figure 5.56 shows the simplification of the computational model to a cuboid of $3D * 3D * 50D$. Further,

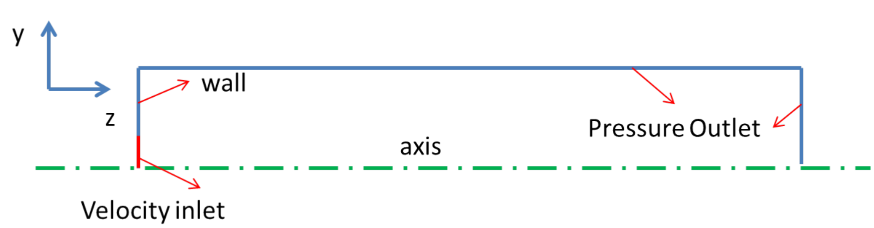

Figure 5.52: The boundary conditions for the two dimensional mercury jet simulation

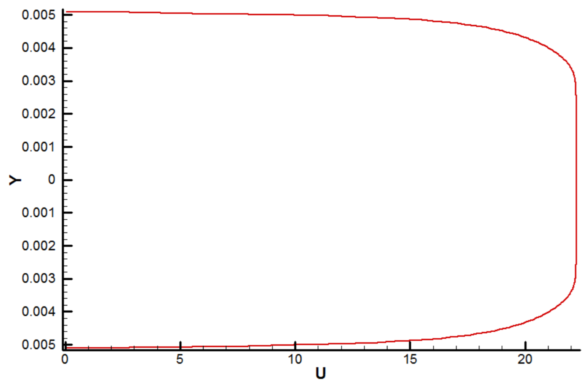

Figure 5.53: The velocity profile at the inlet of the two dimensional mercury jet simulation

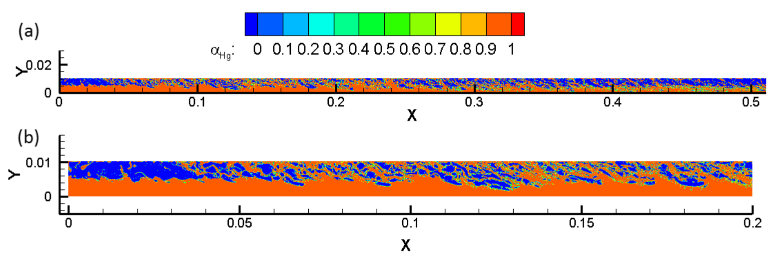

Figure 5.54: Contour of volume fraction of mercury for the two dimensional mercury jet simulation over (a)the whole computational domain (b) $0 < x < 0.2$ for enlarged view

the ILES requires a big number of mesh grids for the three dimensional simulation. With the limited computational resources, we have to use the time-averaged RANS method for the simulation. Therefore, the turbulent model RKE is applied here instead of ILES. Although the unsteady complicated structure on free interface may be time-averaged, it is still possible to analyze the deformation of the jet under different inputs conditions.

The outlet conditions of pipe simulation is assumed at the inlet of the mercury jet simulation. In order to find out the effects of bend and weld on the mercury jet interface deformation, the outlet conditions from a straight nozzle pipe without a weld, a 90°/90° pipe without a weld, and a 90°/90° pipe with a 30° off bend plane weld are used in the section for mercury jet simulation. Therefore, we classify the three dimensional mercury jet simulation into three cases: case 1 uses the outputs of a straight nozzle pipe without a weld, case 2 uses those of a 90°/90° pipe without a weld, and case 3 uses those of a 90°/90° pipe with a 30° off bend plane weld. In the later part of the paper, the names of case 1, case 2,

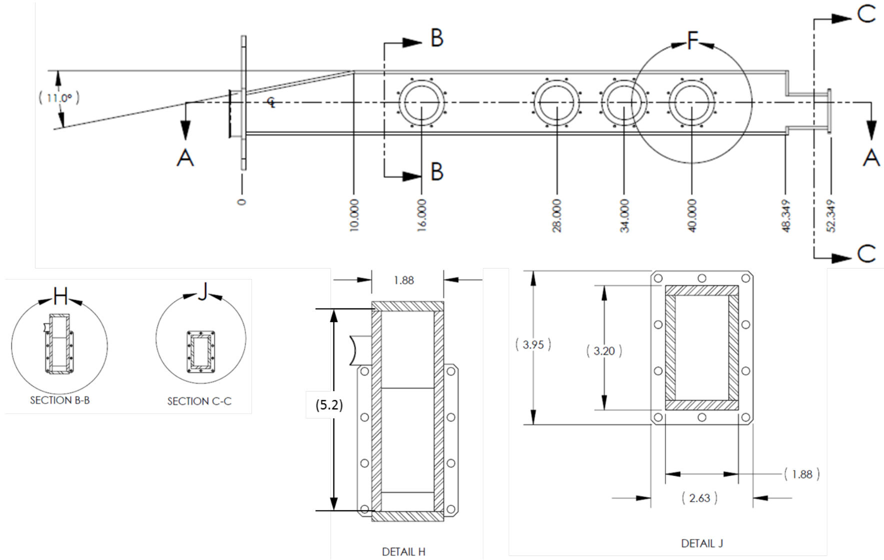

Figure 5.55: Schematics of target delivery system by V. Graves

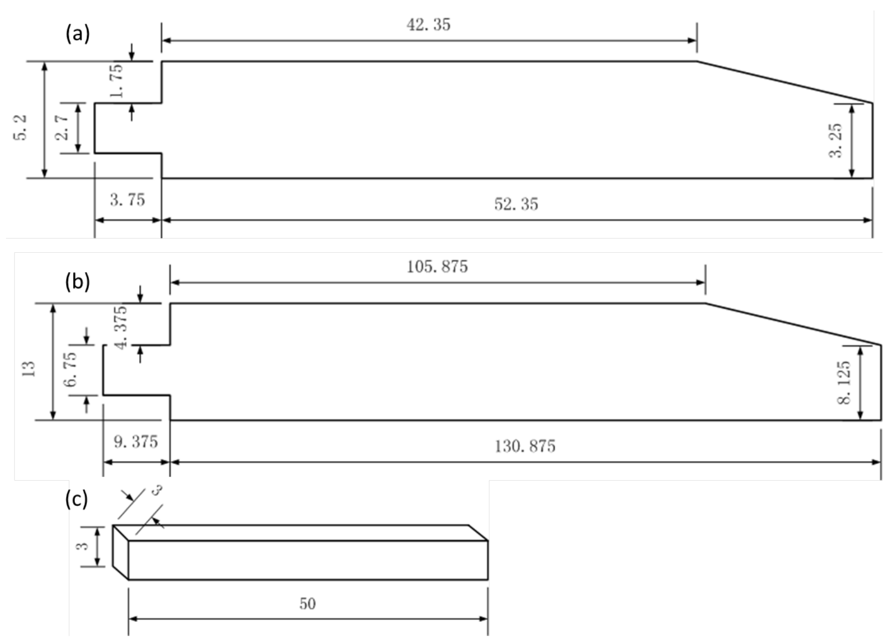

Figure 5.56: Simplification of the three dimensional mercury jet model:(a)dimensional model (unit: inch) (b)non-dimensional model (normalized by jet inlet diameter, D) (c) simplified model with reduced length, width, and height (normalized by jet inlet diameter, D)

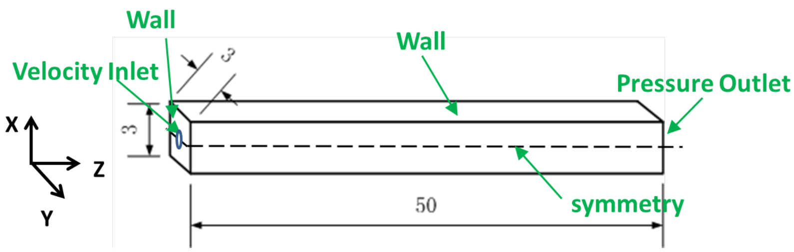

Figure 5.57: The boundary conditions for the three dimensional mercury jet simulation case 1. The dimension shown in the draft is normalized by jet inlet diameter, which is 0.01m. No gravity in the model. Case1: The jet inlet conditions use outputs of straight nozzle pipe without a weld

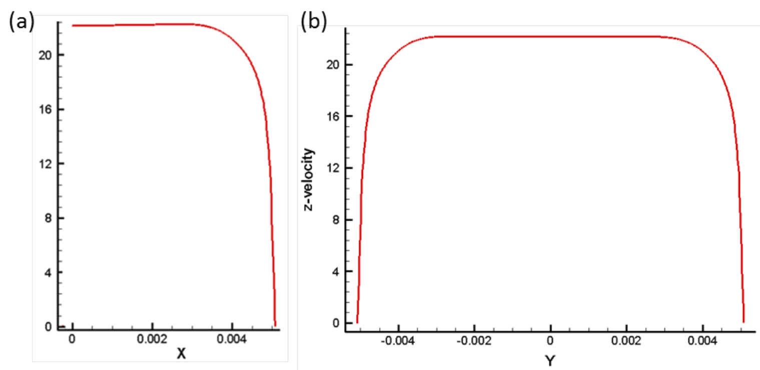

Figure 5.58: The axial velocity profile imposed at the inlet of the three dimensional mercury jet simulation case 1 (a) x line plot (b) y line plot

and case 3 will be called for convenience.

Because of the symmetric outputs from a straight pipe without a weld, halved model can be used in case 1 with a symmetry boundary condition. Figure 5.57 describes the boundary conditions for the case 1 simulation. Velocity profile from the outlet of the straight pipe without a weld (Fig. 5.58) is assumed at the jet inlet. The results of α_{Hg} and U_z are shown in Figs. 5.59 and 5.60. The outputs at the 90°/90° pipe without a weld are also symmetry. Case 2 has the same boundary conditions as case 1 (Fig. 5.57) The velocity profile at the inlet of case 2 jet is shown in Fig. 5.61. The case 2 jet simulation results are shown in Figs. 5.62 and 5.63. The outputs at the 90°/90° pipe with a 30° weld is asymmetric, therefore a complete model should be used for case 3, seen in Fig. 5.64. The velocity profile at the jet inlet is in Fig. 5.65. And results are shown in Figs. 5.66 and 5.67.

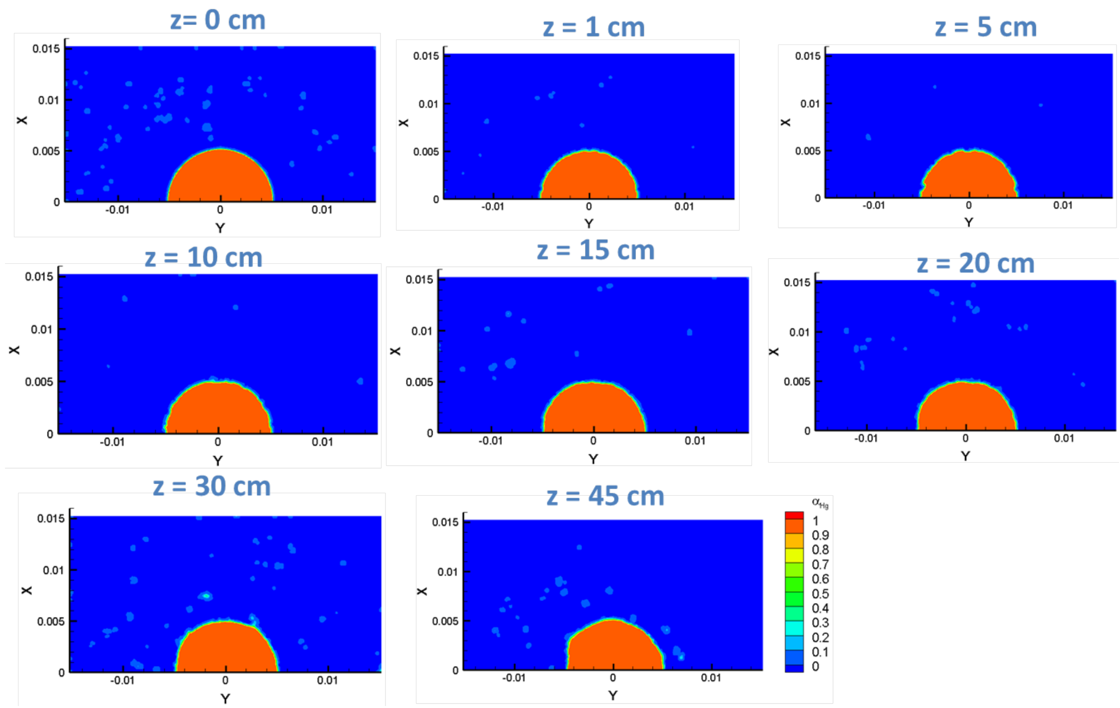

Figure 5.59: Results of volume fraction of mercury, α_{Hg}, for three dimensional mercury jet simulation case 1

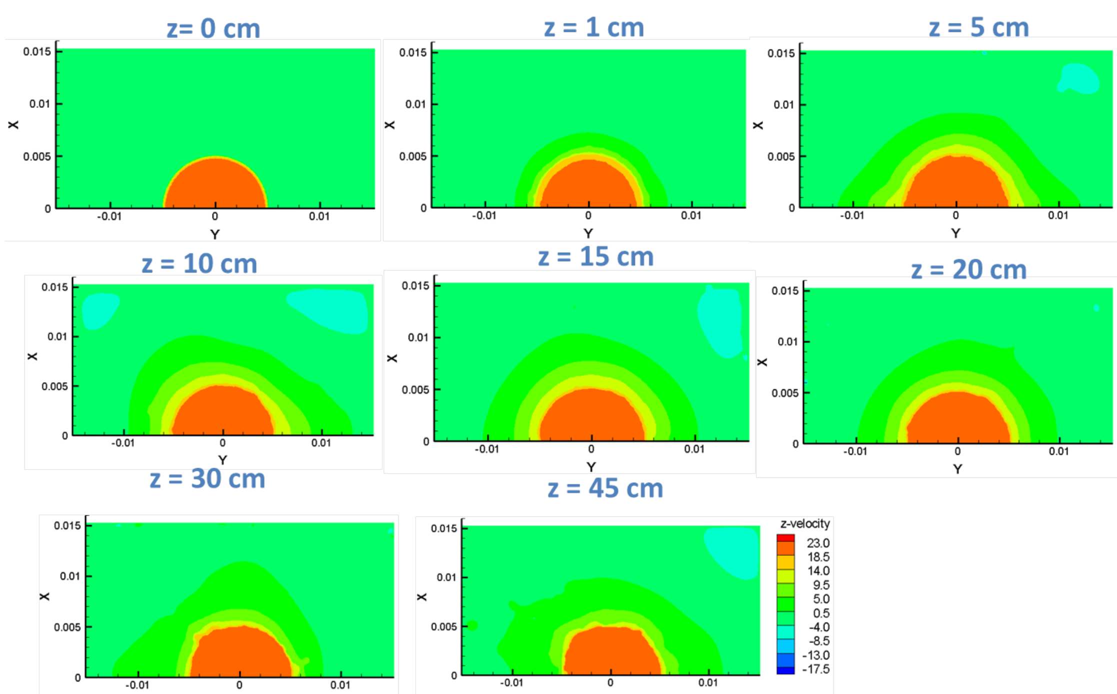

Figure 5.60: Results of axial velocity, U_z, for three dimensional mercury jet simulation case 1

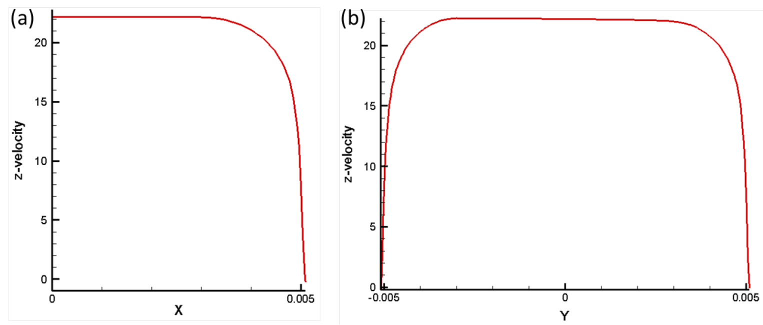

Figure 5.61: The axial velocity profile imposed at the inlet of the three dimensional mercury jet simulation case 2 (a) x line plot (b) y line plot

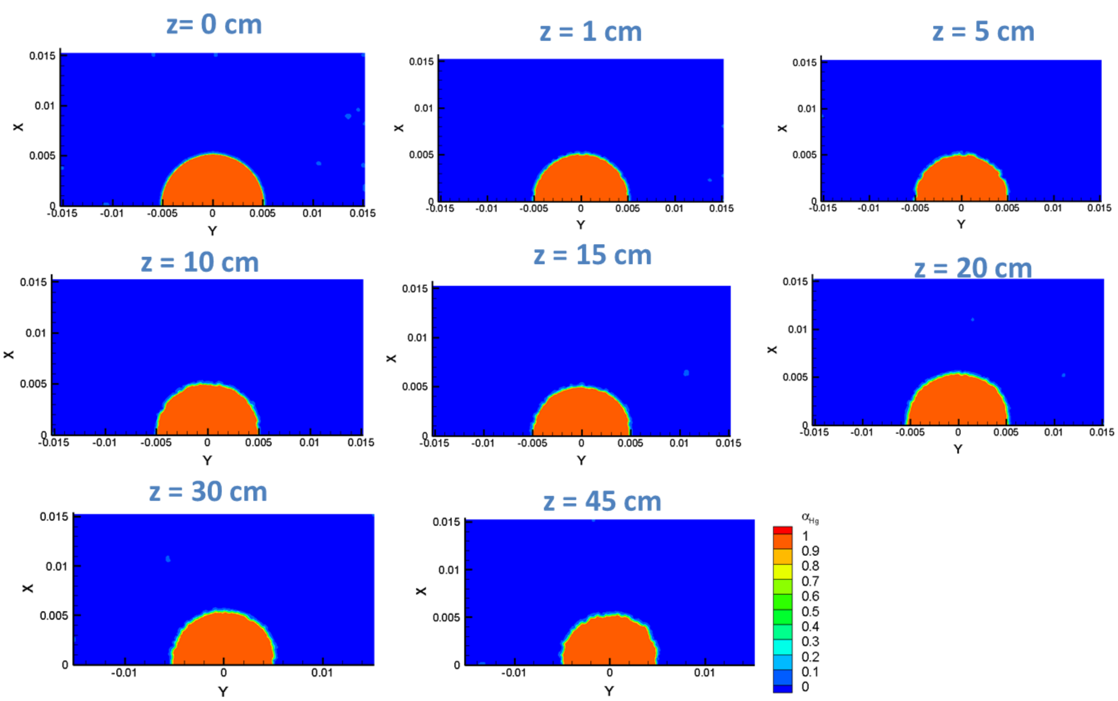

Figure 5.62: Results of volume fraction of mercury, α_{Hg}, for three dimensional mercury jet simulation case 2

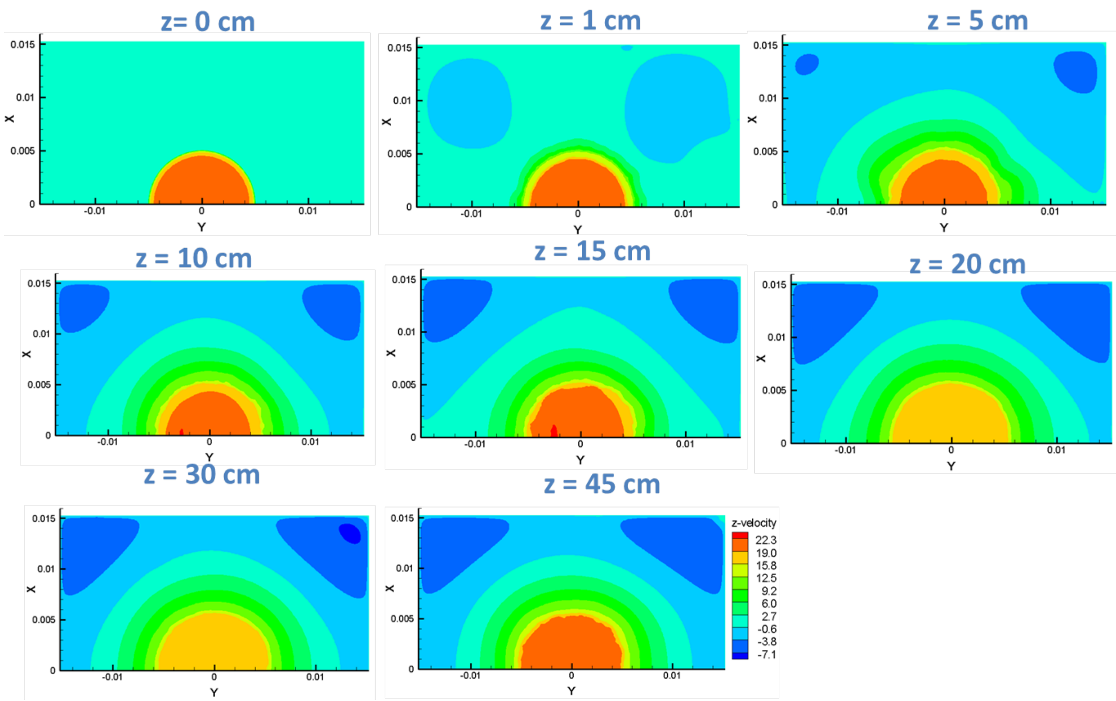

Figure 5.63: Results of axial velocity, U_z, for three dimensional mercury jet simulation case 2

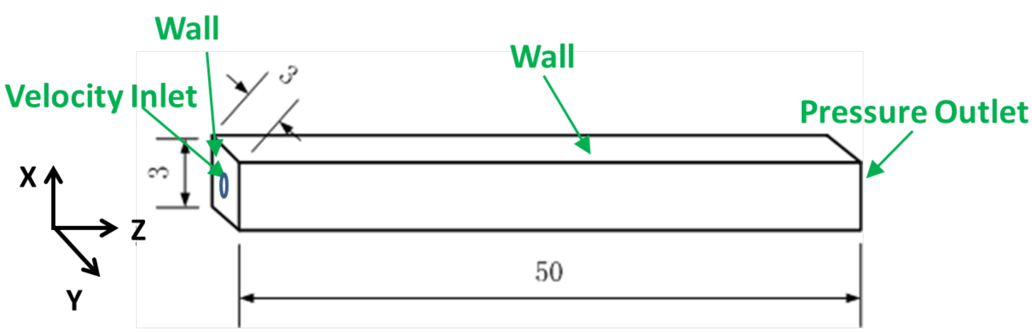

Figure 5.64: The boundary conditions for the three dimensional mercury jet simulation case 3. The dimension shown in the draft is normalized by jet inlet diameter, which is 0.01m. No gravity in the model. Case3: The jet inlet conditions use outputs of 90°/90° pipe with a 30° weld

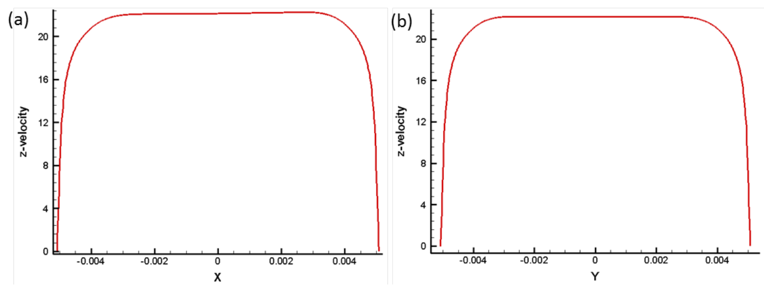

Figure 5.65: The axial velocity profile imposed at the inlet of the three dimensional mercury jet simulation case3 (a) x line plot (b) y line plot

Case 1 is basic case without any influences from bend and weld on jet flow, while case 3 is the most complicated case of the three with combined effects of bend and weld. It is interesting to check what is the differences of the jet deformation under these two cases. Figure 5.68 is the difference of α_{Hg} between case 1 and case 1 at different z locations. The larger values in Fig. 5.68 indicates bigger difference in jet shape. The difference becomes bigger at downstream of the jet. At $z = 45cm$, the bigger difference locates at the positive x (line $y = 0$), the first quadrant, and the second quadrant. Note that the 30° weld centers at the positive x and the first and second quadrants are the inner side of the bend. It seems to indicate some effects or combined effects of the bend and weld on the jet deformation. In order to get a quantitive analysis on the jet deformation, we calculated the ellipticity of the deformed jet for a better idea of the deformation.

5.3.3 Least Squares Fitting of Ellipses

In this section, we will detail the least squares method used to fit an ellipse to given points in the plane, as the draft shown in Fig. (5.69).

In analytic geometry, the ellipse is defined as a collection of points (x, y) satisfying the following implicit equation [132]:

$$\tilde{a_1}x^2 + \tilde{a_2}xy + \tilde{a_3}y^2 + \tilde{a_4}x + \tilde{a_5}y = \tilde{a_6}, \tag{5.9}$$

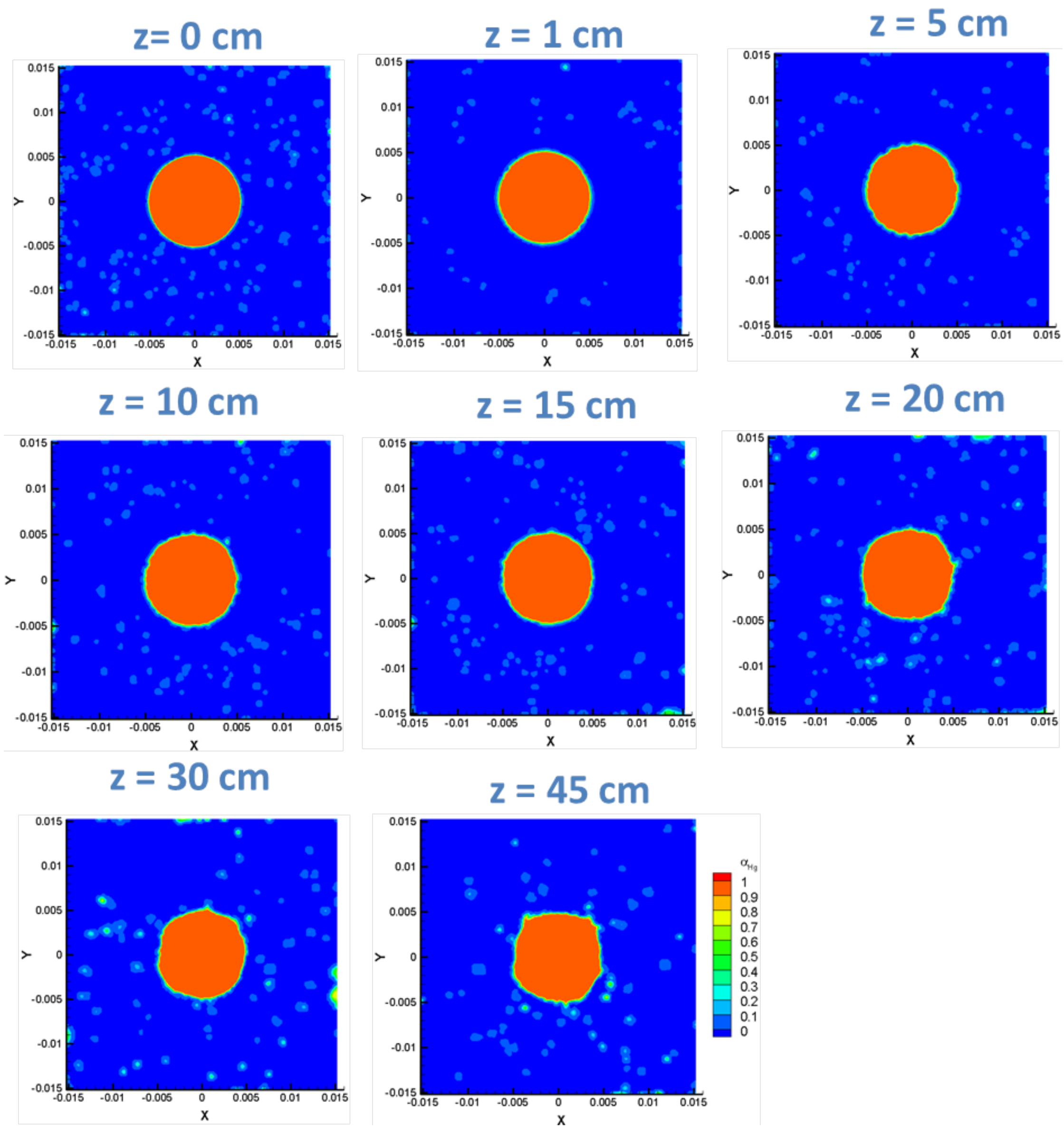

Figure 5.66: Results of volume fraction of mercury, α_{Hg}, for three dimensional mercury jet simulation case 3

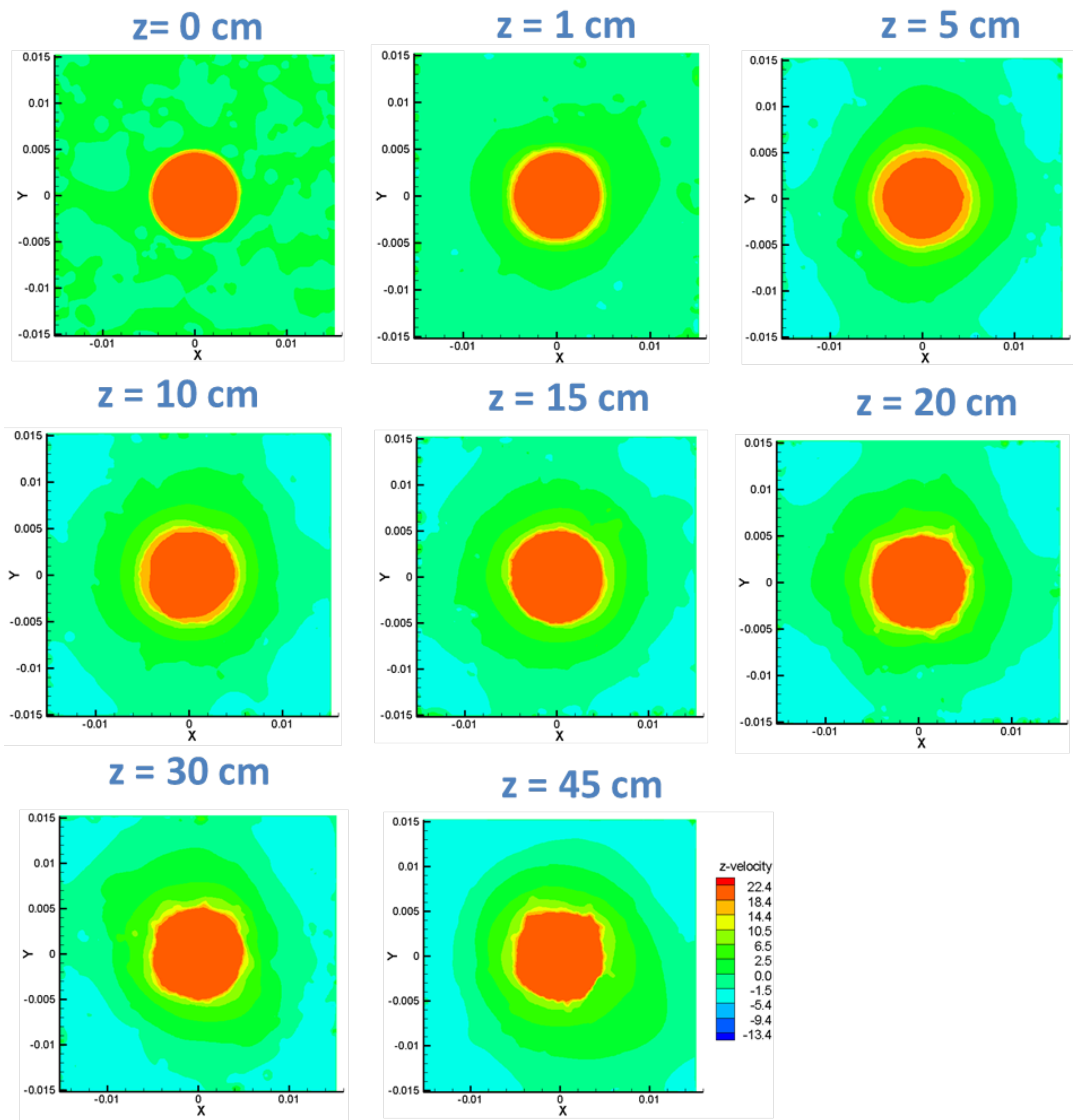

Figure 5.67: Results of axial velocity, U_z, for three dimensional mercury jet simulation case 3

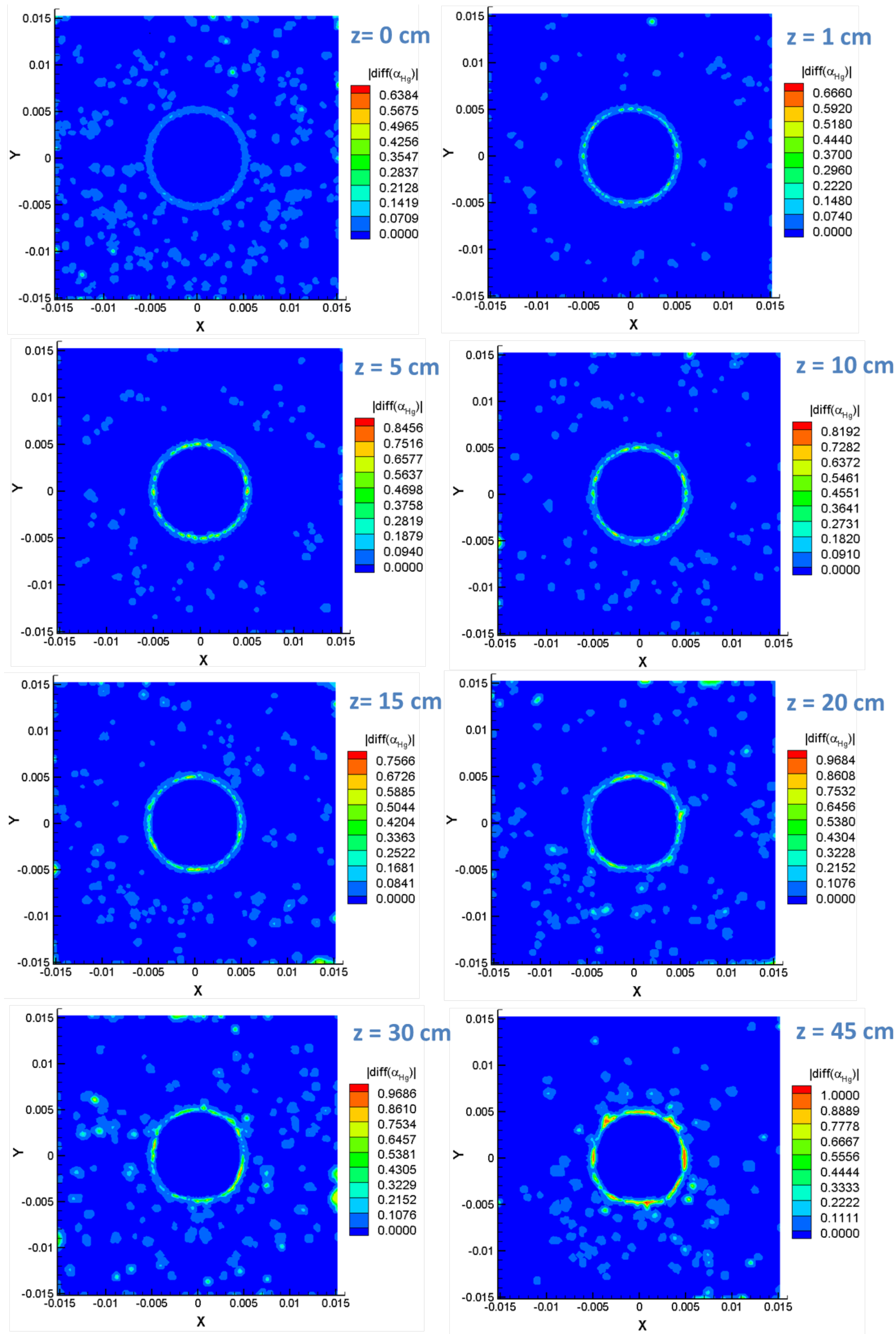

Figure 5.68: Difference of α_{Hg} between three dimensional mercury jet simulation case1 and case3

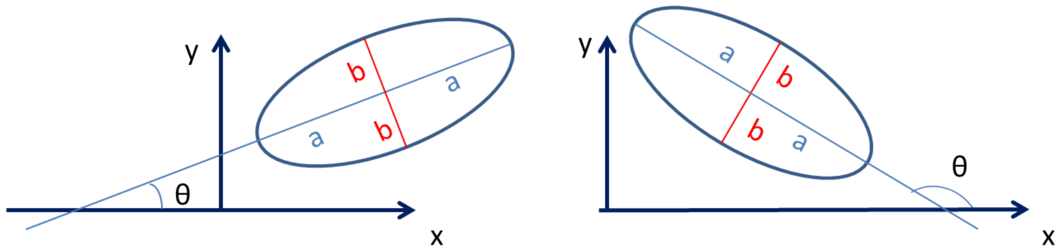

Figure 5.69: Draft of ellipse fitting: a is the major axis, b is the minor axis, and $/theta$ is the rotational angle

where $\tilde{a_6} \neq 0$ and $\tilde{a_2}^2 - 4\tilde{a_1}\tilde{a_3} < 0$.

To simplify the following analysis, we normalize the above implicit form by dividing $\tilde{a_6}$ an both sides of the equality sign, which reduces to

$$a_1x^2 + a_2xy + a_3y^2 + a_4x + a_5y = 1. \tag{5.10}$$

Several new notations needs to be introduced to ease our discussion. For two vectors $\mathbf{s} = (s_1, s_2, \ldots, s_m)^{\mathrm{T}}$ and $\mathbf{t} = (t_1, t_2, \ldots, t_m)^{\mathrm{T}}$, the tensor product between them are defined as

$$\mathbf{s} \otimes \mathbf{t} = (s_1t_1, s_2t_2, \ldots, s_mt_m)^{\mathrm{T}}. \tag{5.11}$$

Assuming n measurements $((x_1, y_1)$, (x_2, y_2), ..., (x_n, y_n) are given, we define $x = (x_1, x_2, \ldots, x_n)^{\mathrm{T}}$ and $y = (y_1, y_2, \ldots, y_n)^{\mathrm{T}}$, then the following cost function needs to be minimized

$$C(\beta) = (X\beta - \mathbf{1})^{\mathrm{T}} (X\beta - \mathbf{1}), \tag{5.12}$$

where $X = [x \otimes x, x \otimes y, y \otimes y, x, y]$ is a n-by-5 matrix, $\beta = (a_1, a_2, a_3, a_4, a_5)^{\mathrm{T}}$ consists of the parameters to be determined, and $\mathbf{1}$ is a n-dimensional column vector with all 1's. Expand the matrix multiplication, we get

$$C(\beta) = \beta^{\mathrm{T}}X^{\mathrm{T}}X\beta - 2\mathbf{1}^{\mathrm{T}}X\beta + n. \tag{5.13}$$

To minimize $C(\beta)$ it is requested that

$$\frac{\partial C(\beta)}{\partial \beta} = 2\beta^{\mathrm{T}} X^{\mathrm{T}} X - 2\mathbf{1}^{\mathrm{T}} X = 0, \tag{5.14}$$

from which we get

$$\beta = \left(X^{\mathrm{T}} X\right)^{-1} X^{\mathrm{T}} \mathbf{1}. \tag{5.15}$$

The next step is to extract geometric parameters of the best-fitting ellipse from the algebraic equation (5.10). We first check the existence of a tilt, which is present only if the coefficient B in (5.10) is non-zero. If that was the case, we first need to eliminate the tilt of the ellipse. Denoting the tilt angle of the ellipse by θ, the following coordinate rotation transformation is employed

$$\begin{cases} x = \cos\theta x' - \sin\theta y' \\ y = \sin\theta x' + \cos\theta y' \end{cases}. \tag{5.16}$$

Substitute the above expressions into Eq. (5.10), we get

$$\begin{aligned} &\left(a_1 c^2 + a_2 cs + a_3 s^2\right) x'^2 + \left(-2a_1 cs + a_2\left(c^2 - s^2\right) + 2a_3 cs\right) x'y' + \\ &\left(a_1 s^2 - a_2 cs + a_3 c^2\right) y'^2 + \left(a_4 c + a_5 s\right) x' + \left(-a_4 s + a_5 c\right) y' + 1 = 0, \end{aligned} \tag{5.17}$$

where $c = \cos\theta$ and $s = \sin\theta$. Let the term before $x'y'$ to be zero, the following equation for θ is achieved

$$-2a_1 \cos\theta \sin\theta + a_2\left(\cos\theta^2 - \sin\theta^2\right) + 2a_3 \cos\theta \sin\theta = 0, \tag{5.18}$$

from which we know $\theta = \frac{1}{2}\arctan\left(\frac{a_2}{a_1 - a_3}\right)$. Now the constants c and s are known, Eq. (5.17) is reduced to

$$a_1' x'^2 + a_3' y'^2 + a_4' x' + a_5' y' = 1, \tag{5.19}$$

where a_1', a_3', a_4' and a_5' are all known constants. The only remaining step for the ellipse fitting is to transform Eq. (5.19) into the following canonical form

$$\frac{(x'-x_0')^2}{b^2}+\frac{(y'-y_0')^2}{a^2}=1, \tag{5.20}$$

in which (x_0', y_0') is the center of the ellipse in the rotated coordinate system, and a and b are the lengths of the semi-axes. Applying a square completion method to Eq. (5.17), we get

$$\frac{(x'+a_4'/\left(2a_1'\right))^2}{(a_6'/a_1')}+\frac{(x'+a_5'/\left(2a_3'\right))^2}{(a_6'/a_1')}=1, \tag{5.21}$$

where $a_6' = 1 + (a_4'^2)/(4a_1') + (a_5'^2)/(4a_3')$. Compare Eqs. (5.20) and (5.21), it easy to notice

$$x_0' = \frac{-a_4'}{2a_1'}, y_0' = \frac{-a_5'}{2a_3'}, a = \sqrt{\frac{a_6'}{a_1'}}, b = \sqrt{\frac{a_6'}{a_3'}}. \tag{5.22}$$

Substitute the above expressions of x_0' and y_0' into Eq. (5.16), we get the coordinate of the ellipse center in the original coordinate system

$$\begin{cases} x_0 = -\cos\theta\frac{a_4'}{2a_1'} + \sin\theta\frac{a_5'}{2a_3'} \\ y_0 = -\sin\theta\frac{a_4'}{2a_1'} - \cos\theta\frac{a_5'}{2a_3'} \end{cases}. \tag{5.23}$$

The mercury jet was considered at $z = 30$ cm and $z = 45$ cm, which are the locations of view port 1 and view port 2, respectively. 40 points were digitized in mercury jet simulations at these z values, shown in Figs. (5.59),(5.62), and (5.66). The results of fitting ellipse to these digitzed points are shown in Figs. (5.70), (5.71), and (5.72).

In the results of ellipse fitting, no big significant differences are found among different cases. To quantify this, uncertainties in the fitting should be estimated. Here we apply an error analysis formulated by Prof. McDonald [133]. It gives a prescription for fitting a set of m points, $\{x_j, y_j\}$, (perhaps from digitization of an image) to an ellipse, with the general

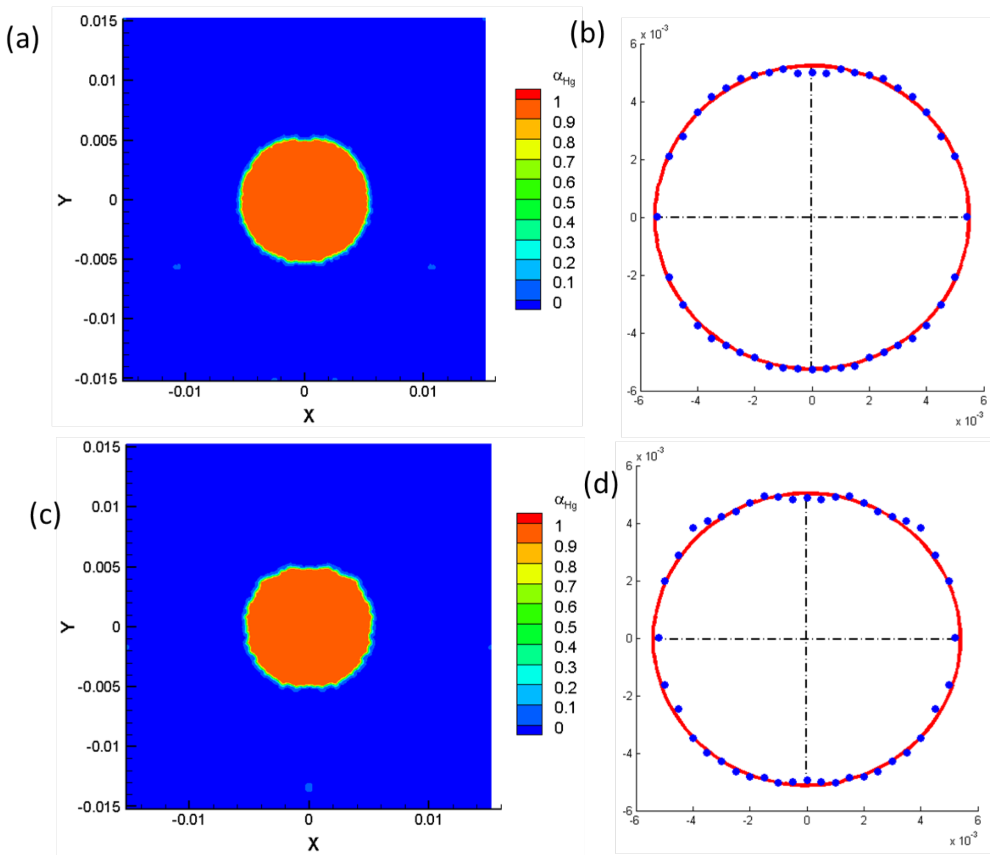

Figure 5.70: Least square fitting of ellipses for 3D mercury jet simulations using as input the output from a straight pipe without a weld: (a) contour of volume fraction of mercury at $z = 30$ cm, (b) ellipse fitting at $z = 30$ cm, (c) contour of volume fraction of mercury at $z = 45$ cm, (b) ellipse fitting at $z = 45$ cm.

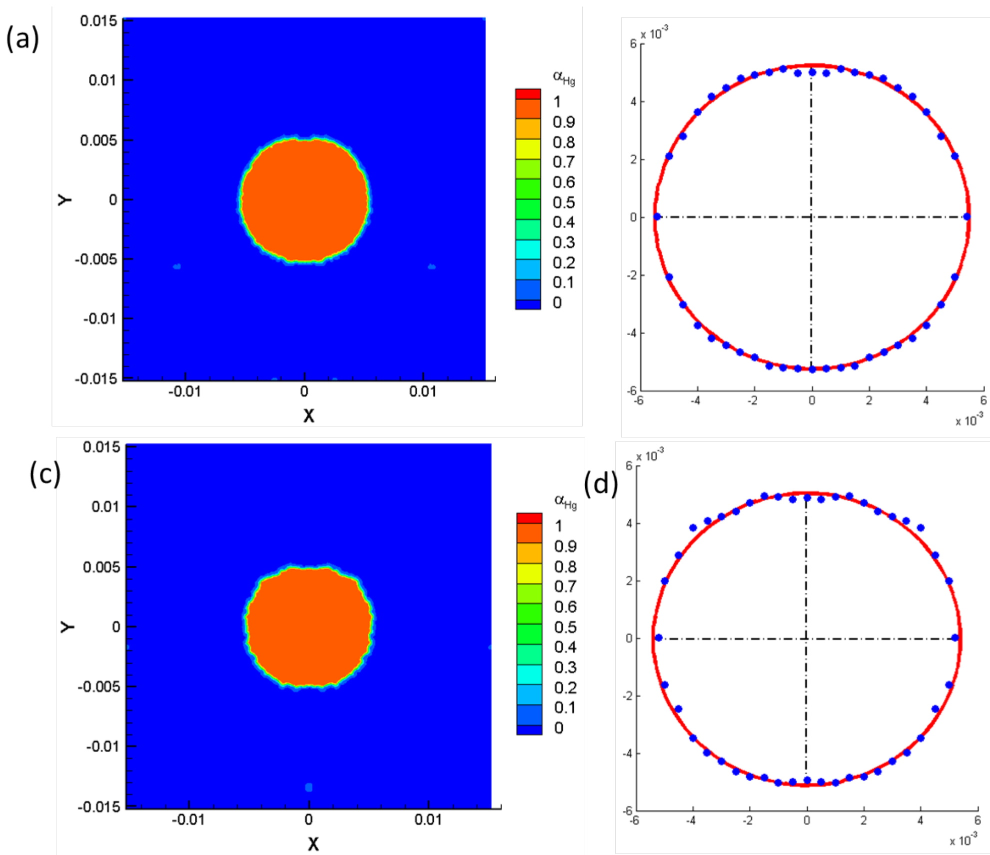

Figure 5.71: Least square fitting of ellipses for 3D mercury jet simulations using as input the output from a 90°/90° pipe without a weld: (a) contour of volume fraction of mercury at $z = 30$ cm, (b) ellipse fitting at $z = 30$ cm, (c) contour of volume fraction of mercury at $z = 45$ cm, (b) ellipse fitting at $z = 45$ cm

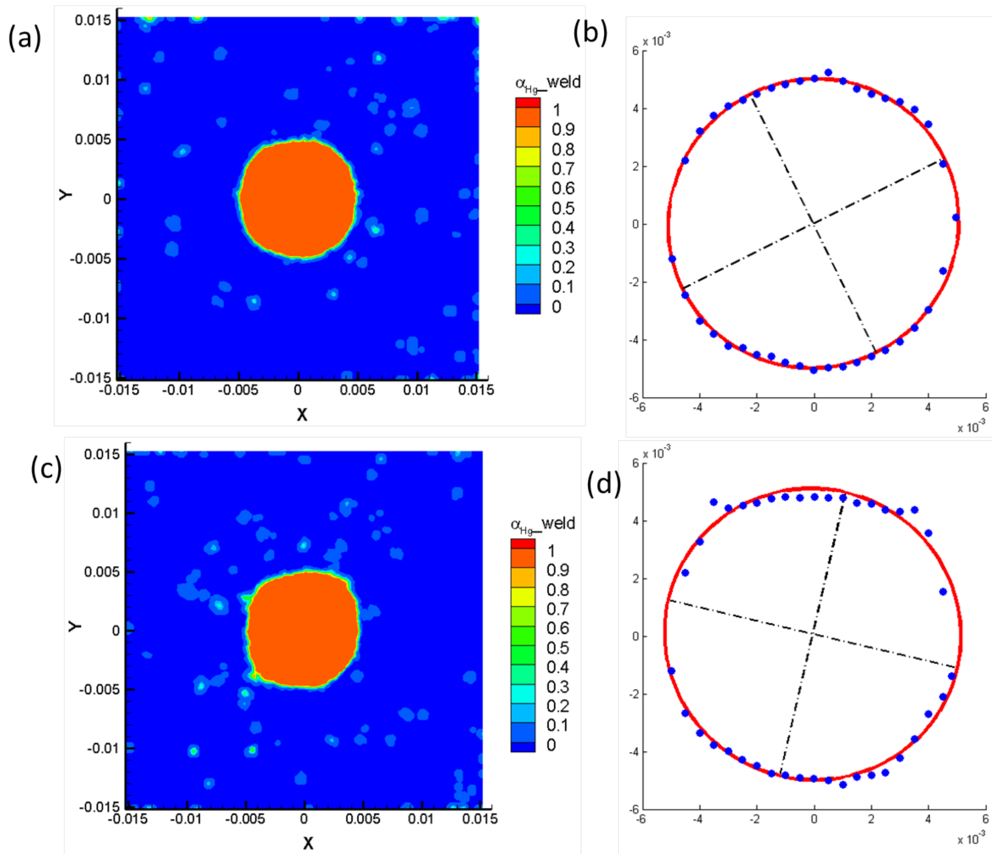

Figure 5.72: Least square fitting of ellipses for 3D mercury jet simulations using as input the output from a 90°/90° pipe with a 30° weld: (a) contour of volume fraction of mercury at $z = 30$ cm, (b) ellipse fitting at $z = 30$ cm, (c) contour of volume fraction of mercury at $z = 45$ cm, (b) ellipse fitting at $z = 45$ cm

form (with 5 parameters a_i),

$$a_1 x^2 + a_2 xy + a_3 y^2 + a_4 x + a_5 y - 1 = 0. \tag{5.24}$$

In addition, we give an estimate of the errors on the best-fit values of the parameters a_i.

(1) Errors on the Parameters of the Quadratic Form (Eq. 5.24). We first define the auxiliary data set $\{z_{ij}\}$, $(i = 1, 5, j = 1, m)$,

$$z_{i,j} = (x_j^2, x_j y_j, y_j^2, x_j, y_j). \tag{5.25}$$

Among many possible measures of the goodness of fit,[1] we adopt the simplest, writing

$$\chi^2 = \sum_{j=1}^{m} \frac{(\sum_{i=1}^{5} a_i z_{ij} - 1)^2}{\sigma_j^2}, \tag{5.26}$$

where σ_j is the measurement uncertainty associated with the data point (x_j, y_j). The best-fit parameters $\hat{a}_i$ are those that minimize the function χ^2 for a set of measurements $\{z_{ij}\}$.

We consider the case that the σ_j are not known, but assumed to have the common value σ. Then, by supposing that the function χ^2 is actually a chi-square [137, 138, 139, 140, 141, 142] with $m - 5$ degrees of freedom, the best-fit (minimum) χ^2 has most probable value $m - 5$. Assuming that the best-fit χ^2 has this value, the unknown σ is determined, and error estimates for the best-fit parameters $_i$ follow via standard procedures.[2]

A great insight is that $\exp(-\chi^2/2)$ can be thought of another way. It is also the (unnormalized) probability distribution that the polynomial coefficients have values a_i when their best-fit values are $\hat{a}_i$ with uncertainties due to the measurements $\{x_j, y_j\}$. Expressing this in symbols,

$$\exp(-\chi^2/2) = \text{const} \times \exp\left(- \sum_{k=1}^{5} \sum_{l=1}^{5} \frac{(a_k - \hat{a}_k)(a_l - \hat{a}_l)}{2\sigma_{kl}^2} \right), \tag{5.27}$$

[1] For a survey of 13 measures, see [134],[135].

[2] For a discussion of this approach for polynomial fitting, see the lab manual of Prof. McDonald [143].

or equivalently

$$\chi^2/2 = \text{const} + \sum_{k=1}^{5}\sum_{l=1}^{5} \frac{(a_k - \hat{a}_k)(a_l - \hat{a}_l)}{2\sigma_{kl}^2}. \tag{5.28}$$

The uncertainty on $\hat{a}_k$ is σ_{kk} in this notation. In Eqs. (5.27) and (5.28) we have introduced the important concept that the uncertainties in the coefficients $\hat{a}_k$ are correlated. That is, the quantity σ_{kl}^2 is a measure of the probability that the values of $\hat{a}_k$ and $\hat{a}_l$ both have positive fluctuations at the same time. In fact, σ_{kl}^2 can be negative indicating that when $\hat{a}_k$ has a positive fluctuation then $\hat{a}_l$ has a correlated negative one.

One way to see the merit of minimizing the χ^2 is as follows. According to Eq. (5.28) the derivative of χ^2 with respect to a_k is

$$\frac{\partial \chi^2}{\partial a_k} = \sum_{l=1}^{5} \frac{a_l - \hat{a}_l}{\sigma_{kl}^2}, \tag{5.29}$$

so that all first derivatives of χ^2 vanish when all $a_l = \hat{a}_l$. That is, χ^2 is a minimum when the coefficients a_i take on their best-fit values $\hat{a}_i$. A further benefit is obtained from the second derivatives:

$$\frac{\partial^2 \chi^2}{\partial a_k \partial a_l} = \frac{1}{\sigma_{kl}^2}. \tag{5.30}$$

For our particular χ^2 (5.26), with $\sigma_j = \sigma$, the first derivatives are

$$\frac{\partial \chi^2}{\partial a_k} = \sum_{j=1}^{m} \frac{z_{kj}(\sum_{i=1}^{5} a_i z_{ij} - 1)}{\sigma^2} = \frac{1}{\sigma^2}\sum_{i=1}^{5}\sum_{j=1}^{m} a_i z_{ij} z_{kj} - \frac{1}{\sigma^2}\sum_{j=1}^{m} z_{kj}, \tag{5.31}$$

and the second derivatives are

$$\frac{\partial^2 \chi^2/2}{\partial a_k \partial a_l} = \frac{1}{\sigma^2}\sum_{j=1}^{m} z_{kj} z_{lj} \equiv \frac{M_{kl}}{\sigma^2}. \tag{5.32}$$

Using the matrix M_{kl} introduced in Eq. (5.32), the condition that the first derivatives (5.31) vanish at the best-fit coefficients $\hat{a}_k$ can be written as

$$\sum_{i=5}^{5} M_{ik}\hat{a}_i = \sum_{j=1}^{m} z_{kj} \equiv V_k. \tag{5.33}$$

We then calculate the inverse matrix M^{-1} and apply it to find the best-fit coefficients $\hat{a}_k$ (which do not depend on the as-yet-unknown value of σ),

$$_k = \sum_{l=1}^{5} M^{-1}_{kl} V_l. \tag{5.34}$$

Comparing eqs. (5.30) and (5.32) we have

$$\frac{1}{\sigma^2_{kl}} = \frac{M_{kl}}{\sigma^2}\,. \tag{5.35}$$

The uncertainty in best-fit coefficient $\hat{a}_i$ is then reported as

$$\sigma_{_i} = \sigma_{ii} = \frac{\sigma}{\sqrt{M_{ii}}}. \tag{5.36}$$

All that remains is to find the value of the unknown uncertainty $\sigma = \sigma_j$ on the measurements. For this, we set the χ^2 for the best-fit parameters $_i$ equal to the number of degrees of freedom, $m - 5$,

$$\chi^2(\hat{a}_i) = m - 5 = \sum_{j=1}^{m} \frac{(\sum_{i=1}^{5} \hat{a}_i z_{ij} - 1)^2}{\sigma^2}\,, \tag{5.37}$$

such that σ is determined to be

$$\sigma = \sqrt{\frac{\sum_{j=1}^{m}(\sum_{i=1}^{5} \hat{a}_i z_{ij} - 1)^2}{m-5}}\,, \qquad \text{and} \qquad \sigma_{_i} = \sigma_{ii} = \sqrt{\frac{\sum_{j=1}^{m}(\sum_{k=1}^{5} \hat{a}_k z_{kj} - 1)^2}{(m-5)\sum_{j=1}^{m} z^2_{ij}}}\,. \tag{5.38}$$

(2) Errors on the Conventional Ellipse Parameters An alternative description of the ellipse of Eq. (5.24) is that it has semimajor axis of length a which makes angle θ to the x-axis,

semiminor axis of length b, and center at (x_0, y_0). The shape parameters a, b and θ depend only on a_1, a_2 and a_3, while the center of the ellipse depends on all five of the a_i. We now deduce the alternative parameters, and their fit errors, in terms of the a_i and the errors on the latter as found in sec. 1.

We first translate the coordinates according to $x' = x - x_0$ and $y' = y - y_0$ such that the resulting parameters a'_i of the quadratic form have

$$a'_1 = a_1, \quad a'_2 = a_2, \quad a'_3 = a_3, \quad a'_4 = 2a_1x_0 + a_2y_0 + a_4, \quad a'_5 = a_2x_0 + 2a_3y_0 + a_5. \tag{5.39}$$

For the ellipse to be centered at $x' = 0 = y'$ we need $a'_4 = 0 = a'_5$, which leads to

$$x_0 = \frac{a_2a_5 - 2a_3a_4}{4a_1a_3 - a_2^2}, \qquad y_0 = \frac{a_2a_4 - 2a_1a_5}{4a_1a_3 - a_2^2}. \tag{5.40}$$

As a check, we note that if $a_4 = 0 = a_5$ then the original ellipse was centered on the origin, and indeed eq. (5.40) implies that $x_0 = 0 = y_0$.

To deduce the error on, say, x_0 we first consider the differential,

$$dx_0 = \frac{a_5da_2 + a_2da_5 - 2a_4da_3 - 2a_3da_4 - x_0(4a_3da_1 + 4a_ada_3 - 2a_2da_2)}{4a_1a_3 - a_2^2}. \tag{5.41}$$

Then, on squaring this we can identify $(dx_0)^2$ with the squared error $\sigma_{x_0}^2$ when we identify the products $da_i\, da_j$ with the σ_{ij}^2 found in Eq. (5.35).

The determine the shape parameters a, b and θ we perform a coordinate rotation by angle θ with respect to the x'-axis[3] (which is parallel to the x-axis),

$$x'' = x'\cos\theta + y'\sin\theta, \qquad x' = x''\cos\theta - y''\sin\theta, \tag{5.42}$$

$$y'' = -x'\sin\theta + y'\cos\theta, \qquad y' = x''\sin\theta + y''\cos\theta, \tag{5.43}$$

[3]We could also make the rotation directly from the (x, y) coordinates, with no affect on the shape parameters, as these don't depend on a_4 and a_5. However, if parameters x_0 and y_0 are deduced only after this rotation, they appear to depend on θ, which complicates the expressions for their errors.

and require that $a_2'' = 0$, in which case $a_1'' = 1/a^2$ and $a_3'' = 1/b^2$. This leads to

$$\tan 2\theta = \frac{a_2}{a_1 - a_3}\,, \quad \cos 2\theta = \frac{a_1 - a_3}{\sqrt{a_2^2 + (a_1 - a_3)^2}}\,, \quad \sin 2\theta = \frac{a_2}{\sqrt{a_2^2 + (a_1 - a_3)^2}}\,, \tag{5.44}$$

$$\sigma_\theta = \frac{\cos^2 2\theta}{2a_1 - a_3}\sqrt{\tan^2 2\theta(\sigma_{11}^2 + \sigma_{33}^2 - 2\sigma_{13}^2) + \sigma_{22}^2 - 2\tan 2\theta(\sigma_{12}^2 - \sigma_{23}^2)}, \tag{5.45}$$

and

$$\frac{1}{a^2} = a_1\cos^2\theta + a_2\sin\theta\cos\theta + a_3\sin^2\theta = \frac{a_1 + a_3 + (a_1 - a_3)\cos 2\theta + a_2 \sin 2\theta}{2}$$
$$= \frac{a_1 + a_3 + \sqrt{a_2^2 + (a_1 - a_3)^2}}{2}\,, \tag{5.46}$$
$$\frac{1}{b^2} = a_1\sin^2\theta - a_2\sin\theta\cos\theta + a_3\cos^2\theta = \frac{a_1 + a_3 - (a_1 - a_3)\cos 2\theta - a_2 \sin 2\theta}{2}$$
$$= \frac{a_1 + a_3 - \sqrt{a_2^2 + (a_1 - a_3)^2}}{2}\,. \tag{5.47}$$

Note that $1/b^2 \le 1/a^2$, which means that b is the semimajor axis, and a is the semiminor axis. Note also that $\tan 2\theta = \tan 2(\theta - \pi/2)$, so there is an ambiguity in Eq. (5.44) as to whether θ is the angle to the semimajor or the semiminor axis.

As a measure of the departure of the ellipse from a circle we introduce the ellipticity (flattening) ϱ,[4]

$$\varrho \equiv \frac{b}{a} \ge 1\,, \qquad \varrho^2 = \frac{a_1 + a_3 + \sqrt{a_2^2 + (a_1 - a_3)^2}}{a_1 + a_3 - \sqrt{a_2^2 + (a_1 - a_3)^2}} \equiv \frac{C_+}{C_-}\,. \tag{5.48}$$

Taking the differential, we have

$$2\varrho\, d\vartheta = \frac{dC_+ - \varrho^2\, dC_-}{C_-} \equiv \frac{C_1\, da_1 + C_2\, da_2 + C_3\, da_3}{C_-}\,, \tag{5.49}$$

[4]If we define $\varrho' = (b - a)/a = \varrho - 1$, so that $\varrho' = 0$ for a circle, then $\sigma_{\varrho'} = \sigma_\varrho$.

where

$$C_\pm = a_1 + a_3 \pm \sqrt{a_2^2 + (a_1 - a_3)^2} = a_1 + a_3 \pm S, \qquad S \equiv \sqrt{a_2^2 + (a_1 - a_3)^2}, \tag{5.50}$$

$$C_1 = 1 - \varrho^2 + \frac{a_1 - a_3}{S}(1 + \varrho^2) = -\frac{2[a_2^2 - 2a_3(a_1 - a_3)]}{SC_-} \equiv -2\frac{D_1}{SC_-}, \tag{5.51}$$

$$C_2 = \frac{a_2}{S}(1 + \varrho^2) = \frac{2a_2(a_1 + a_3)}{SC_-} \equiv 2\frac{D_2}{SC_-}, \tag{5.52}$$

$$C_3 = 1 - \varrho^2 - \frac{a_1 - a_3}{S}(1 + \varrho^2) = -\frac{2[a_2^2 + 2a_1(a_1 - a_3)]}{SC_-} \equiv -2\frac{D_3}{SC_-}. \tag{5.53}$$

Then, the error σ_ϱ on the ellipticity ϱ is given by

$$\sigma_\varrho = \frac{1}{\varrho SC_-^2}\sqrt{D_1^2\sigma_{11}^2 + D_2^2\sigma_{22}^2 + D_3^2\sigma_{33}^2 - 2D_1D_2\sigma_{12}^2 - 2D_2D_3\sigma_{23}^2 + 2D_1D_3\sigma_{13}^2}. \tag{5.54}$$

Of course, the “error” computed this way assumes that the fit is “good”, which might not be the case. A separate judgment should be made as to whether the fit is indeed “good" before taking seriously the error estimates presented here.

The calculations of theta and ellipticity, and their errors, for the six cases are shown in Table 5.1. The ellipticity is not significantly different in any of these cases. However, in some cases the estimated errors are extremely large, which may be a hint that the error-estimation procedure is itself not very accurate.

Table 5.1: Ellipticity and fitting errors

	θ	ϱ	σ_θ	σ_ϱ
Case 1 ($z = 30$cm)	0.00	1.04	6.52×10^{-2}	5.96×10^{-3}
Case 1 ($z = 45$cm)	0.00	1.03	1.52×10^{0}	8.18×10^{-2}
Case 2 ($z = 30$cm)	0.00	1.04	4.24×10^{2}	3.97×10^{1}
Case 2 ($z = 45$cm)	0.00	1.06	1.91×10^{3}	2.46×10^{2}
Case 3 ($z = 30$cm)	0.46	1.03	4.09×10^{-1}	1.80×10^{-2}
Case 3 ($z = 45$cm)	-0.23	1.03	3.85×10^{0}	2.31×10^{-1}

Chapter 6

Concluding Remarks

Since the turbulence of the mercury target flow has a significant influence on the particle produce for the Muon Collider project, this work studies the flow dynamics of mercury flow in target supply pipe and mercury jet flow, with the purpose of achieving the least turbulent target flow.

The theoretical analysis of laminar flow in curved pipes shows the curvature terms representing the rotation flow modes in curved pipes which is different from that in a straight pipe. Realizable $k-\varepsilon$ model is validated as a better turbulence model for simulation of flow in curved pipes than other simpler one- or two-equation RANS approaches, which is applied in this paper. The results of turbulent mercury flow in curved pipes, which take reference from MERIT experiment and consider different half-bend angles and the existence of nozzle at pipe outlet, illustrate that the straight pipe (zero half-bend angle) with a nozzle is the least turbulent flow design. More over, mercury flow in a nozzle with weld beads is studied. Weld causes fluid flows backward and increases the turbulence intensity of the flow. It is found that the turbulence level at the exit of the pipe with a weld is much stronger than that of a pipe without a weld. For a bend pipe without a weld, the turbulence intensity at the exit decreases after the flow passes through the nozzle. These indicates that nozzle plays an opposite role from weld on turbulence intensity: nozzle suppress the turbulence while weld promotes it. Further, the static pressure is found to have almost the same change from inlet to outlet of the pipe with/without a bend/weld.

When starting this problem, FLUENT didn't have the CLSVOF function. A CLSVOF method is developed in this paper by implementing LS method in the FLUENT. The LS method is coupled with the built-in VOF method through UDFs. High order WENO scheme is applied to solve the re-initialization equation in the LS method. The developed CLSVOF method is verified and validated through some successful tests. Due to the limited time after the successful accomplishment of the developed CLSVOF method, the built-in CLSVOF method in FLUENT is used to simulate the two-phase jet flows. The validation of the FLUENT CLSVOF method is verified through laminar and turbulent jet simulations. For mercury jet simulation, the out flow conditions of the pipe flow are considered as the inlet conditions of the jet flow. Rich jet breakups are observed in the two dimensional mercury jet simulation using the ILES method. Since it requires a big number of grid mesh points for the three dimensional mercury jet simulation using ILES, the RKE turbulent model is applied instead. Although RKE averages the unsteady structure on the jet interface, it is still useful in analyzing the deformation of the jet. Jet coming out of a 90°/90° pipe with a 30° off bend plane weld has bigger deformation on the weld and inner bend sides, compared to the jet exhausting from a straight nozzle pipe without a weld. Least square ellipse fitting is used to quantitatively analyze the jet deformation. The magnitude of ellipticity is very close to each jet simulation, which uses three outputs of pipe simulations as jet inputs. From the error of fitting, we can clear see the jet simulation based on the outputs of a 90°/90° pipe with a 30° weld has the largest error. It indicates the biggest influences on jet flow from a bend pipe with a weld.

The developed CLSVOF method has just been worked through. Preliminary successful tests proves its ability in capturing sharp filament. In future, more tests are needed for the developed CLSVOF method, e.g. Rayleigh-Taylor instability. Also, the coordinate transform is considered in the method, which is appropriate for complex geometries. A general curvilinear implementation of the developed CLSVOF method needs to be tested. Further, the current code is in serial implementation. A parallel implementation should be done.

For the three dimensional mercury jet simulation, one more case is suggested to be completed, whose inlet conditions use the the outputs from the 90°/90° pipe with a 30° with 30° weld on the bend plane (note: case3 uses the outputs from the 90°/90° pipe with a 30° weld off the bend plane). Further, the error of fitting analysis needs to be improved.

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