VORTICAL FLOW DYNAMICS AND ACOUSTIC RESPONSE OF GAS-TURBINE SWIRL-STABILIZED INJECTORS

A Thesis in

Mechanical Engineering

by

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Submitted in Partial Fulfillment
of the Requirements
for the Degree of

Doctor of Philosophy

December 2002
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Abstract

The present research focuses on a time-accurate numerical simulation and analysis of the vortical flow dynamics and acoustic characteristics of gas-turbine swirl-stabilized injectors with different swirl numbers. The primary objectives are:

- to establish a comprehensive numerical code, validated against experimental data, to simulate turbulent swirling flows;
- to explore the dominant physical processes and mechanisms involved in such flows;
- to study the effects of inlet conditions, such as swirl number, on flow structures and their dynamic evolution; and
- to investigate the acoustic response of injector dynamics to externally imposed excitation.

The theoretical formulation is based on the complete conservation equations of mass, momentum, and energy in three dimensions. Turbulence closure is achieved by means of a large-eddy-simulation (LES) technique. The governing equations and associated boundary conditions are solved using a finite-volume approach. Both a four-step Runge-Kutta scheme and an Adam-Bashforth predictor-corrector scheme are implemented for temporal integration. A fourth-order central difference scheme along with sixth-order artificial dissipation is employed for spatial discretization of the convective terms. The code is further equipped with a multi-block domain decomposition feature to facilitate parallel processing in a distributed computing environment using the Message Passing Interface (MPI) library.

As part of the model validation effort, the numerical analysis is first implemented to study the turbulent swirling flows in a dump chamber with two different inlet swirl numbers. Good agreement with experimental data is obtained in terms of mean velocities, turbulence intensities, and turbulent kinetic energy. Results show significant effects of the swirl number on the flow evolution. The swirl number not only affects the time-mean topology of the flowfield, such as vortex breakdown, but also strongly
influences the dynamic evolution of the flowfield and acoustic resonance mode of the chamber.

After validation, the analysis is implemented to study the vortical flow dynamics in a gas-turbine swirl-stabilized injector as the second part of the present effort. In this flow configuration, air is radially delivered into the injector through three sets of swirl vanes, which are counter-rotating with each other. Several instability modes with well-defined frequencies, such as vortex breakdown, the Kelvin-Helmholtz instabilities in both the streamwise and azimuthal directions, helical instability, centrifugal instability, and their interactions/competitions, are observed in the flowfields. The flowfield is well organized at a low swirl number, and the vortex shedding due to the Kelvin-Helmholtz instability is the dominant mechanism for driving flow oscillations. The flow structure, however, becomes much more complex at a high swirl number, with each sub flow regime dominated with different frequencies and flow patterns.

The dynamic response of the injector flow to externally imposed oscillations is examined over a broad range of forcing frequency from 400 to 13,000 Hz. The response can be conveniently characterized in terms of the acoustic admittance and mass transfer functions at the exit. Results can be used as an inlet boundary condition in analyzing the combustion instability characteristics of the main chamber. The influences of external excitations on the injector mean flow structures and turbulence properties appear to be limited. However, the unsteady flow evolution in the injector, such as the instantaneous mass flux and pressure distributions, are significantly modulated in both the spatial and spectral domains.
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Nomenclature

- Roman and general symbols

\[ C_l, C_R, C_S \] empirical constants
\[ C_p \] species specific heat at constant pressure, J·kg\(^{-1}\)·K\(^{-1}\)
\[ e \] specific internal energy, J·kg\(^{-1}\)
\[ E \] specific total energy, J·kg\(^{-1}\)
\[ E_v, F_v, G_v \] \(x\)-, \(y\)-, and \(z\)- directional convective-flux vector, respectively
\[ E_v, F_v, G_v \] \(x\)-, \(y\)-, and \(z\)- directional diffusion-flux vectors, respectively
\[ f \] function or frequency, Hz
\[ G \] LES filter function
\[ \hat{G} \] LES filter transfer function
\[ h \] specific enthalpy, J·kg\(^{-1}\)
\[ H \] specific total enthalpy, J·kg\(^{-1}\)
\[ k \] turbulent kinetic energy, m\(^2\)·s\(^{-2}\), or thermal conductivity, W·m\(^{-1}\)·K\(^{-1}\)
\[ n \] normal direction
\[ l \] characteristic length, m
\[ p \] pressure, Pa
\[ Pr \] Prandtl number
\[ r \] radius, m
\[ Re \] Reynolds number
\[ q \] heat flux, W·m\(^{-2}\)
\[ R \] gas constant, J·kg\(^{-1}\)·K\(^{-1}\)
\[ S \] swirl number or swirler angle
\[ S \] surface vector
\[ St \] Strouhal number, dimensionless frequency
\[ T \] temperature, K
\[ t \] time, s
\[ u \] velocity, m/s
\[ V \] volume, m\(^3\)
\[ x, y, z \] spatial coordinate, m
\[ \nabla \] backward difference operator
• Greek symbols

\[ \Delta \] forward difference operator or filter width
\[ \delta_{ij} \] Kronecker delta function
\[ \varepsilon \] turbulence dissipation rate or artificial dissipation coefficient
\[ \phi \] switching parameter of order of spatial difference accuracy
\[ \mu \] viscosity, \( \text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-1} \)
\[ \tau_{ij} \] viscous stress tensor, \( \text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-2} \)
\[ \nu \] kinematics viscosity, \( \text{m}^2 \cdot \text{s}^{-1} \)
\[ \rho \] density, \( \text{kg} \cdot \text{m}^{-3} \)

• Subscripts

\( (\cdot)_{i,j,k} \) spatial coordinate
\( (\cdot)_{K} \) Kolmogorov scale
\( (\cdot)_{L} \) integral scale or laminar property
\( (\cdot)_{\text{ref}} \) reference value
\( (\cdot)_{\text{rms}} \) root mean square
\( (\cdot)_{h} \) turbulent property
\( (\cdot)_{T} \) Taylor scale
\( (\cdot)_{x,r,\theta} \) axial, radial, and azimuthal components, respectively
\( (\cdot)_{\nu} \) viscous term
\( (\cdot)_{\xi,\eta,\zeta} \) each direction in body fitted coordinate system
\( (\cdot)_{F} \) external excitation/forcing

• Superscripts

\( (\cdot)^{L,R} \) left and right sides on the cell boundary, respectively
\( (\cdot)^{\varrho} \) switching parameter of order of artificial damping
\( (\cdot)^{\varpi} \) deterministic unsteady component
\( (\cdot)^{\text{SGS}} \) subgrid scale
\( \bar{(\cdot)} \) time or space average
\( \langle (\cdot) \rangle \) Favre average/density-weighted quantity
\( (\cdot)' \) fluctuation associated with time average
\( (\cdot)'^{\pi} \) fluctuation associated with Favre average
\( \hat{(\cdot)} \) magnitude of the Fourier component
\( \tilde{(\cdot)} \) density-weighted, time-averaged quantity
Acknowledgments

Sincere thanks and gratitude go to my advisor, Professor Vigor Yang, for his invaluable support, guidance, and encouragement throughout my doctorate study in the past four years at Penn State in both professional career and personal life. Working with him, as one of his disciples, has been a pleasant and memorable experience.

Special thanks go to Professors James Brasseur, Dan Haworth, Dom A. Santavicca, and Andre' L. Boehman for kindly providing their expert guidance and for their interest in my work by serving as my Ph.D. committee members.

I extend sincere appreciation to Dr. Shih-Yang Hsieh for many helps in computer coding and Professors Xiyun Lu and Ja Ye Koo for useful discussions. I also thank my colleagues, Dr. Weidong Cai, Dr. Hong-Gye Sung, Dr. Sourabh V. Apte, Dr. Hua Meng, Dr. Eun S. Kim, and Dr. Yuhui Wu, as well as Ms. Danning You, Mr. Ying Huang, Mr. Fuhua Ma, Mr. Nan Zong, and Mr. Yanxing Wang, for their supports, discussions, and comments. I am very thankful to Mrs. Mary Newby and Mr. John Raiser for their administrative help.

This work was sponsored by the NASA Glenn Research Center under Grant NAG 3-2151. The support and encouragement from Mr. Kevin Breisacher is greatly appreciated.

I am indebted to my parents, Mr. and Mrs. Shuchang and Jixiang Wang, for everything they have done and will continue to do for me.

Finally, I take this opportunity to express my deepest love and appreciation to my wife, Aiyu Zhang, for her endless love, patience, and encouragement in the past days and nights.
Chapter 1

Introduction

1.1 Motivation and Objectives

The physiochemical processes in gas-turbine combustors have been studied for more than 60 years. Many problems, however, still exist and must be circumvented in order to develop gas-turbine engines that meet various stringent requirements. For commercial aeroengines, the main challenges are the reduction of NOx and soot at a high-power level, and CO emission at a low-power level. Combustion instability is also a serious problem. For military aeroengines, pattern factor, combustor temperature control, flame stability, and relight capability are of the current concern. For marine and industrial engines, the most serious problems are often related to emission and combustion instability (Yang and Schadow, 1998).

In modern gas turbine engines, swirl-stabilized injectors have been commonly used as an aid to stabilize high-intensity combustion process for efficient clean combustion. One of the most important flow characteristics produced by swirl-stabilized injectors is the central toroidal recirculation zone (CTRZ), which serves as a flame stabilization mechanism (Gupta et al., 1984). Flows in this region are generally associated with high vorticity and turbulent intensity resulting from vortex breakdown, which often leads to irregular large-scale unsteady flow motions. Although this kind of flow oscillation promotes mixing of fuel and air, and extends the range of flame stability, it is usually not a desirable characteristic because of its tendency to drive combustion instabilities. Swirling flows may affect flame stability in two areas. Firstly, large-scale unsteady motions due to high shear layer and vortex breakdown, as well as precessing vortex core (PVC), induce hydrodynamic instability. The ensuing flow oscillations may couple resonantly with acoustic waves in the combustor, and subsequently cause combustion instabilities. Secondly, swirling flows affect the breakup of liquid sheet and droplet size distribution, and consequently influence the fuel distribution in the
combustion chamber. The overall effect on the distribution of equivalence ratio could be significant.

Since the flowfield generated by a swirl-stabilized injector plays an important role in defining the stoichiometry and fluid mechanics of the primary combustion zone, it is necessary to investigate injector dynamics for identifying the root cause of combustion instability.

An example of the vorticity field in a typical swirl-stabilized injector designed for an advanced gas-turbine engine is shown in Fig. 1.1 (Wang et al., 2001). The flowfield involves three characteristics: a central toroidal recirculation zone in the downstream of the centerbody; vortex shedding arising from the Kelvin-Helmholtz instability in the shear layers; and non-axisymmetric structures in the azimuthal direction due to the tangential flow instability.

The present study represents the first step in a systematic treatment of gas-turbine combustion dynamics. The purpose is to conduct a comprehensive numerical analysis of

![Fig. 1.1 Vorticity magnitude contours in a gas-turbine swirl-stabilized injector (Wang, et al., 2001).](image)
the vortical flow dynamics and acoustic response of swirl-stabilized injectors over a broad range of operating conditions by means of a large-eddy-simulation (LES) technique. Important physical processes for driving instabilities will be identified. The responses of the injector to various externally imposed excitations will be investigated in detail. In addition, an efficient and functional methodology for data analysis will be developed to extract salient flow physics from the huge database produced from the LES of complex flowfields.

The study will proceed in three steps:

1. to simulate turbulent swirling flows in a dump chamber for code validation;
2. to investigate the vortical flow dynamics, to explore the dominant physical processes and mechanisms involved, and to study the effect of inlet conditions, such as swirl number, on flow development in swirl-stabilized injectors; and
3. to examine the acoustic response of injector dynamics to externally imposed excitation.

1.2 Literature Review

1.2.1 Turbulence Closure: Large Eddy Simulation (LES)

Turbulence remains a challenge in fluid mechanics research due to its strong nonlinear behavior, although this topic has been studied for more than one hundred years. Numerical simulation of turbulent motions can be classified into three categories, as illustrated in Fig. 1.2.

The most straightforward method is direct numerical simulation (DNS). Given sufficient computing resources, the equations governing flow evolution can be solved without any model, and the entire spectrum of turbulence scales is resolved explicitly. DNS is a good tool to study flow mechanisms; however, the computational requirement of DNS for solving most practical engineering problems far exceeds the current computer capabilities.
Fig. 1.2 Concepts of DNS, LES and RANS.

The Reynolds-averaged Navier-Stokes equations (RANS) have been used for most engineering applications. The computational cost for RANS models is much less than that for DNS because of its lower grid resolution requirement. However, owing to the distinctive behavior between large- and small-scale turbulent motions, it is impossible to achieve a universal model that can cover all turbulent flows (Piomelli, 1999).

Large eddy simulation (LES) (Deardorff, 1970; Pope, 2000) is an intermediate approach between the two aforementioned methods. The largest scales, which contain most energy, are directly simulated. On the other hand, smaller scales, i.e., subgrid scales, are modeled. This method is based on the assumption that small-scale flow evolution tends to be more homogeneous than large-scale flow motions. The inhomogeneity of flow properties decreases with decreasing scales, and eventually disappears at the Kolmogorov scales, i.e., dissipation scales (Batchelor, 1953; Brasseur, 2000). In principle, the grid size of LES should fall in the inertial range.

Subgrid-scale (SGS) modeling is the core of LES. Because the dissipation scales, i.e., Kolmogorov scales, of turbulent flows are not resolved, the main role of SGS models is to transfer energy from resolved scales to unresolved scales through the energy cascade. In other words, the effects of unresolved scales on resolved scales must be modeled. Several SGS models have been developed since the late 1980s, most of which are based on the eddy-viscosity model. Commonly used SGS models include the
Smagorinsky eddy viscosity model, dynamic eddy viscosity model, and similarity and mixed model.

The Smagorinsky SGS model (Smagorinsky, 1963) is widely used because of its simplicity. It predicts fairly accurately from the global dissipation point of view when the integral scales are well resolved. This model, however, has obvious drawbacks because the coefficients are positive constants in its standard form. As a result, the model is too dissipative to accurately predict the SGS stresses in laminar regions or in the viscosity sub-layers of boundary layers, where the SGS stresses should vanish. It cannot predict the backscatter phenomena in the near-wall region either. These drawbacks can be avoided by introducing ad hoc modifications, such as the van Driest damping (van Driest, 1956) and an intermittency function (Piomelli et al., 1990). The van Driest damping function corrects the behavior in the near-wall region and the intermittency function eliminates the SGS stress in the laminar flow region. These ad hoc adjustments require empirical functions.

To avoid the empirical coefficients in the Smagorinsky model, a dynamic eddy viscosity model (Germano et al., 1991) is proposed, which represents a significant progress in subgrid-scale modeling. In the dynamic model, both a test and an LES filters are used, instead of just an LES filter as in the Smagorinsky model. The coefficients of the dynamic model are assumed to be constant in both filters and are computed dynamically during the calculation. The dynamic model yields good predictions of the average subgrid-scale stresses at the local level.

A weakness of the eddy viscosity model is that the principal axis of the strain-rate and SGS stress tensors are aligned. A scale-similar model is introduced by Bardina et al. (1980) to avoid this problem. A dynamic model, including a scale-similar part, has been applied by Zang et al. (1993). These models are based on the recognition that the most active subgrid-scales are generally those close to the cutoff wavenumber, and that the scales with which they interact most are also near the cutoff wavenumber. Meneveau et al. (2000) states that the mixed models are superior, on the whole, to simple eddy viscosity models.
Another promising approach to the LES subgrid-scale modeling is the Monotonically Integrated LES (MILES), which solves the unfiltered Navier-Stokes equations using high-resolution monotone algorithms. In this approach implicit tensorial (anisotropic) SGS models, provided by intrinsic non-linear high-frequency filters built into the convection discretization, are coupled naturally with the resolvable scales of the flow. The MILES approach provides an attractive alternative when seeking improved LES for inhomogeneous (inherently anisotropic) high Reynolds number turbulent flows (Fureby and Grinstein, 1999, 2002; Grinstein et al., 2002).

1.2.2 Swirling Flows

Swirling flows are extensively used as an effective means to stabilize flames and to enhance fuel/air mixing in many combustion devices for propulsion and power-generation applications. Their intensity is usually characterized with a dimensionless parameter: swirl number, defined as the ratio of the angular momentum to the axial momentum in the flow.

There are many unresolved issues of swirling flows, such as vortex breakdown, an inherent dynamic process in swirling flows. This phenomenon manifests itself with an abrupt change in the core of a slender vortex, which usually develops downstream into a recirculating "bubble" or a helical pattern (Shtern and Hussain, 1999). Vortex breakdown has been widely studied since its discovery by Peckham and Atkinson (1957) in their investigation of the flows over the "Gothic" wings. Because of the practical applications of vortex breakdown in destructing wing-tip vortices and stabilizing flames, much effort has been expended on this subject area (Sarpkaya, 1971a,b; Faler and Leibovich, 1977a,b; Garg and Leibovich, 1979; Billant et al. 1998; Pereira et al. 1999).

Sarpkaya (1971a) classified three types of breakdown in swirling pipe flows: bubble, spiral, and double helix. The bubble mode is usually predominant at high swirl numbers, while the spiral mode occurs at low swirl numbers. The double helix mode is formed when the vortex core expands and spirals, and is observed only in a diverging tube (Sarpkaya 1971b). Actually these three types of vortex breakdown are among the seven distinct modes of the vortex core disruption revealed by Leibovich (1978) using
water flow visualization at a variety of Reynolds numbers and swirl numbers. In addition to these types of vortex breakdown observed in laminar flow regime, another fundamental mode of the conical type was identified by Sarpkaya (1995), and Novak and Sarpkaya (2000) for swirling pipe flows at high Reynolds numbers. Recently, Lucca-Negro and O’Doherty (2001) gave a systematic review on vortex breakdown. As indicated in their work, despite the extensive experimental and numerical research conducted in the past few decades, a universally accepted explanation for the appearance of vortex breakdown remains to be established. The presence of turbulence at high Reynolds numbers further complicates the problem. Thus, understanding and characterizing turbulent swirling flows remain fundamental challenges in fluid mechanics.

Swirling flows may also generate other dynamic processes, such as the Kelvin-Helmholtz instability, helical instability, centrifugal instability, and the interactions among these unsteady flow motions. Martin and Meiburg (1996) studied the various nonlinear mechanisms of interactions and competitions among these instabilities by means of a simplified model of swirling jets. An improved understanding of these mechanisms and their mutual coupling is a prerequisite for successful development of active and passive control strategies employing sound, nozzle geometry, flow motion, and micromachines, with the goal of tailoring the flow motion in order to generate desired operation conditions for gas-turbine combustors (Martin and Meiburg, 1996; Paschereit et al., 1998).

Computational fluid dynamics (CFD) has been widely applied to investigate swirling flows. Previous studies, e.g., Rhode et al. (1983), Dong and Lilley (1994), and Lai (1996), mainly focused on the swirl effects on the size of the recirculation zone in two-dimensional axisymmetric configurations with steady incompressible flow assumption based on a RANS technique. Basically, the Reynolds stress components need to be specified with suitable turbulence models. Rhode et al. (1983) suggested that the eddy viscosity model based on the standard $\kappa-\varepsilon$ was inherently inadequate, and a redistribution of the stress magnitudes was necessary. Spall and Gatski (1995) first examined numerically turbulent bubble vortex breakdown by solving three-dimensional
RANS equations coupled with the standard $\kappa-\varepsilon$ and algebraic stress models. Lai (1996) also investigated the predictive capabilities of turbulence models for a confined swirling flow and found some deficiencies by applying RANS equations to predict turbulent quantities.

Because of the progress in LES, it has become a powerful tool in providing fundamental understanding of the physics involved in turbulent swirling flows. Pierce and Moin (1998) studied a confined coaxial jet with the effects of swirl and heat release. A low Mach number variable density formulation was implemented to account for the effect of heat release, along with an assumed PDF approach for modeling the subgrid scale mixture fraction in the limit of fast chemistry. Kim et al. (1999) performed LES of turbulent fuel/air mixing in a gas turbine combustor and focused on accurately capturing the dynamics of turbulent fuel/air mixing with a conventional LES technique. Cannon et al. (2000) examined the combustion dynamics in a liquid-fueled flammetube combustor using a two-dimensional LES simulation. Those studies show that the LES is favorable in light of the calculated characteristics of turbulent swirling flows.

In spite of the vast research performed in the general field of swirling flows, a comprehensive understanding of vortical dynamics in the turbulent swirling flows is still lacking. In particular, the mutual couplings among different instability mechanisms involved in complex flowfields need to be explored. Earlier work using conventional turbulence closure (RANS) or 2D LES lacks detailed information about the unsteady flow evolution.

1.3 Work Scope and Method of Approach

The present study investigates the vortical flow dynamics and acoustic characteristics of swirl-stabilized injectors by means of three-dimensional large eddy simulations. The entire flowfield under consideration is extremely complicated, involving many intricate characteristics. The high-intensity turbulent swirling flows give rise to strong vortical stretching effects; the presence of swirling enhances the helical-mode flow motions; the strong shear flows in the azimuthal direction induce the Kelvin-Helmholtz instability; the unstable radial stratification originating from swirling flows
generates centrifugal instability; and the precessing vortex core (PVC) may arise from swirling flows in many applications. All of these phenomena are inherently non-axisymmetric; therefore, a three-dimensional analysis with effective turbulence modeling must be conducted to study these highly unsteady flow motions.

To unveil the difference between an axisymmetric simulation with the inclusion of the azimuthal velocity component and a fully three-dimensional simulation, snapshots of the vorticity magnitude fields resulting from these two different types of simulations are presented in Fig. 1.3. The flow conditions for the simulations are identical. It is quite clear that the flow structures showing the dynamic evolution of vortex breakdown in the axisymmetric case are much larger than those in the three-dimensional simulation. One major factor contributing to this difference is the vortex stretching effect, which does not exist in the two-dimensional simulation. Although this effect is considered to certain extent in the axisymmetric case by considering the azimuthal velocity, it is still undervalued due to the axisymmetric assumption. To correctly predict this characteristic, a three-dimensional simulation is essential.

Fig. 1.3  Snapshots of vorticity magnitude contours (a) an axisymmetric simulation and (b) a three-dimensional simulation. Logarithmic contour levels are drawn.
In the present work, the following questions must be resolved: (1) how to develop and validate an accurate numerical code to simulate highly complex turbulent swirling flows; (2) how to identify the dominant physical mechanisms underlying the flow evolution; (3) how to study the effects of inlet conditions, such as the swirl number; (4) how to characterize the acoustic response of the injectors; and (5) how to process the huge data set resulting from the calculations. Accordingly this thesis is organized as follows:

- An LES simulation of turbulent swirling flows in a dump chamber is first performed. The flow evolution in the chamber is investigated. The configuration under consideration matches the geometry and flow conditions used in the experimental study of Favaloro et al. (1989, 1991). Several reduced-order data analyses are developed and implemented to extract the flow physics from the huge data set of calculated results.
- After code validation, the vortical flow dynamics in a gas-turbine swirl-stabilized injector is studied. The unsteady motions associated with different instability mechanisms at two different swirl numbers are identified and studied in detail.
- Finally, externally periodic excitations are imposed at the inlet of the radial swirlers to generate traveling acoustic waves in the injector. The effects of acoustic and vortical motions on flow evolution are carefully examined. Several response functions are obtained to characterize the acoustic response of the injector.

Chapter 2 focuses on the models and methodologies employed to account for the full three-dimensional conservation equations of mass, momentum, and energy. The Smagorinsky subgrid-scales (SGS) model proposed by Erlebacher et al. (1992) and the dynamic model by Germano et al. (1991) are implemented for turbulence closure.

The governing equations presented in Chapter 2 are discretized by means of a density-based, finite-volume approach described in Chapter 3. The basic formulation is presented along with the relevant numerical issues and analyses that characterize the fundamental algorithmic properties. Spatial discretization is obtained using a fourth-order central differencing scheme developed by Rai and Chakravarthy (1993) and a sixth-order artificial dissipation term employed to prevent numerical oscillation and
subsequently improve numerical convergence. Both the four-step Runge-Kutta and Adam-Bashforth predictor-corrector methods are employed for the temporal integration. A scheme-error estimation based on the von Neumann analysis and a post-calculation evaluation are presented. The implementation of parallel processing in the present work is addressed in detail. Finally, the methodology for the data analysis is discussed.

Chapter 4 presents a study for turbulent swirling flows in a dump chamber for code validation. The effects of swirl number are investigated, and the computational results are compared with experimental data. A variety of data analysis methods are employed to examine the flow physics, including the proper orthogonal decomposition (POD) method and a finite-element code for acoustic waves.

Chapters 5 and 6 present a series of case studies of the vortical flows in a gas-turbine swirl-stabilized injector. Several flow instability mechanisms, including vortex breakdown, the Kelvin-Helmholtz instability, helical instability, and centrifugal instability, appearing in the flow evolution are studied. In Chapter 5 the flows without external periodical excitation at two different swirl numbers are investigated. The effects of swirl number on the flowfield are examined carefully. After establishing a solid foundation for large-scale computations of the flowfields, external excitations are implemented to study the acoustic response of the injector in Chapter 6. A triple decomposition technique is applied in data analysis. Three response functions, including an acoustic admittance function and two mass transfer functions, are introduced to characterize the acoustic behaviors of the injector.
Chapter 2
Theoretical Formulation

2.1 Governing Equations

The formulation is based on the full conservation equations of mass, momentum, and energy in Cartesian coordinates:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_j u_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}
\]

\[
\frac{\partial \rho E}{\partial t} + \frac{\partial [(\rho E + p) u_i]}{\partial x_j} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial (u_i \tau_{ij})}{\partial x_j}
\]

where the specific total energy \( E \) is given by

\[
E = e + \frac{u_j u_j}{2}
\]

\[
e = h - \frac{p}{\rho}
\]

\[
h = h_{\text{ref}} + \int_{T_{\text{ref}}}^{T} C_p dT
\]

The equation of state for an ideal gas is used.

\[
p = \frac{R_u \rho T}{m}
\]

The universal gas constant, \( R_u \), is 8314.36 J kmol\(^{-1}\)K\(^{-1}\) and \( m \) the molecular weight. The \textit{Newtonian fluid} and \textit{Stokes assumptions} are implemented for the viscous stress tensor, \( \tau_{ij} \),

\[
\tau_{ij} = -\frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]
The heat flux $q_i$ is modeled using the *Fourier law* (Kundu, 1990)

$$ q_i = -k \frac{\partial T}{\partial x_i} \quad (2.9) $$

### 2.2 Large Eddy Simulation

A large eddy simulation (LES) technique is implemented in the present work for turbulence closure. In LES techniques (Deardorff, 1970; Lesieur, 1997), flow motions are treated in two different ways depending on their sizes. Large-scale turbulence is directly simulated, whereas turbulence smaller than the grid or filter size is modeled to represent the effects of unresolved motions on resolved scales.

#### 2.2.1 Filter Operation

The first step in large eddy simulation lies in the filter operation. The filtered (or resolved, large-scale) variable can be obtained as follows

$$ \widetilde{f}(x) = \int_{-\infty}^{\infty} f(x') G(x-x') dx' \quad (2.10) $$

where $G$ is the filter function and $\int_{\infty}^{\infty} G(x) dx = 1$. The filter function determines the size and structure of the small scales. Leonard (1974) indicated that if $G$ is only a function of $x-x'$, the differentiation and filtering operations could commute with each other. Commutation of the filtering operation with spatial differentiation is strictly valid only for uniform grid systems (Ghosal and Moin, 1995; Ven, 1995). The commutation error is usually neglected for moderately stretched grids, and can be lumped with the subgrid model (Ribault *et al.*, 1999; Moin, 1997). The modeling error is found to be generally smaller than the discretization error (Ribault *et al.*, 1999).

The filter function $G$ could be any function defined in an infinite domain and satisfies the following requirements

1. $G(x) = G(-x)$;
2. $\int_{-\infty}^{\infty} G(x)dx = 1$;

3. $\int_{-\infty}^{\infty} G(x) |x|^n dx < \infty$, $\forall n \geq 0$; and

4. $G(x)$ is small while $|x| > \Delta$.

where $\Delta$ stands for the filter size. The most commonly used filter functions are summarized as follows.

- **Tophat:**
  This filter is popularly employed in the physical space, defined as

  $$G(x) = \begin{cases} 
  1/\Delta^3 & \text{if } |x| \leq \Delta/2 \\
  0 & \text{otherwise}
  \end{cases}$$

  (2.11)

  For example, in the finite-volume approach, the cell-averaged variables are defined as

  $$\bar{f} = \frac{1}{\Delta V} \int_{\Delta V} f(x)dx$$

  (2.12)

  Thus, a tophat filter results in a cell-averaged quantity.

- **Gaussian filter:**

  $$G(x) = \frac{6}{\pi \Delta^2} \exp\left(-\frac{6 |x|^2}{\Delta^2}\right)$$

  (2.13)

- **Cutoff Filter:**

  $$\hat{G}(k) = \begin{cases} 
  1 & \text{if } |k| \leq \pi/\Delta \\
  0 & \text{otherwise}
  \end{cases}$$

  (2.14)

  The cutoff filter is a tophat filter in spectral space.

  To capture all of the flow scales resolved by a given grid system, and to model the effects of unresolved scales, the concepts of decomposition and filtering are introduced. Based on the Favre-averaging (Favre, 1969), any instantaneous variable ($f$) can be expressed as the sum of a Favre-averaging filtered scale ($\tilde{f}$) and a subgrid scale ($f''$)

  $$f = \tilde{f} + f''$$

  (2.15)
where
\[ \tilde{f} = \frac{\rho f}{\rho} \]  
(2.16)

Because of \( \tilde{f} \neq 0 \) and \( \tilde{f}^* \neq 0 \) in this spatial filtering process, the filter operation in LES is different from the conventional Reynolds average in time domain. Therefore, the relationships derived from the time averaging in the RANS concept are not always true in the filter operations of LES.

2.2.2 Favre Filtered Governing Equations

After applying the Favre-averaging on Eqs. (2.1)-(2.3), the conservation equations can be written as:

\[ \frac{\partial \rho \tilde{u}_i}{\partial t} + \frac{\partial (\rho \tilde{u}_i \tilde{u}_j)}{\partial x_j} = 0 \]  
(2.17)

\[ \frac{\partial \rho \tilde{u}_i}{\partial t} + \frac{\partial (\rho \tilde{u}_i \tilde{u}_j)}{\partial x_j} = - \frac{\partial \rho}{\partial x_i} + \frac{\partial (\tilde{\tau}_{ij} - \tau_{ij}^{SGS} + D_{ij}^{SGS})}{\partial x_j} \]  
(2.18)

\[ \frac{\partial \rho \tilde{E}}{\partial t} + \frac{\partial (\rho \tilde{E} + \rho \tilde{u}_i \tilde{u}_i)}{\partial x_i} = - \frac{\partial}{\partial x_i} \left[ \tilde{q}_i + \tilde{u}_j \tilde{\tau}_{ij} + \sigma_{ij}^{SGS} - H_i^{SGS} \right] \]  
(2.19)

where the subgrid closure terms are

\[ \tau_{ij}^{SGS} = \rho (\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j) \]  
(2.20)

\[ D_{ij}^{SGS} = (\tilde{\tau}_{ij} - \tilde{\tau}_{ij}) \]  
(2.21)

\[ H_i^{SGS} = \rho (\tilde{E} \tilde{u}_i - \tilde{E} \tilde{u}_i) + (\tilde{p} \tilde{u}_i - \tilde{p} \tilde{u}_i) \]  
(2.22)

\[ \sigma_{ij}^{SGS} = (\tilde{u}_i \tilde{\tau}_{ij} - \tilde{u}_j \tilde{\tau}_{ij}) \]  
(2.23)

Those terms arising from the unresolved scales must be modeled in terms of resolved scales. Because the filter scale of LES falls in the turbulence inertial range, the modeling of the subgrid terms is relatively universal in comparison with the RANS modeling. This apparently is the biggest advantage of LES. The subgrid-scale models will be discussed in detail in the following section.
2.2.3 Subgrid-Scale Models

The SGS modeling for the unresolved terms in Eqs. (2.20)–(2.23) is one of the central issues in LES and must be carefully treated. Because the small eddies, which are less than the filter size and unresolved in LES, dissipate most turbulent kinetic energy, SGS models are introduced to account for the energy transfer from the largest scales to smaller ones. In most cases, the equilibrium assumption for sub-grid scales is made to simplify the problem. Most of the SGS models are based on the eddy-viscosity model as follows

\[
\tau_{ij}^{SGS} - \frac{\delta_{ij}^{SGS}}{3} \tau_{kk}^{SGS} = -2\nu_t \tilde{\rho} \tilde{S}_{ij}
\]  

(2.24)

where \( \nu_t \) is the eddy viscosity. The unresolved terms, \( \tau_{ij}^{SGS} \), are related to the resolved strain-rate tensor, \( \tilde{S}_{ij} \), defined as

\[
\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_j}{\partial x_i} + \frac{\partial \tilde{u}_i}{\partial x_j} \right).
\]  

(2.25)

2.2.3.1 Smagorinsky Model

The Smagorinsky model (Smagorinsky, 1963) can be written as

\[
\nu_t = (C \Delta)^2 |\tilde{S}| \]  

(2.26)

where \( \Delta \) is the filter width and

\[
|\tilde{S}| = (\tilde{S}_{ij} \tilde{S}_{ij})^{1/2}
\]  

(2.27)

The coefficient \( C \) can be determined from the isotropic turbulence decay or a prior test.

Erlebacher et al. (1992) extended the Smagorinsky model to include flow compressibility effect. The SGS stresses in Eq. (2.20) are separated into two parts, i.e., deviatoric and isotropic parts. The deviatoric part of the SGS stresses is treated using the
Smagorinsky model, Eq. (2.26), while $\tau_{kk}$ is modeled with a formulation proposed by Yoshizawa (1986),
\begin{equation}
\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -2C_R \bar{\Delta}^2 \bar{p} \left| \bar{S} \right| \left( \bar{S}_{ij} - \frac{\delta_{ij}}{3} \bar{S}_{kk} \right) = 2v_t \bar{p} \left( \bar{S}_{ij} - \frac{\delta_{ij}}{3} \bar{S}_{kk} \right) \tag{2.28}
\end{equation}
\begin{equation}
\tau_{kk} = 2\bar{p}k^{SGS} = 2C_i \bar{\Delta}^2 \left| \bar{S} \right|^2 \tag{2.29}
\end{equation}
where
\begin{equation}
v_t = C_R \bar{\Delta}^2 \left| \bar{S} \right|^2 \tag{2.30}
\end{equation}
denotes SGS kinematic viscosity. The dimensionless quantities $C_R$ and $C_I$ are the compressible Smagorinsky model constants. Yoshizawa (1986) proposed an eddy-viscosity model for weakly compressible turbulent flows, using a multi-scale, direct-interaction approximation method and suggested $C_R = 0.012$ and $C_I = 0.0066$ basing on theoretical arguments.

The subgrid energy flux terms, $H_j^{SGS}$, is modeled as
\begin{equation}
H_j^{SGS} = -\bar{p} \frac{v_t \frac{\partial \tilde{H}}{\partial x_j}}{Pr_t} = -\bar{p} \frac{v_t}{Pr_t} \left( \frac{\partial \tilde{h}}{\partial x_j} + \tilde{u}_i \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{1}{2} \frac{\partial k^{SGS}}{\partial x_j} \right) \tag{2.31}
\end{equation}
where the $\tilde{H}$ and $Pr_t$ represent the filtered specific total enthalpy and turbulent Prandtl number, respectively. The turbulent Prandtl number $Pr_t$ is fixed (e.g., $Pr_t = 0.7$ of Zang et al., 1992). The subgrid-scale kinetic energy term, $k^{SGS}$, is
\begin{equation}
k^{SGS} = \frac{1}{2} \left( \tilde{u}_i \tilde{u}_i - \tilde{u}_i \tilde{u}_i \right) \tag{2.32}
\end{equation}
The SGS viscous diffusion terms, $\sigma_i^{SGS}$, is neglected in the present study due to its small contribution to the total energy equation (Martin et al., 1999). At the same time, the nonlinearity of viscous stress terms $D_i^{SGS}$ is invariably neglected (i.e., $\bar{\tau}_{ij} - \bar{\tau}_{ij} = 0$) (Piomelli, 1999)

The Erlebacher model is an algebraic model. It predicts the overall dissipation well; however, its drawback is also obvious. The model is purely dissipative because of
its positive viscosity coefficient. Another deficiency is the lack of universality of the model coefficients. In a laminar flow region or the viscous sub-layer of a boundary layer, the SGS stress predicted by the Erlebacher model does not vanish, rendering incorrect results in those flow regions. To overcome this drawback, the van Driest damping function (van Driest, 1956; Piomelli et al. 1988) is introduced in the present study. The concept of the damping function is to scale turbulence mixing length through a damping factor recommended by Piomelli et al. (1988)

\[ D(y^+) = 1 - \exp\left[ -\left( \frac{y^+}{A^+} \right)^3 \right] \]  \hspace{1cm} (2.33)

where

\[ y^+ = \frac{u_\tau y}{v}, \quad u^+ = \frac{\tilde{u}}{u_\tau}, \quad u_r = \sqrt{\frac{\tau_w}{\bar{p}}}, \quad A^+ = 25 \]  \hspace{1cm} (2.34)

Calculation of the shear stress at the wall, \( \tau_w \), depends on the grid resolution and will be discussed in Section 2.2.4. The filter size, \( \Delta \), implemented in Eqs. (2.28) and (2.29) is scaled as

\[ \tilde{\Delta}' = D(y^+) \tilde{\Delta} \]  \hspace{1cm} (2.35)

The scaled filter size \( \tilde{\Delta}' \) will replace the \( \tilde{\Delta} \) in Eqs. (2.28) and (2.29). The prime appearing in the above equation will be omitted in the following sections for clarity. The van Driest damping function leads to a correct flow behavior in the near wall region.

2.2.3.2 Dynamic Model

Among the various SGS turbulence models, such as the mixed model (Fureby 1996) and the two-parameter mixed model (Salvetti et al. 1995), the dynamic SGS model for compressible flow turbulence offers the best tradeoff between accuracy and cost (DesJardin et al. 1998), and is thus employed in the present study in addition to the Smagorinsky model.

The introduction of dynamic model (Germano et al., 1991) has spurred significant progress in the subgrid-scale modeling of non-equilibrium flows. Moin et al. (1991)
proposed a modification of the eddy viscosity model (Eqs. (2.28) and (2.29)) in which the two model coefficients are determined as the calculation progresses, instead of being treated as input parameters \textit{a priori}. In order to calculate the model parameters $C_R$ and $C_l$ dynamically, the test filter, $\hat{G}$, whose width $\hat{\Delta}$ is generally larger than the grid filter-width $\Delta$, is introduced.

$$\hat{f} = \int_{\alpha} \hat{G}(x - x') f(x') dx'$$  \hfill (2.36)

Application of the test filter $\hat{G}$ with a characteristic width $\hat{\Delta}$ to Eqs. (2.17)-(2.19) yields the subtest-scale stresses, $T_{ij}$, defined as

$$T_{ij} = \hat{\rho} \hat{u}_i \hat{u}_j - \hat{\rho} \hat{\bar{u}}_i \hat{\bar{u}}_j$$  \hfill (2.37)

where

$$\hat{\bar{f}} = \hat{\rho} \hat{f} / \hat{\rho}.$$  \hfill (2.38)

Both the subgrid stresses, $\tau_{ij}^{SGS}$, and the subtest-scale stresses, $T_{ij}$, are modeled using the aforementioned compressible Smagorinsky model, Eq. (2.28).

$$\tau_{ij}^{SGS} - \frac{\delta_{ij}}{3} \tau_{kk}^{SGS} = -2C_R \hat{\Delta}^2 \hat{\rho} |\hat{S}| \left( \tilde{S}_{ij} - \frac{\delta_{ij}}{3} \tilde{S}_{kk} \right) = C_R \alpha_{ij}$$  \hfill (2.39)

$$T_{ij} - \frac{\delta_{ij}}{3} T_{kk} = -2C_R \hat{\Delta}^2 \hat{\rho} |\hat{S}| \left( \tilde{S}_{ij} - \frac{\delta_{ij}}{3} \tilde{S}_{kk} \right) = C_R \beta_{ij}$$  \hfill (2.40)

where

$$\alpha_{ij} = -2\hat{\Delta}^2 \hat{\rho} |\hat{S}| \left( \tilde{S}_{ij} - \frac{\delta_{ij}}{3} \tilde{S}_{kk} \right)$$  \hfill (2.41)

$$\beta_{ij} = -2\hat{\Delta}^2 \hat{\rho} |\hat{S}| \left( \tilde{S}_{ij} - \frac{\delta_{ij}}{3} \tilde{S}_{kk} \right).$$  \hfill (2.42)

The \textit{resolved turbulent stresses} is defined as
\( L_{ij} = T_{ij} - \hat{\tau}_{ij} \). \hspace{2cm} (2.43)

Assume that the flow behavior in the test filter region varies smoothly, \textit{i.e.}, scale invariance; as a result, the coefficients are constant in the test filter, \textit{i.e.}, \( \overline{C_{ij}} = \overline{C_{ij}} \hat{f} \).

Substitution of the test-filter into Eq. (2.39) and application of Eq. (2.40) onto Eq. (2.43) yields

\[
L_{ij} = C_R \left( \beta_{ij} - \hat{\alpha}_{ij} \right) + \frac{\delta_{ij}}{3} (T_{kk} - \hat{r}_{kk}) = C_R M_{ij} + \frac{\delta_{ij}}{3} L_{kk}
\]

where

\[
M_{ij} = \beta_{ij} - \hat{\alpha}_{ij}
\]

Notice that \( L_{ij} \) involve only one unknown variable, \( C_R \), but five independent equations. Here one equation is deducted from Eq. (2.44) because the track of the matrix \( L = \frac{1}{3} L_{kk} \) is zero. To obtain a single coefficient from a system of five independent equations, Lilly (1992) proposed that Eq. (2.44) be least-squared with respect to \( C_R \)

\[
\frac{\partial \Delta E^2}{\partial C_R} = 0
\]

where

\[
\Delta E^2 \triangleq \left( L_{ij} - C_R M_{ij} - \frac{\delta_{ij}}{3} L_{kk} \right) \left( L_{ij} - C_R M_{ij} - \frac{\delta_{ij}}{3} L_{kk} \right).
\]

The deviatoric part model coefficient becomes

\[
C_R = \frac{\langle L_{ij} M_{ij} \rangle}{\langle M_{kl} M_{kl} \rangle} - \frac{1}{3} \frac{\langle L_{mm} M_{nn} \rangle}{\langle M_{kl} M_{kl} \rangle}
\]

where the brackets \( \langle \cdot \rangle \) denote an appropriate average to ensure the stability of numerical calculations (Moin \textit{et al.} 1991; Germano \textit{et al.} 1991). In the current work, the \( \langle \cdot \rangle \) operator is locally smoothed using the same test filter employed by Fureby (1996) and DesJardin \textit{et al.} (1998).
Following the same procedure through Eqs. (2.39)–(2.48), the isotropic model coefficient $C_I$ is

$$C_I = \frac{\langle L_{kk} \rangle}{\langle \beta - \alpha \rangle} \quad (2.49)$$

while

$$\tau_{kk}^{SGS} = 2C_I \bar{\rho} \hat{\Delta}^2 \left| \hat{S} \right|^2 = C_I \alpha \quad (2.50)$$

$$T_{kk} = 2C_I \bar{\rho} \hat{\Delta}^2 \left| \hat{S} \right|^2 = C_I \beta . \quad (2.51)$$

The same procedure can be applied to the SGS energy flux, Eq. (2.22), to obtain the turbulent Prandtl number in Eq. (2.31). The SGS heat flux terms are given by

$$Q_j^{SGS} - \bar{\rho} \bar{u}_j \bar{T} - \bar{\rho} \bar{u}_j \bar{T} = -\bar{\rho} v_t \frac{\partial \bar{T}}{\partial x_j} = -C_r \frac{\hat{\Delta}^2 \bar{\rho} \langle \hat{S} \rangle \partial \bar{T}}{Pr_r \frac{\partial \bar{x}_j}{\partial x_j}} \quad (2.52)$$

where $v_t$ is the eddy viscosity coefficient in Eq. (2.30). The turbulent Prandtl number $Pr_r$ can be fixed (e.g., $Pr_r = 0.7$ in Zang et al., 1992), or adjusted dynamically. The subtest-scale heat flux is presented as

$$\Theta_j = \bar{\rho} \bar{u}_j \bar{T} - \bar{\rho} \bar{u}_j \bar{T} \quad (2.53)$$

and

$$H_j = \Theta_j - \hat{\Theta}_j = \bar{\rho} \bar{u}_j \bar{T} - \bar{\rho} \bar{u}_j \bar{T} = \bar{\rho} \bar{u}_j \bar{T} - \bar{\rho} \bar{u}_j \bar{T} / \bar{\rho} - \bar{\rho} \bar{u}_j \bar{T} / \bar{\rho} \quad (2.54)$$

Then the turbulent Prandtl number $Pr_r$ is determined dynamically as

$$Pr_r = C_r \frac{\langle T_j T_j \rangle}{\langle H_j T_k \rangle} \quad (2.55)$$

where

$$T_j = -\hat{\Delta}^2 \bar{\rho} \langle \hat{S} \rangle \frac{\partial \bar{T}}{\partial x_j} - \hat{\Delta}^2 \bar{\rho} \langle \hat{S} \rangle \frac{\partial \bar{T}}{\partial x_j} \quad (2.56)$$
Both the Smagorinsky model and dynamic model are implemented in the current study. The dynamic model does not require empirical constants, but be implemented at the expense of computational time. The grid resolution of the dynamic model is normally stricter than the Smagorinsky model because the scales of the test filter must fall in the turbulence inertial subrange.

### 2.2.4 Wall Bounded Turbulent Flows

Wall affects turbulent flows in several ways. Firstly, the wall constrains small scales. Secondly, in the near-wall regions, small scales may produce significant turbulent kinetic energy. Finally, the length scale of the large structures near the wall depends on the Reynolds number (Piomelli, 1998).

The aforementioned SGS models are valid for outer flows, but may fail in the near-wall region. Two methods can be used to handle the flow in the near-wall region. First, the grid size is fine enough to resolve the viscous sub-layer directly. Therefore, modeling is unnecessary and the non-slip wall boundary condition can be employed directly. The cost for such a direct resolution of viscous sub-layer, however, is usually too expensive to be realizable for very high Reynolds number flows. The second method requires modeling of the wall layer, such as wall functions. Obviously, wall modeling introduces further empiricism. Most wall models assume that the dynamics of the wall layer are universal, and that some generalized law-of-the-wall are implemented. This assumption remains questionable for swirling flows near curved surfaces or separation flows. In the present work, all near-wall regions are resolved directly in order to avoid the uncertainties resulting from the wall modeling. Because the flow Reynolds numbers of concern are moderately high in the present study, direct resolution is possible.

The wall function introduced here may be used for future study of very high Reynolds number flows. The mean shear stress at the wall is calculated as a function of the friction velocity, $u_\tau$. The composite formula derived by Spalding (1961) as a transcendental equation is given as
\[ y^+ = u^+ + e^{-kB} \left[ e^{-kB} - 1 - \kappa u^+ + \frac{1}{2} (\kappa u^+)^2 - \frac{1}{6} (\kappa u^+)^3 \right] \]  \hspace{1cm} (2.57)

where \( \kappa = 0.41 \) is the von Karman constant and \( B = 5 \). Equation (2.57) is employed when the first grid point off the wall falls in the interval of \( 2 \leq y^+ \leq 150 \). Because the wall shear stress in the above equation is implicit, Eq. (2.57) must be solved iteratively. Implementation of the wall function also implies that the no-slip boundary condition cannot be strictly employed on the wall boundary.
Chapter 3

Numerical Method and Data Analysis

An accurate numerical scheme is essential for resolving turbulent flows with a variety of time and length scales. This chapter will address the numerical method for solving the theoretical model described in the previous chapter. In Section 3.1 the governing equations are rewritten in a vector form for the convenience of discretization. Spatial derivatives are discretized using a fourth-order finite-volume method in Section 3.2. A sixth-order artificial dissipation is employed in the discretized formulation in order to prevent numerical oscillation and subsequently to improve numerical convergence. In Section 3.3 both a four-step Runge-Kutta and a two-step predictor-corrector Adam-Bashforth schemes are employed for temporal discretization. The numerical stability and accuracy of the scheme are analyzed theoretically using the von Neumann analysis in Section 3.4. The concepts of parallel processing and its implementation in the present study are described in Section 3.5. Finally, a methodology for data processing and analysis is presented in Section 3.6.

3.1 Governing Equations

The Favre-filtered mass, momentum, and energy conservation equations in the Cartesian coordinates can be expressed in a general vector form as follows:

$$
\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = \frac{\partial E_v}{\partial x} + \frac{\partial F_v}{\partial y} + \frac{\partial G_v}{\partial z}
$$

(3.1)

The vector $Q$ contains dependent variables and is defined as

$$
Q = [\rho, \rho u, \rho v, \rho w, \rho \tilde{E}]^T
$$

(3.2)

where the superscript $T$ stands for the transpose of a vector. The convective flux vectors $E$, $F$, and $G$ in the $x$-, $y$-, and $z$-directions, respectively, take the form
The diffusion-flux vectors $E_v$, $F_v$, and $G_v$ in the $x$-, $y$- and $z$-directions, respectively, are

$$
E_v = \begin{bmatrix}
\tilde{\rho}\tilde{u}
\tilde{\rho}\tilde{u}^2 + \bar{\rho}
\tilde{\rho}\tilde{u}\tilde{v}
\tilde{\rho}\tilde{u}\tilde{w}
(\bar{\rho}\tilde{E} + \bar{p})\tilde{u}
\end{bmatrix}, \\
F_v = \begin{bmatrix}
\tilde{\rho}\tilde{v}
\tilde{\rho}\tilde{v}^2 + \bar{\rho}
\tilde{\rho}\tilde{v}\tilde{w}
(\bar{\rho}\tilde{E} + \bar{p})\tilde{v}
\end{bmatrix}, \\
G_v = \begin{bmatrix}
\tilde{\rho}\tilde{w}
\tilde{\rho}\tilde{w}^2 + \bar{\rho}
\tilde{\rho}\tilde{w}\tilde{v}
(\bar{\rho}\tilde{E} + \bar{p})\tilde{w}
\end{bmatrix}
$$

(3.3)

The resultant integral conservation equation takes the following form

$$
\Omega_x = \tilde{u}\tilde{\tau}_{xx} + \tilde{v}\tilde{\tau}_{xy} + \tilde{w}\tilde{\tau}_{xz} + \bar{q}_x - H_x^{SGS} \\
\Omega_y = \tilde{u}\tilde{\tau}_{yx} + \tilde{v}\tilde{\tau}_{yy} + \tilde{w}\tilde{\tau}_{yz} + \bar{q}_y - H_y^{SGS} \\
\Omega_z = \tilde{u}\tilde{\tau}_{zx} + \tilde{v}\tilde{\tau}_{zy} + \tilde{w}\tilde{\tau}_{zz} + \bar{q}_z - H_z^{SGS}
$$

(3.5)

3.2 Spatial Discretization

3.2.1 Finite-Volume Approach

The governing equations are solved numerically by means of a finite-volume approach. This method allows for the treatment of arbitrary geometry, and avoids problems with metric singularities usually associated with finite-difference methods. To initiate the finite-volume approach, we first integrate the conservation equations over a small control volume $V$ enclosed by the surface $S$. The volume integral for the flux vector is then converted to a surface integral by means of the Gauss divergence theorem. The resultant integral conservation equation takes the following form
\[
\int_V \frac{\partial \mathbf{Q}}{\partial t} dV + \oint_S \mathbf{W} \cdot n \, dS = 0 \quad (3.6)
\]

where the flux tensor, \( \mathbf{W} \), is
\[
\mathbf{W} = (\mathbf{E} - \mathbf{E}_v) \mathbf{e}_i + (\mathbf{F} - \mathbf{F}_v) \mathbf{e}_j + (\mathbf{G} - \mathbf{G}_v) \mathbf{e}_k \quad (3.7)
\]

and \( n \) is the outward unit vector normal to each surface. For a three-dimensional hexahedral cell as shown in Fig. 3.1, the governing equations can be written as follows:
\[
\int_V \frac{\partial \mathbf{Q}}{\partial t} dV + \int_{\xi} W \cdot n_\xi \, dS_\xi + \int_{\eta} W \cdot n_\eta \, dS_\eta + \int_{\zeta} W \cdot n_\zeta \, dS_\zeta = 0 \quad (3.8)
\]

The subscripts \( \xi \), \( \eta \), and \( \zeta \) represent quantities aligned with the axial, radial, and azimuthal directions, respectively. The unit vectors normal to the surfaces in the \( \xi \)-, \( \eta \)-, and \( \zeta \)- directions are respectively defined as

Fig. 3.1 Three-dimensional cells in finite-volume discretization.
\[ n_\xi = \frac{(S_\xi e_i + S_\xi e_j + S_\xi e_k)}{|S_\xi|} \]
\[ n_\eta = \frac{(S_\eta e_i + S_\eta e_j + S_\eta e_k)}{|S_\eta|} \]
\[ n_\zeta = \frac{(S_\zeta e_i + S_\zeta e_j + S_\zeta e_k)}{|S_\zeta|} \]  
(3.9)

where

\[ S_\xi = \frac{1}{2} r_{72} \times r_{56} = \frac{1}{2} \begin{vmatrix} e_i & e_j & e_k \\ x_2 - x_7 & y_2 - y_7 & z_2 - z_7 \\ x_6 - x_3 & y_6 - y_3 & z_6 - z_3 \end{vmatrix} = S_\xi e_i + S_\xi e_j + S_\xi e_k \]  
(3.10)

\[ S_\eta = \frac{1}{2} r_{86} \times r_{75} = \frac{1}{2} \begin{vmatrix} e_i & e_j & e_k \\ x_6 - x_8 & y_6 - y_8 & z_6 - z_8 \\ x_5 - x_7 & y_5 - y_7 & z_5 - z_7 \end{vmatrix} = S_\eta e_i + S_\eta e_j + S_\eta e_k \]  
(3.11)

\[ S_\zeta = \frac{1}{2} r_{74} \times r_{83} = \frac{1}{2} \begin{vmatrix} e_i & e_j & e_k \\ x_4 - x_7 & y_4 - y_7 & z_4 - z_7 \\ x_3 - x_8 & y_3 - y_8 & z_3 - z_8 \end{vmatrix} = S_\zeta e_i + S_\zeta e_j + S_\zeta e_k \]  
(3.12)

The magnitude of each surface vector represents the cell interface area and can be obtained with the following formulas.

\[ |S_\xi| = \sqrt{S_{\xi x}^2 + S_{\xi y}^2 + S_{\xi z}^2} \]
\[ |S_\eta| = \sqrt{S_{\eta x}^2 + S_{\eta y}^2 + S_{\eta z}^2} \]
\[ |S_\zeta| = \sqrt{S_{\zeta x}^2 + S_{\zeta y}^2 + S_{\zeta z}^2} \]  
(3.13)

\[ \Delta V = \frac{1}{3} r_7 \cdot (S_\xi + S_\eta + S_\zeta) \]  
(3.14)

Substitution of Eq. (3.9) in Eq. (3.8) yields

\[ \int \frac{\partial Q}{\partial t} dV + \int_{S_\xi} \left[ S_{\xi x} (E - E_x) + S_{\xi y} (F - F_y) + S_{\xi z} (G - G_z) \right]/|S_\xi| dS_\xi \]
\[ + \int_{S_\eta} \left[ S_{\eta x} (E - E_x) + S_{\eta y} (F - F_y) + S_{\eta z} (G - G_z) \right]/|S_\eta| dS_\eta \]
\[ + \int_{S_\zeta} \left[ S_{\zeta x} (E - E_x) + S_{\zeta y} (F - F_y) + S_{\zeta z} (G - G_z) \right]/|S_\zeta| dS_\zeta = 0 \]  
(3.15)
Rewrite Eq. (3.15) as

\[
\int_V \frac{\partial Q}{\partial t} dV + \oint_{\Omega_k} \left[ S_{\xi x} (E - E_v) + S_{\xi y} (F - F_v) + S_{\xi z} (G - G_v) \right] d\eta d\zeta \\
+ \int_{\Gamma_{\xi v}} \left[ S_{\eta x} (E - E_v) + S_{\eta y} (F - F_v) + S_{\eta z} (G - G_v) \right] d\zeta d\xi \\
+ \int_{\Gamma_{\xi v}} \left[ S_{\zeta x} (E - E_v) + S_{\zeta y} (F - F_v) + S_{\zeta z} (G - G_v) \right] d\xi d\eta = 0
\]  

(3.16)

Assuming that the increments in the general coordinate system are unity, i.e.,

\[
\Delta\xi = \Delta\eta = \Delta\zeta = 1
\]  

(3.17)

and substituting Eq. (3.17) into Eq. (3.16) yields the following governing equation at the cell \((i, j, k)\) in the general coordinates:

\[
\frac{\partial \hat{Q}}{\partial t} + (\hat{E} - \hat{E}_v)_{i+1/2,j,k} + (\hat{F} - \hat{F}_v)_{i,j+1/2,k} + (\hat{G} - \hat{G}_v)_{i,j,k+1/2} = 0
\]  

(3.18)

where the vectors \(\hat{Q}, \hat{E}, \hat{F}, \hat{G}, \hat{E}_v, \hat{F}_v, \) and \(\hat{G}_v\) are defined as:

\[
\hat{Q} = \Delta V Q \\
\hat{E} = S_{\xi x} E + S_{\xi y} F + S_{\xi z} G \\
\hat{F} = S_{\eta x} E + S_{\eta y} F + S_{\eta z} G \\
\hat{G} = S_{\zeta x} E + S_{\zeta y} F + S_{\zeta z} G
\]

(3.19)

The indices \(i \pm 1/2, j \pm 1/2\) or \(k \pm 1/2\) represent the cell interfaces.

### 3.2.2 Evaluation of Inviscid Fluxes

Because the problem of concern does not involve any discontinuity, such as shock or flame, a fourth-order central difference scheme along with a sixth-order artificial dissipation is employed to evaluate the inviscid flux terms (Rai et al., 1993):

\[
\hat{E}_{i+1/2} = \frac{1}{2} \left[ \hat{E}(Q^L_{i+1/2}) + \hat{E}(Q^R_{i+1/2}) \right] - d_{i+1/2,j}
\]  

(3.20)
where \( L \) and \( R \) denote the states of left and right, and \( d_{i+1/2,j} \) the artificial dissipation.

\[
Q^L_{i+1/2} = Q_i + \phi^{(2)} \left( \frac{3\nabla Q_{i+1} + \nabla Q_i}{8} \right) + \phi^{(4)} \left( -\frac{5\nabla Q_{i+2} + 7\nabla Q_{i+1} + \nabla Q_i - 3\nabla Q_{i-1}}{128} \right)
\]

(3.21)

\[
Q^R_{i+1/2} = Q_{i+1} - \phi^{(2)} \left( \frac{\nabla Q_{i+2} + 3\nabla Q_{i+1}}{8} \right) + \phi^{(4)} \left( \frac{3\nabla Q_{i+3} - \nabla Q_{i+2} - 7\nabla Q_{i+1} + 5\nabla Q_i}{128} \right)
\]

(3.22)

and

\[
\nabla(\cdot) = (\cdot)_i - (\cdot)_{i-1}
\]

\[
\Delta(\cdot) = (\cdot)_{i+1} - (\cdot)_i
\]

(3.23)

### 3.2.3 Evaluation of Viscous Fluxes

A central difference scheme is employed to evaluate the viscous terms. This procedure requires calculations of the gradients of \( u, v, w, \) and \( T \) at the interfaces. To be consistent with the finite-volume formulation, auxiliary cells, as shown schematically by the dash-dotted lines in Fig. 3.1, are constructed with their centers located at the midpoints of the cell interfaces under consideration. These cells with solid lines are called the primary cells. Now apply the Gauss divergence theorem to transform the following volume integral of vector \( \mathbf{f} \) to a surface integral:

\[
\int_V \nabla \cdot \mathbf{f} dV = \oint_S \mathbf{f} \cdot n dS.
\]

(3.24)

For a small control volume, \( \Delta V \), this equation can be approximated as

\[
\nabla \cdot \mathbf{f} = \frac{1}{\Delta V} \oint_S \mathbf{f} \cdot n dS
\]

(3.25)

Application of Eq. (3.25) to the auxiliary cell gives

\[
(\nabla \cdot \mathbf{f})_{i+1/2,j,k} = \frac{1}{V_{i+1/2,j,k}} \begin{bmatrix}
(f \cdot S_\xi)_{i+1/2,j,k} & -(f \cdot S_\xi)_{i,j,k} \\
+(f \cdot S_\eta)_{i+1/2,j+1/2,k} & -(f \cdot S_\eta)_{i+1/2,j-1/2,k} \\
+(f \cdot S_\zeta)_{i+1/2,j,k+1/2} & -(f \cdot S_\zeta)_{i+1/2,j,k-1/2}
\end{bmatrix}
\]

(3.26)
If we take \( \mathbf{f} = f \cdot \mathbf{e}_i \), then

\[
\left( \frac{\partial f}{\partial x} \right)_{i+\frac{1}{2},j,k} = \frac{1}{V_{i+\frac{1}{2},j,k}} \left[ f S_{\phi} \bigg|_{i+1,j,k} - f S_{\phi} \bigg|_{i,j,k} + f S_{\phi} \bigg|_{i+\frac{1}{2},j+1/2,k} - f S_{\phi} \bigg|_{i+\frac{1}{2},j-1/2,k} \right] \tag{3.27}
\]

Similarly, let \( \mathbf{f} = f \cdot \mathbf{e}_j \) or \( \mathbf{f} = f \cdot \mathbf{e}_k \) to obtain

\[
\left( \frac{\partial f}{\partial y} \right)_{i+\frac{1}{2},j,k} = \frac{1}{V_{i+\frac{1}{2},j,k}} \left[ f S_{\phi} \bigg|_{i+1,j,k} - f S_{\phi} \bigg|_{i,j,k} + f S_{\phi} \bigg|_{i+\frac{1}{2},j+1/2,k} - f S_{\phi} \bigg|_{i+\frac{1}{2},j-1/2,k} \right] \tag{3.28}
\]

\[
\left( \frac{\partial f}{\partial z} \right)_{i+\frac{1}{2},j,k} = \frac{1}{V_{i+\frac{1}{2},j,k}} \left[ f S_{\phi} \bigg|_{i+1,j,k} - f S_{\phi} \bigg|_{i,j,k} + f S_{\phi} \bigg|_{i+\frac{1}{2},j+1/2,k} - f S_{\phi} \bigg|_{i+\frac{1}{2},j-1/2,k} \right] \tag{3.29}
\]

Note that \( f \) could be \( u, v, w \) or \( T \) in this case.

Within the finite-volume approach, physical variables with integer indices are well defined at the cell center, but those having one-half indices need to be interpolated from the quantities at the neighboring cell centers. If a simple average is used, then

\[
f_{i+1/2,j+1/2,k} = \frac{1}{4} (f_{i,j,k} + f_{i+1,j,k} + f_{i,j+1,k} + f_{i+1,j+1,k}) \tag{3.30}
\]

\[
f_{i+1/2,j,k+1/2} = \frac{1}{4} (f_{i,j,k} + f_{i+1,j,k} + f_{i,j,k+1} + f_{i+1,j,k+1})
\]

The surface vectors associated with the auxiliary cell can also be approximated by averaging the neighboring surface vectors associated with the primary cells.

\[
S_{\xi,i,j,k} = \frac{1}{2} \left( S_{\xi,i+1/2,j,k} + S_{\xi,i-1/2,j,k} \right)
\]

\[
S_{\eta,i,j,k} = \frac{1}{2} \left( S_{\eta,i,j+1/2,k} + S_{\eta,i,j-1/2,k} \right)
\]

\[
S_{\zeta,i,j,k} = \frac{1}{2} \left( S_{\zeta,i+1/2,j+1/2,k} + S_{\zeta,i+1/2,j-1/2,k} + S_{\zeta,i-1/2,j+1/2,k} + S_{\zeta,i-1/2,j-1/2,k} \right)
\]
3.2.4 Approach of High Order Scheme

When the neighboring cells are extremely distorted or stretched, for example, near the wall region, the above simple average, Eqs. (3.30) and (3.31), introduces significant error, depending on the degree of non-uniformity. Consequently, an appropriate interpolation technique should be employed, at the expense of considerable computational efforts. In order to calculate a gradient at the mid-point of a surface, the solution is first interpolated at each vertex of the cell. Then, the gradient of the solution is obtained at the mid-point by applying the Gauss theorem. At the same time, the multipoint Gaussian quadrature should be implemented for the flux integrals on the cell boundaries to achieve sufficiently high-order accuracy.

Regarding the cost of high-order finite-volume schemes, it should be noted that the use of these high order algorithms would be more costly than a corresponding finite-difference scheme. The higher cost of the finite-volume scheme is largely attributed to the use of cell average (Shu, 2001).

3.2.5 Artificial Dissipation

Numerical dissipation is required in central difference schemes to avoid artificial oscillations in regions with discontinuity and to improve numerical stability and convergence. The numerical dissipation model used in this work is of a non-metric type:

\[ d = -(-1)^{q/2} \frac{S_{\xi}}{8} (D_{\xi}^q + D_{\eta}^q + D_{\zeta}^q)Q \]  

(3.32)
\[ D_q^4 = \nabla \Delta \nabla \Delta \nabla \Delta Q \quad (3.33) \]
\[ D_q^6 = \nabla \Delta \nabla \Delta \nabla \Delta \nabla \Delta Q \quad (3.34) \]

The superscript \( q \) represents the order of artificial damping, \textit{e.g.}, \( q = 4 \) and \( q = 6 \) for the fourth- and sixth-order artificial dissipation terms, respectively. The fourth-order artificial dissipation term is associated with the second-order convection term, while the sixth-order artificial dissipation term is allied with the fourth-order convection term. The coefficients used in the present study are \( \xi_2 \sim 0.1 \), \( \xi_4 \sim 0.01 \), and \( \xi_6 \sim 0.001 \).

### 3.3 Temporal Integration

The integral conservation equation, Eq. (3.6), is repeated here for convenience.

\[ \int_V \frac{\partial Q}{\partial t} dV + \oint_S W \cdot ndS = 0 \quad (3.6) \]

Assuming the cell volume is \( \Delta V \), we have

\[ \frac{\partial Q}{\partial t} + \frac{1}{\Delta V} \oint_S W \cdot ndS = 0 \quad (3.35) \]

Rewrite the upon equation as

\[ \frac{\partial Q}{\partial t} = R(Q) \quad (3.36) \]

with

\[ R(Q) = -\frac{1}{\Delta V} \oint_S W \cdot ndS . \quad (3.37) \]

Two time integration methods, \textit{i.e.}, the four-step Runge-Kutta method and the Adam-Bashforth predictor-corrector method are implemented in the current study to solve Eq. (3.36).
3.3.1 Four-Step Runge-Kutta Scheme

The four-step Runge-Kutta (RK4) scheme proceeds in the following four steps:

\[
Q^1 = Q^n + \frac{\Delta t}{4} R^n
\]
\[
Q^2 = Q^n + \frac{\Delta t}{3} R^1
\]
\[
Q^3 = Q^n + \frac{\Delta t}{2} R^2
\]
\[
Q^{n+1} = Q^n + \Delta t R^3
\]  

This scheme has been widely used in the simulation of turbulent flows (e.g., Hsieh and Yang, 1997) owing to its low memory requirement, low dissipation, and high-order time accuracy.

3.3.2 Adam-Bashforth Predictor-Corrector Scheme

The Adam-Bashforth predictor-corrector scheme (AB) involves the following two steps:

Predictor step:

\[
Q^* = Q^n + \frac{\Delta t}{2} [3R(Q^n) - R(Q^{n+1})]
\]  

Corrector step:

\[
Q^{n+1} = Q^n + \frac{\Delta t}{12} [5R(Q^*) + 8R(Q^n) - R(Q^{n+1})]
\]

In comparison with the RK4 scheme, the greatest advantage of the AB scheme is only two steps in each temporal marching instead of four steps in the RK4 scheme. The AB scheme also has third-order time accurate because of the implementation of \(Q^{n+1}\), as shown in Appendix B. Although this scheme needs more memory storage for \(Q^{n+1}\), this problem can be easily solved using modern distributed hardware architecture.
3.4 Numerical Stability and Error Analysis

Estimation of computational errors in turbulence simulations has recently been addressed by Ghosal (1996), Fabignon et al. (1997), Apte (2000), and Apte and Yang (2001). Ghosal (1996) has analyzed the truncation errors of the various terms in finite-difference equations and compared the contributions of the errors at a given time with the exact terms for incompressible flow equations. A model turbulence spectrum was used to facilitate the comparison. His study found that the errors introduced by finite-difference approximation of the convection terms generally dominate the errors generated by the other terms in the governing equation. The convection terms are important in turbulence simulation at high Reynolds numbers. Fabignon et al. (1997) also used the von Neumann stability analysis to assess the importance of the errors associated with the convection terms by introducing a reference spectrum obtained from homogenous, isotropic turbulence theory.

The validity of the present numerical scheme is studied by means of the von Neumann analysis and post-computation data evaluation.

3.4.1 Theoretical Analysis

3.4.1.1 von Neumann Stability Analysis

A one-dimensional Euler equation is employed to address the numerical stability and dissipation of the present scheme.

\[
\frac{\partial Q}{\partial t} + A \frac{\partial Q}{\partial x} = 0
\]  

(3.41)

where
The eigenvalues of the Jacobian matrix, $A$, are

$$\lambda_{1,2,3} = u+c, u, u-c$$

for the perfect gas. An elementary solution of Eq. (3.41) can be expressed in a Fourier series expansion as (Fabignon et al., 1997; Merkle and Yu, 1997):

$$Q_l(x,t) = \sum_{k=-\infty}^{\infty} \hat{Q}_{k,l} e^{i(kx-\lambda_l t)}, \ l = 1, 2, 3$$

where $k$ denotes the wavenumber and $\hat{Q}$ the Fourier component. The amplification factor of the numerical discretization applied to Eq. (3.41) is defined as

$$G_{k,l} = \frac{\hat{Q}_{k,l}^{n+1}}{\hat{Q}_{k,l}^n} = \exp(-ik\tilde{\lambda}_l \Delta t) = \exp(-i\tilde{\omega}_l \Delta t)$$

where $G_{k,l}$ is the amplification factor matrix and $\tilde{\omega}_l$ the complex frequency. To achieve a stable numerical solution, the norm of $G$ must satisfy

$$\|G\| < 1 + O(\Delta t)$$

The numerical stability and error analysis are carried out following Fabignon et al. (1997), and Apte and Yang (2001). The amplification factors, $G$, of the RK4 and AB schemes become

$$G_{RK4} = 1 + Z + Z^2 / 2 + Z^3 / 6 + Z^4 / 24$$

$$G_{AB}^2 - (I + \frac{13}{12} Z + \frac{5}{8} Z^2) G_{AB} + (\frac{1}{12} Z + \frac{5}{24} Z^2) G_{AB} = 0,$$
\[ Z = -i \frac{A \Delta t}{\Delta x} \left[ 8 \sin(k \Delta x) - \sin(2k \Delta x) \right] - \varepsilon_6 \left[ 1 - \cos(k \Delta x) \right]^3 I \]  

(3.49)

for a fourth-order central difference scheme (4CD) along with sixth-order artificial dissipation. \( A \Delta t/\Delta x \) can be represented in terms of the Courant number, \( \sigma_{1,2,3} \)

\[
\begin{bmatrix}
\sigma_1 \\
\sigma_2 \\
\sigma_3
\end{bmatrix} = \frac{\Delta t}{\Delta x} \begin{bmatrix}
\lambda_1 \\
\lambda_2 \\
\lambda_3
\end{bmatrix}
\]  

(3.50)

The derivation of Eq. (3.47) can be found in Beddini et al. (1997) and that of Eq. (3.48) in Appendix B.2.

Figure 3.2 shows the amplification factors for the RK4-4CD and AB-4CD with sixth order artificial dissipation, \( i.e. \)

\[
\frac{\partial Q}{\partial t} + A \frac{\partial Q}{\partial x} = \varepsilon_6 \Delta x^6 \frac{\partial^6 Q}{\partial x^6}
\]  

(3.51)

The stability domain of the RK4-4CD scheme is larger than that of the AB-4CD scheme. However, the best CFL number should be unity for time-accurate calculations. The amplification factors associated with the vortical waves, \( i.e. \), \( u \), of the two schemes are quite approximate. This indicates that the two schemes have similar performance in simulating vortical waves and turbulence at low Mach numbers.

### 3.4.1.2 Homogeneous Turbulence Spectrum Temporal Evolution

To study the dissipation of the AB and RK4 schemes in turbulent flow simulation, the evolution of the energy spectrum of homogeneous turbulence in one eddy lifetime is investigated. The initial dimensionless spectrum of energy is given as (Beddini \textit{et al.}, 1997)

\[
E(k, 0) = \alpha(\delta \text{Re}_c)^{-5/4} (k\eta)^{-5/3} \exp \left[ -\frac{1.5 \pi \beta \sqrt{\alpha(k\eta)^{4/3}}}{\delta \text{Re}_c} \right]
\]  

(3.52)
and the time-marching step to achieve one eddy lifetime is

\[
I_\tau = \delta^{1/4} \frac{M + 1}{\xi M \sigma} \text{Re}_c^{3/4}
\]  

(3.53)

where \( \alpha \) and \( \beta \) denote the Kolmogorov constants and are 1.5 and 0.3, respectively (Fabignon et al., 1997). \( \xi \) represents the ratio of the grid size to the Kolmogorov length scale. \( \delta \) is the scaling between the turbulent Reynolds number, \( \text{Re}_t \), and the centerline Reynolds number, \( \text{Re}_c \), and is defined as

\[
\text{Re}_t = u' l / \nu \approx \delta \text{Re}_c \text{ and } \text{Re}_c = \bar{u} c h / \nu
\]  

(3.54)

where \( u' \), \( \bar{u}_c \), \( h \), and \( l \) denote the RMS velocity of the fluctuations, the mean velocity at the centerline, the half-height of the channel, and the integral length scale, respectively. After one eddy lifetime, the energy spectrum becomes

\[
E(k, \tau) = ||G_{k,\omega}||^2 t \cdot E(k, 0)
\]  

(3.55)

---

**Fig. 3.2** Variation of amplification factors for RK4-CD4 and AB-CD4 schemes with sixth-order artificial dissipation, \( \varepsilon_6 = 0.05 \).
Fig. 3.3 Comparison of the effects of RK4-CD4 and AB-CD4 schemes on the energy spectrum after one large eddy lifetime, a spatial fourth-order central difference scheme with sixth-order artificial dissipation is implemented, $\varepsilon_6 = 0.05$, $\sigma_{\text{max}} = 0.9$, $\text{Re} = 4.51 \times 10^6$. (a) $M = 0.8$ and (b) $M = 0.3$. 
The dimensionless turbulence energy spectra corresponding to the RK4 and AB schemes are shown in Fig 3.3. The RK4 scheme is only slightly better than the AB scheme when the Mach number is 0.8. The minor difference almost disappears at the Mach number of 0.3, which indicates similar performance of the two schemes in low Mach number flow simulation. Because the characteristic flow speed in the present study is at a low Mach number and the AB scheme can save up to 50% of computer time in comparison with the RK4 scheme, the AB scheme is used as the primary workhorse.

To examine the effect of computational errors on subgrid-scale modeling, an investigation was carried out based on the Smagorinsky eddy viscosity model (Apte and Yang 2001). Their work extended the previous work of Ghosal (1996) and Fabignon et al. (1997) to study the effects of the SGS model and artificial dissipation for numerical stabilization on the turbulence energy spectrum. Results demonstrated that the present numerical method could reasonably predict turbulent flows.

### 3.4.2 Post-Calculation Data Analysis

In addition to the theoretical analysis of numerical dissipation in the above section, the turbulent kinetic energy spectrum is post-evaluated as part of the scheme and simulation validation.

#### 3.4.2.1 Taylor Hypothesis

Two-point velocity correlation, $R_{ij}(r)$, is required to obtain the turbulence energy spectrum. It is, however, not feasible in the present work if we need $R_{ij}(r)$ for the entire range of scales, $r$. The “flying hot wire” concept is thus introduced to approximately calculate $R_{ij}(r)$ with a single probe (Pope, 2000). Assume that the probe moves in parallel with the $e_i$ axis at a speed of $V$

$$X(t) = x_0 + e_i V t$$

The temporal correlation becomes
\[ R^m_{ij}(s) = u_i(\mathbf{X}(t), t)u_j(\mathbf{X}(t+s), t+s) \]
\[ = u_i(\mathbf{X}(t), t)u_j(\mathbf{X}(t) + \mathbf{e}_r, t + r/V) \]  

(3.57)

where \( r \equiv s V \) represents distance that the probe traverses in a time interval of \( s \). Taylor (1938) assumed that the turbulence was statistically homogenous in the \( e_1 \) direction and \( V \) tended to be infinity, yielding

\[ R^m_{ij}(s) = u_i(x_0, 0)u_j(x_0 + e_r, 0) \]
\[ = R_{ij}(e_r, x_0, 0) \]  

(3.58)

where \( R_{ij} \) is the spatial correlation. Equation (3.58) is only an approximation in real flows because of the finite speed \( V \). Equation (3.58) is commonly known as the Taylor’s hypothesis (Taylor 1938). To further simplify Eq. (3.58), we assume

\[ r_i = \bar{U}_i s \]  

(3.59)

where \( \bar{U}_i \) is the mean velocity in the \( e_i \) direction. (Pope 2000)

The accuracy of Taylor’s hypothesis depends upon both the flow properties and the statistics to be measured, such as the statistical homogeneity of turbulence and the turbulence intensity compared with the mean velocity (Pope 2000). Although Taylor’s hypothesis was established for homogeneous turbulence, it can still serve as a reference in the current study.

### 3.4.2.2 Turbulent Kinetic Energy Spectrum

In the present work, the mean axial velocity, \( U \), is on the order of 60 m/s, the mean grid size inside injector, \( \Delta x \), 0.2 mm, and the Kolmogorov scale 0.003 mm. Figure 3.4 shows the frequency spectrum of turbulent kinetic energy obtained from the RK4 and AB schemes under the identical flow condition. Both schemes give rise to the Kolmogorov-Obukhov spectrum (-5/3 law) (Kolmogorov, 1941) in the high wavenumber region with the grid size locating in the inertial subrange. The spatial resolution in the present calculations is sufficient to capture the flow property variation in the inertial subrange. Because the turnover times of those eddies with scales comparable to the
numerical grid size is much longer than the time-marching step of the numerical simulation, the effects of the scheme time accuracy appears to be small in this situation, leading to similar results for both schemes. The AB method is thus used in the present work because of its computational efficiency.

One point should be noted is that the turbulent energy spectrum shown in Fig. 3.4 follows the $-5/3$ law even when the corresponding flow scales are close to the Kolmogorov scales, which is much smaller than the grid size. As a consequence of the limitation of grid resolution, small-scale flow motions cannot be resolved at all; therefore, the $-5/3$ behavior near the Kolmogorov scales is not correct and the turbulent kinetic energy spectrum is trivial in this regime. This phenomenon also points out that the numerical time-marching step is much less than the eddy turnover time mentioned above. In other words, a more efficient numerical method can be implemented in future study, such as the preconditioning method (Choi and Merkle, 1993; Hsieh and Yang, 1997), which can predict the dynamic evolution of resolved eddies accurately.

![Fig. 3.4](image-url) Comparison of the $tke$ spectra at a probe achieved through RK4-CD4 and AB-CD4 schemes.
3.5 Implementation of Parallel Computation

3.5.1 Parallel Architecture

Flynn (1966) classified the computing architecture into four types in terms of instruction and data streams:

- Single Instruction and Single Data (SISD), such as IBM PC and IBM RS/6000 workstation;
- Multiple Instructions and Single Data (MISD), which is seldom used in practice;
- Single Instruction and Multiple Data (SIMD), including the MasPar MP-2 and Thinking Machines CM-5, which is a hybrid of the SIMD and MIMD machine; and
- Multiple Instruction and Multiple Data (MIMD), including CRAY T3E and Beowulf.

Figure 3.5 shows the differences among the various computing architectures. MIMD is the dominant architecture in the current high-performance computing (HPC) community because of its flexibility. Bell (1994) further classified MIMD-type machines into two types, i.e., shared-memory parallel computer and distributed-memory parallel computer, based on the memory access mode.

![Diagram showing examples of operations of classified computing architectures](Hurley, 1994).
Shared-Memory Parallel Computer

The shared memory is accessible for multiple processors, so that data sharing among different tasks is fast. Programming for computer of this kind resembles that for vector computers, on which the programming is easier than that for distributed-memory computers. However, its scalability is limited due to the limitation of system bus and memory access. Typical shared-memory parallel computers are the CRAY T90, SGI Power Challenger, and PCs or workstations based on symmetric multiprocessors (SMP).

Distributed-Memory Parallel Computer

Memory of such a computer is physically distributed among processors; each local memory is directly accessible only by its processor. Message passing among processors is required for accessing remote memory, which saves the data at the request of a local processor. Because of its unlimited scalability, it is widely implemented in massively parallel processing systems (MPP), which is one of the most important trends in high performance computing. On the other hand, this kind of computer has two disadvantages. First, latency time for message passing is normally long owing to a software layer required to access remote memory. Second, handling of message passing is the responsibility placed on a programmer. The programmer must explicitly implement the data distribution scheme, all inter-process communication, and synchronization.

3.5.2 Message Passing

The message passing among processors, such as sending or receiving a message, is explicitly implemented by programmers in the code. The message-passing operations are executed by calling a message-passing library. Typical message-passing libraries include public-domain packages that do not target any specific machine (e.g., PICL, PVM, PARMACS, P4, MPI, etc.), and machine-dependent vendor implementations (e.g., MPL, NX, CMMD, etc.). NX is the Intel/Paragon native message-passing library. Parallel Virtual Machine (PVM) is a public domain package available from the Oak
Ridge National Laboratory. Message Passing Interface (MPI) has the strongest capabilities in terms of portability, performance, functionality, vendor support, dynamic control, and parallel input/output. In view of these advantages, MPI is selected for this study.

3.5.3 Beowulf System

A Beowulf system is a sort of high-performance massively parallel, distributed memory MIMD computer built primarily out of commodity hardware components such as PC, running a free-software operating system such as Linux or FreeBSD, interconnected by a private high-speed network. The primary advantage of a Beowulf system is its high performance/price ratio in comparison with other dedicated MPP systems.

The Beowulf project was started by Donald Becker in early 1994 (Beowulf, 2002) and was built by and for researchers with parallel programming experience. An important characteristic of Beowulf clusters is compatibility. The changes of node and network system, including software and hardware, will not affect the programming model. Another key component to forward compatibility is the system software used on Beowulf. With the maturity and robustness of Linux, GNU (GNU's Not Unix) software and the standardization of message passing via PVM or MPI, programmers now have a guarantee that the programs they write will run on future Beowulf clusters.

The present work is implemented on an in-house Beowulf system consisting of 350 Pentium II/III processors. Figure 3.6 summarizes the royalty-free software implemented on the Beowulf system. The system hardware, as shown in Fig. 3.7, is based on PCs and high-speed intranet network. Two graphics workstations are used for graphics processing. The hardware characteristics dictate the use of message passing in the numerical code.
<table>
<thead>
<tr>
<th>Component</th>
<th>Description</th>
<th>Website</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Operation System:</strong></td>
<td>Linux, distributed by RedHat, Inc.</td>
<td><a href="http://www.redhat.com">http://www.redhat.com</a></td>
</tr>
<tr>
<td><strong>Parallel Environment:</strong></td>
<td>Massage Passing Interface (MPICH)</td>
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<tr>
<td><strong>Compiler:</strong></td>
<td>Fortran 90 (Absoft/PG Fortran), C++ (GCC)</td>
<td><a href="http://www.absoft.com">http://www.absoft.com</a></td>
</tr>
<tr>
<td><strong>Queue System:</strong></td>
<td>Public Batch System (PBS)</td>
<td><a href="http://www.openpbs.org">http://www.openpbs.org</a></td>
</tr>
<tr>
<td><strong>Node Installation:</strong></td>
<td>KickStart (RedHat)</td>
<td><a href="http://www.redhat.com">http://www.redhat.com</a></td>
</tr>
<tr>
<td><strong>File System:</strong></td>
<td>Network File System (NFS)</td>
<td><a href="http://nfs.sourceforge.net/">http://nfs.sourceforge.net/</a></td>
</tr>
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<td><strong>User Account Manager:</strong></td>
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</tr>
<tr>
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<td>Security Shell (SSH, Internet)</td>
<td><a href="http://www.openssh.org">http://www.openssh.org</a></td>
</tr>
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<td></td>
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<tr>
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<td><a href="http://www.ntp.org">http://www.ntp.org</a></td>
</tr>
</tbody>
</table>

Fig. 3.6  Software schematic of the Beowulf system at Yang’s laboratory, the Pennsylvania State University.
Fig. 3.7 Hardware schematic of the Beowulf system at Yang’s laboratory, the Pennsylvania State University.
3.5.4 Domain Decomposition Method

Because the time-marching scheme applied in the current work is explicit, \textit{i.e.}, only the neighboring data instead of the data from the whole computational domain is required during computation, the data dependence is weak. This application is best suited for domain decomposition, which is also a common implementation for distributed-memory computers. In the field of computational fluid dynamics (CFD), it is generally referred to as multi-block technique or mesh partitioning based on the geometric substructure of the computational domain.

In the domain-decomposition technique, the physical domain is divided into several subdomains. Variables are updated only for each computing cell. In order to calculate the spatial derivatives near the subdomain boundaries, ghost cells or halo data around the computing cells are introduced. Figure 3.8 shows a two-dimensional example with fourth-order spatial accuracy.

Because the ghost cell of a subdomain is also located in another subdomain, message passing of the ghost cell is required to synchronize the data between different

![Diagram of ghost cells in a two-dimensional domain](image)

Fig. 3.8 Schematic of ghost cells in a two-dimensional domain (fourth-order spatial accuracy).
subdomains. Figure 3.9 shows an example of the inter-processor communication. Overlapped regions, where information must be obtained from neighboring processors, exist on each side of the local domain. Likewise, these processors would also need to send some data to their neighbors. It is noted that data at the eight corners of the overlapped regions are exchanged with that at the diagonally opposite corner to evaluate viscous fluxes at that corner. The communication overhead is directly proportional to the volume-to-surface ratio of that subdomain. An increase in the computation-to-communication ratio, i.e., increasing the grain size of each node, leads to a higher parallel execution efficiency.

3.6 Data Analysis and Data Mining for Complex Flowfield

In a three-dimensional numerical simulation of complex flow evolution, a common problem is how to handle and analyze the huge database produced from the large-scale computation. The limitation of computer storage prevents us from storing every piece of information calculated by the program. On the other hand, after obtaining
a huge data set describing the evolution information of the flowfield, we may be buried in an avalanche of data. Thus, how to extract useful information from the huge database is the objective of data mining. The concept of data mining originates from a selection of methods for machine learning and statistics that provide models of various kinds of data sets. In order to achieve a physics-based understanding of flow evolution, a kind of data mining should be implemented and a good methodology/procedure for the data analysis should be established in light of the huge computational expenses.

Several data analysis techniques employed in the current study are presented in the following.

Probes

The time histories of the instantaneous flow properties at each probe are stored and analyzed. This method is commonly used in both experiments and simulations, and is helpful for analyzing the dynamic flow evolution of the flowfield. The spectral information obtained can be used to identify the dynamics of the system.

Resolved turbulence statistic properties

The Reynolds averaging method can be used to obtain resolved turbulence properties. For example, the resolved axial velocity component can be decomposed as

\[ \tilde{u} = \bar{u} + \tilde{u}' \]  

(3.60)

where \( \bar{u} \) and \( \tilde{u}' \) denote the time-mean Reynolds averaged and resolved fluctuating velocity, respectively. Because a time-mean instead of a spatial-averaged quantity is used, we have

\[ \bar{\bar{u}} = \bar{u} \quad \text{and} \quad \bar{u}' = 0 \]  

(3.61)

Therefore, both \( \int_{t_0}^{t_f} \tilde{u}^2 dt \) and \( \int_{t_0}^{t_f} \tilde{u} dt \) can be computed during the calculation and the final resolved turbulence intensity can be determined through the well known Reynolds averaging relationship

\[ \bar{\left(\bar{u}^2\right)} = \bar{u}^2 - \bar{u}'^2 \]  

(3.62)
**Snapshot of flowfield**

Snapshots are used to aid understanding complex flow structures and evolution. For three-dimensional flowfield visualization, powerful graphics hardware and software is definitely indispensable. It can greatly improve the data processing efficiency. The animation achieved from the sequential snapshots can impressively demonstrate the dynamic evolution of flow structures.

**Spatial averaging**

To obtain insight into the complex three-dimensional flowfield, a spatial averaging in the azimuthal direction is widely used to identify the flow pattern in the present study. The resultant two-dimensional flow structures can be further averaged into a one-dimensional field to provide useful information about the wave motions along a given axis. The flow patterns can sometimes be easily visualized in a one-dimensional domain. It is useful to establish a spatial averaging procedure to deduce data from 3D $\rightarrow$ 2D $\rightarrow$ 1D.

**Proper orthogonal decomposition (POD)**

In addition to the analysis presented above, the method of proper orthogonal decomposition (POD) (Lumley, 1981) is employed. The POD is commonly used for extracting energetic coherent structures from data, either experimental or computational. Given a set of the calculated flowfield as a function of space and time, the POD determines a basis set of orthogonal functions of space that span the data optimally in the $L^2$-sense. A detailed description can be found in Appendix C.

**Response functions**

In order to characterize the response of the flowfield to the externally imposed excitation, response functions, such as the acoustic admittance and transfer functions, are introduced. These functions provide quantitative information about the dynamic characteristics of the flowfield.
Part I

Vortical Flow Dynamics in a Dump Chamber
Chapter 4

Turbulent Swirling Flows in a Dump Chamber

In this chapter, turbulent swirling flows in a dump chamber as shown schematically in Fig. 4.1 are investigated. The study has two objectives: 1) to validate numerical code developed in the current work; and 2) to achieve a better understanding of the swirling flow characteristics in a confined chamber.

The present computational case is designed to match the experimental setup used by Favaloro et al. (1989, 1991), described in Section 4.1. The grid system and boundary conditions are presented in Sections 4.2 and 4.3, respectively. A thorough comparison of experimental data and computational results, including the mean velocity profiles, turbulence intensities, and turbulent kinetic energy (tke), is carried out in Section 4.4. Furthermore, an analysis of the flow structure is given in Section 4.5 to investigate the flow behavior in the recirculation zone and the dynamic evolution of the entire flowfield. Section 4.6 addresses the acoustic motions and their relationship with the vortical dynamics for two different swirl numbers. Finally, a brief summary is presented in Section 4.7.

Fig. 4.1 Schematic of a dump chamber with a swirler housing.
4.1 Problem Description

The physical model of concern is shown in Fig 4.1. A swirler with 12 circular inlet guide vanes is located at 50.8 mm upstream of the dump plane. The leading edge of each blade is designed to be tangential to the incoming flow and perpendicular to the centerline of the chamber. The chamber consists of a plexiglas pipe measuring 152.4 mm in internal diameter and 1850 mm in length. A laser Doppler velocimeter (LDV) is used to measure the three velocity components and turbulence quantities. The centerline velocity in the inlet pipe is 19.2 m/s, the inlet temperature 300 K, and pressure 1 atm. The Reynolds number is $1.25 \times 10^5$ based on the inlet radius. The swirl number in the experiment is defined as

$$S = \frac{\int_{R_h}^{R_{in}} \tilde{u}_x \tilde{u}_\theta r^2 dr}{\int_{R_h}^{R_{in}} \tilde{u}_x^2 rd\theta}$$  \hspace{1cm} (4.1)

where subscripts $h$ and $in$ denote the swirl hub and inlet pipe, respectively; and $R_h = 9.5$ mm and $R_{in} = 54.8$ mm. The present calculation considers two swirl numbers of 0.3 and 0.5. Most results are based on the swirl number of 0.5 unless otherwise indicated because of the occurrence of vortex breakdown in this case. The situation with $S = 0.3$ is also discussed for comparison, in which the vortex breakdown is not observed.

4.2 Computational Domain and Grid System

The computational domain consists of the inlet immediately downstream of the swirler and the dump chamber. A three-dimensional grid is generated by rotating a two-dimensional grid with respect to the centerline. The total grid number is $161 \times 75 \times 81$ (1 million) in the axial, radial, and azimuthal directions, respectively, as shown in Fig 4.2. The grid is uniform in the azimuthal direction but stretched in the axial and radial directions in order to resolve strong shear layer and near wall region. The computational domain is divided into 28 subdomains as shown in Fig. 4.3 and assigned to 28 processors for parallel processing.
Fig. 4.2  Schematic of computational grid system, the presented grid has fewer points than those used in the calculations, but the distribution of points is similar.

Fig. 4.3  Multi-block structure of domain decomposition with 28 blocks.
4.3 Boundary Conditions

Numerical algorithms based on high-order approaches can provide spectral-like resolution and very low numerical dissipation (Thompson, 1987; Poinsot and Lele, 1992). The accuracy and applications of these schemes are constrained by the treatment of boundary conditions that must be included in the final numerical schemes. In the present study, the method of characteristics (MOC) is used to specify the boundary conditions.

- Inlet boundary

An axial swirler is used in the present work to generate swirling flows. Four variables, including the velocity \((u_x, u_r, u_\theta)\) and total temperature \((T_0)\), are specified. The pressure \((p)\) is extrapolated from the interior region using a simplified axial momentum equation. The axial velocity follows the one-seventh-power law for a fully developed turbulent pipe flow. The azimuthal velocity is determined by the angle of swirler vanes, and the radial velocity is zero:

\[
\tilde{u}_x = u_0 \left(1 - \frac{r}{R_i}\right)^{1/7} \tag{4.2}
\]
\[
\tilde{u}_\theta = \tilde{u}_x \tan(S_V) \tag{4.3}
\]
\[
\tilde{u}_r = 0 \tag{4.4}
\]

where \(S_V\) is the angle of the swirler vanes. The pressure is determined using the simplified axial momentum equation:

\[
\frac{\partial \tilde{p}}{\partial x} = -\rho \frac{\partial \tilde{u}_x}{\partial x} \tag{4.5}
\]

Turbulence at the inlet is provided by superimposing a white noise on the velocity profile with a turbulence intensity of 10%.

- Outlet boundary

For the exit boundary conditions, extrapolation of primitive variables from the interior region may cause undesirable reflection waves in a confined chamber. The non-reflecting boundary condition based on the characteristic equations, proposed by Poinsot
and Lele (1992), is applied. The derivation of the non-reflection boundary conditions is presented in Appendix D.

- Wall boundary

The grid near the wall boundary is stretched to be fine enough to resolve the near-wall region to avoid the uncertainties resulting from the wall modeling. In the current case, $y^+$ for the first grid point varies in the range of 4-12. Because the physics properties in the finite-volume approach are defined in the center of each cell, the spatial resolutions of these first cells are in the range of 2-6, which is located in the viscous sub-layer region. Hence, the no-slip wall condition can be directly employed as:

$$
\vec{u} \big|_{wall} = \vec{v} \big|_{wall} = \vec{w} \big|_{wall} = 0
$$

(4.6)

Adiabatic and zero-pressure-gradient conditions are applied along the solid walls, *i.e.*,

$$
\frac{\partial \rho}{\partial n} = \frac{\partial T}{\partial n} = 0
$$

(4.7)

### 4.4 Mean Flowfield and Turbulence Behavior

To validate the code and to characterize turbulent swirling flows, comparison between experimental data (Favaloro *et al.* 1989) and computational results in terms of mean velocity profiles, turbulence intensities, and turbulent kinetic energy is given in this section.

Figures 4.4 and 4.5 show the streamline patterns in a longitudinal plane based on the mean axial and radial velocity components at swirl numbers of 0.5 and 0.3, respectively, to illustrate the global flow patterns. When the swirl number is 0.5, shown in Fig. 4.4, a small separation bubble appears behind the centerbody and the associated separated flow is recovered in the near downstream of the bubble. Approximately at $x = 60$ mm, a CTRZ is formed in the central region originating from the swirling effect, and the separated bubble is closed around $x = 250$ mm. Both the primary and secondary separation bubbles are generated downstream of the backward step. When the swirl number is 0.3, as shown in Fig. 4.5, the vortex breakdown phenomenon is not observed.
The length of the corner recirculation zone (CRZ) increases due to smaller expansion of the flow resulting from the centrifugal force (Favaloro et al., 1989).

### 4.4.1 Mean Velocity Profiles

The mean velocity profile is obtained by means of spatial averaging in the azimuthal direction. The calculated and measured mean axial, radial and azimuthal velocity components at the swirl number of 0.5 are compared at several axial locations, as shown in Figs. 4.6-4.8.

Good agreement is obtained for the mean axial velocity profiles at three measurement locations, $x = 64.5$, 101.6 and 152.4 mm, as shown in Fig. 4.6. The negative mean axial velocity appearing near the central region indicates the existence of a CTRZ. Some minor differences between the measurements and computations are observed at $x = 64.5$ and 101.4 mm, where the primary and secondary separation bubbles
are formed, as shown in Fig. 4.4. At \( x = 152.4 \) mm, both the calculated and measured results are in good agreement. The velocity profile at \( x = 64.5 \) mm is similar to that of a swirling jet, and its distribution changes smoothly to a parabolic profile in the downstream location of \( x = 152.4 \) mm.

Figure 4.7 shows distributions of the mean radial velocity. Both the calculated and measured results agree quantitatively well, even at \( x = 64.5 \) and 101.6 mm in the backward-step recirculation region, where the velocity profiles vary rapidly.

The mean azimuthal velocity distributions at \( x = 64.5, 101.6 \) and 152.4 mm are shown in Fig. 4.8. Qualitatively good agreement is obtained with experimental data in the central region. The numerical results, however, under-predict the azimuthal velocity near the chamber wall. The reason for this deficiency may be attributed to the lack of reliable data specifying the inlet flow conditions. The inlet velocity profiles in the axial, radial, and azimuthal directions would have significant influences on the results. Figure 4.8 shows that the mean azimuthal velocity behaves like a solid-body rotation near the centerline, which is similar to that of a potential vortex away from the centerline. This behavior was also observed by Panda and McLaughlin (1994) in a free swirling jet.

![Fig. 4.6 Comparison of computational and experimental results, mean axial velocity (line: computation; symbol: experiment): (a) \( x = 64.5 \) mm, (b) \( x = 101.6 \) mm, and (c) \( x = 152.4 \) mm. \( S = 0.5 \).]
Fig. 4.7 Comparison of computational and experimental results, mean radial velocity (line: computation; symbol: experiment): (a) $x = 64.5$ mm, (b) $x = 101.6$ mm, and (c) $x = 152.4$ mm. $S = 0.5$.

Fig. 4.8 Comparison of computational and experimental results, mean azimuthal velocity (line: computation; symbol: experiment): (a) $x = 64.5$ mm, (b) $x = 101.6$ mm, and (c) $x = 152.4$ mm. $S = 0.5$. 
4.4.2 Turbulence Intensities and Turbulent Kinetic Energy

Calculated turbulence properties are compared with experimental results at three axial locations, \( x = 101.6, 152.4 \) and 203.2 mm. Figures 4.9–4.11 show the resolved turbulence intensities in the axial, radial and azimuthal directions, respectively. In these figures, the inlet centerline velocity, \( U = 19.2 \) m/s, and the height of the backward step, \( H = 25.4 \) mm, are used to normalize the turbulence properties. Excellent agreement is obtained for turbulence intensities in the axial and radial directions, as shown in Figs. 4.9 and 4.10. Two high peaks associated with the shear layers originating from the centerbody and the backward step are observed in Fig. 4.9. Figure 4.11 shows the calculated profiles of the azimuthal turbulence intensity, which agree qualitatively well with experimental data, although some discrepancy appears at \( x = 101.6 \) and 152.4 mm due to the uncertainties in specifying the azimuthal velocity at the inlet.

Fig. 4.9 Comparison of computational and experimental results, axial turbulent intensity (line: computation; symbol: experiment): (a) \( x = 101.6 \) mm, (b) \( x = 152.4 \) mm, and (c) \( x = 203.2 \) mm. \( S = 0.5 \).
Fig. 4.10 Comparison of computational and experimental results, radial turbulent intensity (line: computation; symbol: experiment): (a) $x = 101.6$ mm, (b) $x = 152.4$ mm, and (c) $x = 203.2$ mm. $S = 0.5$.

Fig. 4.11 Comparison of computational and experimental results, azimuthal turbulent intensity (line: computation; symbol: experiment): (a) $x = 101.6$ mm, (b) $x = 152.4$ mm, and (c) $x = 203.2$ mm. $S = 0.5$. 
Figure 4.12 Comparison of computational and experimental results, turbulent kinetic energy (line: computation; symbol: experiment): (a) \(x = 101.6\) mm, (b) \(x = 152.4\) mm, and (c) \(x = 203.2\) mm. \(S = 0.5\).

Figure 4.12 shows that the computation agrees well with measurement in the \(tke\) distribution. Near the inlet, the high \(tke\) motions are concentrated in the CTRZ. Due to the influence of convection and centrifugal force, this profile becomes uniform in the downstream.

The resolved turbulence intensities and \(tke\), as shown in Figs. 4.9-4.12, reveal that high intensity turbulence is generated from the CTRZ and the surrounding shear layers. The region of high intensity turbulence spreads radially because of the growing shear layers and vortex breakdown. At the same times, turbulence intensity decays with the downstream distance due to viscous dissipation. Strong turbulence intensity in the CTRZ can stabilize flame and practically promote mixing, and will consequently lead to better blow-off limits and lower pollutant emission.
4.5 Flow-Structure Analysis

The mean flowfield with a swirl number of 0.5 is addressed in this section to evaluate the flowfield and entrainment characteristics of the CTRZ. The instantaneous velocity and vorticity fields are presented to visualize flow evolution at swirl numbers of 0.3 and 0.5.

4.5.1 Vortex Breakdown and Its Dynamic Evolution

A simplified radial momentum equation illustrates that a radial pressure gradient is required to balance the centrifugal force arising from the swirling effect

\[
\frac{\partial p}{\partial r} = \frac{\rho u_\theta^2}{r}. \tag{4.8}
\]

Strong swirl motions can generate a significant radial pressure gradient. As the swirling flow expands and the azimuthal velocity decays with the downstream distance, the pressure recovers in the downstream. In a high swirling flow, the strong pressure gradient in the axial direction may lead to a recirculation flow in the central region.

Most previous investigations on vortex breakdown focused on low Reynolds number, laminar flows (Grabowski and Berger, 1976; Spall and Gatski, 1991; Spall, 1996). However, in most practical applications such as swirling flows in combustion chambers, vortex breakdown occurs within the turbulent regime. Extension of the laminar results to turbulent vortex breakdown is questionable. Sarpkaya (1995) and Sarpkaya and Novak (1998) presented experimental results for vortex breakdown in noncavitating, high Reynolds number turbulent swirling flows and considered the resulting "conical" breakdown to be fundamentally distinct from the various forms of laminar breakdown (Leibovich, 1984; Sarpkaya, 1971a,b). They showed that the conical form of breakdown actually results from a rapid precessing, in which the vortex core slightly deviates from the tube centerline.

The flow pattern of \( S = 0.5 \) in the present study is a typical turbulent vortex breakdown. The mean flow pattern corresponding to the CTRZ is shown in Fig. 4.4. Figure 4.13 shows the contours of the mean azimuthal velocity component, which is one
of the key factors dictating the occurrence of vortex breakdown. The strongest azimuthal velocity occurs at $x \approx 20 \sim 40$ mm near the axis due to the conservation of angular momentum. The high azimuthal velocity further generates a low-pressure field and subsequently a CTRZ starting from $x \approx 60$ mm, as explained by Eq. (4.8).

The streamline pattern, shown in Fig. 4.4, illustrates that several separation bubbles are generated in the central region. These vortical bubbles can be regarded as turbulent vortex breakdown originating from swirling effect. Actually, it is hard to classify the vortex breakdown of this kind in any specific forms (e.g., bubble, spiral, or conical) observed in previous experimental studies.

To illustrate the dynamic evolution of the CTRZ, Fig. 4.14 shows the snapshots of the instantaneous streamline fields, spatially averaged in the azimuthal direction, during a typical flow evolution period. The time increment between sequence snapshots is approximately 0.61 ms. In Figs. 4.14a and b, a new vortical bubble is generated before a braid of vortical bubbles. Then these bubbles coalesce with each other as shown in Figs. 4.14c and d. At the same time, the bubble located in the downstream of the vortical braid is separated into two (Fig. 4.14d): one still stays at the same location, and the other is convected to the downstream and finally disappears due to viscous dissipation, as shown in Figs. 4.14e-h. During this period, the coalesced vortical bubble is separated into two, as seen in Figs. 4.14e-g, and another new vortical bulb appears at the upstream again, shown in Fig. 4.14h. The snapshots demonstrate that the vortex bubble evolution in the central region is very complicated.
Fig. 4.14 Time evolution of streamlines based on the mean axial and radial velocity components spatially averaged in the azimuthal direction (time increment 0.61 ms). $S = 0.5$, (a)-(d).
Fig. 4.14 Sequence of the streamlines based on the mean axial and radial velocity components averaged in the azimuthal direction (time increment 0.61 ms). $S = 0.5$, (e)-(h).
4.5.2 Vorticity Dynamics

In turbulent swirling flows, large-scale coherence structures, particularly arising from vortex breakdown, the Kelvin-Helmholtz instability, helical instability, and centrifugal instability (Panda and McLaughlin, 1994; Martin and Meiburg, 1996), significantly influence the flowfield. In order to study the vorticity dynamics and the effect of the swirl number, the snapshots of velocity and vorticity fields at different swirl numbers are investigated.

Figure 4.15 shows the contours of instantaneous axial velocity at swirl numbers of 0.3 and 0.5. Two peripheral shear layers are created from the centerbody and the backward step, and shed downstream in the form of vortex due to the Kelvin-Helmholtz instability, as shown in a longitudinal plane. The evolution of shear layers in the azimuthal direction is illustrated in two $r$-$\theta$ cross-sections, $x = 60$ and 90 mm. When $x = 60$ mm, i.e., right downstream of the backward step, strong shear layer resulting from the backward-step flows is observed. Only minor non-axisymmetric structures appear in this region. These strong unstable shear layers roll up and form large non-axisymmetric structures at $x = 90$ mm.

To unveil the effects of the shear layer in the azimuthal direction, the contours of instantaneous azimuthal velocity are shown in Fig. 4.16. Two strong shear layers in the azimuthal direction are observed at $x = 60$ mm. The outer one corresponds to the backward-step flows while the other represents the motions associated with the CTRZ. Because of the strong shear layers in the azimuthal direction, the Kelvin-Helmholtz instability also appears in this direction. The structures are very clearly shown in the cross-sections in both the axial and azimuthal velocity contours, especially at $x = 90$ mm. While the flows convect to the downstream, the large coherence structures are dissipated due to turbulence and viscous effects. Due to the appearance of the Kelvin-Helmholtz instability in the azimuthal direction, the development of the unstable motions in the $x - r$ plane is also accelerated. At the swirl number of 0.5, the strength of the shear layer around the axis significantly augments due to the increase of the azimuthal velocity and the decrease of the effective flow area, resulting from the appearance of the CTRZ. This
can be demonstrated by the vortical bulbs appearing at the boundary of the CTRZ, shown in the cross-section view of Fig. 4.16.

As indicated by Pullin and Saffman (1998), because the flow is determined entirely by the distribution of vorticity, it is a truism to say that the evolution of a turbulent velocity distribution is a problem of vortex dynamics. Figure 4.17 shows the iso-surfaces of the instantaneous vorticity magnitude fields at swirl numbers of 0.3 and 0.5. Helical structures, which are counter-rotating with the mean swirling flows, are clearly observed in Fig. 4.17. They stand for different flow mechanisms at different swirl numbers. The helical structure in $S = 0.5$ represents the flow pattern arising from the vortex breakdown, and that in $S = 0.3$ is attributed to the precessing vortex core (PVC), i.e., non-axisymmetric vortical structures appearing in swirling flows. The vortical structures originating from the vortex breakdown in $S = 0.5$ are much larger than those corresponding to the PVC in $S = 0.3$. To obtain a clearer view, the iso-surfaces of the fluctuation vorticity magnitude are also shown in Fig. 4.18. The vorticity in the CTRZ is mainly generated from the vortex shedding arising from the centerbody.

Figures 4.14–4.18 show that strong shear layers have been produced near the centerbody and the backward step. Usually, the shear layer unstable frequency is very sensitive to external low amplitude distributions. Given a suitable external excitation, the shear layer unstable frequency may switch to a specific acoustic nature frequency associated with the dump chamber geometry. Detailed discussion will be carried out in the following section.
Fig. 4.15 Instantaneous axial velocity contours in a longitudinal plane and cross-sections, $x = 60$ and $90$ mm. Contour levels between -12 and 33 m/s at increment of 3. Solid lines: positive values; dashed lines: negative values. (a) $S = 0.5$ and (b) $S = 0.3$. 
Fig. 4.16 Instantaneous azimuthal velocity contours in a longitudinal plane and cross-sections, $x = 60$ and $90$ mm. Contour levels between -24 and 6 m/s at increment of 3. Solid lines: negative values; dashed lines: positive values. (a) $S = 0.5$ and (b) $S = 0.3$. 
Fig. 4.17 Iso-surfaces of instantaneous vorticity magnitude. Dark lines represent streamlines. The iso-value is $1.5 \times U / H$. (a) $S = 0.5$ and (b) $S = 0.3$.

Fig. 4.18 Iso-surfaces of vorticity fluctuation magnitude. The iso-value is $1.5 \times U / H$. (a) $S = 0.5$ and (b) $S = 0.3$. 
4.6 Acoustic Analysis

Acoustics is a fundamental element in combustion instabilities. Investigations of chamber acoustics characterized by pressure oscillations have substantially improved the general understanding of combustion instabilities. Analysis of the pressure oscillations in the dump chamber could provide detailed physical descriptions of acoustic motions and its interaction with the shear layer instability. In the present work, some preliminary analyses of acoustics, including the pressure oscillation and the identification of acoustic mode, are addressed.

4.6.1 Pressure Oscillation

4.6.1.1 Pressure Field Evolution

Figure 4.19 shows the contours of an instantaneous pressure fluctuation field at $S = 0.5$. The different flow scales from the inlet to the downstream are clearly indicated. High fluctuation appears in the near downstream of the centerbody, where high vorticity magnitude is observed as shown in Fig. 4.17. The three-dimensional pressure-fluctuation field is extremely complicated; therefore, specific averaging is used to illustrate the global behavior. Two reduced approaches are employed by means of spatial averaging in the present study.

Figure 4.20 shows the contours of pressure oscillation in a longitudinal plane based on the flowfields spatially averaged in the azimuthal direction. In comparison with the complicated three-dimensional instantaneous flow structures, shown in Fig. 4.19, the spatially averaged pressure oscillation patterns, shown in Fig. 4.20, clearly demonstrate the pressure evolution in the dump chamber. The pressure fields, shown in Fig. 4.20, are further reduced to a one-dimensional quantity along the axial direction by taking spatial averaging in the radial direction.

Figure 4.21 shows the reduced one-dimensional pressure oscillation profiles. It clearly shows that a negative peak is formed and travels to the downstream intermittently. The profiles from $t = 34.377$ ms to $35.598$ ms indicate that this peak moves...
approximately at the speed of sound. At the same time, a positive pressure fluctuation follows each negative peak during this propagation process. Two negative pressure peaks are observed in Fig. 4.21 at $t = 35.903$ ms. Because the evolution patterns of the two fluctuations are almost same, we can conclude that the frequency of the peak generation is approximately 655 Hz based on the distance between the two negative pressure peaks at $t = 35.903$ ms. The peak signal moves out of the computational domain without reflected wave due to the implementation of a non-reflecting boundary condition at the exit. The generation of this pressure fluctuation signal may relate with local hydrodynamic evolution.

![Contour plots](image)

**Fig. 4.19** Contours of an instantaneous pressure fluctuation field in a longitudinal plane and cross-sections, $x = 10, 20, 30, \text{ and } 40 \text{ mm}$. Contour levels between -300 and 300 at increment of 15. Solid lines: positive values; dashed lines: negative values. $S = 0.5$. 
Fig. 4.20 Time evolution of two-dimensional pressure fluctuation contours spatially averaged in the azimuthal direction. Contour levels between -300 and 300 at increment of 15. Solid lines: positive values; dashed lines: negative values. $S = 0.5$. 
Fig. 4.21 Time evolution of one-dimensional spatially averaged pressure fluctuation. $S = 0.5$.

4.6.1.2 Spectral Analysis

Probes are used in the flowfield to measure the time histories of the instantaneous flow properties. Figure 4.22 shows the pressure spectra of probes at $y = 1.4$ mm and $z = 1.7$ mm with different axial locations, $x = 65, 106.5$ and $284.5$ mm. The frequency of the highest fluctuation magnitude is $1,380$ Hz. Other characteristic frequencies include $660, 2,040,$ and $3,420$ Hz. These frequencies fall within the low-frequency unstable regime and their amplitudes decrease with the downstream distance. Although the low-frequency unstable modes might be affected by many factors, such as the interaction between flame and vortex, and combustor geometry, it is still reasonable to predict them using cold-flow calculations.
Fig. 4.22 Pressure spectra at (a) $x = 60.5$ mm, (b) $x = 106.5$ mm, and (c) $x = 284.5$ mm, and $y = 1.4$ mm, $z = 1.7$ mm. $S = 0.5$.

Fig. 4.23 Probe locations, $S = 0.3$. The background is the vorticity magnitude contours.

The probes are also employed at $S = 0.3$ as shown in Fig. 4.23. The dominant frequency of the whole flowfield in term of pressure oscillation is 3,900 Hz, as shown in Fig. 4.24. An intensive spectral analysis is carried out to discover the trigger of this
oscillation mode, i.e., velocity fluctuation at the same frequency. Only near the surface of the swirler housing and its downstream (probes 23:19 and 23:20), the local dominant frequency of velocity fluctuation is the same as the global dominant frequency. Neglecting the trivial low frequency components due to insufficient time window in the Fourier transform, the 3,900 Hz fluctuation dominates the pressure and radial velocity spectra in this region. The 3,900 Hz mode is very weak in the spectrum of the axial velocity and can be observed in the spectrum of the azimuthal velocity at probe 23:19. The correlation between the radial velocity and pressure oscillation will be further discussed in Chapter 5. The variation of the radial velocity represents the oscillation of the shear layer, which is anchored at the tip of the backward step. Because of the oscillation at this region, a mixed first tangential/first radial acoustic mode is excited in the dump chamber at $S = 0.3$ and will be addressed in Section 4.6.2.2 in detail.

4.6.2 Acoustic Mode Analysis

The eigen-frequency of acoustic mode in the dump chamber is calculated based on the geometry and mean flow properties. The eigen-frequency associated with the chamber closed at both sides can be calculated by

$$f_{lmn} = \frac{c}{2\pi} \sqrt{\frac{\lambda_{\text{mn}}^2}{R_c^2} + \frac{l^2\pi^2}{L_c^2}}, \quad l, m, n = 0, 1, 2, \ldots$$  \hspace{1cm} (4.9)

where $c$, $R_c$, $L_c$, $\lambda_{\text{mn}}$, and $f_{lmn}$ denote the speed of sound, chamber radius, chamber length, eigenvalue, and acoustic eigen-frequency, respectively. $l$, $m$ and $n$ are the longitudinal, tangential, and radial model numbers, respectively.

In addition to the theoretical analysis presented in Eq. (4.9), the method of proper orthogonal decomposition (POD) (Lumley, 1981) is employed for identifying acoustic mode. The POD is commonly used for extracting energetic coherent structures from data, either experimental or computational. For example, if the pressure, $p(x, t)$, is a function of space and time, then POD can determine the orthogonal functions $\varphi_j(x)$, $j=1,2,\ldots$, so that the projection of $p$ onto the first $n$ functions
Fig. 4.24 Pressure and velocity Spectra at (a) $x = 59.7$ mm, $y = 41.4$ mm, $z = 0$ mm, and (b) $x = 59.7$ mm, $y = 49.5$ mm, $z = 0$ mm. $S = 0.3$. 

 Probe 23:19

 Probe 23:20
\[ \hat{p}(x,t) = \bar{p}(x) + \sum_{j=1}^{n} a_j(t) \varphi_j(x) \quad (4.10) \]

has the smallest error, defined by \( E(\|p - \hat{p}\|^2) \). Here, \( a_j(t) \) represents the time trace of the \( j \) mode, \( E(\cdot) \) time average, and \( \| \cdot \| \) the \( L^2 \) norm on functions of space (Rowley et al., 2000). A brief introduction of the POD is presented in Appendix C, and a rigorous version can be found in Berkooz, Holm and Lumley (1993). Different acoustic modes are observed at swirl numbers of 0.3 and 0.5, and are discussed separately in the following sections.

4.6.2.1 Swirl Number of 0.5

The first tangential acoustic mode, \( \lambda_{10} = 1.8412 \), is considered at swirl number of 0.5. To simplify the prediction of the acoustic eigen-frequency, assume

\[ c = 340 \text{ m/s }, r_c = 76.2 \text{ mm}, \text{ and } r_i = 50.8 \text{ mm} \quad (4.11) \]

where the subscript \( c \) and \( i \) represent the chamber and inlet/swirler housing, respectively. Substitution of Eq. (4.11) into Eq. (4.9) yields two eigen-frequencies

\[ f_c = 1,350 \text{ Hz } \text{ and } f_i = 2,000 \text{ Hz} \quad (4.12) \]

These two transversal acoustic modes may interact with each other and generate subharmonic and superharmonic, \( \text{e.g., } f_{S1} = f_i - f_c = 650 \text{ Hz } \text{ and } f_{S2} = f_i + f_c = 3,350 \text{ Hz} \).

Compared to the pressure spectra shown in Fig. 4.22, the predicted eigen-frequencies as well as their harmonics are very close to those dominant frequencies in the pressure spectra. The 1,380 Hz frequency, corresponding to the highest peak in the pressure spectra, is very close to the chamber's eigen-frequency \( f_c = 1,350 \text{ Hz} \), and another peak frequency at 2,040 Hz approximates the inlet pipe's eigen-frequency \( f_i = 2,000 \text{ Hz} \). Furthermore, the 655 Hz frequency associated with the pressure fluctuation evolution in Fig. 4.21 is close to the subharmonic at \( f_{S1} = 650 \text{ Hz} \), which may resonate with the flowfield and result in a longitudinal acoustic mode, as shown in Fig. 4.21.
The generation of longitudinal acoustic modes is relevant to the dynamic evolution of the flowfield. Based on linear theory approximation (Lighthill, 1978), the linear wave equation derived from the Navier-Stokes equations is

\[
\frac{\partial^2 p}{\partial t^2} - c^2 \frac{\partial^2 p}{\partial x_i \partial x_j} = c^2 \frac{\partial^2 T_{ij}}{\partial x_i \partial x_j}
\]

(4.13)

where

\[
T_{ij} = \rho u_i u_j + [(p - p_0) - c^2 (\rho - \rho_0)] \delta_{ij} - \frac{4}{3} \mu \frac{\partial u_i}{\partial x_k} \delta_{ij},
\]

(4.14)

\(p_0\) and \(\rho_0\) are the reference values of pressure and density, respectively.

The viscous terms in Eq. (4.14) can be omitted because the dilatation effect is negligible due to the low speed of the bulk flow in the chamber. The dominant term in the source term of Eq. (4.14) is \(\rho u_i u_j\), in which the dilatation is also neglected. As a result, the pressure oscillation mainly arises from the vorticity evolution.

As aforementioned, the vorticity in the central region results from the incoming swirling flow, and vortices shed from the centerbody and the backward step. The latter accounts for the main contribution to the vorticity field, as shown in Fig. 4.17. The strong shear layer originating from the centerbody, as shown in Fig. 4.15, is very sensitive to external forcing frequency (Wu et al., 1998). The concept of the most unstable mode of the shear layer can enhance a physical understanding of the flow dynamic evolution. The most unstable frequency is referred to as the natural frequency of the shear layer and denoted by \(f_s^0\). In the downstream of the shear layer, due to vortex pairing, the magnitudes of subharmonic modes, such as \(f_s^0/2\) and \(f_s^0/4\), would increase and further dominate flow evolution.

The non-dimensional shear layer frequency is defined as

\[
St_s = \frac{f_s \delta}{U}, \quad U = \frac{1}{2}(U_1 + U_2)
\]

(4.15)
where $\delta$ is the momentum thickness of the layer, and $U_1$ and $U_2$ the velocities at the two sides of the shear layer. The mean averaged axial velocity $\bar{U}$ is approximately 10 m/s, as shown in Fig. 4.6. The most unstable mode of an unforced straight shear layer occurs at $St_s \approx 0.032$ for laminar flows, and at $St_s \approx 0.044-0.048$ for turbulent flows (Ho and Huerre 1984). The momentum thickness $\delta$ is one-fourth of the vorticity thickness, which is calculated from the axial velocity profile at a given axial station (Panda & McLaughlin, 1994). Based on Eq. (4.15), the most unstable natural frequency, $f_s^0$, is approximately on the order of $10^3$ Hz near the downstream of the centerbody.

The dominant frequency at the swirl number of 0.5, shown in Fig. 4.22, is 1,380 Hz on the order of $10^3$ Hz. Therefore, the response frequency ($f_s^R$) of the shear layer could be considered as 1,380 Hz. In other words, the response unstable frequency of the shear layer originating from the centerbody is locked to $f_s^R = 1,380$ Hz. At this response frequency, the shear layer rolls up into discrete vortices, which would further pair with each other in the downstream at subharmonic frequency, $f_s^R / 2 = 690$ Hz. This subharmonic frequency is also close with the interacted subharmonic frequency, $f_{S1} = 650$ Hz. The vortices rolling up and pairing procedure affects the pressure oscillation by means of Eq. (4.13) and consequently triggers the first tangential acoustic mode in the dump chamber at $f_c = 1,350$ Hz. Thus the pressure oscillation is stimulated by a quasi-periodic disturbance at a specific frequency, around the response frequency $f_s^R$ or its subharmonic frequency $f_s^R / 2$. The latter has been identified approximately 655 Hz from the reduced one-dimensional pressure profiles shown in Fig. 4.21.

4.6.2.2 Swirl Number of 0.3

The POD analysis for the instantaneous pressure fields has been performed to study the acoustic mode at swirl number of 0.3. For simplicity, the POD analysis is only conducted on two planes instead of the whole three-dimensional flowfield. 220 snapshots extending over a time period of 13 ms are used.
Figure 4.25 shows the most energetic POD modes in an x-r plane. In the first POD mode, a 2L/1R mode is observed in the dump chamber while a 1L mode appears in the swirler housing. The spectra of the time traces associated with the first six most energetic modes are shown in Fig. 4.26. A dominant frequency at 3,900Hz is clearly observed in the spectrum of the first POD mode, which represents the first longitudinal (1L) mode in the swirler housing and the second longitudinal and first radial (2L/1R) mode in the chamber. This suggests that the flow motion corresponding to the first POD mode varies at a frequency of 3,900Hz. Figure 4.27 shows the normalized energy occupied by each POD mode. Obviously, the first mode is dominant and represents more than 20% of the total energy.

![Mode 1](image1)

![Mode 2](image2)

![Mode 3](image3)

Fig. 4.25 First three POD modes in an x-r plane, pressure contours, $S = 0.3$. 
Fig. 4.26 Spectra of time traces of the first four POD modes in the $x-r$ plane, $S = 0.3$.

Fig. 4.27 Energies of POD modes in the $x-r$ plane, $S = 0.3$. 
To further unveil the flow structures in the azimuthal direction, *i.e.*, tangential mode, the most energetic POD modes in the \( r-\theta \) plane are presented in Fig. 4.28. This cross-section is located right at the downstream of the dump plane, \( x = 80 \) mm. The first mode represents the axisymmetric mode while the second and third modes are associated with the first tangential and first radial (1T/1R) mode. This result is consistent with the previous observation, *i.e.*, 2L/1R mode observed in the \( x-r \) plane. The time traces of the two 1T/1R POD modes imply that the tangential mode is counter-rotating with the swirling flow. This conclusion has been proved in Fig. 4.17 and is consistent with the conclusion that the \( m = -1 \) helical mode is more unstable in comparison with \( m = 1 \) mode for swirl jet (Lessen *et al.*, 1974; Martin and Meiburg, 1996). Figure 4.29 represents the spectra of time traces and a 3,900 Hz dominant frequency is also observed. The normalized energy of the POD modes is shown in Fig. 4.30.

![Fig. 4.28 First four POD modes in the \( r-\theta \) plane, pressure contours, \( S = 0.3 \).](image-url)
Fig. 4.29 Spectra of time traces of the first four POD modes in the $r-\theta$ plane, $S = 0.3$.

Fig. 4.30 Energies of POD modes in the $r-\theta$ plane, $S = 0.3$. 

Percent energy in mode k

Energy sum from mode 1 through k

Mode number k
After combining the POD modes in both the $x$-$r$ and $r$-$\theta$ planes, we conclude that the 1L/1T mode leads in the swirler housing and that the 2L/1T/1R mode dominates in the dump chamber at $S = 0.3$. In order to validate this conclusion, $\lambda_{10} = 1.8412$ and $\lambda_{11} = 5.3314$ are substituted into Eq. (4.9). The eigen-frequency of the 2L/1T/1R mode, $f_{211}$, in the dump chamber is 3827 Hz, and that of 1L/1T mode in the swirler housing, $f_{110}$, is 3,879 Hz. Obviously, the two frequencies are very close to the dominant frequency of the flowfield, $f = 3,900$ Hz.

4.6.2.3 Validation and Discussions

To further identify and validate the calculated acoustic mode, the POD modes are compared with the pure acoustic mode shapes calculated with ANSYS, commercial finite-element software. Figures 4.31 and 4.32 show the acoustic mode shapes, which are calculated based on the same geometry and flow conditions presented in Eq. (4.11).

Figure 4.31 shows the acoustic mode shape at eigen-frequency of 1300 Hz. As expected, only a 1T mode with an eigen-frequency of $f_{010} = 1,960$ Hz is observed in the swirler housing. In the dump chamber, a 1T mode is observed and the eigen-frequency, based on Eq. (4.9), is $f_{010} = 1,350$ Hz, which is close to the natural frequency of the acoustic mode calculated through ANSYS, $f = 1,300$ Hz.

Figure 4.32a) is a global view of the acoustic mode shape at eigen-frequency of 3,982 Hz. A 1L/1T mode is clearly observed in the swirler housing shown in Figs. 4.32b) and c). Its eigen-frequency, $f_{110} = 3,879$ Hz, is close to the eigen-frequency, 3982 Hz, of the system, shown in Fig. 4.32a). A 1L/1T/1R mode is observed in the dump chamber and its eigen-frequency is $f_{111} = 3,795$ Hz. Because the non-reflecting boundary condition is implemented at the chamber, the longitudinal acoustic mode of the dump chamber is trivial. For the reader’s convenience, a close-view of the mode shapes associated with the first POD modes in the $x$-$r$ plane and $r$-$\theta$ cross-section is shown in Fig. 4.33. The two patterns are similar except for a phase difference in the azimuthal direction.
Fig. 4.31 Acoustic mode shapes corresponding to $f_0 = 1,300$ Hz, calculated by means of ANSYS. Solid lines: positive values; dash lines: negative values. (a) 3D view, (b) $x-r$ plane, and (c) $r-\theta$ cross-sections.

As aforementioned in Section 4.6.1.2, when $S = 0.3$, the spectral analysis shows that the flow region, in which the local dominant frequency of velocity is the same as the global dominant frequency of pressure, is near the tip of the backward step and its downstream. The strong shear layer in this region induces the Kelvin-Helmholtz instability near this surface. The spectra at probe 23:19, shown in Fig. 4.24, demonstrate a 3,900 Hz frequency motion existing in the radial velocity spectrum. This indicates an oscillation of the shear layer in the radial direction. Obviously, this flow motion excites the radial acoustic mode from zero to one in the dump chamber. Because this is a very important position in the flowfield, it could resonate the system frequency at this frequency. Owing to relative weak unsteady motions near the central region at $S = 0.3$, the importance of the Kelvin-Helmholtz instability near the surface of the swirler housing increases. Therefore, the acoustic mode stimulated by the 3,900 Hz mode suppresses that associated with the 1,380 Hz mode, which appears at $S = 0.5$. 
Fig. 4.32 Acoustic mode shapes corresponding to $f_0 = 3,982 \text{ Hz}$, calculated by means of ANSYS. Solid lines: positive values; dash lines: negative values. (a) 3D view, (b) $x-r$ plane, and (c) $r-\theta$ cross-sections.

Fig. 4.33 Close-view of the first mode in the $x-r$ plane and second mode in $r-\theta$ cross-section, $S = 0.3$. 
In the $S = 0.5$ case, due to strong vortex shedding from the centerbody and the dynamical evolution of the vortex breakdown, the system frequency is locked in a lower frequency, \textit{i.e.}, 1,380 Hz, and its subharmonic and superharmonic frequencies.

The results reveal two facts in the two connected chambers, \textit{i.e.}, the swirler housing and the dump chamber. First, the acoustic tangential mode numbers must match each other at the interface, \textit{i.e.}, dump plane. For example, both the two acoustic modes in the swirler housing and the dump chamber have a 1T mode and this phenomena appear at both swirl numbers. This point is obvious from the continuity perspective. Although the acoustic mode number in the radial direction is zero in the swirler housing, the 1R mode appears in the dump chamber. The trigger for this change is that a large area variation at the dump plane. Second, the frequencies corresponding to the acoustic modes in the two sections must match each other. The point can be explained by the factor of the consistency of the global system. For example, when $S = 0.3$, the 3,900 Hz dominant frequency is close to the individual eigen-frequencies of the acoustic modes in the dump chamber, $f_{211} = 3,827$ Hz, and in swirler housing, $f_{110} = 3,879$ Hz. When $S = 0.5$, a multi-frequency spectrum, including the eigen-frequencies of different acoustic modes and their subharmonic/supharmonic modes, is observed.

\subsection*{4.7 Summary}

Turbulent swirling flows injected into a dump chamber are numerically studied by means of three-dimensional LES. The simulation is designed to match the geometry and flow conditions used in the experimental study of Favaloro \textit{et al.} (1989). The present computational predicted results agree with the experimental data (Favaloro \textit{et al.} 1989) very well. It demonstrates that the code implemented in the present study is confident in simulating turbulent swirling flows.

Based on the present calculation, some insight into fundamental phenomena, including turbulent behaviors, vortex breakdown, the Kelvin-Helmholtz instability, and helical instability, are addressed. The calculated mean resolved velocities, turbulence intensities, and turbulent kinetic energy are in good agreement with experimental results when the swirling number is 0.5, at which the vortex breakdown phenomenon
occurrences. It is difficult to categorize the flow pattern to any type of vortex breakdown found in previous experiments. The vortex breakdown phenomenon is not observed at the swirl number of 0.3, although the helical precessing vortex core appears.

Some typical low-frequency unstable modes are identified. The natural transversal acoustic modes can resonate with the flowfield and lock it into the eigen-frequencies of these acoustic modes or their harmonics. On the other hand, unstable shear layers also induce flow oscillation at the response frequency, which will stimulate pressure oscillations.

A theoretical analysis, POD analysis, and commercial software, ANSYS, are used for comparison in the present study. The results show the significant effects of swirl number on the acoustic mode. The local vortical wave moves along the shear layer affect the global acoustic wave in the dump chamber. At $S = 0.5$, the 1T acoustic mode in the dump chamber at $f_c = 1,350$ Hz excites the unsteady evolution of the shear layer from the centerbody. The vortices pairing would induce the subharmonic mode, $f_{S1}^R / 2 = 675$ Hz. The low frequency vortical dynamic evolution affects the dynamic evolution of vortex breakdown, and resonates with the interaction mode between the 1T acoustic modes in the swirler housing and dump chamber, $f_{S1} = 650$ Hz. Finally, a dominant frequency at 655 Hz is observed in the real calculation at the swirl number of 0.5. The dominant frequency of the system shifts to 3,900 Hz when the swirl number is 0.3. The 1T/1L acoustic mode is identified in the swirler housing and the 1T/1R/2L mode in the dump chamber. The eigen-frequencies associated with the two acoustic modes are close to each other.
Part II

Vortical Flow Dynamics and Acoustic Response of a Gas-Turbine Swirl-Stabilized Injector
Chapter 5

Vortical Flow Dynamics in a Gas-Turbine Swirl-Stabilized Injector

In this section, the vortical flow dynamics in a gas-turbine swirl-stabilized injector, as shown in Fig. 5.1, is studied. The effects of swirl number on the flow patterns are investigated in detail. Section 5.1 describes the design motivation and injector configuration. The boundary conditions implemented in the present study are addressed in Section 5.2. Section 5.3 presents the grid system and a grid independence study. A simple description of the overall flow motions is carried out in Section 5.4. The mean flowfield and turbulence properties are studied in Section 5.5. In Section 5.6, the detailed mechanisms underlying the unsteady flow motions are discussed. A spectral analysis of flow properties at selected positions is conducted in Section 5.7 to identify the dynamics of the system. A proper orthogonal decomposition (POD) method is implemented in Section 5.8 to achieve a structure-based physical understanding of the vortical flow dynamics. Finally, a summary is given in Section 5.9.

Fig. 5.1 Schematic of a gas-turbine swirl-stabilized injector with a tri-radial-swirler.
5.1 Background and Computational Case Description

The physical model considered herein is a gas-turbine swirl-stabilized injector. The injector consists of a mixing duct and fuel orifices located coaxially upstream of the mixing duct, as shown in Fig. 5.1 (Graves, 1997). The mixing duct includes a center cylindrical passage and two annular passages, which are spaced radially outward from the axis. Three radial air swirlers, denoted as $S_1$, $S_2$, and $S_3$, are located upstream of the air-passages. The second swirler, $S_2$, is counter-rotating relative with the others to the longitudinal axis. Fuel is discharged from a number of fuel orifices, and the liquid jet emanating from the fuel orifices is directed toward the prefilmer surface, on which a liquid film is formed (Cohen and Rosfjord, 1993). This liquid film is subsequently sheared by the swirler airstreams. The airflows through swirlers $S_1$ and $S_2$ flow along the liquid film and generate waves on its surface, which further induce the instability of the liquid film. The airflow through swirler $S_3$ acts on the liquid film at the edge of the prefilmer surface. The performance of atomizer of this type is affected mostly by the shear stress between the air jets. Once vaporization occurs, the fuel and air mix and burn in the shear layers formed at the edges of the central toroidal recirculation zone (CTRZ) and corner recirculation zone (CRZ).

This swirl-stabilized injector is also referred to as a high-shear nozzle/swirler (HSNS) and has four major advantages. First, it reduces smoke through inducing high swirl from the first passage. Second, the second swirler is implemented to generate strong shear layers in both the axial and azimuthal directions and to reduce the overall swirl angle, consequently to improve fuel/air mixing. The introduction of the second passage makes it easy to control the magnitude and the initial swirl angle of the flow. Third, a richer CTRZ is generated, which increases the relight stability. Finally, the relight stability and the total flow can be decoupled by shifting the airflow through the third passage (Graves, 1997).

The mixing duct measures a length of 28 mm, and the first duct outlet has a diameter of 32 mm. The baseline flow condition in the current study includes an ambient pressure of 1 atm, an inlet temperature of 293 K, and an inlet mass flow rate of 0.077
kg/s. The corresponding Reynolds number is $2 \times 10^5$ based on the diameter and the flow bulk velocity at the injector outlet.

### 5.2 Boundary Conditions

The method of characteristics (MOC) is used to specify the boundary conditions.

- **Inlet boundary**
  
The inlet flow is subsonic, thus four variables are specified with the other parameters extrapolated from the flowfield. The specified variables are the total temperature ($T_0$), mass flow rate ($\dot{m}$), the axial velocity ($u_z$), and the angle between the radial ($u_r$) and azimuthal velocity ($u_\theta$). The pressure is determined through a simplified radial momentum equation:

$$\frac{\partial \rho u_r}{\partial t} + \frac{\partial \rho u_r^2}{\partial r} + \frac{\rho u_\theta^2}{r} = -\frac{\partial p}{\partial r}$$  \hspace{1cm} (5.1)

Turbulence at the inlet is provided by superimposing white noise with the intensity of 10% of the mean average velocity. The disturbance is implemented at every few time steps and space cells to avoid high frequency dissipation.

- **Outlet boundary**
  
  Because the outlet flow is also subsonic, only one variable is required to be specified. The back pressure at the outlet of the computational domain is not constant due to the high azimuthal velocity. A constant back pressure could induce an unphysical recirculation zone near the boundary. Therefore, the static temperature is specified in this study and the other variables are extrapolated, *i.e.*,

$$\bar{T} = T_{\text{ambient}}$$  \hspace{1cm} (5.2)

and

$$\frac{\partial \bar{u}_r}{\partial n} = 0$$  \hspace{1cm} (5.3)

$$\frac{\partial \bar{p}}{\partial n} = 0$$  \hspace{1cm} (5.4)
• **Wall boundary**
  
  Adiabatic and zero-pressure-gradient conditions are applied along the walls, *i.e.*, 
  
  \[
  \frac{\partial p}{\partial n} = \frac{\partial T}{\partial n} = 0
  \]  
  (5.5)
  
  The no-slip condition is also used
  
  \[
  \tilde{u} \mid_{wall} = \tilde{v} \mid_{wall} = \tilde{w} \mid_{wall} = 0
  \]  
  (5.6)

• **Far-field**
  
  Because the air flows directly into the ambience after passing through the injector, entrainment of the surrounding air occurs along the far-field boundary of the computational domain. The pressure, total temperature, and axial velocity are specified as:
  
  \[
  \rho = P_{back}
  \]  
  (5.7)
  
  \[
  \bar{T}_0 = T_0 \mid_{back}
  \]  
  (5.8)
  
  \[
  \tilde{u}_x = 0
  \]  
  (5.9)
  
  The conservations of mass and angular momentum are employed to determine the radial and azimuthal velocities, respectively, as
  
  \[
  \frac{1}{r} \frac{\partial (\rho \tilde{u}_r)}{\partial r} = 0
  \]  
  (5.10)
  
  and
  
  \[
  \frac{\partial (\rho \tilde{u}_\theta)}{\partial r} = 0
  \]  
  (5.11)

### 5.3 Grid System and Validation

#### 5.3.1 Grid system and Computational Domain

A three-dimensional grid system is generated by rotating a two-dimensional grid with respect to the centerline, as shown in Fig. 5.2. The external region downstream of
Fig. 5.2 Grid system: (a) longitudinal direction, (b) cross section view, and (c) Overall computational domain.

The injector is also considered to provide a complete description of the flow development. The length and outside diameter of the computational domain are 15 times and 8 times of the injector outlet diameter, respectively. The computational domain is carefully chosen so that the outer boundaries in the axial and radial directions are sufficiently far from the injector exit to minimize the propagation of boundary-induced disturbances into the injector.

The selection of grid size in the injector region is based on the turbulent kinetic energy spectrum. Assuming the large/integral length scale \( L \) is the injector outlet diameter, 32 mm, and the associated Reynolds number, \( \text{Re} \), \( 2\times10^5 \). The Kolmogorov and Taylor microscales, \( l_K \) and \( l_T \), are

\[
l_K = L \cdot \text{Re}^{-3/4} \approx 0.003 \text{ mm} \tag{5.12}
\]
and

\[ l_T = L \cdot \text{Re}^{-1/2} \approx 0.07 \text{ mm} \quad (5.13) \]

respectively (Brasseur, 2000). The average grid size in the injector interior is around 0.2 mm, which is of the order of the Taylor microscale or the turbulence inertial subrange. The entire grid system has 2 million points, of which 0.9 million points are located within the injector. 54 computational blocks/subdomains, as shown in Fig. 5.3, are submitted to 54 processors for parallel processing.

Figure 5.4 shows the frequency spectra of the turbulent kinetic energy at four positions. Results in the high-frequency region follow the Kolmogorov-Obukhov spectrum (-5/3 law), which is based on the equilibrium hypothesis for homogeneous turbulence at large Reynolds numbers (Kolmogorov, 1941). Deviations from this ideal energy spectrum may also be extended to inhomogeneous turbulence. The results illustrate that the spatial resolution in the present calculations is sufficient to capture the turbulence inertial subrange.

![Multi-block structure of domain decomposition with 54 blocks](image_url)
Fig. 5.4 Spectrum of turbulent kinetic energy.
In order to avoid the uncertainties resulting from the near-wall modeling, the stretched grid near the wall is used to resolve the flow motions in the near-wall region. Most of the first layer grids near the wall fall in the range of \( y^+ = 6 \sim 20 \). Because the flow variables in the finite-volume method are defined at the center of each control volume, the distance of the first resolved variables to the wall is \( y^+ = 3 \sim 10 \), which fall in the joint between the viscous sub-layer and the buffer zone (Piomelli, 1994).

### 5.3.2 Grid Independence Study

A detailed grid independence study has been performed based on mesh sizes of 2.0 million and 3.2 million to capture the details of the turbulent motions. In comparison with the coarse mesh case, the grid numbers of the fine mesh case in axial and radial directions increase 1.2 and 1.3 times, respectively. At the same time, the computational domain is also expanded in the fine mesh case to validate the effects of the boundary. The mean axial velocity and turbulent kinetic energy contours of the two cases are shown in Fig. 5.5. They agree with each other very well with minor differences; therefore, the coarse grid system is implemented in the present work.

### 5.4 Description of Flow Phenomena

In the current study, the flowfields corresponding to two sets of tri-radial-swirlers at different swirler angles, i.e., low swirl number (LSN) and high swirl number (HSN) swirlers, are investigated separately. The two configurations are presented in Table 5.1.

<table>
<thead>
<tr>
<th>Radial Swirler</th>
<th>High Swirl Number (HSN)</th>
<th>Low Swirl Number (LSN)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S_1 )</td>
<td>45°</td>
<td>30°</td>
</tr>
<tr>
<td>( S_2 )</td>
<td>-60°</td>
<td>-40°</td>
</tr>
<tr>
<td>( S_3 )</td>
<td>70°</td>
<td>50°</td>
</tr>
<tr>
<td>Swirl Number</td>
<td>0.49</td>
<td>0.34</td>
</tr>
</tbody>
</table>

Table 5.1 Swirl vane angles at injector inlet and swirl numbers defined at injector exit.
Fig. 5.5 Comparison of flowfields based on two sets of meshes. (a) azimuthal velocity contours and streamlines; and (b) turbulent kinetic energy contours.

The swirl number is defined as

$$ S = \frac{\int_0^{R_{out}} \bar{u}_x \bar{u}_\theta r^2 dr}{R_{out} \int_0^{R_{out}} \text{sign}(\bar{u}_x) |\bar{u}_s| r dr} \tag{5.14} $$

where \( \text{sign}(x) = \begin{cases} 1 & x \geq 0 \\ -1 & x < 0 \end{cases} \) in order to avoid counting the recirculation flow.

Figure 5.6 shows the snapshots of the vorticity magnitude contours on the \( x-r \) and \( r-\theta \) planes for the low and high swirl number cases, respectively. The flow patterns exhibit four common features as follows.

First, because of strong radial-entry swirling flows, vortex breakdown phenomena occur in the downstream of the centerbody. Since the flows accelerate through the turning section, the flow separation points are fixed at the tip of the centerbody.
Meanwhile, owing to the strong shear layer between the inlet passage and the CTRZ, a strong vorticity layer is produced starting from the tip of the centerbody, and subsequently rolls, tilts, stretches, and breaks up into small bulbs. These small vorticity bulbs interact and merge with the surrounding flow structures while traveling downstream. The flow motions associated with the dynamic evolution of vortex breakdown are large, disorganized, coherent structures.

Second, due to the velocity differences at the trailing edges of the guide vanes, strong shear layers exist in the downstream. The Kelvin-Helmholtz instabilities and subsequent vortex shedding are observed. In comparison with the large disorganized
coherent structures resulting from the dynamic evolution of vortex breakdown, the flow structures of vortex shedding originating from the Kelvin-Helmholtz instabilities are smaller and well organized.

Third, large non-axisymmetric structures appear in the azimuthal direction. Three mechanisms, including helical instability, centrifugal instability, and the Kelvin-Helmholtz instability in the azimuthal direction, account for these non-axisymmetric patterns. The helical instability appears in the azimuthal direction and is clearly observed in the internal region of the injector, which will be discussed later. The presence of swirling flows could result in an unstable radial stratification, and consequently lead to centrifugal instability (Martin and Meiburg, 1996). The narrow strong shear layer near the joint between the first and second passages surrounding the axis also induces the Kelvin-Helmholtz instability in the azimuthal direction.

Finally, the four aforementioned different flow instabilities, i.e., vortex breakdown, the Kelvin-Helmholtz instabilities, centrifugal instability, and helical instability, interact and compete with each other in the injector. While the swirl number varies, the dominant instability mode may change correspondingly. For example, in the HSN flow, the flow motions associated with vortex breakdown and Kelvin-Helmholtz instability in the azimuthal direction are enhanced, hence suppress the development of the Kelvin-Helmholtz instability in the axial direction.

The detailed analyses corresponding to these flow patterns will be carried out in the following sections.

5.5 Mean Flowfield and Turbulence Properties

The properties of the mean flowfields and turbulence properties are shown in Figs. 5.7-5.13, which present the streamlines, contours of the axial velocity, pressure, azimuthal velocity, centrifugal force, angular momentum, and turbulent kinetic energy (tke), respectively.

Several points must be emphasized here. First, a CTRZ, where the mean axial velocity is negative near the axis, appears in both low and high swirl number flows,
although their sizes are different. The presence of a CTRZ is a typical characteristic of 
vortex breakdown and the formation of this phenomenon has been discussed in Chapter 
4. Because of higher azimuthal velocity in the HSN case, the size of its CTRZ is larger 
accordingly.

Second, the streamline topologies of the two cases are different near the 
centerbody, as shown in Fig. 5.7. In the LSN case, the highest axial velocity region, 
shown in Fig. 5.8, is near the surface of the centerbody, while vortex breakdown occupies 
the same region in the HSN case. The pressure contours, shown in Fig. 5.9, of the LSN 
case indicate the existence of a low-pressure core at this region with the lowest pressure 
around 78000 Pa. This low-pressure core significantly affects the flow pattern in the 
neighborhood region. The lowest pressure in the HSN case is around 88000 Pa. This 
contrast may conflict with the fact that higher swirl-number flows generally induce 
higher pressure-gradient, or lower pressure, in the core regions.
Fig. 5.8 Contours of mean axial velocity at two swirl numbers.

Fig. 5.9 Contours of mean pressure at two swirl numbers.
This phenomenon results from the change of the topology of mean flow pattern due to different swirl numbers. In the HSN case, the vortex breakdown occurs right in the downstream of the centerbody because of high swirling strength. The swirling strength in the LSN case, however, is not strong enough to push the inlet flow out of the central region, thus the inlet flow can penetrate into the axis region. Because of the angular momentum conservation, the azimuthal velocity near the axis increases rapidly while the flow moves toward the centerline, thus the extremely high swirling flow in the downstream of centerbody produces a low-pressure core. On the other hand, due to the constraint of the wall, the flow azimuthal velocity near the surface of the centerbody is slow and the pressure is relatively high; therefore, a high-speed wall jet is induced in the axial direction by this high-pressure gradient (Shtern and Hussain, 1999).

The confliction in the pressure fields also can be qualitatively explained by the centrifugal force. The maximum mean azimuthal velocities, shown in Fig. 5.10, in the HSN and LSN cases are 157 m/s and 151 m/s, respectively. Although the two values are very close, the radii at which the maximum azimuthal velocity locates are quite different, which are 5.0 mm and 2.3 mm for the HSN and LSN cases, respectively. The mean

![](image)

*Fig. 5.10 Contours of mean azimuthal velocity at two swirl numbers.*
centrifugal force, shown in Fig. 5.11, can be estimated as

\[ f_c \sim \frac{\bar{\rho} \bar{u}_\theta^2}{r} = \frac{\Omega^2}{\bar{\rho} r^3}. \]  

where

\[ \Omega = r \bar{\rho} \bar{u}_\theta \]  

represents the angular momentum and is shown in Fig. 5.12.

Although the mean azimuthal velocity of the HSN case is higher than that of the LSN case, the minimum pressure due to the centrifugal force is higher. Batchelor (1999) indicated that the circulation around a material curve, \textit{i.e.}, streamline, was constant in \textit{steady}, \textit{axisymmetric}, \textit{incompressible}, \textit{inviscid} flow. This can be demonstrated qualitatively in Fig. 5.12. At the region, in which the turbulence intensity is low and the assumption is tenable, the contours of circulation are consistent with the streamlines. Figure 5.12 also illustrates the penetration effect of the angular momentum near the centerbody in the LSN case.
Finally, there are two regions with high turbulent kinetic energy in both cases in different profiles, shown in Fig. 5.13. The turbulent kinetic energy in the regions near the centerline and the second guide vane of the injector is much higher than that in the other regions. The high turbulent kinetic energy region near the axis results from the dynamic evolution of vortex breakdown while the other undergoes the vortex shedding due to the Kelvin-Helmholtz instability. These two high turbulent kinetic energy regions merge at the exit of the injector in the HSN case but are isolated in the LSN case. This phenomenon implies the interaction between vortex breakdown and the Kelvin-Helmholtz instability in the HSN case.

In the HSN case, the highest turbulent kinetic energy region is near the location of the fuel nozzles, where liquid jet is injected into the injector. High intensive flow motion appears since the flow separates at this region. This flow pattern definitely aids the breakup of the liquid jet and improves the performance of the atomization. From the turbulent kinetic energy point of view, high swirl number flows speed up the atomization processing in this geometry. Given higher swirl number or tuned centerbody geometry, the turbulent motions could enhance the atomization processing.
5.6 Flow Dynamics

The typical unsteady motions involved in the present work include the CTRZ, vortex shedding, non-axisymmetric flow pattern, and so on. Detailed flow dynamics associated with aforementioned flow motions, such as vortex breakdown, the Kelvin-Helmholtz instabilities, helical instability, and interaction among each other, will be explored in this section thoroughly.

5.6.1 Vortex Breakdown

Figure 5.14 shows the instantaneous iso-surfaces of the azimuthal velocity. A bubble-form vortex breakdown is clearly observed in the downstream of the centerbody for the LSN case. In the HSN case, vortex breakdown still occurs, but becomes difficult to identify a succinct structure due to the complex flow evolution involved. Since the flow accelerates at the turning section, the flow separation point is fixed at the tip of the centerbody. Therefore, for the HSN case, the vortex breakdown occurs from the flow
separation point, \textit{i.e.}, the tip of the centerbody, instead of the downstream of the centerbody in the LSN case.

The difference in vortex breakdown between the two cases is also shown in Fig. 5.7, representing the streamlines of the mean flowfields. The streamline topologies of the two cases are disparate. Only a single breakdown is observed in the HSN case, while two breakdowns occur in the LSN case. This phenomenon may be attributed to the effects of the end-wall (Escudier, 1984) since the flow from the swirler S\textsubscript{1} can enter the axial region directly in the LSN case.

Figure 5.8 indicates the existence of the wall jet associated with the vortex breakdown in the LSN case, as mentioned and explained in Section 5.5. The phenomenon also represents a competition between the convergent radial flows restrained by geometry constraints and the divergent flows due to the centrifugal force arising from the swirling flows. The latter dominates the HSN case, while the former leads the LSN case. This is a common phenomenon appearing in the radial-swirler injector.

![Fig. 5.14 Instantaneous iso-surfaces of azimuthal velocity, (a) LSN and (b) HSN.](image)
Two points should be noted here. First, the centerbody exerts strong influence on the vortex breakdown through its end-wall effect, which consequently influences the streamline topology and the injector dynamics. This suggests that a slight change in injector geometry may notably affect the flow topology, which should be kept in mind in the injector design. Second, the streamline topology dictates that the effective flow area depends on the local flow structure and the size of the recirculation zone. It may further affect the hydrodynamic instability of the system.

In order to further visualize the dynamic evolution of the CTRZ, the streamlines of instantaneous flowfields, which are spatially averaged in the azimuthal direction for the HSN case, are shown in Fig. 5.15. Obviously, the flow structures in Fig. 5.15 are much clearer in comparison with the three-dimensional flowfields, which are too complex for an insight analysis.

Basically, two large vortices exist downstream of the centerbody. One is located just in the downstream of the centerbody and the other is in the downstream of the first vortex. The vortices evolve in three forms. First, a small vortex separates from the large vortex at the upstream, travels to the downstream, and eventually coalesces with the other

![Fig. 5.15 Snapshots of streamline lines based on spatially averaged flowfields at HSN.](image-url)
large vortex located at the downstream. Second, a small vortex is generated near the centerbody, and the large vortex, which is normally anchored at the centerbody, detaches from the centerbody. The flow topology, consequently, switches from one pattern to another at a intermittent time period. This flow pattern is similar to the mean flow pattern of the LSN case, which induces a strong wall jet near the surface of the fuel nozzle. Finally, the evolution of the large vortex induces the change of the effective flow area of the injector, and further affects the injector dynamics.

5.6.2 Kelvin-Helmholtz Instabilities

The Kelvin-Helmholtz instability is used to describe the instability where the variations of velocity and density are continuous and occur over a finite thickness. In general, the vortices are concentrated during the evolution of the Kelvin-Helmholtz instability. Figure 5.6 contains the snapshots of the vorticity magnitude contours on the $x$-$r$ and $r$-$\theta$ planes at different swirl numbers. Vortex shedding due to the Kelvin-Helmholtz instability is observed in both LSN and HSN cases at the trailing edge of the guide vanes. It is clear that the primary vortex shedding results from the Kelvin-Helmholtz instability of the mixing layer, which is arises from the velocity differences between the flows from different passages.

Figure 5.16 shows the iso-surfaces of the azimuthal velocity in the phase space, in which the three components of Cartesian coordinates, $(x, y, z)$, are converted from the axial, radial, and azimuthal coordinate components, $(x, \theta, r)$, in the physical space. For the LSN case, a sinuous spanwise instability of Kelvin-Helmholtz billows develops in the upstream of the mixing layer. Then, hairpin vortices appear as the billows are carried to the downstream, and longitudinal vortices form during the same time. The Kelvin-Helmholtz billows are highly distorted while hairpin vortices appear and finally transit to small-scale three-dimensional turbulence in the downstream of the mixing layer.

The unstable frequency of the shear layer is sensitive to the forcing arising from the surrounding environment. The order of the frequency of the vortex shedding due to Kelvin-Helmholtz instability in the streamwise direction is estimated as follows (Ho and
Fig. 5.16 Iso-surface of azimuthal velocity, \( u_t = 10 \text{ m/s} \), in phase space. (a) LSN and (b) HSN.

Huerre, 1984): the Strouhal number, \( S_t \), is 0.044-0.048 for turbulent flows, and the mean velocity, \( \bar{U} \), is 50 m/s, the thickness of the momentum boundary layer, \( \theta \), is around 0.2 mm, the frequency of the most unstable mode is

\[
f_n = S_t \frac{\bar{U}}{\theta} = \frac{(0.045)(50)}{0.0002} = 1.1 \times 10^4 \text{ Hz}
\]

(5.17)

A later spectrum analysis shows that the frequency of the vortex shedding is 13,000 Hz, which is the dominant frequency in the LSN flow. Therefore, the result is consistent with the above estimation and demonstrates that the dominant flow mechanism in this region is the Kelvin-Helmholtz instability in the streamwise direction for the LSN case. This frequency is also observed in a previous axisymmetrical simulation.

In the HSN case, due to the stronger shear layer in the azimuthal direction, which enhances the azimuthal direction unstable modes, such as the Kelvin-Helmholtz instability, helical instability, and centrifugal instability, the flows become highly disordered as soon as they mix with each other. Well-organized large structures appearing at the upstream soon break into small structures at the downstream.

Due to the counter-rotating swirling flows between the first and second passages, a strong shear layer appears in the azimuthal direction near their joint surrounding the
axis. This strong shear layer further induces the Kelvin-Helmholtz instability in the azimuthal direction. Figure 5.17 shows the azimuthal velocity contours of the LSN case, indicating the development of Kelvin-Helmholtz instabilities in the azimuthal direction. In the upstream of the injector, \( x = 11 \) mm, the azimuthal velocity profile is only slightly non-uniform. While these flow structures travel downstream, large non-axisymmetric structures appear. At the injector outlet, \( x = 27.5 \) mm, periodical flow structures appear in the azimuthal direction. In comparison with the LSN case, the development of the Kelvin-Helmholtz instability in the HSN case is much obvious. Because of the larger difference in the swirler vane angles, the shear layer strength at the cross-section of the HSN case is stronger than that of the LSN case, and consequently enhances the Kelvin-Helmholtz instability in the azimuthal direction. The azimuthal velocity contours of the HSN case, as presented in Fig. 5.17, clearly show well-organized structures appearing in the azimuthal direction. When the structures are convected to the downstream, they tend to be disorganized.

![Fig. 5.17 Snapshots of azimuthal velocity contours in four \( r-\theta \) cross sections (a) LSN and (b) HSN.](image-url)
5.6.3 Helical Instability

Any flow variable can be represented in a cylindrical \((x, r, \theta)\) coordinate system by a Fourier series in the azimuthal direction as

\[
f(x,r,\theta,t) = \sum_{m=-\infty}^{\infty} f_m(x,r) \exp[i(m\theta - \omega t)]
\]

(5.18)

where \(m\) is the wavenumber in the azimuthal direction, \(\omega\) the complex frequency, and \(f_m\) Fourier coefficients. The \(m = 0\) and \(m \neq 0\) modes represent axisymmetrical and helical modes, respectively. In Fig. 5.16, helical structure super-imposing on the Kelvin-Helmholtz billows is clearly observed upstream of the mixing layer for the LSN case. Figure 5.18 shows the instantaneous iso-surfaces of axial vorticity at different swirl
numbers, and the helical structures are clearly presented. The associated animations show that the large coherent helical structures appear intermittently.

Fig. 5.18 Instantaneous iso-surfaces of axial vorticity component, (blue: $-1 \times 10^7$ 1/s, yellow: $2 \times 10^4$ 1/s). (a) LSN and (b) HSN.

Fig. 5.19 Pressure contours of the first two POD modes, based on kinetic energy in a cross-section ($x = 15$ mm). Solid line: positive, dash line: negative. (a) 1st mode and (b) 2nd mode, LSN.
The proper orthogonal decomposition (POD) method is employed to analyze the helical mode appearing in the flowfield. Figures 5.19 and 5.20 represent the first and second most energetic modes and their time traces in a cross-section perpendicular to the axis. These two modes are responsible for the $m = -1$ helical mode. This negative mode represents the helical wave is counter-rotating relative to the swirling flow. A similar phenomenon is described in Chapter 4.

In the HSN case, the azimuthal velocity contours show that large oscillations appear in the mix layer zone. This pattern indicates the interaction between the Kelvin-Helmholtz instability and helical instability. However, we do not observe helical structures that are as clear as those in the LSN case. The explanation for this phenomenon is that the flow structures in the HSN case are more complex due to the higher swirling velocity difference; therefore, we cannot expect a clear helical mode to exist in the flowfield.
5.6.4 Mode Interaction/Competition

As aforementioned, three major flow patterns exist and interact with each other in the injector. Three different kinds of interactions/competitions are identified. First, the Kelvin-Helmholtz instability in the streamwise direction interacts with the vortex breakdown shown in Fig. 5.6. In the high swirl number flow, the vortex shedding arising from the Kelvin-Helmholtz instability is significantly suppressed by the irregular, large-scale organized structures originating from the vortex breakdown, although they coexist well in the LSN case. The vortex shedding appears while the core of the vortex breakdown shrinks and is suppressed while the vortex breakdown core grows, i.e., vorticity bulbs move to the outside of the core. Moreover, in the high swirl number flow, some of the vorticity bulbs, generated by the shear layer at the boundary of the CTRZ, travel along the surface of the guide vane and interact directly with the shed vortices at a low frequency.

Second, the Kelvin-Helmholtz instabilities in different directions also compete with each other. In the LSN case, the Kelvin-Helmholtz instability in the streamwise direction dominates the flowfield; therefore, the structures of Kelvin-Helmholtz billows and consequent hairpin-vortice structures are clearly observed. The Kelvin-Helmholtz instability in the azimuthal direction is not obvious until the flows convect to the downstream of the mixing layer. In the HSN case, a rather different pattern appears. The Kelvin-Helmholtz instability in the azimuthal direction is enhanced; therefore, the Kelvin-Helmholtz billows generated from the Kelvin-Helmholtz instability in the streamwise direction are suppressed, and flow structures are highly distorted.

Finally, the Kelvin-Helmholtz instability interacts with the centrifugal instability. The presence of swirling flows can result in an unstable radial stratification, thereby leading to centrifugal instability. Furthermore, the swirling flow can give rise to standing or propagating nonlinear inertial waves, similar to the internal waves observed in flows with density stratification (Martin and Meiburg, 1996). The gradient of the centrifugal force is stronger in a higher swirl-number flow and can result in strong instabilities in the azimuthal direction. Martin and Meiburg (1996) gave a detailed analysis on this phenomenon. The swirling flow tends to promote the evolution of a counter-rotating
vortex-ring. A higher azimuthal velocity gradient increases the centrifugal instability in the azimuthal direction and consequently further suppresses the Kelvin-Helmholtz instability in the streamwise direction, as demonstrated in Fig. 5.17. There are two separated regions where strong model competition exists. In the outer region, Kelvin-Helmholtz instabilities are dominant; therefore, the interaction between the two instabilities is obvious. On the other hand, in the region near the axis, the vortex breakdown primarily interacts with the centrifugal instability.

5.7 Spectral Analysis

The spectral analysis is implemented to study the flow dynamics. Figure 5.21 presents the probe locations in the current study in a longitudinal plane. The results associated with the LSN and HSN cases are presented and discussed as follows.

Fig. 5.21 Probes location (point: probe, yellow line: probe line, blue line: cross-section for POD).
5.7.1 Low Swirl Number Flow

In the LSN case, the flow patterns in the injector are dominated by the high-frequency Kevin-Helmholtz instability in the streamwise direction. Figure 5.22 shows the frequency spectra of pressure oscillations at the low swirl number.

Following the probes along Line 1, we observed a dominant mode at $f = 13,000$ Hz, which achieves its maximum magnitude at probe 1-2 due to the vortex shedding. Line 2 presents a similar characteristic. Because of the geometry constraint, the spectrum of probe 2-1 at 13,000 Hz reaches the maximum.

Line 3 presents the flow passage through the swirler $S_3$, the dominant frequency at $f = 13,300$ Hz is also observed. The strong shear layer that exists at the trailing edge of the second and third guide vanes induces the Kelvin-Helmholtz instability in this region too. Vortex shedding, however, is not apparent in this region due to the complex flow structures.

The probes near the centerline are shown along Line 4. A 5,783 Hz mode, which corresponds to the vortex shedding from the center body, is observed. As the flow travels downstream, the amplitude of the 5,783 Hz mode decreases. At the same time, because of the vortex breakdown in this region, the frequency spectra become broadband.

Line 5 represents the probes along the exit of the injector. Two peaks present, at the frequencies of 13,300 and 13,000Hz, on the spectrum plot of the probes near the guide vane. They may correspond to the Kelvin-Helmholtz instabilities associated with the flows through $S_1$ & $S_2$, and $S_2$ & $S_3$, respectively. As for the probes near the centerline, the strength of low-frequency components increases; however, no dominant frequency is observed in this region.
Fig. 5.22 Frequency spectra of pressure oscillations, LSN.
Fig. 5.22  Frequency spectra of pressure oscillations, LSN, cont'.
Fig. 5.22 Frequency spectra of pressure oscillations, LSN, cont'.
Fig. 5.22 Frequency spectra of pressure oscillations, LSN, cont'.
Fig. 5.22 Frequency spectra of pressure oscillations, LSN, cont'.
5.7.2 High Swirl Number Flow

The frequency spectra of pressure oscillations in the HSN case are shown in Fig. 5.23. The flow structures in the HSN case are much more complex than those in the LSN case. For example, several different dominant frequencies are observed in different regions instead of a single dominant frequency in the entire flowfield.

On Line 1, which corresponds to the main passage of the airflows, a 500 Hz peak near the inlet is observed. The mechanism is still unknown. In the downstream region, a 4,000 Hz mode resulting from the vortex breakdown dominates.

A broadband spectrum with a peak around 1,500 Hz is observed on Line 2, which corresponds to the prefilmer surface, i.e., the inner surface of the guide vane between S₂ and S₃. This frequency may result from the interaction between the Kelvin-Helmholtz instability and vortex breakdown. A study in Chapter 6 indicates that the 1,500 Hz could be considered the resonant frequency of the injector at high swirl number.

Line 4 represents the path of the shear layer originating from the centerbody. At probe 4-1, separated flows dominate and are characterized by irregular large-scale organized structures. In the downstream, a 4,000 Hz structure clearly develops, which is attributed to the dynamic evolution of the CTRZ.

Because of the interaction between the Kelvin-Helmholtz instability and vortex breakdown, the spectrum of the probe near the guide vane has a broad distribution. A 4,000 Hz mode is clearly presented at probes 5-2 and 5-3, which are located at the boundary of the CTRZ where strong shear layer and vortex evolution exist. The driving mechanism for the 4,000 Hz motion is same as that along Line 4.
Fig. 5.23 Frequency spectra of pressure oscillations, HSN.
Fig. 5.23 Frequency spectra of pressure oscillations, HSN, cont'.
Fig. 5.23 Frequency spectra of pressure oscillations, HSN, cont'.

Probe 3-1 (P16:2)

Probe 3-2 (P16:4)

Probe 3-3 (P21:2)

Probe 3-4 (P21:1)
Fig. 5.23 Frequency spectra of pressure oscillations, HSN, cont'.
Fig. 5.23 Frequency spectra of pressure oscillations, HSN, cont'.

Probe 5-1 (P10:14)

Probe 5-2 (P13:10)

Probe 5-3 (P14:10)

Probe 5-4 (P15:10)
5.7.3 Velocity and Pressure Oscillations

Figure 5.24 shows the spectra of velocity and pressure oscillations in the HSN case at two probes, which are located in the vortex breakdown region. The dominant frequencies of the pressure and radial velocity are same at two probes while the strengths of the other velocity components at the same frequency are weak. This phenomenon can be schematically explained through Fig. 5.25. Due to the strong radial pressure gradient, $\frac{\partial \bar{p}}{\partial r}$, arising from swirling effects, a small disturbance in the radial direction, $u'_r$, could induce a small displacement of fluid particle, $\Delta r$. Consequently, this small displacement would cause a relatively large pressure disturbance, $\Delta p$. Another reason is that the radial velocity fluctuation may change the effective flow area, which further influences the pressure variation.

![Fig. 5.24 Frequency spectra of velocity and pressure oscillations, HSN.](image-url)
Fig. 5.24 Frequency spectra of velocity components and pressure oscillations, HSN, cont'.

Fig. 5.25 Schematic of pressure oscillation due to swirling effects.
The strong coupling between the pressure and radial velocity component is an interesting phenomenon. In general, the axial and azimuthal velocity components, rather than the radial velocity component, are measured in experiments. This study shows that the radial velocity component is also a critical variable.

5.8 Proper Orthogonal Decomposition

In addition to the analyses presented above, the POD analysis is also employed for the instantaneous velocity fields. For similarity, the analysis is only performed on three cross-sections instead of the whole three-dimensional flowfield. 850 snapshots extending over a time period of 8.5 ms and 1000 snapshots extending over 10 ms are used for the LSN and HSN cases, respectively. The reason of processing these considerable snapshots is the broad time-scale range involved in the flow motions.

5.8.1 Low Swirl Number Flow

The POD results of the flow structures in the $x$-$r$ plane of the LSN case are shown in Figs. 5.26-5.29. Figures 5.26 and 5.27 present the normalized eigenvalues and

![Fig. 5.26 Energies of POD modes in an x-r plane, LSN.](image)
Fig. 5.27 First six POD modes in the $x$-$r$ plane, azimuthal velocity contours, LSN.

eigenfunctions/mode shapes, respectively. The eigenvalues of the first two modes are approximate (0.210 vs. 0.206) and account for more than 40% of the energy of the flow in the region of concern. This indicates that the flow structures, originating from vortex shedding in the streamwise direction, are the dominant pattern in the injector. The associated eigenfunctions and time traces suggests that the phase differences between the first two modes in both space and time are $\pi/2$. The mean velocity, wavelength, and frequency are consistent, which demonstrate that the vortex shedding travels downstream in the form of vortical wave, and that this unsteady flow pattern is well organized.

The spectra of the time traces of the first six modes are shown in Fig. 5.28. The peaks of the first two modes are at $f_0 = 13,000$ Hz. The $2f_0$ harmonic modes are also found in the 8th and 9th POD modes, which are not presented. Another important frequency is 5783 Hz, shown in Fig. 5.28 as the 3rd POD mode. The associated POD mode shape, shown in Fig. 5.27, illustrates that this mode is responsible for the flow structures dominated by the vortex breakdown and breakup procedures. A 350 Hz
frequency dominating the 4th mode corresponds to strong oscillations along the centerline. The POD based on pressure oscillation in the cross section also confirms the existence of this frequency, which may result from the dynamic evolution of the wall jet.

In the POD analysis of the cross-section perpendicular to the injector axis, as shown in Fig. 5.29, a high frequency (13,000Hz) peak is observed. The corresponding POD modes clearly show the mode shapes, associated with the mixed first tangential and first radial (1T/1R) acoustic mode. The natural frequency of this acoustic mode can be estimated with Eq. (4.9)

\[ f_{\text{mode}} = \frac{c}{2\pi} \sqrt{\frac{\lambda_{mn}^2}{R_c^2} + \frac{l^2 \pi^2}{L_c^2}}, \quad l, m, n = 0, 1, 2, \ldots \]  

(4.9)

For calculation simplicity, assume that the sound speed is 340 m/s and the radius of the convergent injector 19 mm, and the eigenvalue of the 1T/1R mode, \( \lambda_{11} \), is 5.33. Thus, the acoustic natural frequency of the 1T/1R mode, \( f_{11} \), is \( 1.5 \times 10^4 \) Hz, which is close to the dominant frequency of the flowfield. Considering the impacts of the centerbody and the
existence of the CTRZ, the real frequency of the 1T/1R acoustic mode in the injector would be less than $1.5 \times 10^4$ Hz$^*$. This result suggests that the vortex shedding originating from the Kelvin-Helmholtz instability resonates with the 1T/1R acoustic mode. Similar phenomena have also been observed in Chapter 4 and by Ying et al. (2002). In a confined cavity, such as an injector or a combustion chamber, the natural acoustic frequency depends on the acoustic modes, such as 1L, 1T, 1R, 1T/1R, and so on. If there is not strong flow fluctuation, a small flow oscillation arising from hydrodynamic instability, such as the Kelvin-Helmholtz instability at the shear layer, could resonate an acoustic mode. In other words, the flow oscillation can pick up a special acoustic mode, which satisfies the lock in requirement. Other mechanisms may also contribute to excite this specific acoustic mode in this case. For example, the swirling flow enhances the helical instability, i.e., tangential mode (1T), of the flowfield. The flow through the second passage, $S_2$, could trigger the radial acoustic mode (1R) due to the special geometry and flow conditions. Therefore, the 1T/1R mode dominants the flow pattern in the cross-section.

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$^*$ The high frequency transverse acoustic mode of this kind may considerably add to surface heat transfer in the rocket engine, called “screaming” (Male et al., 1954).
5.8.2 High Swirl Number Flow

The normalized eigenvalues and eigenfunctions of the flow structures for the $x$-$r$ plane in the HSN case are shown in Figs. 5.30 and 5.31. The flow structures of the first two POD modes are very large and correspond to low-frequency flow oscillation. The dominant frequencies include 1,500 Hz and 4,000 Hz, as shown in Fig. 5.32. The magnitudes of fluctuations near the vortex breakdown region and the guide vane are very high. They are responsible for different flow mechanisms along with different frequencies, 1,500 Hz or 4,000 Hz. To identify the mixed frequencies, higher modes are examined. In the third and fourth modes, the dominant flow structures with a frequency of 1,500 Hz are near the guide vane; therefore, the frequency of the similar flow pattern appearing in the first and second modes is 1,500 Hz too. The flow structures near the vortex breakdown region appearing in the first two modes consequently can be referred to as a flow oscillation at the 4,000 Hz. The first two modes also show that the flow structures near the guide vane may strongly interact with the flow pattern resulting from the vortex breakdown because the two flow structures are very close. This further verifies the mode interactions observed in Fig. 5.6 and discussed in the previous sections.

Fig. 5.30 Energies of POD modes in an $x$-$r$ plane, HSN.
Fig. 5.31 First six POD modes in the $x-r$ plane, azimuthal velocity contours, HSN.

Fig. 5.32 Spectra of the time traces of POD modes in the $x-r$ plane, HSN.
The spectra of the time traces shown in Fig. 5.32 indicate that the fifth and sixth modes correspond to a high frequency pattern at 14,000 Hz, \textit{i.e.}, vortex shedding resulting from the Kelvin-Helmholtz instability. The associated flow pattern, shown in Fig. 5.31, is similar to the first two POD modes in the LSN case.

Figure 5.30 shows the energy associated with each POD mode of the HSN case. No dominant pattern/mode is identified; therefore, the energy distribution is quite smooth in comparison with the LSN case.

The flow structures of the POD modes in the cross-section perpendicular to the axial axis are shown in Fig. 5.33 for the HSN case. Compared to the LSN case, these structures are much more complicated. Near the outside boundary, the alternated organized structures represent the flow structures originating from the Kelvin-Helmholtz instability in the azimuthal direction. Dipole structures appear near the axis in the first two modes while quadrupole structures exist in the fourth and fifth modes. These

![Fig. 5.33 First six POD modes in an $r$-$\theta$ plane, pressure contours, HSN.](image-url)
structures stand for the first and second tangential modes whose corresponding frequencies are 2,000 Hz and 4,000 Hz, respectively. Obviously, these modes are not acoustic modes because the frequency of the lowest acoustic tangential mode of the injector is around 5000 Hz. They may be responsible for helical modes associated with the hydrodynamic instabilities.

The 1T/1R acoustic mode, appearing in the LSN case, is not observed in the HSN case. It may be attributed to the irregular, large-scale organized, coherent structures arising from the vortex breakdown. While the vorticity bulbs originating from the evolution of the vortex breakdown are convected to downstream, the vortex shedding due to the Kelvin-Helmholtz instability in the streamwise direction is seriously interrupted, thus cannot stimulate the 1T/1R acoustic mode.

By means of the POD analysis, the complex flow structures are separated into several basic modes and various flow scales, i.e., large and small structures. The decomposition of this type is helpful for achieving a structure-based understanding of the complex flow evolution. Further studies, such as a three-dimensional POD analysis (Freund and Colonius, 2002), are required to provide more insight of the physics.

5.9 Summary

A comprehensive numerical analysis has been conducted to investigate the vortical flow dynamics in a gas-turbine swirl-stabilized injector. Results show that this swirl-stabilized injector is effective in mixing the fuel and air. Several unsteady flow characteristics, such as vortex breakdown, the Kelvin-Helmholtz instabilities in both the axial and azimuthal directions, centrifugal instability, and helical instability, as well as their interactions, are investigated.

The swirl strength significantly affects the flow patterns inside the injector. In the LSN case, the vortex shedding originating from the Kelvin-Helmholtz instability in the streamwise is clearly observed, and the helical mode, \( m = -1 \), is identified. This helical mode also corresponds to the mixed first tangential and first radial acoustic mode, which resonates with vortex shedding resulting from the Kelvin-Helmholtz instability in the
streamwise direction. The associated high frequency is 13,000 Hz, which dominates the flowfield. An apparent bulb style vortex breakdown is also observed in the LSN case while the mean flowfield shows a double vortex breakdown near the centerbody of the injector.

In the HSN case, a higher azimuthal velocity enhances the flow patterns resulting from vortex breakdown, the Kelvin-Helmholtz instability in the azimuthal direction, and centrifugal instability. The vortex shedding due to Kelvin-Helmholtz instability in the streamwise is suppressed in the HSN case and the helical mode also weakens. The flowfield inside the injector is dominated by the irregular, large-scale coherent structures, generated by the vortex breakdown. A uniform dominant frequency is not observed in the HSN case while it appears in the LSN case. Instead, several dominant frequencies are observed in different flow regions, which show that different instability mechanisms may dictate each sub flow region. Because of more complex dynamic evolution in the HSN case, the style of the vortex breakdown cannot be identified.
Chapter 6

Acoustic Response of a Swirl-Stabilized Injector to External Excitation

6.1 Introduction

The dynamics of a system can be conveniently studied by imposing external forcing to the system. Ho and Huerre (1984) conducted a detailed review of perturbed free shear layers. They stated that monochromatic excitation could suppress the broadband background noise and lead to well-organized vortical structures. In addition, single-frequency forcing could considerably delay the appearance of other discrete frequency components, which were observed in free forcing flows.

Brereton et al. (1990) carried out a thorough investigation into the effects of unsteadiness on a well-developed flat-plate turbulent boundary layer by imposing periodic fluctuations downstream. They reported that statistical descriptions of turbulent motions in boundary layers under conditions with and without free-stream oscillations were equivalent to each other over a broad range of forcing frequency.

In contrast to Brereton’s observation for boundary layers, forced oscillations may cause resonance or other profound response within confined cavities, such as combustion chambers of rocket and air-breathing engines. Apte and Yang (2002) studied the unsteady flow evolution in a porous-walled chamber with impressed periodic excitations. They found that periodic excitations led to an earlier laminar-to-turbulence transition than that observed in stationary flows, and that the coupling between the turbulent and acoustic motions resulted in significant changes in the unsteady flow evolution.

In this chapter, the acoustic response of a gas-turbine swirl-stabilized injector studied in Chapter 5 is investigated by imposing periodical external forcing. The computational conditions and data analysis method are described in Section 6.2. In Section 6.3 the responses of the instantaneous flowfields at different forcing frequencies are examined. The resultant mean flowfield and turbulence properties are addressed in
Section 6.4. Several reduced-order data analyses are conducted in Section 6.5, including the spectral analysis of the pressure and velocity data at selected locations and the response function analysis for flow properties at the outlet of the injector. An acoustic admittance function and two mass transfer functions are obtained to characterize the injector dynamics. In addition, the effect of external excitations on the flow structure of the central toroidal recirculation zone is discussed in this section. Finally, a summary is presented in Section 6.6.

6.2 Computational Case Description

The same gas-turbine swirl-stabilized injector studied in Chapter 5 is investigated in this chapter. Chapter 5 illustrates that, when the swirl-stabilized injector is at the high swirl number (HSN), several dominant frequencies are observed in different regions and are associated with different flow instability mechanisms. The injector becomes a distributed dynamic system over a broadband frequency range. This implies that an external excitation implemented on this system might induce considerable response. Therefore, the HSN case, i.e., $S_1 = 45^\circ$, $S_2 = -60^\circ$, and $S_3 = 70^\circ$, is used as the base case in the current study. All external excitations are implemented under this flow condition.

The grid system implemented in the present study is identical to that used in Chapter 5, as well as the numerical discretization and boundary conditions. The externally imposed oscillation is employed by changing the mass flow rate at the inlet as

$$\dot{m} = \dot{m}_0 \left[ 1 + \alpha \sin \left( 2\pi f_F t \right) \right]$$ (6.1)

where $\dot{m}_0$ denotes the mean mass flow rate, $\alpha$ the amplitude, and $f_F$ the forcing frequency. $\alpha$ fixes at 10% in the present work.

A triple decomposition method is used for data analysis in order to examine the effects of the periodical external excitation. This method introduced by Hussain and Reynolds (1970) for incompressible flows is extended to include compressibility effects using density-weighted, i.e., Favre-averaged, ensemble- and time-averaging techniques given below (Apte, 2000):
\[ \bar{u}(x,t) = \bar{u}(x) + u'(x,t) = \bar{u}(x) + u''(x,t) \]

where \( \bar{u}(x) \) represents the density-weighted long time average and \( u'(x,t) \) the fluctuation. \( u'(x,t) \) is further decomposed into \( u''(x,t) \) and \( u''(x,t) \), where \( u''(x,t) \) is the density-weighted phase averaged (ensemble averaged) oscillation and stands for the periodical fluctuation, and \( u''(x,t) \) the turbulent fluctuation.

The externally imposed frequencies are over a broad range from 400 to 13,000 Hz since the nature spectrum of the turbulent swirling flow is broadband in the swirl-stabilized injector at high swirl number. The vortical and acoustic responses to these external excitations will be explored in the following sections.

### 6.3 Responses of Instantaneous Flow Structure

The magnitude of the vorticity fluctuation, including phase averaged oscillation and turbulent fluctuation, at \( f_F = 500, 1,500, 4,000, \) and 13,000 Hz is shown in Fig. 6.1. When the forcing frequency is higher than 1,500 Hz, well-defined vortical structures appear at the forward section of the injector and are convected to the downstream with the local flow velocity, \( i.e., \) a vortical wave, which is stimulated by the high-frequency oscillation of mass flow rate at the inlet.

To investigate the flow pattern associated with the vortical wave, the contours of velocity and pressure fluctuations at \( f_F = 13,000 \) Hz are shown in Fig. 6.2. It illustrates that the vortical wave is mainly allied with the velocity fluctuation in the azimuthal direction and that the pressure fluctuation is associated with the longitudinal acoustic wave. This decoupled phenomenon can be explained by that the transmission of the azimuthal velocity fluctuation is primarily attributed to convection while the axial velocity, radial velocity, and pressure fluctuations at this region are coupled with acoustic oscillation.

When the forcing frequency is 1,500 Hz or lower, it is difficult to observe the aforementioned flow pattern due to the long vortical and acoustic wavelengths associated
with these low forcing frequencies. A reference frequency, \( f_L \approx 11,000 \) Hz, is defined in Section 6.5.2.2 to normalize the forcing frequency.

Figure 6.1 also reveals another interesting phenomenon related with the energy distribution. When the forcing frequency is higher than 1,500 Hz, the magnitude of vorticity fluctuation is redistributed, compared with the flow without forcing. External excitations tend to give rise to a more uniform flowfield. The vorticity field is strengthened in the forward section of the injector, but weakened near the boundary of the CTRZ, a situation opposite to the free-oscillation case.

Two mechanisms account for this phenomenon. First, high frequency oscillation in the time domain results in spatial flow oscillation; therefore, the vorticity field in the forward section strengthens. Second, the high frequency forcing influences the turbulence evolution. For instance, it enhances the energy transfer from the low-frequency/large-scale motions to the high-frequency/small-scale motions, \( i.e. \), it accelerates the energy transfer process in the energy cascade of turbulent flows. In order to explain this mechanism, the triple decomposition is employed on the momentum equations (Brereton et al., 1990; Apte, 2000; Cai, 2001). The induced external excitation leads to an additional pathway to transfer energy between the mean flowfield and turbulent motions. Following their approach, the differential equations describing the transport of variance of turbulent and periodic velocity can be deduced in its component form, yielding coupled time-averaged ‘energy’ equation,

\[
\frac{D}{Dt} \left( \rho u_a^a u_a^a \right) = \cdots - \rho u_a^a u_a^a \frac{\partial U_a^a}{\partial x_i} - \rho u_a^a u_a^a \frac{\partial u_a^a}{\partial x_i} 
\]

\[
\frac{D}{Dt} \left( \rho u_a^a u_a^a \right) = \cdots - \rho u_a^a u_a^a \frac{\partial U_a^a}{\partial x_i} + \rho u_a^a u_a^a \frac{\partial u_a^a}{\partial x_i} 
\]
Fig. 6.1  Magnitude of vorticity fluctuation under conditions without and with external forcing at four different frequencies. \( f_F = 500, 1,500, 4,000, \) and \( 13,000 \) Hz. The fluctuation includes phase averaged oscillation and turbulent motions.
Fig. 6.2 Snapshots of vorticity fluctuation magnitude, velocity, and pressure contours at $f_F = 13,000$ Hz. The fluctuation includes phase averaged oscillation and turbulent motions.
where $D/Dt$ denotes the substantial derivative following the organized motion of fluid, and repeated English subscripts $i$ imply summation while Greek letters imply no summation. Additional terms, such as pressure-strain, diffusion and dissipation are not explicitly written for clarity. In turbulent kinetic energy Eq. (6.3), the $-\rho u^i u^i_\alpha \partial U_\alpha / \partial x_i$ term is responsible for energy transfer of mean flow to turbulent flow, and the $\rho u^i u^i_\alpha \partial u^\alpha / \partial x_i$ term accounts for an additional energy transfer mechanism, which represents the energy transfer from the organized flow oscillations to turbulent motions. The latter term also could be found in Eq. (6.4) except an opposite sign. In organized flow oscillation kinetic energy equation, i.e., Eq. (6.4), the energy transferred from the mean flow to organized flow is accomplished by $-\rho u^i u^i_\alpha \partial U_\alpha / \partial x_i$ term. Obviously, the introduction of the organized flow oscillation provides an additional energy transfer path, as shown in Fig. 6.3, compared to stationary turbulent flows.

When the forcing frequency increases, the length scales of the phase averaging components, $u^i_\alpha$, decrease. Hence, the derivations of these components, i.e., $\partial u^i_\alpha / \partial x_j$, $i, j=1,2,3$, enlarge and consequently improve the energy transfer from large-scale to small-scale turbulent motions.

![Energy exchange mechanism among mean, periodic, and turbulent flowfields.](image)
6.4 Responses of Mean Flowfield and Turbulence Properties

Figures 6.4 and 6.5 show the mean axial and azimuthal velocity contours at \( f_r = 500, 1,500, 4,000, \) and 13,000 Hz. From the mean flowfield point of view, no discernible difference is observed between the flows with and without external forcing except the region near the prefilmer surface at the 13,000 Hz externally imposed excitation. When the forcing frequency is 13,000 Hz, the mean azimuthal velocity magnitude at the probes near the prefilmer region, such as probe 10:03, decreases almost by half. It indicates that the length of the mixing region, induced by the counter-rotating swirling flows, shortens. Dismissing this exception, the effects of forced oscillation on mean flow properties in the injector appear to be slight.

The turbulence properties under the four external excitation frequencies are presented in Figs. 6.6-6.8, representing turbulence intensities in the axial and azimuthal directions, and turbulent kinetic energy, respectively. In comparison with the free oscillation flow, the turbulent kinetic energy with forcing increases slightly, so are the turbulence intensities. There are only a few exempt points. First, when the forcing frequency is 13,000 Hz, the turbulence intensities in the downstream of the two guide vane lips, \( i.e., \) probes 05:01 and 21:01, change considerably. Because the natural frequencies of the strong shear layers in these regions are very close to the forcing frequency, the mixing process at the two shear layers are enhanced. The turbulence intensities and the turbulent kinetic energy accordingly increase. At the same time, due to the more rapid mixing process, the length of the mixing region decreases as shown in Fig. 6.5. Second, when the forcing frequency is 4,000 Hz, the turbulence intensities of flow region near the fuel nozzle, \( i.e., \) probe 09:04, increase apparently. Because the mean flow separation point anchors in this region, it is a critical point to the structure of the whole flowfield. This phenomenon implies that the influence of the forced oscillation on the dynamic flow motions in the injector may be significant, which will be investigated in detail in the following section.
Fig. 6.4 Axial velocity contours of mean flowfields (spatially averaged in the azimuthal direction) under conditions without and with external forcing at four different frequencies. $f_F = 500$, 1,500, 4,000, and 13,000 Hz.
Fig. 6.5 Azimuthal velocity contours of mean flowfields (spatially averaged in the azimuthal direction) under conditions without and with external forcing at four different frequencies. $f_F = 500$, 1,500, 4,000, and 13,000 Hz.
Free oscillation

f_F = 500 Hz

f_F = 1500 Hz

f_F = 4000 Hz

f_F = 13000 Hz

Fig. 6.6 Axial component of turbulence intensity (spatially averaged in the azimuthal direction) under conditions without and with external forcing at four different frequencies. f_F = 500, 1,500, 4,000, and 13,000 Hz.
Fig. 6.7 Azimuthal component of turbulence intensity (spatially averaged in the azimuthal direction) under conditions without and with external forcing at four different frequencies. $f_F = 500, 1,500, 4,000, \text{ and } 13,000 \text{ Hz.}$
Fig. 6.8  Contours of turbulent kinetic energy (spatially averaged in the azimuthal direction) without and with external forcing at four different frequencies. $f_F = 500, 1,500, 4,000,$ and 13,000 Hz.
Although there are some minor differences in the mean flowfield and turbulence properties under different external excitations, it is still proper to conclude that the statistical descriptions of the turbulent motions in the swirl-stabilized injector, with and without externally imposed oscillations, appear to be equivalent over a broad range of forcing frequency from the global viewpoint. Two reasons may account for this phenomenon. First, the flow structures in these regions are very complex and their intensities are relatively high; therefore, a weak forced oscillation could not adjust the mean flow patterns considerably. Because of the distributed system characteristics of the flowfield, we cannot expect that the external forcing at a single frequency could induce a noticeable response on the mean flowfield unless that frequency happens to cause resonance of the injector (Brereton et al., 1990). Second, the acoustic wavelengths of the forcing frequencies except 13,000 Hz are much longer than the injector dimensions, thus it is difficult to observe considerable change from the mean flowfield point of view.

### 6.5 Dynamic Response

In order to investigate the dynamic response of the system, the spectral analyses of the pressure and velocity, and several response functions are carried out in this section.

#### 6.5.1 Spectral Analysis

Figure 6.9 (a-f) shows the spectra of the pressure oscillations under 500, 1,500 and 4,000 Hz forced oscillations at six selected probes, 07:01, 25:01, 05:04, 10:09, 14:05, and 14:09, respectively. The probe locations are shown in Fig. 5.21. Probes 07:01 and 25:01 are located in the main passage of the injector; probes 05:04 and 10:09 in the region leaded by the vortex shedding originating from the Kelvin-Helmholtz instability; and probes 14:04 and 14:09 near the boundary of the CTRZ, in which vortex breakdown is the dominant flow pattern.

In comparison with the free forcing flow, a dominant peak corresponding to the forcing frequency, i.e., 500Hz, 1,500Hz, or 4,000Hz, is clearly observed in pressure spectra, shown in Fig. 6.9, in the forcing flows. It indicates that the forcing affects the
dynamic behavior of the flowfield considerably. At each probe, the oscillation magnitude achieves the maximum at $f_F = 1500$ Hz, which implies that the system response reaches to the maximum at this forcing frequency. The following sections will verify this statement from several different ways. This forcing frequency also excites the spectral range close to 1,500 Hz as shown in Fig. 6.9, which is not noticeable in the forcing studies at other excitation frequencies, such as 500 or 4,000 Hz. Although the dominant peak is observed in each pressure spectrum at 500 or 4,000 Hz frequency forcing, the excited range is normally narrow except the probes near the CTRZ at 4,000 Hz forcing, where the natural frequency of the CTRZ is 4,000 Hz.

Figure 6.10 is the velocity component spectra of probes 13:06, 14:10, and 10:03 at forcing frequency $f_F = 4000$ Hz. At probe 13:06, the responses of the axial and azimuthal velocities are very high. The forcing frequency, however, is difficult to identify at probe 14:10, which is located at the boundary of the CTRZ. In other words, in comparison with the intensity of natural vortical dynamic evolution, the response arising from the external excitation in the vortex breakdown flow region appears to be very small. The similar behavior is also observed at probe 10:03 although the strong vortical dynamic evolution in this region originates from the Kelvin-Helmholtz instabilities.

This reason for the different responses is that probe 13:06 is located out of the two high turbulent kinetic energy regions, while probes 10:03 and 14:10 are in. Because the flow motion at probe 13:06 is comparatively simple, the mass and angular momentum conservations can preserve the axial and azimuthal velocity oscillations convecting from the upstream. In contrast, the natural flow fluctuations resulting from the inherent hydrodynamic instabilities at probes 10:03 and 14:10 are very strong; therefore, the external excitations at the upstream do not cause significant response at these regions. At probe 14:10, the strong recirculation flow further disturbs the incoming excitation from the injector inlet.
Fig. 6.9  Comparison of pressure spectra, (a) probe 07:01.

Fig. 6.9  Comparison of pressure spectra, (b) probe 25:01.
Fig. 6.9  Comparison of pressure spectra, (c) probe 05:04.

Fig. 6.9  Comparison of pressure spectra, (d) probe 10:09.
Fig. 6.9  Comparison of pressure spectra, (e) probe 14:05.

Fig. 6.9  Comparison of pressure spectra, (f) probe 14:09.
Fig. 6.10 Comparison of velocity spectra, (a) probe 13:06.
Fig. 6.10 Comparison of velocity spectra, (b) probe 14:10.
Fig. 6.10 Comparison of velocity spectra, (c) probe 10:03.
One point needs to be noted at here. The pressure field is more sensitive to the external forcing compared to the velocity. The forcing frequency always prevails in the pressure spectrum, but it disappears in the velocity spectrum at some probe locations, such as \( f_\text{F} = 4,000 \text{ Hz} \) at probe 14:10. The velocity responses, especially the radial and azimuthal components, are very weak in the recirculation or strong shear layer zone. While the flow fluctuations travel to the downstream via the vortical waves, the azimuthal and radial velocity oscillations decrease due to viscous dissipation and turbulence. The pressure oscillation, on the other hand, propagates at the local acoustic wave speed, which is not very sensitive to these damping effects.

### 6.5.2 Response Functions

Besides the discretized information obtained in the spectral analysis, an admittance function and two transfer functions, which are associated with the mass flux and flow rate, are examined in this section to study the acoustic response of the injector from the global viewpoint.

#### 6.5.2.1 Admittance Function

The admittance function, \( A \), is defined as

\[
A(f) = \frac{\hat{a}^v / \bar{a}}{\hat{p}^v / \gamma \bar{P}}
\]

where \( \bar{a} \) and \( \gamma \bar{P} \), denoting the mean acoustic speed and mean modified static pressure, are introduced for normalization. The admittance function is the reciprocal of the impedance function and is usually used to assess the velocity fluctuation arising from the pressure fluctuation. Because the primary and secondary breakups of the spray are strongly coupled with the velocity fluctuation, the admittance function is an important parameter in studying the change of the velocity fluctuations induced by the pressure oscillation, which usually exists in the combustor chamber while the combustion instability occurs.
Figure 6.11 shows the radial distribution of the admittance function at the injector exit, $x = 28$ mm, at four different forcing frequencies, i.e., 500, 900, 1,500, and 4,000 Hz. This cross-section is the interface between the injector and the combustor chamber, so the result can conveniently be used as the acoustic boundary conditions of the combustor chamber in future reduced-order mode analysis.

A common phenomenon in Fig. 6.11 is that the magnitude of the admittance function near the upper boundary is higher than that in the central region. This phenomenon may be attributed to the large pressure oscillation in the CTRZ, in which both the evolution of the large coherent structures resulting from the vortex breakdown and high pressure gradient originating from the strong swirling flow near the axis region could induce high pressure oscillation. Another important observation is that the admittance function magnitude achieves its maximum at 500 Hz forcing, especially near the upper boundary/prefilmer where the breakup of liquid film occurs. This implies that a small pressure oscillation at 500 Hz may result in a large velocity disturbance; the
velocity disturbance could consequently influence the spray breakup process at this region. This characteristic of the injector could be a potential trigger of a low frequency combustion instability appearing in the combustor chamber (Cohen and Hibshman, 1997).

### 6.5.2.2 Transfer Functions

The transfer function is commonly implemented to investigate the correlation between the output and input of a system. In this study, it presents the oscillation response at the exit of the injector to the external forcing at the inlet. Two transfer functions related with mass flux and mass flow rate are studied individually.

- **Mass flux distribution**

  The transfer function of the normalized mass flux is defined as

  \[
  T(f) = \frac{\tilde{m}_{out}^a \cdot A_{out}}{\tilde{m}_{in}^a \cdot A_{in}}
  \]  

  (6.6)

  where \( A_{out} \) and \( A_{in} \), representing the areas of the outlet and the inlet of injector, respectively, are introduced for the purpose of normalization. The inlet reference point is at probe 02:01 and the outlet is defined at \( x = 28 \text{ mm} \). This function is in aid of examining the dynamic distribution of mass flux.

  The mass flux transfer function, shown in Fig. 6.12, clearly demonstrates that the distribution of mass flux oscillation is significantly adjusted by the external excitation. For the 500 Hz frequency forcing, the magnitude is almost uniform in the range of 0.85 ~ 1.23. And it is in the range of 0.91 ~ 1.45 and achieves the maximum near the boundary of the recirculation zone for the 900 Hz forcing. The phase difference is around \( \pi \) indicating that the compressibility effect is extremely weak.

  When the forcing frequency is 1,500 Hz, the magnitude of the transfer function is greater than 2 near the upper boundary and less than unity near the recirculation zone. This phenomenon suggests that the 1,500 Hz forcing boosts the flow oscillation near the upper boundary where the dominant frequency without external forcing is 1,500 Hz, as
Fig. 6.12 Transfer function I (x = 28 mm): normalized mass flux distribution at 500, 900, 1,500, and 4,000 Hz external excitations.

presented in Fig. 5.23. The 1,500 Hz flow motion is considered as the competition between the vortex breakdown and the Kelvin-Helmholtz instability as described in Chapter 5. An external excitation at this frequency may dictate the dominant flow mechanism in the flowfield, so the 1,500 Hz external forcing modulates the flow motion in the injector considerably.

In a striking contrast, the 4,000 Hz frequency forcing does not exert discernible influence near the upper boundary since the magnitude is very low. Although a peak exists near the boundary of the central recirculation zone, where the natural frequency is around 4,000 Hz, the response within the central recirculation zone is still weak. The phase difference associated with the 4,000 Hz forcing disparts from $\pi$ noticeably, suggesting a considerable compressibility effect. The phase difference will be studied using the second transfer function in detail.

The present results demonstrate that the dynamic distribution of mass-flux fluctuation greatly depends on the forcing frequency although the profiles of the mean
mass flux are almost identical. This mass flux dynamic redistribution process could change the air/fuel distribution and mixing in the downstream, and further influence the combustion instability, emission, and soot generation.

- Mass flow rate

Besides the investigation of the mass flux distribution, the total mass flow rate is also studied as the second transfer function for exploring the overall acoustic characteristics. The response of the total mass flow rate at the exit is defined as

\[ M(f) = \frac{\hat{m}_{\text{out}}^a}{\hat{m}_{\text{in}}^a} \]  

(6.7)

Figure 6.13 shows the mass flow rate as a function of the forcing frequency. The fluctuations of the inlet and outlet mass flow rates are almost in-phase at the forcing frequency of 500 Hz because the flow is almost incompressible at this frequency. A

![Graph showing mass flow rate as a function of forcing frequency](image)

Fig. 6.13 Transfer function II \((x = 28 \text{ mm})\): normalized mass flow rate at 500, 900, 1,500, and 4,000 Hz external excitations. (a) magnitude and (b) phase.
phase shift, \( i.e. \), the compressible effects, is observed when the forcing frequency is 1,500 Hz or higher.

A characteristic frequency based on the flow conditions in the injector is estimated to study the phase-shift phenomenon. Assume the streamwise length from the inlet to the outlet is \( L \approx 30 \text{ mm} \) and the speed of sound \( \bar{a} \approx 340 \text{ m/s} \), then the phase difference, \( \theta \), of a traveling acoustic wave between the inlet and outlet satisfies

\[
\theta = \frac{2\pi L f_f}{\bar{a}} = 2\pi \frac{f_f}{f_L} \tag{6.8}
\]

where the acoustic characteristic frequency \( f_L \) is given by

\[
f_L = \frac{\bar{a}}{L} \approx 11,000 \text{Hz}. \tag{6.9}
\]

Because \( f_L \) is linked with the acoustic characteristics of the baseline conditions, it can be considered as a reference frequency for studying the acoustic behavior of the injector.

Figure 6.13 illustrates a very good agreement between acoustic analysis, Eq. (6.8), and numerical simulation, Eq. (6.7), and demonstrates that the oscillation of the mass flow rate propagates in the form of acoustic wave. The magnitude of the mass flow rate transfer function achieves its maximum at 1,500 Hz as expected, so it further proves that the 1,500 Hz is the dominant response frequency of this injector. The mean mass flow rate is well conserved in the simulation; however, the large disparity of the mass flow rate fluctuations between inlet and outlet is observed in the instantaneous flowfield, especially at 1,500 Hz forcing. In summary, the forcing frequency affects not only the spatial distribution of mass flux, but also the spectral distribution of the mass flow rate.

### 6.5.3 Dynamic Evolution of CTRZ

To the author’s knowledge, the effects of the external excitation on the CTRZ have not been studied up-to-date. Considering the importance of the CTRZ in swirling flows, it is necessary to investigate its dynamic response to the external excitation.
Fig. 6.14 Normalized radius fluctuation of CTRZ versus the forcing frequency. (a) magnitude and (b) phase.

The radius of the CTRZ, \( r_c \), based on the spatially averaged flowfield, is introduced to examine the effects of external forcing process on the overall CTRZ structures. The definition of \( r_c \) is

\[
\bar{\rho} \bar{u}_r r \, dr = 0
\]

(6.10)

at the exit of the injector, \( x = 28 \) mm. The operator \( \bar{\cdot} \) represents the spatial averaging in the azimuthal direction. The above equation implies that the net mass flow rate between the flowfield \( 0 \leftrightarrow r_c \) is zero. The normalized radius is defined as

\[
R_c(f) = \frac{\bar{\rho}^a / \bar{\rho}_c}{\bar{\rho}^a / \bar{\rho}_c} = \frac{\bar{\rho}^a / \bar{\rho}_c}{\bar{\rho}^a / \bar{\rho}_c}
\]

(6.11)

where \( R_c \) denotes the normalized CTRZ radius fluctuation as a complex and is shown in Fig. 6.14.
The phase of the radius fluctuation is out of phase ($\pi$) with that of the mass flow rate at the injector outlet, which suggests that not only the flow mass flux magnitude but also the effective passage area varies while excitation is implemented. The detailed oscillating process is shown in Fig. 6.15, which represents the streamlines of the spatially averaged flowfields in a period at 1,500 Hz external forcing. The variation of the CTRZ structure in one cycle is very clear: the CTRZ size shrinks to the minimum when the mass flow rate achieves to the maximum, and vice versa. This represents an interaction between the CTRZ and the mass flow rate due to the external excitation, and indicates that further efforts are required to uncover the effects of the external imposed excitation on the vortex breakdown.

The above observation seems to conflict with the results of the spectral analysis studied in Section 6.5.1, where we do not observe strong velocity response near the boundary of the CTRZ at the 1,500 Hz forcing. This is contributed to the reduced-order data analysis, implemented to process the complex three-dimensional data. The turbulent swirling flow is fully three-dimensional along with strong helical structures, large-scale intermittent vortical evolution, and high background noise, so the information at a single point used in the spectral analysis may not correctly present the real flow evolution. The spatial averaging in the azimuthal direction efficiently screens the influence of helical motions, and reduces the background noise originating from the turbulent fluctuations. Therefore, this reduced-order data analysis improves the understanding of the complex flowfield and phenomena.

6.6 Summary

The acoustic responses of a gas-turbine swirl-stabilized injector over broadband externally imposed excitations are investigated comprehensively in this chapter. The baseline flow condition is the high swirl number flow studied in Chapter 5.
Fig. 6.15 Instantaneous flowfield evolution in a cycle at 1,500 Hz external forcing frequency (spatial averaged in the azimuthal direction). The blank circle on the dash line denotes the time mean CTRZ radius.
The convection of vortical waves arising from the external excitation is clearly observed at high forcing frequency. The external forcing influences the turbulence evolution by means of an additional path to transfer energy between the mean flowfield and turbulent motions. Higher frequency forcing improves this energy transfer process.

Results of the forced oscillation flows indicate that the effects of imposed oscillations on the mean flow and turbulence properties appear to be rather small. The response of the flow in the main effective passage is sensitive to the forcing oscillation while that in either the central recirculation or the vortex shedding zone is not. The vortex breakdown phenomenon is also insensitive to forced oscillations from the spectral analysis point of view.

The admittance function is introduced to study the acoustic response. The results show that the magnitude of the admittance function reaches a maximum value near the second flow splitter at a forcing frequency of 500 Hz, suggesting a potential triggering mechanism for low-frequency instability in a combustion chamber.

Two transfer functions corresponding to the mass flux and mass flow rate show that the dynamic flow distribution is significantly modulated by the external imposed excitation in both spatial and spectral domains. The flow motion response achieves the maximum at 1,500 Hz forcing frequency. Meanwhile, the transfer function of the mass flow rate illustrates the existence of the compressibility effects, although the mean flow velocity in most flow regions falls in the incompressible flow regime, i.e., $\bar{M} < 0.3$.

A reduced-order data analysis successfully demonstrates that the radius of the central recirculation zone varies at a phase shift of $\pi$ with the mass flow rate at the injector exit, which indicates that the total mass flow rate oscillation consists of two parts, the mass flux and the effective flow area variations.
Chapter 7
Conclusions and Future Work

7.1 Conclusions

The present work has addressed a wide variety of basic and practical issues related to the modeling and analysis of flow dynamics in gas-turbine swirl-stabilized injectors. The approach accounts for fundamental physics, and takes advantages of recent advances in parallel computing architecture. A unique aspect of this work is its comprehensive investigation into the flow dynamics and acoustic response of swirl-stabilized injectors on which very little has been studied to date. The present study also demonstrates the capability of large eddy simulation (LES) for studying the unsteady evolution of highly complex turbulent swirling flows.

The theoretical formulation includes complete conservation equations of mass, momentum, and energy in three dimensions, along with a large eddy simulation technique for turbulence closure. A density-based, finite-volume approach with low-dissipation explicit time marching is employed in this numerical simulation. The program is further parallelized using a domain decomposition method (DDM) in conjunction with the message-passing interface (MPI) library.

The code was first validated against the experimental data for the swirling flow in a dump chamber in terms of mean flow quantities and turbulence properties. After validation, the flow evolution in both a dump chamber and a swirl-stabilized injector were investigated in detail. Several instability mechanisms, such as vortex breakdown, the Kelvin-Helmholtz instabilities in both the streamwise and azimuthal directions, and helical instability, as well as the interactions and competitions among those instability modes, are clearly identified. The swirl number plays a critical role in determining the dominant flow mechanism. It influences the competitions among different unsteady flow motions, and consequently dictates the dominant flow pattern that could eventually alter the acoustic resonance modes.
Because the frequency spectrum of the intrinsic flowfield is broadband, the influences of external excitations on the mean flow structures and turbulence properties appear to be limited. The dynamic behavior, such as the instantaneous mass flux distribution and acoustic admittance characteristics, however, are significantly modulated in both the spatial and spectral domains. Information of these kinds can be used effectively to characterize the dynamic behavior of the injector. Results are critical to injector design optimization in terms of the mixing, flame stabilization, and combustion stability characteristics.

Several data analysis techniques are developed and implemented for processing the numerical results of the complex flowfields. For example, the data reduction procedure based on a spatial averaging technique helps extract information about the flow development and dominant flow mechanisms; the proper orthogonal decomposition (POD) method identifies the strongest energy-carrying flow structures; and the spectral analysis for both point data and multi-dimensional POD fields gives rise to a structure-based physical understanding. Various important flow patterns are clearly revealed through the above methods, further verifying the effectiveness of these data analysis methods in analyzing complex flow evolution.

7.2 Future Work

Since the flowfield in a gas-turbine injector involves a broad range of time and length scales characterizing the local flow evolution and its acoustic and vortical behavior, a more efficient time-marching scheme, such as a preconditioning method, should be considered in the future.

After a comprehensive study of the single-phase flow is conducted, an analysis will be carried out to explore the spray-field dynamics and its associated combustion. An Eulerian-Lagrangian approach that accommodates the mass, momentum and energy exchange in a manner completely consistent with the LES framework will be employed.

Finally, a high-performance numerical method taking advantage of contemporary and projected massive parallel computing architecture should be established to study the two-phase chemically reacting flows in gas-turbine combustors.


Kundu, P. (1990), Fluid Mechanics, Academic.


Appendix A

Closure of Filtered Total Energy Term

To calculate $\bar{\rho} E$ term in Eq. (2.19) through averaged valuables $\bar{\rho}$ and $\bar{u}_i$, we apply

$$
\bar{\rho} E = \bar{\rho} \left( \bar{e} + \frac{1}{2} \bar{u}_i \cdot \bar{u}_i \right)
= \bar{\rho} \left( \bar{e} + \frac{1}{2} \bar{u}_i \cdot \bar{u}_i \right) + \frac{1}{2} \bar{\rho} (u_i \cdot u_i - \bar{u}_i \cdot \bar{u}_i)
= \bar{\rho} \left( \bar{e} + \frac{1}{2} \bar{u}_i \cdot \bar{u}_i \right) + \frac{1}{2} \tau_{ii}^{SGS}
$$

(A.1)

The Smagorinsky compressible flow SGS model

$$
\tau_{ii}^{SGS} = 2 \bar{\rho} \kappa^{SGS} = 2 C_f \bar{\rho} \Delta^2 \bar{S}_{ij} \bar{S}_{ij}
$$

(A.2)
Appendix B

Properties of Adam-Bashforth Predictor-Corrector Scheme

B.1 Scheme Accuracy

The Adam-Bashforth predictor-corrector scheme includes two steps: predictor step and corrector step. It is repeated here for the reader's convenience as follows:

Predictor step:

\[
Q^* = Q^n + \frac{\Delta t}{2} (3R(Q^n) - R(Q^{n-1})) \tag{3.39}
\]

Corrector step:

\[
Q^{n+1} = Q^n + \frac{\Delta t}{12} (5R(Q^*) + 8R(Q^n) - R(Q^{n-1})) \tag{3.40}
\]

Taking the Taylor series expansion of Eq. (3.39) at the time \( n \) step and substituting \( \frac{d}{dt}(\cdot) \) into Eq. (3.39), then Eq. (3.39) can be rewritten as

\[
Q^* = Q^n + \frac{\Delta t}{2} \left[ 3 \frac{dQ^n}{dt} - \left( \frac{d^2Q^n}{dt^2} \Delta t + \frac{d^3Q^n}{dt^3} \frac{\Delta t^2}{2} + O(\Delta t^3) \right) \right]. \tag{B.1}
\]

Application of \( d(\cdot)/dt \) on both sides of Eq. (B.1) yields

\[
\frac{dQ^*}{dt} = \frac{dQ^n}{dt} + \frac{d^2Q^n}{dt^2} \Delta t + \frac{d^3Q^n}{dt^3} \frac{\Delta t^2}{2} - O(\Delta t^3) \tag{B.2}
\]

Substitution of Eq. (B.2) into Eq. (3.40) gives
\[ Q^{n+1} = Q^n + \frac{\Delta t}{12} \left( 5 \frac{dQ^n}{dt} + 8 \frac{dQ^n}{dt} - \frac{dQ^n}{dt} \right) \]

\[ = Q^n + \frac{\Delta t}{12} \left[ 5 \left( \frac{dQ^n}{dt} + \frac{d^2Q^n}{dt^2} \right) - \frac{d^3Q^n}{dt^3} \Delta t \right] + O(\Delta t^4) \]  

(B.3)

\[ = Q^n + \frac{dQ^n}{dt} \Delta t + \frac{d^2Q^n}{dt^2} \frac{\Delta t^2}{2} + \frac{d^3Q^n}{dt^3} \frac{\Delta t^3}{3} + O(\Delta t^4) \]

B.2 von Neumann Stability Analysis

Following the procedure of von Neumann analysis (Merkel and Yu, 1997) and assuming

\[ R^n = AQ^n \]  

(B.4)

and

\[ Q^{n+1} = GQ^n = G^2Q^{n-1} \]  

(B.5)

where the matrix \( A \) depends on the spatial discretization of the convection and artificial dissipation terms. In the Navier-Stokes equations, both the viscous and sgs modeling terms will be involved. Substitution of Eqs. (B.4) and (B.5) into Eqs. (3.39) and (3.40) yields

\[ Q^* = Q^n + \frac{\Delta t}{2} (3AQ^n - AQ^{n-1}) \]  

(B.6)

\[ Q^{n+1} = Q^n + \frac{\Delta t}{12} (5AQ^* + 8AQ - AQ^{n-1}) \]  

(B.7)

After substituting Eq. (B.6) into Eq. (B.7) and reorganizing, we have

\[ G - \left( I + \frac{13}{12} Z + \frac{15}{24} Z^2 \right) + \left( \frac{1}{12} Z + \frac{5}{24} Z^2 \right) G^{-1} = 0 \]  

(B.8)

where \( Z = \Delta t \cdot A \).
The amplification factor is the maximum absolute value or norm between the two roots of Eq. (B.8). The matrix $G$ should be diagonalized in order achieve the norm of the amplification factor:

$$\hat{G} = M^{-1}GM$$

where $M$ and $\hat{G}$ are the modal matrix and diagonalized form of $G$. If only the one-dimensional Euler equations are concerned, we have

$$\hat{G}^{i,2} = \frac{-b_i \pm \sqrt{b_i^2 - 4a_ic_i}}{2a_i} \quad i = 1, 2, 3$$  \hspace{1cm} (B.9)

where

$$a_i = 1$$

$$b_i = -1 - \frac{13}{12} \lambda_i - \frac{15}{24} \lambda_i^2$$

$$c_i = \frac{1}{12} \lambda_i + \frac{5}{24} \lambda_i^2$$

$$\lambda_i, 1, 2, 3 = u + c, u, u - c$$  \hspace{1cm} (B.10)
Appendix C

Proper Orthogonal Decomposition

The Proper Orthogonal Decomposition (POD) (Holmes, Lumley and Berkooz, 1998) uses data to generate a set of basis functions/modes that optimally represent the flow’s energy as defined by user-selected norm. The basis is optimal in the sense that a finite number of these orthogonal modes represent more of the flow energy than any other set of orthogonal modes. For this reason, the POD is often used to identify the most energetic contribution and to obtain the spatial structure of the corresponding mode.

Given a set of data, represented as a function of space and time, the POD determines a basis set of orthogonal functions of space that span the data optimally in the $L^2$ sense. For example, if the pressure, $p(x, t)$, is a function of space and time, then POD can determine the orthogonal functions $\varphi_j(x)$, $j=1,2,\ldots$, so that the projection onto the first $n$ functions

$$\hat{p}(x, t) = \bar{p}(x) + \sum_{j=1}^{n} a_j(t) \varphi_j(x) \quad (C.1)$$

has the smallest error, defined by $E(\|p - \hat{p}\|^2)$. Here, $a_j(t)$ represents the time trace of the $j$ mode, $E(\cdot)$ and $\|\cdot\|$ denote time average and the $L^2$ norm on functions of space, respectively (Rowley et al., 2000).

C.1 $L^2$ Norm and Inner Production

The selection of the $L^2$ norm affects the final POD modes. For incompressible flows, it is relatively simple and the fluctuation kinetic energy is typically taken as the $L^2$ norm (Freund and Colonius, 2002). In the present study, the acoustic is also our concern; therefore, the pressure field is also included. The $L^2$ norm is defined as
\[ \| q \| = \int_{\Omega} \left( \alpha_1 u'^2 + \alpha_2 v'^2 + \alpha_3 w'^2 + \alpha_4 p'^2 \right) dV \] (C.2)

where \( \Omega \) is the region of the concern and the constants \( \alpha = (\alpha_1, \alpha_2, \alpha_3, \alpha_4) \) determine the specific form of the \( L^2 \) norm. For example, \( \alpha = (1, 1, 1, 0) \) and \( \alpha = (0, 0, 0, 1) \) represent the fluctuation kinetic energy and pressure norms, respectively.

The inner production associated with the \( L^2 \) norm, defined in Eq. (C.2), is

\[ \left\langle q_i, q_j \right\rangle = \int_{\Omega} \left( \alpha_1 u_i' u_j' + \alpha_2 v_i' v_j' + \alpha_3 w_i' w_j' + \alpha_4 p_i' p_j' \right) dV \] (C.3)

where

\[ q_i \equiv q(x, t_i) \] (C.4)

This integration is easy to achieve in a uniform grid system. As for the non-uniform grid, such as the grid implemented in the present work, a weight, \( \Delta V \), associated with each cell must be involved. Therefore, the numerical implementation of Eq. (C.3) is

\[ \left\langle q_i, q_j \right\rangle = \sum_{l=1}^{k} \left( \alpha_1 u_i' u_j' + \alpha_2 v_i' v_j' + \alpha_3 w_i' w_j' + \alpha_4 p_i' p_j' \right) \Delta V_n_i \] (C.5)

where \( n_i, l = 1, 2, \ldots, k \) represent the cell of concern, and \( \Delta V \) the volume of the cell.

### C.2 Procedure of Calculating POD Modes and Simple Properties

The method of snapshots is employed in the present work to compute the POD modes. Assume that a total of \( T \) snapshots is used to compute the POD modes and each timestamp is denoted as \( t_i \).

- **POD modes**

  In order to obtain the POD modes, we must calculate the eigenvalue, \( \lambda_k \), and eigenvector, \( a^k = [a_1^k, a_2^k, \ldots, a_T^k]^T \), of matrix \( M \) firstly

\[ Ma^k = \lambda_k a^k \] (C.6)

where matrix \( M \) is the inner product of the snapshots
\[ M_q = \langle q_i, q_j \rangle \]  
\hspace{1cm} (C.7)

and

\[ a_i^\top a_j = \delta_{ij}, \quad \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r \]  
\hspace{1cm} (C.8)

Then, the \( j \)th POD mode is

\[ \varphi^j(x) = \sum_{i=1}^r a_i^j q_i \]  
\hspace{1cm} (C.9)

- **Snapshot reconstruction**

  Multiplying eigenvector \( a_i^j \) and summing index \( j \) on both sides of Eq. (C.9) yields

\[ q_i = \sum_{j=1}^r a_i^j \varphi^j(x) \]  
\hspace{1cm} (C.10)

The eigenvector \( a_i^j \) also is the projection of \( q \) onto the \( j \)th POD mode.

- **POD mode property**

  Based on Eqs. (C.6)-(C.10), we have

\[ \langle \varphi^j, \varphi^j \rangle = \left( \sum_{i=1}^r a_i^j q_i, \sum_{m=1}^r a_m^j q_m \right) \]
\[ = \sum_{i=1}^r a_i^j \sum_{m=1}^r \langle q_i, q_m \rangle a_m^j \]
\[ = \sum_{i=1}^r a_i^j M_{im} a_m^j \]
\[ = \sum_{i=1}^r a_i^j \lambda_i a_i^j \]
\[ = \lambda_j \delta_{ij} \]  
\hspace{1cm} (C.11)

- **Average mean energy**

  In order to check the averaged mean energy of \( q \) over the domain reconstructed by the first \( N \) POD modes, we define
\[ E^{(N)} = \frac{1}{2} \langle q^{(N)} , q^{(N)} \rangle = \frac{1}{2T} \sum_{i=1}^{T} \langle q_{i}^{(N)} , q_{i}^{(N)} \rangle \]
\[ = \frac{1}{2T} \sum_{i=1}^{T} \left( \sum_{n=1}^{N} \alpha_{i}^{n} \varphi^{n} \right) \sum_{m=1}^{N} \alpha_{i}^{m} \varphi^{m} \]
\[ = \frac{1}{2T} \sum_{n=1}^{N} \sum_{m=1}^{N} \langle \varphi^{n} , \varphi^{m} \rangle \sum_{i=1}^{T} \alpha_{i}^{n} \alpha_{i}^{m} \]
\[ = \frac{1}{2T} \sum_{n=1}^{N} \lambda_{n} \]
Appendix D

Non-Reflection Boundary Conditions in Generalized Coordinates

The three-dimensional Euler equations in the generalized coordinate can be written in terms of linearized vector form as:

\[
\frac{\partial \tilde{Q}}{\partial t} + A \frac{\partial \tilde{Q}}{\partial \xi} + B \frac{\partial \tilde{Q}}{\partial \eta} + C \frac{\partial \tilde{Q}}{\partial \zeta} = 0
\] (D.1)

with Jacobian matrix

\[
A = \frac{\partial E}{\partial \tilde{Q}}, \quad B = \frac{\partial F}{\partial \tilde{Q}}, \quad C = \frac{\partial G}{\partial \tilde{Q}}
\] (D.2)

where

\[
\tilde{Q} = \frac{Q}{J} \\
\hat{E} = (\xi, E + \xi, F + \xi, G)/J \\
\hat{F} = (\eta, E + \eta, F + \eta, G)/J \\
\hat{G} = (\zeta, E + \zeta, F + \zeta, G)/J \\
J^{-1} = \frac{\partial(x, y, z)/\partial(\xi, \eta, \zeta)}
\] (D.3)

The Jacobian matrix \( A \) can be transformed to a diagonal matrix by the similarity transformation defined by

\[
A = M_{\xi} \Lambda_{\xi} M^{-1}_{\xi}
\] (D.4)

where \( \Lambda_{\xi} \) is the diagonal matrix of eigenvalue associated with the Jacobian matrix \( A \). The eigenvalues \( \lambda_i, i = 1, 2, \ldots, 5 \) are in an ascending sequence. Matrices \( M_{\xi} \) and \( M^{-1}_{\xi} \) represent the right and left eigenvector of matrix \( A \), respectively. Substituting Eq. (D.4) into (D.1), and multiplying by \( M^{-1}_{\xi} \) yields
\[ M^{-1}_\xi \frac{\partial \hat{\Theta}}{\partial t} + \Lambda_\xi M^{-1}_\xi \frac{\partial \hat{\Theta}}{\partial \xi} + M^{-1}_\xi D = 0 \]  \hspace{1cm} \text{(D.5)}

where

\[ D = B \frac{\partial \hat{\Theta}}{\partial \eta} + C \frac{\partial \hat{\Theta}}{\partial \xi}. \]  \hspace{1cm} \text{(D.6)}

Define a new function \( V \) by

\[ dV = M^{-1}_\xi d\hat{\Theta} + M^{-1}_\xi D dt \]  \hspace{1cm} \text{(D.7)}

and Eq. (D.5) is written in terms of \( V \)

\[ \frac{\partial V}{\partial t} + \Lambda_\xi \frac{\partial V}{\partial \xi} = 0 \]  \hspace{1cm} \text{(D.8)}

Equation (D.8) is a set of wave equations for waves with characteristic velocity \( \lambda_i \). For a perfectly nonreflecting boundary condition, the amplitude of the incoming wave must be independent of time at the boundary, \( i.e., \) no incoming wave. Mathematically, this condition can be expressed as

\[ \left. \frac{\partial V}{\partial t} \right|_{\text{boundary}} = 0 \text{ for incoming waves} \]  \hspace{1cm} \text{(D.9)}

The outgoing waves depend only on information at and within boundary. Thus those equations in the form of Eq. (D.5), which represents outgoing waves, can be solved as is. The general form for the boundary condition can be written as

\[ M^{-1}_\xi \left. \frac{\partial \hat{\Theta}}{\partial t} + \Gamma + M^{-1}_\xi D \right|_{\text{boundary}} = 0 \]  \hspace{1cm} \text{(D.10)}

where

\[ \Gamma = \begin{cases} \Lambda_\xi M^{-1}_\xi \frac{\partial \hat{\Theta}}{\partial \xi} & \text{for outgoing waves} \\ 0 & \text{for incoming waves} \end{cases} \]  \hspace{1cm} \text{(D.11)}
The condition for constant pressure at infinity is used to obtain the amplitude variation of the incoming wave. If the pressure at the far field is not close to the back pressure, $p_{\infty}$, reflected waves will enter the domain through the outlet to bring the mean pressure back to a value close to $p_{\infty}$. To simulate this information, Poinset and Lele (1992) have proposed that $L$ for the incoming waves in Eq. (D.11) is replaced by

$$
\Gamma = K(p - p_{\infty}) \tag{D.12}
$$

where

$$
K = \sigma(1 - M^2)c/\xi_c. \tag{D.13}
$$

Here, $M$ represents the maximum Mach number in the computational domain, $\xi_c$ the characteristic axial length of the domain in generalized coordinates, $c$ the local speed of sound, and $\sigma$ a constant ranging from 0.25 to 0.5 (Posinot and Lele, 1992; Baum et al., 1994).

Equation (D.10) can be discretized in the following using Runge-Kutta scheme

$$
M_\xi^{-1}(\tilde{Q}^i - \tilde{Q}^a) = -\Delta t \sum_{k=1}^{i} \alpha_{ik} \left( \Lambda_\xi M_\xi^{-1} \frac{\partial \tilde{Q}}{\partial \xi} + M_\xi^{-1} D \right)^{k-1} \tag{D.14}
$$

where $i = 1, 2, \ldots, N$ represents the $N$-step Runge-Kutta scheme. For a subsonic outflow condition, the outgoing characteristic equations are solved by

$$
L^* M_\xi^{-1}(\tilde{Q}^i - \tilde{Q}^a) = -L^* \Delta t \sum_{k=1}^{i} \alpha_{ik} \left( \Lambda_\xi M_\xi^{-1} \frac{\partial \tilde{Q}}{\partial \xi} + M_\xi^{-1} D \right)^{k-1} \tag{D.15}
$$

And the incoming characteristic equation is solved by

$$
L M_\xi^{-1}(\tilde{Q}^i - \tilde{Q}^a) = -L \Delta t \sum_{k=1}^{i} \alpha_{ik} (M_\xi^{-1} D)^{k-1} \tag{D.16}
$$
where $L^+$ and $L^-$ are selection matrices

$$
L^+ = \begin{bmatrix}
0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1
\end{bmatrix}
\quad \text{and} \quad
L^- = \begin{bmatrix}
1 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0
\end{bmatrix}
$$

Combining Eqs. (D.15) and (D.16) yields

$$
M_{\xi}^{-1}(\tilde{Q} - \bar{Q}) = -L^+ \Delta t \sum_{k=1}^{i} \alpha_k \left( \frac{\partial \tilde{E}}{\partial \xi} + \frac{\partial \tilde{F}}{\partial \eta} + \frac{\partial \tilde{G}}{\partial \zeta} \right)^{k-1}
$$

$$
- L^- M_{\xi}^{-1} \Delta t \sum_{k=1}^{i} \alpha_k \left( \Gamma + \frac{\partial \tilde{F}}{\partial \eta} + \frac{\partial \tilde{G}}{\partial \zeta} \right)^{k-1}
$$

(D.18)
Vita

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