
A Study of the Internal Flow of Dense Vapours used in Organic Rankine Cycle (ORC) Turbines

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*I declare this thesis to be my own work and the appropriate citations are included
to acknowledge the work of others.*

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Abstract

An Organic Rankine Cycle (ORC) is a thermodynamic cycle utilizing a heat source at low-temperature. It can be used for the waste heat recovery of vehicle engines, industrial processes, solar thermal power plants, and geothermal power plants, leading to reduction of CO₂ emissions. The turbine expander is a key component of this cycle, and its efficiency is critical to the system performance. To improve the design of an ORC turbine, the internal flow of the turbine should be studied. Unlike the fluids in conventional turbines, the fluids used in ORC turbines are dense vapours. These vapours have complex molecules and relatively large molecular weights, and they operate at states close to thermodynamic critical points or saturation line. Therefore, the thermodynamic behaviours of dense vapours are far from those of ideal air. However, the influence of these effects on the internal flows is not well understood. The fundamental flow behaviours of dense vapours, including gasdynamic behaviours in blade-shaped nozzle flows and turbulent behaviours in wall-bounded flows, are the focus of this work.

A supersonic cascade using R1233zd(E) as working fluids is designed by the method of characteristics. The designed geometry is able to achieve a nearly uniform outlet flow at about $Ma = 2$, which is checked in an RANS simulation. A blade-shaped nozzle is designed using the blade shape of this cascade, and the preliminary test results of this nozzle is presented. This nozzle is tested with both nitrogen and R1233zd(E) as working fluids. In the test with nitrogen, an adverse pressure gradient is measured on both nozzle surfaces downstream of the nozzle throat, and a shock train is observed at the corresponding position. Similar to the nitrogen test, the adverse pressure gradient is also found in the tests with R1233zd(E), but the Schlieren images cannot clearly show the shock train due to the disturbance of two-phase flows.

A Direct Numerical Simulation (DNS) method for dense vapours is developed to obtain detailed information on turbulence. A modified Steger-Warming splitting is proposed to considering the strong non-ideal effects of gases, and the Span-Wagner EoS [1] is used for studied dense vapours. The first studied benchmark case of wall-bounded flow is the supersonic fully-developed channel flow. Both the mean flow fields and the turbulent fluctuation fields are analysed. The mean profile and the fluctuation of thermodynamic properties are significantly affected by both molecular-

complexity effects and non-ideal effects, and the sound-wave mode can be the dominant mode for generating fluctuations of thermodynamic properties (T' , ρ') in dense vapours. Important modelling issues for dense vapours are also discussed, including the Strong Reynolds Analogy (SRA) and assumptions required for the $k-\varepsilon$ RANS method. The second studied benchmark case of wall-bounded flow is the bypass laminar-turbulent transition over a flat plate under a supersonic incoming flow. At the same incoming non-dimensional numbers (Ma_∞ and Re_x), the breakdown of laminar flow starts earlier in dense vapours than in air. The mechanism of breakdown for both dense vapours and air is due to the interaction of two streamwise vortices in opposite rotational directions, leading to Kelvin-Helmholtz (KH) instability in a high shear layer. Proper Orthogonal Decomposition (POD) is also used to support the findings in vortex structure analysis.

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Nomenclature

Greeks

α	Blade angle	°
α	Dimensionless Helmholtz energy, $\mathbf{a}/RT$	-
δ_1	Displacement thickness	m
δ_{99}	99% velocity thickness	m
η_k	Kolmogorov length scale	m
Γ	Fundamental derivative	-
γ	Specific heat ratio, c_p/c_v	-
λ	Heat conductivity	W/(m·K)
μ	Dynamic viscosity	Pa·s
ν	Prandtl-Meyer function	-
ω	Acentric factor	-
ρ	Density	kg/m ³
σ	Entropy generation rate	W/(m ³ ·K)
τ	Inverse reduced temperature, T_{cr}/T	-
τ_w	Wall shear stress, $[\mu(\partial u/\partial y)]_w$	Pa
$\tau_{i,j}$	Viscous stress tensor	Pa
θ	Flow angle	°
θ	Momentum thickness	m
θ	Reduced density, ρ/ρ_{cr}	-
ε	Dissipation	kg/m ³
ε^p	Total pressure loss coefficient	-
ε^s	Entropy loss coefficient	-

Latins

$\mathbf{a}$	Helmholtz energy	J/kg
$\mathbf{M}$	Molecular weight	L/kg
c	Speed of sound	m/s
C_f	Skin friction coefficient	-

c_p	Isobaric specific heat capacity	J/(kg·K)
c_v	Isochoric specific heat capacity	J/(kg·K)
e	Specific inner energy	J/kg
E_{uu}	Energy spectrum of u	-
Ec	Eckert number, $u^2/c_p T$	-
H	Blade height	m
h	Specific enthalpy	J/kg
k	Kinetic energy	m ² /s ²
l_b	Blade length	m
Ma	Mach number, u/c	-
p	Pressure	Pa
Pr	Prandtl number, $c_p \mu / \lambda$	-
q_i	Heat flux	J/(m ² ·s)
R	Specific gas constant	J/(kg·K)
$R_{\alpha\beta}$	Correlation coefficients between two parameters	-
R_{uu}	Self-coefficients of u	-
Re	Reynolds number, $\rho u l / \mu$	-
s	specific entropy	J/(kg·K)
S_c	Blade pitch	m
T	Temperature	K
t	Time	s
T_t	Trailing-edge thickness	m
U	Mean velocity	m/s
u_τ	Wall friction velocity $\sqrt{\tau_w} / \bar{\rho}_w$	m/s
u_τ^*	Semi-local wall friction velocity $\sqrt{\tau_w} / \bar{\rho}$	m/s
u_i or u, v, w	Velocity components	m/s
V	Specific volume	m ³ /kg
x_i or x, y, z	Distance in three directions	m
y^*	Non-dimensional semi-local wall distance, $\bar{\rho} u_\tau y_{wall} / \overline{m u}$	-
y^+	Non-dimensional wall distance, $\bar{\rho}_w u_\tau y_{wall} / \overline{m u}_w$	-
Z	Compressibility factor	-

Superscripts and Subscripts

∞	Far upstream
θ	Boundary layer edge

B	Bulk parameters
br	Breakdown
bs	Blowing and suction
c	At channel center
cr	At thermodynamic critical point
e	At the edge
G	Parameters at characteristic thermodynamic state
in	At inlet
lam	Laminar
o	Ideal-gas part
p	Period
r	Real-gas part
ref	At reference states
rms	Root mean square
sw	Sound wave mode
t	Turbulent
th	At the throat
vor	Vorticity mode
w	At wall surface
0	Total thermodynamic state

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Chapter 1

Introduction

1.1 Research Background

Reducing global CO₂ emissions has become a critical issue for all countries in the world, and the UK government has agreed to achieve 'Net Zero' CO₂ emissions in 2050 [2]. The indicative plan for reducing CO₂ emissions in the UK is shown in Figure 1.1 [2]. In this plan, reducing CO₂ emissions in the transport and industry sectors is a major goal. Improving the thermal efficiency of industrial processes and vehicle engines and saving energy to reduce CO₂ emissions, and waste heat recovery (WHR) has been considered as an effective technology to achieve this goal.

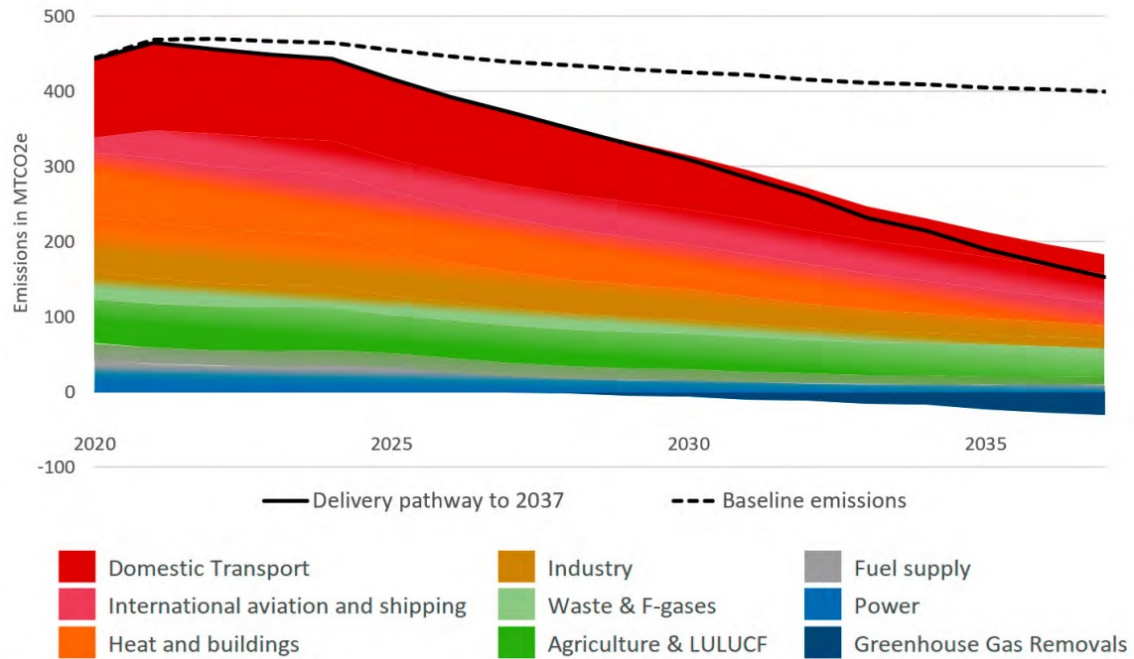


Figure 1.1: Indicative CO₂ emissions pathway in UK to 2037 [2].

The Organic Rankine Cycle (ORC) system is a WHR technology that has the advantage of utilizing low-temperature thermal energy. Figure 1.2 [3] shows that ORC technology is more suitable for low-temperature and small-scale power plants compared with steam Rankine cycle technology. It can recover low-temperature ($<350\text{ }^{\circ}\text{C}$) waste heat directly or work as the bottom cycle of a combined cycle to recover high-temperature waste heat. For industry, Campana [34] reported that ORC has the potential to recover 20 TW·h waste heat and reduce 7.6Mt of CO_2 emissions per year in four European industrial sectors. For the transport sector, Freymann [35] showed that the thermal efficiency of vehicle internal combustion engines can be improved by about 10% by installing the ORC system to recover the waste heat of engine. Meanwhile, ORC technology is also applied in renewable energy power plants, such as solar-thermal power plants and geothermal power plants. This makes ORC a research focus recently [36, 37, 38, 39].

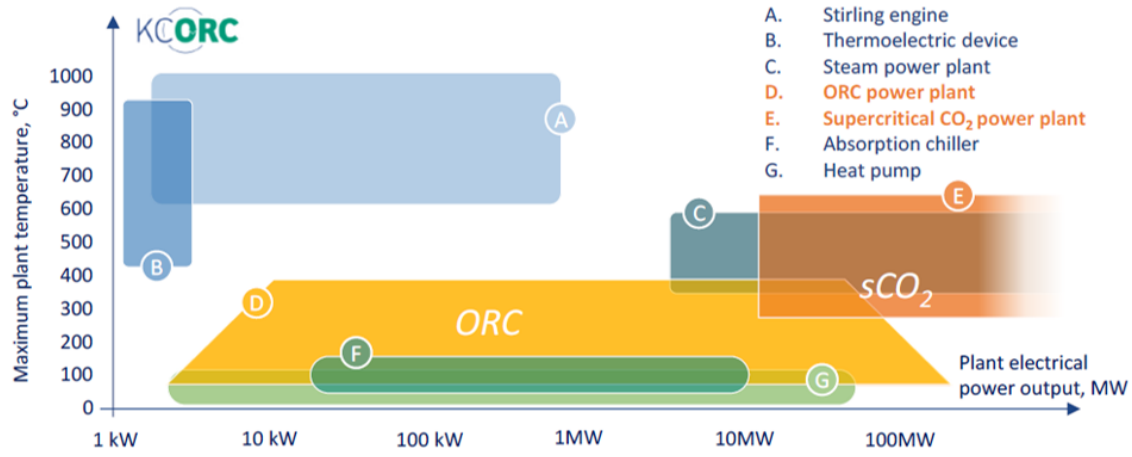


Figure 1.2: Comparison of ORC versus other technologies for utilizing thermal energy.[3]

A typical ORC system consists of four main components: an evaporator, a condenser, a pump and an expander. The system layout and thermodynamic process are shown in Figure 1.3.

In the pumping process (1 to 2), a liquid working fluid is pressurised and pumped. The mass flow rate of the system is normally controlled by the pump.

In the evaporation process (2 to 3), the thermal energy of the heat source is transferred to the working fluid of the system and evaporates them from liquid to superheated vapour, with no significant change in the pressure. The evaporator here is collectively referred to a preheater, an evaporator and a superheater, which are normally found in various types of heat exchangers. It can take energy directly from the heat source (e.g., industrial hot water and sunlight) or through an intermediate medium (e.g., thermal oil).

In the expansion process (3 to 4), the superheated vapour under high-pressure expands in a nearly isentropic process, and the thermal energy is converted into mechanical energy by the

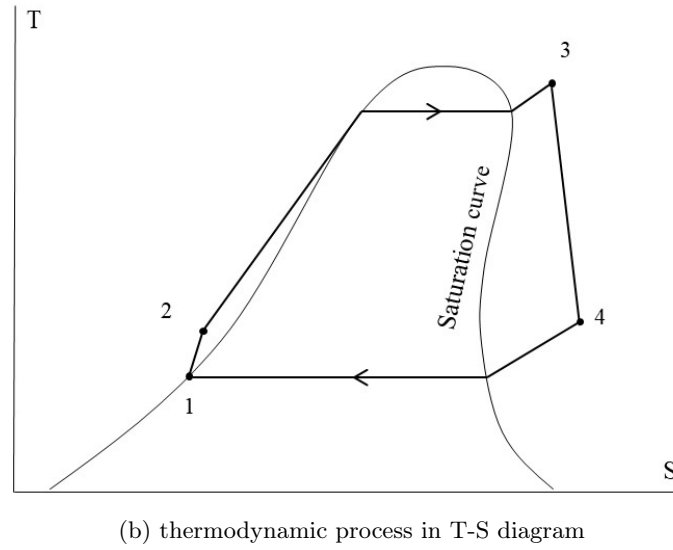
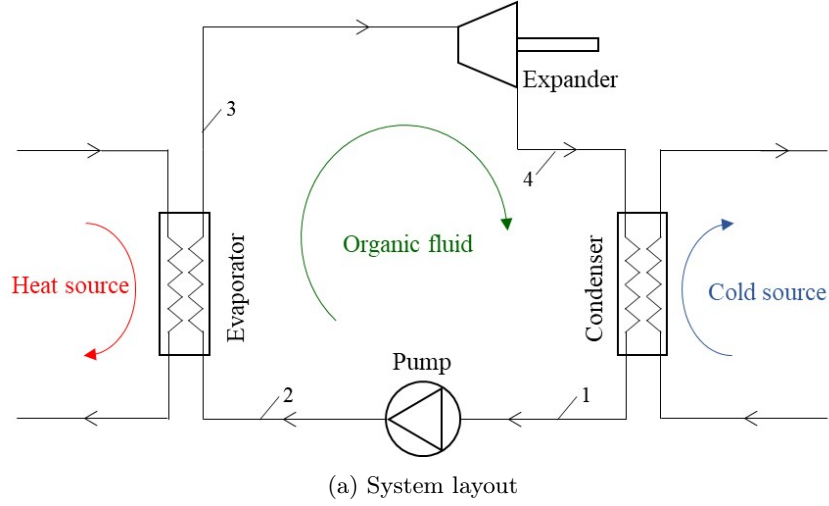


Figure 1.3: (A) system layout and (b) thermodynamic process temperature-entropy (T-S) diagram of a typical ORC system.

expander. In the condensation process (4 to 1), the low-pressure vapour releases heat to a cold source (usually the environment) and condenses to a liquid. In some applications, a liquid-receiver tank is placed downstream of the condenser to ensure stable operation of the system.

In addition, in advanced ORC systems, a recuperator is commonly used to improve the thermal efficiency of the system when the temperature at point 4 is greater than at point 2, $T_4 > T_2$ (Figure 1.3(b)). For more advanced cycle architectures, see Lecompte's review [40].

The temperature of the heat source of ORC systems is in a wide range (from 20°C to 450°C) [40], so a larger number of organic fluids can be considered as working fluids. Common refrigerants usually selected as ORC working fluids include chlorofluorocarbons (CFCs), hydrofluorocarbons (HFCs), hydrochlorofluorocarbons (HCFCs) and hydrofluoro-olefins (HFOs). In addition, hydrocarbons, alcohols, perfluorocarbons and siloxanes are also considered. From them, the most suitable

fluid for a particular application can be selected by following the selection guidelines [41]. Some researchers also use mixed fluids to reduce energy loss in heat exchangers.

These organic fluids have larger molecules than air or steam, their molecular weight is higher, and their molecular complexity level is also higher. The intermolecular force cannot be ignored in their vapour phase (in expansion process), especially when their thermodynamic state is close to the critical point or vapour saturation line, where the ideal gas assumption is no longer valid. The gases with complex molecules and operating close to the critical point or saturation line is also called dense vapours, and the molecule-complexity effects and non-ideal effects on internal flows should be paid more attentions in the analysis and development of ORC systems, especially the expanders.

Among the various types of ORC expanders, turbines have the advantage of high efficiency and small size [42]. Both axial and radial turbines are used in ORC systems. The conventional stage layouts of these two types are shown in Figure 1.4 [4]. Gases expand and accelerate in the stators and then drive the rotors. The single stage turbine is usually used in small-scale ORC systems because of its small size, which requires a high expansion ratio within one stage. Consequently, the flow velocity at the outlet of the stator is very high and the Mach number can be higher than 2 [43]. This supersonic flow of organic gases is a characteristic of ORC turbines.

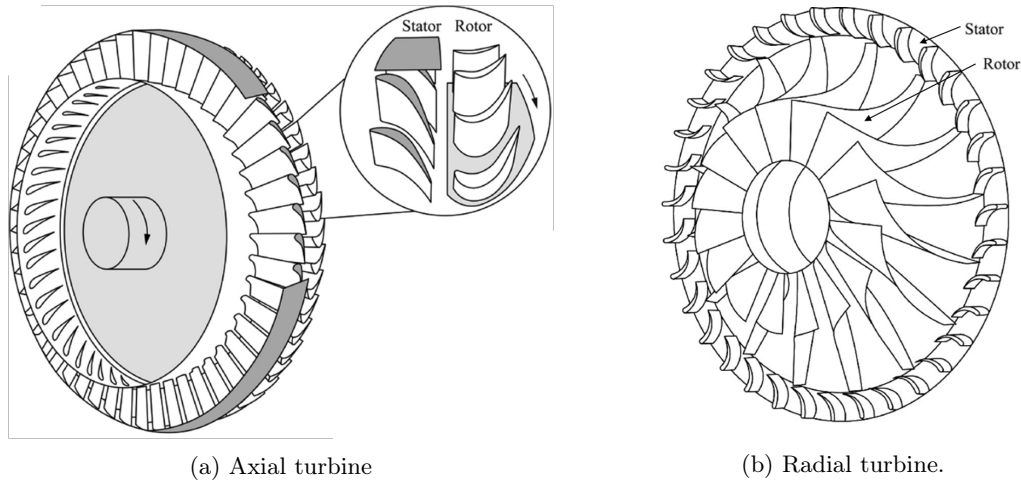


Figure 1.4: Turbine stage layout [4].

Understanding basic flow phenomena of the dense vapours used in ORC turbines is the focus of this dissertation. The the supersonic gasdynamic behaviour and wall-bounded turbulent behaviour of dense-vapour flows are the two crucial issues for the internal flows of an ORC turbine, and the understanding of them can help improve the analysis and design of an ORC turbine, so they are the main research interests of this dissertation.

1.2 Industry Collaboration

This PhD research is a continuation of an industrial research project funded by Innovate UK. The project title is 'Mobile Organic Rankine Cycle Power system with Electrified Ancillaries for Reduced Parasitics (MORCEA)' as a part of IDP 9 - Technology challenge in low carbon vehicles [44]. This project aims to develop an ORC system applied to a 15L diesel engine for the electrification of engine ancillary components to reduce the engine's fuel consumption.

The lead partner in the MORCEA project is Caterpillar Inc., and Imperial College London is the university partner for the development of turbine design and analysis. In the project, a radial turbine has been designed and a blowdown facility for dense vapours is established. In this thesis, the initial study of the MORCEA project is extended and expanded to understand the turbulence behaviour and gasdynamic behaviour in the ORC turbine. The MORCEA project developed the blowdown facility used in this project, the numerical analysis and the cascade testing is unique to this thesis and separate from the MORCEA project.

1.3 Aim and Objectives

This thesis aims to improve the understanding of fundamental internal flow phenomena of dense vapours used in ORC turbines, including the understanding of supersonic gasdynamic behaviours and wall-bounded turbulent behaviours. To achieve this aim, the main research objectives of this work are as follows:

1. The development of a DNS solver for non-ideal-gas flows, which can consider strong non-ideal effects and apply the state-of-the-art Equation of States (EoS).
2. The establishment of an experimental test facility for a supersonic nozzle using dense vapours (measuring the pressure distribution and Schlieren images), and the preliminary test of a supersonic nozzle.
3. The study of fully-developed turbulent boundary layers in a channel, allowing to understand the molecular-complexity effects and non-ideal effects on wall-bounded turbulent behaviours and turbulent modelling issues.
4. The understanding of the bypass type laminar-turbulent transition over a flat plate in the present of fluids with molecular complexity and non-ideal effects.

1.4 Thesis Outline

This thesis is organised as follows:

Chapter 1: Introduction - This chapter introduced the background, motivation and aim of this thesis.

Chapter 2: Literature Review - This chapter reviews recent published research associated with the internal flows of dense vapours used in ORC turbines. The research of ORC systems applications, non-ideal thermodynamics, dense-vapour fluid dynamics and ORC turbines are summarised to support the current understanding, and knowledge gaps are presented.

Chapter 3: Methodology - This chapter establishes the research methods used in this thesis. The numerical methods, including a highly accurate DNS method and a steady RANS method for dense vapours, are presented together with the corresponding data analysis methods. The experimental method of a supersonic nozzle for measuring the pressure distribution and the Schlieren imaging is introduced.

Chapter 4: Design of a Supersonic Cascade and Preliminary Test of a Blade-Shaped Nozzle using the Designed Geometry - This chapter designs a supersonic cascade with R1233zd(E) as working fluids. Method of characteristic is used to designed the geometry of the cascade, and the performance of the cascade is checked by RANS simulation method. A blade-shaped nozzle, which used the blade shape of the designed cascade, is tested with two fluids: nitrogen and R1233zd(E). The preliminary test results are presented in this chapter.

Chapter 5: Study of Supersonic Fully-Developed Turbulent Channel Flows of Dense Vapours using DNS Method - This chapter studies the fully-developed turbulent channel flows of two organic gases by DNS. The impact of molecule-complexity effects and non-ideal effects on turbulent behaviours is analysed, and the turbulence modelling issues is also discussed in dense vapours.

Chapter 6: Study of Bypass Laminar-Turbulent Transition on a Flat Plate of Dense Vapours using DNS Method - This chapter studies the bypass laminar-turbulent transition on a flat plate by DNS. The impact of molecule-complexity effects and non-ideal effects on the transition flow structure is analysed and discussed.

Chapter 7: Conclusion and Future Work - This chapter summarises main conclusions of this thesis and briefly discusses the future work.

To claim, the experiment plan of the blade-shaped nozzle was interrupted by the unexpected breakdown caused by COVID 19. The research focus has to be turn from the experimental work to the numerical work. Therefore, the theoretical basis of RANS simulation method - the turbulent behaviours - is studied from a scientific way using DNS method.

1.5 Scholarly Output

During the author's PhD period, the publications of articles in journals and conferences are listed below:

T. Chen, P.J. Newton, M.C. Robertson, R.F. Martinez-Botas. "Analysis of Transonic Nozzle Loss Generation in Organic Rankine Cycle (ORC) Turbines", 5rd International Seminar on ORC Power Systems, Paper ID 105, September 9-11, 2019, Athens, Greece.

T. Chen, B. Yang, M.C. Robertson, R.F. Martinez-Botas. "Direct Numerical Simulation of Real-Gas Effects within Turbulent Boundary Layers for Fully-Developed Channel Flows", Journal of the Global Power and Propulsion Society, 5, 216-232, 2021.

T. Chen, B. Yang, R.F. Martinez-Botas. "DNS of Fully-Developed Supersonic Turbulent Channel Flows with Real Gases", Journal of Fluid Mechanics. (under reviewing)

M.C. Robertson, P.J. Newton, T. Chen, R.F. Martinez-Botas. "Development and Commissioning of a Blowdown Facility for Dense Gas Vapours", Turbo Expo: Power for Land, Sea, and Air. Vol. 58608. American Society of Mechanical Engineers, 2019.

M.C. Robertson, P.J. Newton, T. Chen, A. Costall, R.F. Martinez-Botas. "Experimental and Numerical Study of Supersonic Non-ideal Flows for Organic Rankine Cycle Applications", Journal of Engineering for Gas Turbines and Power 142(8), 2020.

Chapter 2

Literature Review

This chapter reviewed recent research on the internal flows of the dense vapours used in ORC turbines. In Chapter 2.1, the demand of using ORC systems to reduce global CO₂ emissions is pointed out, and the applications of ORC systems are reviewed in different fields.

2.1 Environmental Context

2.1.1 Global Emissions

Reducing global CO₂ emissions is critical to solving the problem of climate change and is accepted by most nations of the world. The Intergovernmental Panel on Climate Change (IPCC) [45] reported that the global surface temperature in 2011 - 2020 was 1.09°C higher than in 1850-1900, and that well-mixed greenhouse gases (GHGs) produced by humans contributed to 1.0°C to 2.0°C of warming. The United Nations Environment Programme (UNEP) has analysed the GHG emissions until 2020 (see Figure 2.1) and warned that global warming will rise to 2.7°C by the end of this century unless stricter regulations are put in place[5]. To achieve the target of the Paris Agreement (in Conference of the Parties, Paris, COP 21): to "Limit the global warming to well below 2°C, preferably to 1.5°C, compared to pre-industrial levels," global 'net zero' emissions should be achieved by mid-century. 120 countries have updated their Nationally Determined Contribution (NDC) to the United Nations Framework Convention on Climate Change (UNFCCC), and 12 G20 members have declared a clear path to 'net zero' pledges, including the UK. CO₂ accounts for the largest share of the GHG emissions (see Figure 2.1), making 'net-zero' CO₂ the important target for achieving 'net zero' GHG emissions [5, 2].

In UK's 'net zero' plan [2], emission reduction targets in six sectors are included (see Table 2.1).

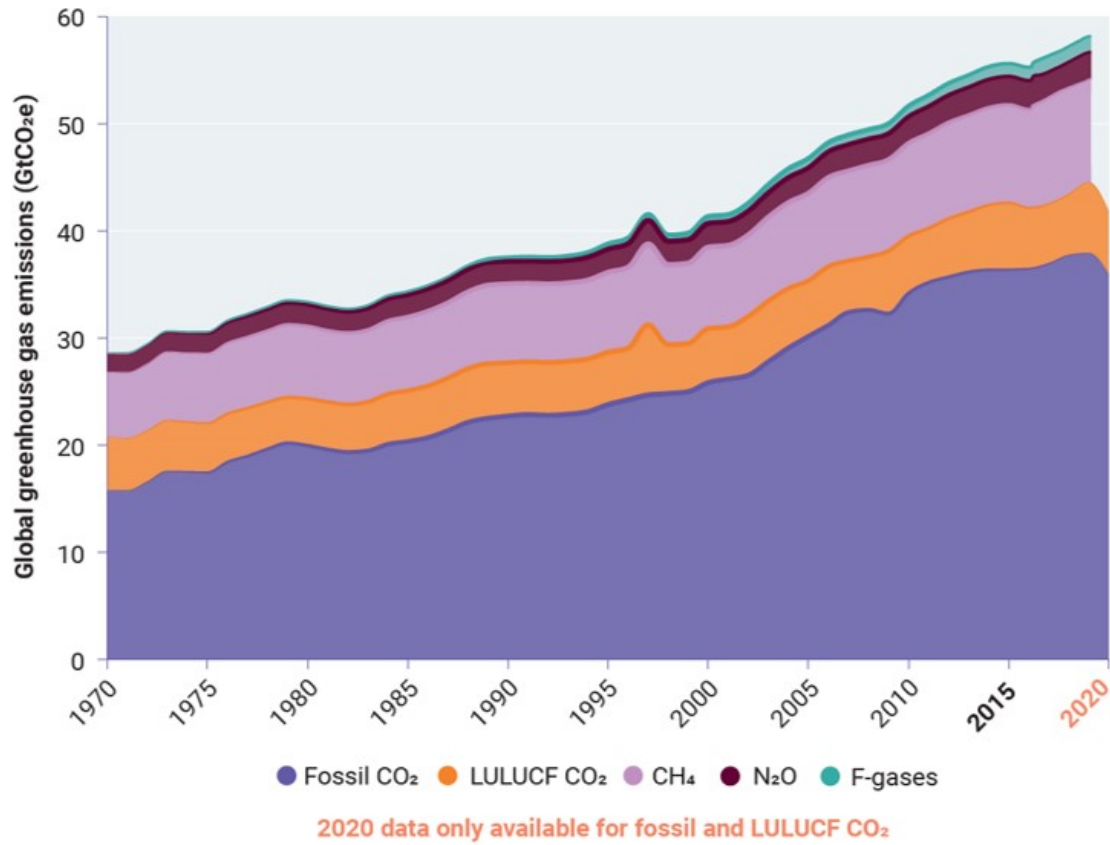


Figure 2.1: Global greenhouse gas emissions [5].

ORC systems have the potential to reduce the CO₂ emissions in four sectors: Power, Industry, Heat and Buildings, and Transport, and the ORC systems applications in these sectors are reviewed in the following part.

Sector	% of UK emissions in 2019	Expected reduction by 2035 from 1990
Power	11%	80-85%
Fuel supply and Hydrogen	5%	53-60%
Industry	15%	63-76%
Heat and Buildings	17%	47-62%
Transport	32%	47-59%
Natural Resources	20%	39-51%

Table 2.1: A breakdown of GHG emissions in 2019 and the emission reduction target by 2035 from 1990 [2].

2.1.2 ORC Systems Applications for CO₂ Emission Reduction

Power

ORC systems can be used to generate electrical energy from renewable sources (e.g solar thermal energy, geothermal power, and biomass energy) to partially replace fossil fuels in the power generation. About 86% of all ORC installed capacity in the world is in this field, and geothermal ORC systems take the largest share, followed by biomass ORC systems and solar ORC systems [46].

In solar ORC systems, concentrated solar power is absorbed by heat transfer fluids (or directly by ORC working fluids) and converted into electrical energy by ORC systems. ORC systems can be coupled with various solar thermal collectors that have a wide range of heating temperatures from 80°C to 500°C [47]. Cost-effective thermal energy storage can be applied in this system, which is a key advantage over photovoltaic technology [48]. Most solar ORC systems are in small scale (<100kW) [48], and the large-scale systems (>1MW) have been reported by Arizona Public Service (APS) [49], Cimarron Cement Group [50], National Renewable Energy Laboratory (NREL) [51], ORC-PLUS [52], and AALBORG CSP [53].

Geothermal energy is contained in the pressurised underground water in geothermal reservoirs, and 68% of the energy is low-temperature resources (<130°C), which can generate 209GW of electrical power and 4400GW of thermal energy [54]. The installed capacity of geothermal power plants is 15,950.46MW at the end of 2020[55], and about 3,125MW is taken by the ORC power plants[56]. The total capacity of ORC power plants shows a strong growth, since it increased by about 75% from that in 2014[57, 56]. The percentage of ORC power plants in the total geothermal power plants (considering the installed capacity) increased from 14.2% to 19.5% in 2014-2020. ORMAT, Exergy, TAS, Turboden and General Electric have most applications of geothermal ORC power plants so far, all of which have the total installed capacity larger than 100MW [46, 56] (other manufactures can be seen in the summary by Wieland[56]).

Although the biomass boiler still produces CO₂ emissions, biomass-fired ORC can still help reduce the use of fossil fuels, especially in rural electrification. Thermal oil is used to absorb heat from the biomass boiler and transfer the heat to ORC systems for electricity generation; meanwhile, thermal energy (up to 120°C) is also supplied [58]. 332 biomass ORC power plants have been installed and the total installed capacity has reached 301MW by 2017 [46], most of which are combined heat and power (CHP) plants. The electric capacity of biomass ORC CHP systems is mostly between 500kW and 2MW, and the thermal capacity is between 2MW and 8MW, which makes them suitable for district heating applications (more than half of biomass ORC applications). In addition, hybrid solar-biomass ORC is also considered as a potential technology for distributed

power generation [59, 60].

Industry

Waste heat recovery (WHR) from industrial processes can reduce industrial power consumption and thus reduce CO₂ emissions. Knowledge Center on Organic Rankine Cycle (KCORC) [3] estimated the potential capacity for electricity generation from industrial processes WHR in EU28, and showed that approximately 150 TWh/year electricity can be generated, which is about 5 % of the yearly electricity production in European Union countries. It[3] also indicated that about 45 Mt/year of CO₂ can be reduced when considering the average emissions in EU28 (CO₂ emission in the power generation field is 294 g/kWh in 2017 [61]). To be mentioned, some other research have more positive estimations, which estimated that 280 TWh/year[62] and 300 TWh/year [63] electricity can be generated from the waste heat in industrial processes.

The waste heat from industrial processes is at different temperature levels, and the distribution of these potential electricity generation is shown in Table 2.2 [3]. More electricity can be generated from high-temperature (>500 °C) and moderate-temperature (200 - 500 °C) waste heat, while the low-temperature (<100 °C) waste heat is also important. It means that the variable heat source temperature for WHR-ORC system should be paid more attentions.

Temperature level	Potential electricity generation
°C	TWh/year
<100	32.2
100 - 200	9.5
200 - 500	61.7
>500	47.2

Table 2.2: Potential electricity generation from industrial processes in European Union countries. [3]

By 2017, the installed capacity of ORC WHR systems in industry worldwide was about 130MW [46]. Moreover, the applications of ORC WHR are predicted to grow faster in the future due to the stricter regulations on CO₂ emissions in major industrialised countries [34, 64, 65].

Transport

The internal combustion engine is still important for transportation, especially for heavy-duty truck engines and for marine engines. Recovery of waste heat from vehicle engines can reduce transportation-related CO₂ emissions. More than 50% of the fuel energy is in the engine exhaust

gases and coolant, and ORC systems can help convert this waste heat into electrical energy (or mechanical energy) with a thermal efficiency of 8-20% [66]. Therefore, ORC systems can help increase the overall thermal efficiency of engine to over 50% [67]. The ORC system has already been considered by engine manufacturers, and it has a potentially larger number of applications as regulations become more stringent in the future [68, 35, 69, 67].

Heat and Building

Recent research has shown that ORC systems can also help reduce energy consumption in buildings. Dumont [70] designed and tested a reversible heat pump (HP)/ORC unit to obtain a 'net-zero' energy building with a 120m² thermal solar roof and a geothermal heat exchanger. Dong [71] suggested that the ORC CHP system can be combined with an evaporative cooling-assisted outdoor air system to work as the centralized ventilation system in high-rise residential buildings, and that it reduces annual primary energy consumption by 28%.

In summary, ORC can reduce CO₂ emissions in various sectors and has already been installed on a large scale and at a high growth rate.

2.2 Thermodynamic Characteristics of Dense Vapours

The researched fluids in this dissertation are organic fluids operating in vapour phase (or supercritical phase). The intermolecular forces and the molecular volume are no longer negligible, and they significantly influence the relationship between fluids properties. Therefore, the ideal gas assumption is not valid, and real-gas equation of states should be used to accurately relate the properties of fluids. The nature of fluids, molecular complexity, is also important for the thermodynamic of dense vapours, which is reviewed as well.

2.2.1 Ideal Gas Assumption

The relationship between the properties of a ideal gas is given as:

$$p = \rho RT. \quad (2.1)$$

This equation can be achieved by either classical or quantum statistical mechanics, when assuming that the volume of molecule the intermolecular force are ignored [72], and this relation is commonly accepted at low pressures based on experimental evidences [73].

The relationship between the thermal energy and temperature of ideal gases can be represented

as follows:

$$de = c_v dT, \quad dh = c_p dT, \quad (2.2)$$

where c_v and c_p depend on temperature. If c_v and c_p are constant, the gas is also called a perfect gas, and the specific heat ratio $\gamma \equiv c_p/c_v$ is also constant.

In addition to Equation 2.1 and 2.2, other EoSs are needed in the analysis of flows of perfect gases, relating the speed of sound, dynamic viscosity, and thermal conductivity to temperature, as follows:

$$c = c(T) = \sqrt{\gamma RT}, \quad (2.3)$$

$$\mu = \mu(T), \quad (2.4)$$

$$\lambda = \lambda(T). \quad (2.5)$$

For perfect gases, the Sutherland viscosity law [74] is often used as the exact expression of Equation 2.4:

$$\mu = \mu_{ref} \left(\frac{T}{T_{ref}} \right)^{3/2} \frac{T_{ref} + T_s}{T + T_s}, \quad (2.6)$$

where μ_{ref} is the dynamic viscosity at the reference temperature T_{ref} , and T_s is a constant (e.g., $T_s=110.4$ K for air). The Prandtl number, $Pr \equiv c_p \mu / \lambda$, is usually assumed to be constant, so the exact expression of Equation 2.5 follows:

$$\lambda = \frac{c_p \mu}{Pr}. \quad (2.7)$$

2.2.2 Equation of States for Dense Vapour

For dense vapours, the ideal gas assumption no longer holds, therefore the compressibility factor is defined as a correction factor to quantitatively show the deviation from ideal-gas behaviour:

$$Z \equiv \frac{p}{\rho RT}. \quad (2.8)$$

Z is smaller than unity when the gas is at states near the critical point and vapour saturation line. More complicated EoSs (also called real-gas EoSs) have to be used to accurately describe the relationships between fluids properties. The EoS is important for modelling the fluids in computational fluid dynamics and analysing fluid dynamic behaviours, so two main types of real-gas EoSs are briefly reviewed here: the virial EoS and the cubic EoS.

The virial EoS is the equation using the power series expansions to model the compressibility

factor [75]:

$$Z(T, \rho) = 1 + B\rho + C\rho^2 + \dots, \quad (2.9)$$

$$\text{or } Z(T, p) = 1 + B'p + C'p^2 + \dots, \quad (2.10)$$

where $B, C, B', C' \dots$ are the second or higher-order virial coefficients. These coefficients depend on the temperature and the nature of the gas, and the second- and third-order coefficients were determined by using the experimental database [76]. This virial EoS is accurate only when the gas density is low or moderate [75].

The cubic EoS is a class of EoS originating from Van de Waals (VDW) EoS[77]. In the VDW EoS, the molecular volume and intermolecular forces are taken into consideration:

$$p = \frac{RT}{V - b} - \frac{a}{V^2}, \quad (2.11)$$

where V is the specific volume, and the parameters a and b are constants which depend on the nature of the fluids. a is related to the intermolecular force, and b is related to the hard-core molecular volume. In applications, they are calculated by the properties at the critical point of the fluid:

$$a = \frac{27R^2T_{cr}^2}{64p_{cr}}, \quad (2.12)$$

$$b = \frac{RT_{cr}}{8p_{cr}}. \quad (2.13)$$

Based on this concept, a number of cubic EoSs are proposed to improve the VDW EoS, such as the Soave-Redlich-Kwong equation [78], Peng-Robinson equation [79], Peng-Robinson-Stryjek-Vera [80], Patel-Teja equation [81], Elliott-Suresh-Donohue equation [82], Martin-Hou equation [83], Benedict-Webb-Rubin equation [84] and Span-Wagner equation [1]. In general, the more coefficients an EoS uses the more accurate it is. The state-of-the-art EoSs for commonly-used fluids are summarised by the National Institute of Standards and Technology (NIST) [7]. However, a large number of coefficients will slow down the calculation process of CFD. The cubic EoSs provide a good tradeoff between accuracy and computational cost, so they have been widely used to analyse the ORC turbine internal flows. P. Colonna [85] compared different EoSs inside a 2D nozzle blade of an ORC turbine using siloxane MDM as the working fluid and found that a cubic EoS should be used instead of the ideal-gas law to achieve an acceptable accuracy.

The Peng-Robinson (PR) EoS and Span-Wagner (SW) EoS are present here, of which the former (lower computational cost) is used in the RANS simulation in Chapter 4 and the latter (more accurate) is used in the DNS method in Chapter 5 and 6.

The PR EoS has the expression as following expression [79]:

$$p = \frac{RT}{V-b} - \frac{a\alpha}{V(V+b)+b(V-b)}, \quad (2.14)$$

where

$$a = 0.45724 \frac{R^2 T_{cr}^2}{p_{cr}}, \quad (2.15)$$

$$b = 0.07780 \frac{RT_{cr}}{p_{cr}}, \quad (2.16)$$

$$\alpha = [1 + (1 - T_r^{0.5})(0.37464 + 1.54226\omega - 0.26992\omega^2)]^2, \quad (2.17)$$

and

$$T_r = \frac{T}{T_{cr}}. \quad (2.18)$$

Here, ω is the acentric factor. PR EoS only needs one more parameter than VDW EoS.

The SW EoS is a modification of the Benedict-Webb-Rubin EoS [84]. This EoS relates $\mathbf{a}$ - ρ - T instead of p - V - T , where $\mathbf{a}$ is the Helmholtz energy. In SW EoS, Helmholtz energy consists of a ideal-gas part (superscript o) and a real-gas part (superscript r):

$$\alpha(\delta, \tau) = \alpha^o(\delta, \tau) + \alpha^r(\delta, \tau), \quad (2.19)$$

where α is the dimensionless Helmholtz energy, $\alpha = \mathbf{a}/RT$; δ is the reduced density, $\delta = \rho/\rho_{cr}$; and τ is the inverse reduced temperature, $\tau = T_{cr}/T$. The ideal-gas part is shown as follows:

$$\alpha^o(\delta, \tau) = \frac{h_{ref}^o}{RT_c} \tau - \frac{s_{ref}^o}{R} - 1 + \ln \left(\frac{\delta \tau_{ref}}{\delta_{ref} \tau} \right) - \frac{\tau}{R} \int_{\tau_{ref}}^{\tau} \frac{c_p^0}{\tau^2} d\tau + \frac{1}{R} \int_{\tau_{ref}}^{\tau} \frac{c_p^0}{\tau} d\tau, \quad (2.20)$$

where h_{ref}^o and s_{ref}^o are enthalpy and entropy at reference states, and c_p^0 is the heat capacity c_p at zero pressure ($\lim p \rightarrow 0 c_p(T)$). The real-gas part includes polynomial terms, exponential terms and 'hard-sphere' & 'well-sphere' terms:

$$\begin{aligned} \alpha^r(\delta, \tau) = & \sum_{k=1}^{I_{pol}} N_k \tau^{t_k} \delta^{d_k} + \sum_{k=1+I_{pol}}^{I_{pol}+I_{exp}} N_k \tau^{t_k} \delta^{d_k} \exp(-\delta^{l_k}) \\ & + \sum_{k=1+I_{pol}+I_{exp}}^{I_{pol}+I_{exp}+I_{sph}} N_k \tau^{t_k} \delta^{d_k} \exp[-\eta_k(\delta - \varepsilon_k)^2 - \beta_k(\tau - \gamma_k)^2]. \end{aligned} \quad (2.21)$$

All parameters in these equations are based on the nature of the fluid in question and are determined by experimental data from various studies. For example, the parameters for the refrigerant R1233zd(E) and the siloxane MDM were determined by M.E. Mondeja [86] and P.Colonna [87],

respectively. From the Helmholtz equation, pressure, inner energy and speed of sound are derived [1]:

$$p(\rho, T) = \rho^2 \left(\frac{\partial \mathbf{a}}{\partial \rho} \right)_T = \rho RT \left(1 + \delta \frac{\partial \alpha^r}{\partial \delta} \right), \quad (2.22)$$

$$e(\rho, T) = \mathbf{a} + Ts = RT\tau \left(\frac{\partial \alpha^o}{\partial \tau} + \frac{\partial \alpha^r}{\partial \tau} \right), \quad (2.23)$$

$$c(\rho, T) = \sqrt{\left(\frac{\partial p}{\partial \rho} \right)_s} = \sqrt{RT \left[1 + 2\delta \frac{\partial \alpha^r}{\partial \delta} + \delta^2 \frac{\partial^2 \alpha^r}{\partial \delta^2} - \frac{(1 + \delta \frac{\partial \alpha^r}{\partial \delta} - \delta \tau \frac{\partial^2 \alpha^r}{\partial \tau \partial \delta})^2}{\tau^2 \left(\frac{\partial^2 \alpha^o}{\partial \tau^2} + \frac{\partial^2 \alpha^r}{\partial \tau^2} \right)} \right]} \quad (2.24)$$

In addition to either PR EoS or SW EoS, the relation between c_p^0 and T has to be given. A fourth-order polynomial expression is used for PR EoS in this dissertation:

$$\frac{c_p^o}{R} = \sum_{i=0}^5 A_i T^i, \quad (2.25)$$

and a more complicated expression is used for SW EoS here:

$$\frac{c_p^o}{R} = 4 + \sum_{i=1}^2 v_i \left(\frac{u_i}{T} \right)^2 \frac{\exp(u_i/T)}{[\exp(u_i/T) - 1]^2}. \quad (2.26)$$

Coefficients A_i , v_i and u_i depend on the nature of fluids, and they are determined by experimental data.

Viscosity and thermal conductivity of dense vapours depend not only on temperature but also on density (or pressure). They can also be divided into an ideal-gas part (sometimes called a dilute-gas part) and a real gas part:

$$\mu(\rho, T) = \mu^o(T) + \mu^r(\rho, T), \quad (2.27)$$

$$\lambda(\rho, T) = \lambda^o(T) + \lambda^r(\rho, T). \quad (2.28)$$

Exact expressions of Equations 2.27 and 2.28 were developed by TH. Chung et al [88, 89], from which the averaged absolute deviation is 4% for viscosity and 6% for thermal conductivity. M.L. Huber [90] proposed a modified extended corresponding states (ECS) model based on the ECS model of J.F. Ely and H.J.M. Hanley [91]. The principle of the ECS model is to relate the properties of a fluid to those of a reference fluid (e.g., R134a). This model is more practical, especially when analysing a wide range of fluids and multi-component fluids. The averaged absolute deviation of the Huber ECS model is less than 5.68% for viscosity and 6.78% for thermal conductivity [90].

2.2.3 Discussion of Non-Ideal Effects

Non-ideal effects refer to the thermodynamic characteristics different from those of ideal gases. One characteristic of non-ideal gas is that the $\rho - p - T$ relation does not follow ideal gas assumption (Equation 2.1), and this deviation from ideal gas assumption is quantified by the compressibility factor Z . However, the non-ideal behaviour is complex and only the value of Z cannot represent all non-ideal characteristics.

Another characteristic is that some thermodynamic properties (e.g. inner energy, enthalpy, heat capacity, speed of sound, viscosity and thermal conductivity) depend not only on temperature but also on other properties (e.g. density or pressure). In other words, these properties are functions of two variables (e.g. temperature and density) in non-ideal gases. For example, the differential changes in the internal energy is given as: $de = c_v dT$ in ideal gases, but it is given as: $de = c_v dT + \left(\frac{\partial e}{\partial V}\right)_T dV$ in non-ideal gases.

Next characteristic is that some dimensionless thermodynamic derivatives are no longer constant. For example, a typical normalised derivative such as $\widehat{\left(\frac{\partial p}{\partial T}\right)}_\rho \equiv \left(\frac{\partial p}{\partial T}\right)_\rho / \left(\frac{p}{T}\right)$ is equal to unity in ideal gases, but its value is variable and a function of two properties (e.g. temperature and density) in non-ideal gases. Different dimensionless derivatives have different non-ideal behaviours, which makes this characteristic is also difficult to be qualified by a single parameter.

In this dissertation, non-ideal effects are qualitatively described as "strong" when the state of gas is in the region close to critical point, and they are described as "weak" when the state of gas is in the region with low pressure.

2.2.4 Molecular Complexity of Dense Vapour

The dense vapour used in an ORC system is a pure organic substance or the mixture of different organic substances. The pure organic substance is the focus here. Commonly-used organic substances (also called organic fluids) are listed in Table 2.3. To claim, some fluids in Table 2.3 is no longer used in applications due to the more and more strict environmental restriction, but they are valuable for research. It shows that the molecular weight has positive relation with the number of atom N_{atom} in each group, and the number of atom also influence thermodynamic properties: heat capacity c_v and fundamental derivative of gasdynamics Γ .

The number of available degrees of freedom N_{avail} is associated to the number of atoms N_{atom} : $N_{avail} = 6N_{atom} - 5 - \epsilon$, where $\epsilon = -2, 0, 1$ stands for monatomic linear polyatomic and nonlinear polyatomic molecules, respectively [92]. At a given temperature, the degrees of freedom N is lower

Fluid name	Chemical name	Chemical formula	Group	Molecular weight g/mol
R134a	1,1,1,2-tetrafluoroethane	C ₂ F ₂ H ₄	Refrigerants	102.03
R1234yf	2,3,3,3-tetrafluoropropene	CH ₂ =CFCF ₃	Refrigerants	114.04
R1233zd(E)	Trans-1-chloro-3,3,3-trifluoropropene	C ₃ H ₂ ClF ₃	Refrigerants	130.50
R245fa	1,1,1,3,3-pentafluoropropane	C ₃ H ₃ F ₅	Refrigerants	134.05
MM	Hexamethyldisiloxane	C ₆ H ₁₈ OSi ₂	Siloxanes	162.38
MDM	Octamethyltrisiloxane	C ₈ H ₂₄ O ₂ Si ₃	Siloxanes	236.53
D ₆	Dodecamethyl-cyclohexasiloxane	C ₁₂ H ₃₆ Si ₆ O ₆	Siloxanes	444.92
PP10	Perfluoro-perhydrofluorene	C ₁₃ F ₂₂	Perfluorocarbons	574.10
PP11	Perfluoro-perhydrophenanthrene	C ₁₄ F ₂₄	Perfluorocarbons	624.11
Pentane	Pentane	C ₅ H ₁₂	Hydrocarbons	72.15
Toluene	Toluene	C ₇ H ₈	Hydrocarbons	92.14

Table 2.3: Common organic fluids in ORC systems.

than N_{avail} . The ratio of the gas constant to the heat capacity c_v is defined as:

$$\delta \equiv \frac{R}{c_v}. \quad (2.29)$$

This ratio is related to the number N of active degrees of freedom of molecules according to the energy equipartition principle [92]: $\delta = 2/N$, therefore, the number of atom has a positive relation with the heat capacity. Figure 2.2(a) shows heat capacity $c_{v,\infty}^{cr}$ versus molecular weight $\mathcal{M}$ for the organic fluids listed in Table 2.3. Here, $c_{v,\infty}^{cr}$ is the heat capacity at critical temperature and dilution limit, $c_{v,\infty}^{cr} \equiv \lim_{V \rightarrow \infty} c_v(T_{cr}, V)$. It shows a clear positive relation between molecular weight and heat capacity in each group of organic fluids.

The molecular complexity will also influence the minimum value of the fundamental derivative of gasdynamics Γ in dense vapours [33]. The expression of Γ is given as follows:

$$\Gamma(\rho, s) \equiv \frac{c^4}{2V^3} \left(\frac{\partial^2 V}{\partial p^2} \right)_s = \frac{1}{c} \left(\frac{\partial \rho c}{\partial \rho} \right)_s = 1 + \frac{c}{V} \left(\frac{\partial c}{\partial p} \right)_s, \quad (2.30)$$

For ideal gases, Equation 2.30 can be simplified, and it shows that Γ is determined only by the

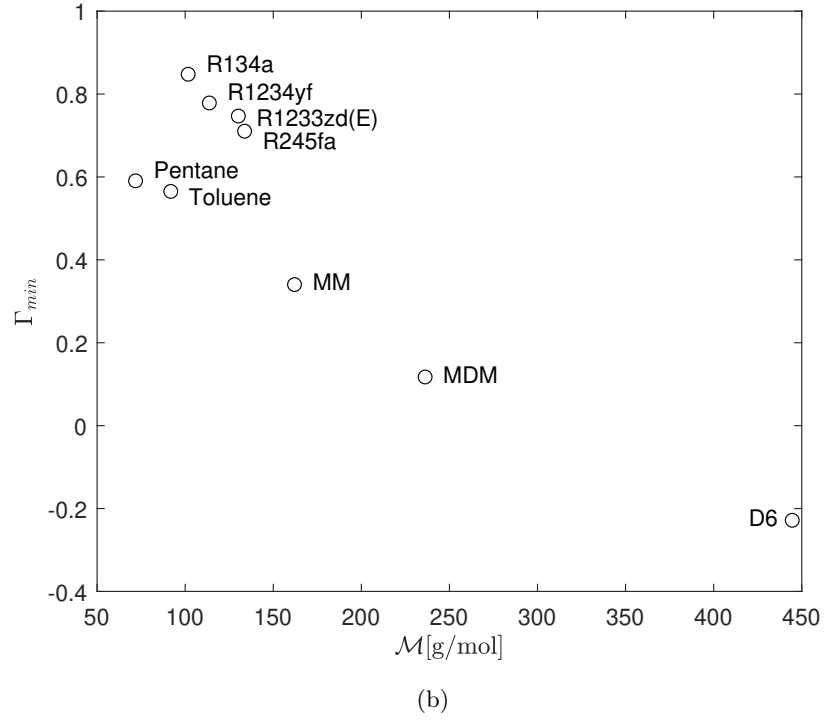
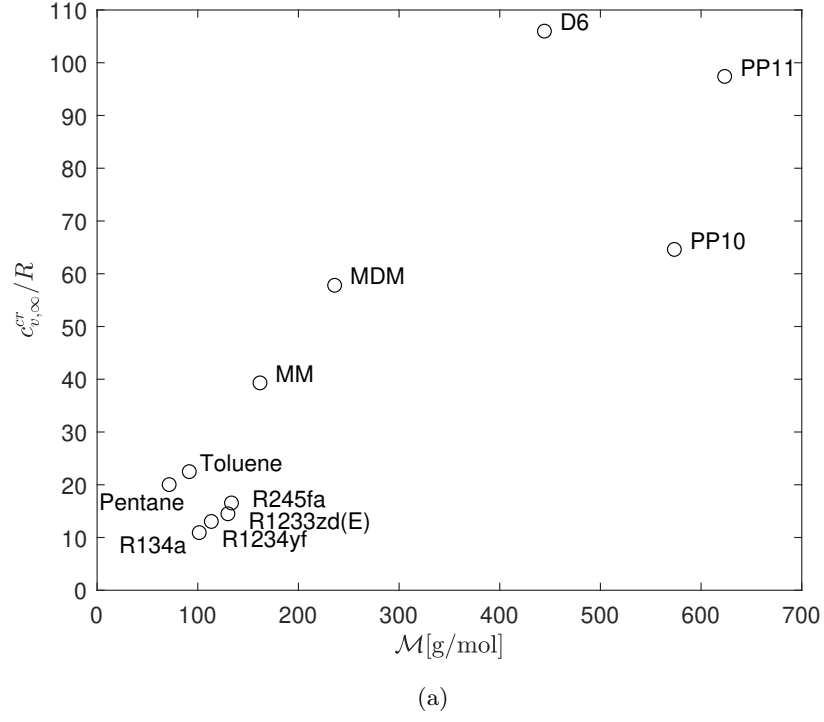


Figure 2.2: Heat capacity and minimum Γ of organic fluids versus gas molecular weight. Data are from reference [6, 7].

specific heat γ :

$$\Gamma = \frac{1}{2}(\gamma + 1). \quad (2.31)$$

Therefore, Γ is always greater than 1 in ideal gases, since γ is greater than 1. However, in non-ideal gases, Γ is closer to or even less than zero. P. Colonna [33] studied the relation between fluid molecular weight and Γ using VDW EoS. They found that if N is larger than 7.57, a $\Gamma < 1$ region possibly exists in vapour phase; and if N is larger than 33.33, a $\Gamma < 0$ region possibly exists in vapour phase. If the state-of-the-art EoS is used, the minimum value of Γ in vapour phase for the organic fluids in Table 2.3 is calculated and shown in Figure 2.2(b) (PP10 and PP11 are not considered in this figure). It shows that Γ_{min} has negative relation with molecular weight $\mathcal{M}$ in each group of organic fluids.

2.3 Fundamental Fluid Dynamics of Dense Vapours

The understanding of fundamental compressible fluid dynamics is usually based on ideal-gas law, and dilute air is the mostly researched gas. Therefore, the conservation equations are closed by Equations 2.1 & 2.2. However, in dense vapours, molecular-complexity effects and non-ideal effects lead to quantitative and even qualitative changes. Current research of the gasdynamic behaviours and turbulent behaviours in dense vapours is reviewed here.

2.3.1 Gasdynamics

The study of gasdynamic behaviours in dense vapour is a research interest, because non-classical gasdynamic behaviours can possibly exist in dense vapour if the fundamental derivative of gasdynamic Γ is negative (in theory). According to the definition (Equation 2.30), the sign of Γ represents the sign of the curvature of isentrope, see the schematic $p - V$ diagram Figure 2.3 [8]. Meanwhile, if Γ is smaller than unity, the speed of sound increases with the decreasing of pressure in isentropic process, $\left(\frac{\partial c}{\partial p}\right)_s < 0$. Based on these, the classification of gasdynamics is summarised in Table 2.4 [33]. First, the theoretical studies of non-classical gasdynamic behaviours in the fluids with $\Gamma < 0$ region are briefly reviewed here; then the pursuit for experimental evidence of these non-classical gasdynamic behaviours is reviewed, even the evidence is still not reported; after these, the classical non-ideal gasdynamic behaviours are discussed.

Theoretical Study of Non-Classical Gasdynamic Behaviours

In 1971, Thompson [8] summarised a series of theoretically possible non-classical gasdynamic behaviours existing in $\Gamma < 0$ region. In one-dimensional isentropic transonic flows, the cross area will increase then decrease (divergent-convergent nozzle) in the region $\Gamma < 0$, see Figure 2.4 (a). In two-dimensional supersonic flows, the absolute angel, $\mu + \theta$ ($\mu \equiv \sin^{-1} 1/Ma$ is the Mach angle,

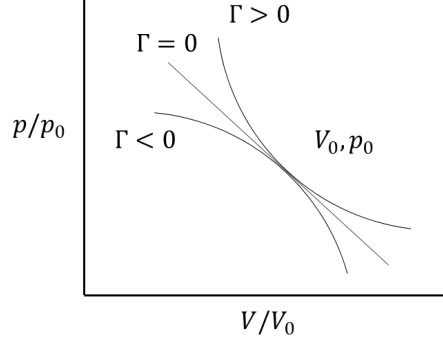


Figure 2.3: Sketch of the curvature of isentrope in $p - V$ diagram [8].

Value of Γ	Value of $\left(\frac{\partial c}{\partial p}\right)_s$	Classification
$\Gamma > 1$	$\left(\frac{\partial c}{\partial p}\right)_s > 0$	Classical ideal gasdynamic
$\Gamma = 1$	$\left(\frac{\partial c}{\partial p}\right)_s = 0$	Classical non-ideal gasdynamic
$0 < \Gamma < 1$	$\left(\frac{\partial c}{\partial p}\right)_s < 0$	
$\Gamma = 0$	$\left(\frac{\partial c}{\partial p}\right)_s < 0$	Non-classical gasdynamic
$\Gamma < 0$	$\left(\frac{\partial c}{\partial p}\right)_s < 0$	

Table 2.4: Classification of gasdynamics [33].

and θ is the streamline angle), of the Mach lines along a turning streamline will decrease if $\Gamma d\theta < 0$. For example, in Figure 2.4 (b), $\mu + \theta$ will decrease along a up-turning streamline ($d\theta > 0$) if $\Gamma < 0$. Therefore, at a sharp corner in $\Gamma < 0$, rarefaction shock and compression fans will exists (see Figure 2.4 (c)). In the unsteady supersonic flow, the rarefaction waves will steepen and compression waves will spread out if $\Gamma < 0$, see Figure 2.4 (d).

The fluids with theoretical $\Gamma < 0$ region in vapour phase is also called BZT fluids (named after Bethe [93], Zel'dovich [94] and Thompson [8]), and the $\Gamma < 0$ region is found closed to vapour saturation line when applying real-gas EoSs to BZT fluids (see Figure 2.5). Non-classical gasdynamic behaviours in BZT fluids are discussed in a series of research, where an expansion process or a shock wave can start inside or outside the $\Gamma < 0$ region and can end inside or outside the $\Gamma < 0$ region.

Thompson [95] studied the rarefaction shocks forming from plane waves, for example, a plane wave in which the pressure decrease from point A to point F along an isentropic line in Figure 2.5. They found that a rarefaction shock wave can form (see Figure 2.6(a)), and its upstream and downstream (points 1 and 2) are in the $\Gamma > 0$ region; meanwhile, the Mach number at both points

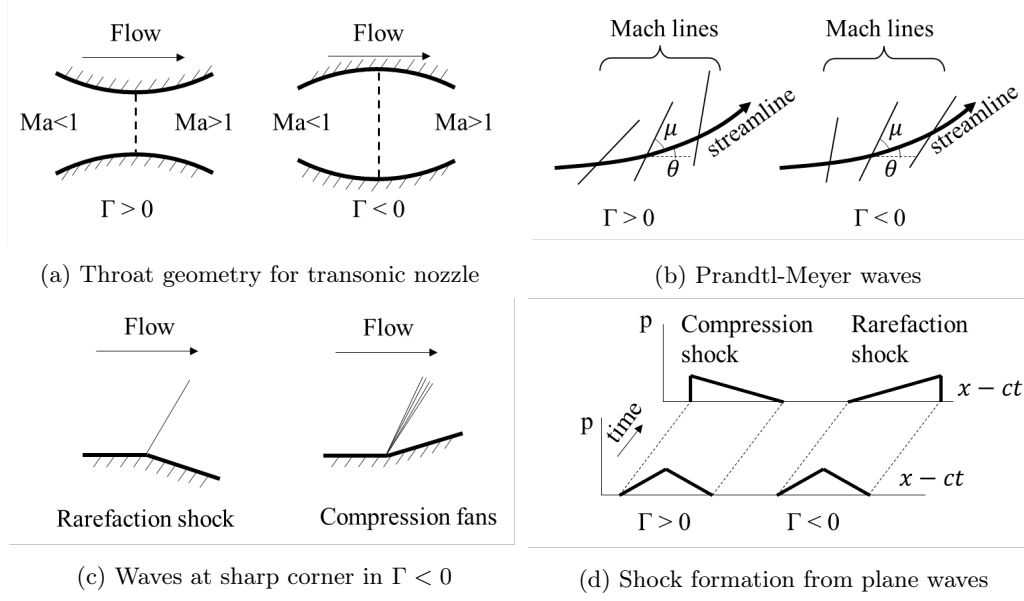


Figure 2.4: Non-classical gasdynamic behaviour in $\Gamma < 0$ region [8].

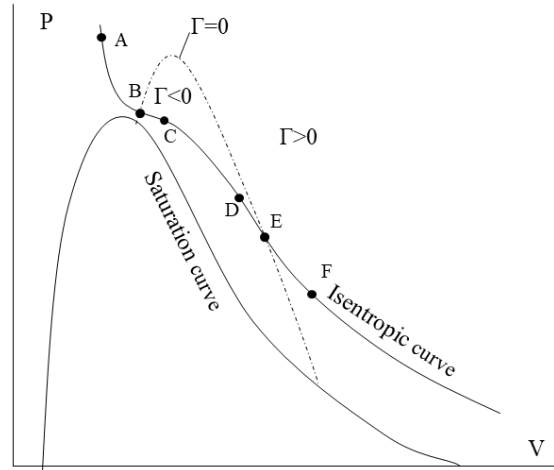


Figure 2.5: The $\Gamma < 0$ region in a typical BZT fluids. (sketch $p - V$ diagram)

1 and 2 are equal to unity, so it is called a double-sonic shock (or a double Chapman-Jouguet shock). Cramer [96] found that the Mach number can decrease in an isentropic expansion. They defined a non-dimensional number j ,

$$j \equiv 1 - \Gamma - 1/Ma^2, \quad (2.32)$$

and they derived the gradient of Mach number within an isentropic expansion:

$$\frac{dMa}{d\rho} = \frac{Ma}{\rho} j. \quad (2.33)$$

If $\Gamma < 0$, $j > 0$ always holds in supersonic flows, so Mach number decreases along an expansion. Cramer and Kluwick [97] studied the small-amplitude waves around $\Gamma \approx 0$ and proposed that the entropy jump in shock is fourth order (instead of third order) of the shock strength, $[s] \propto [p]^4$. Cramer [98] found that a compression shock may split by a compression fan, if the thermodynamic states of the shock cross the $\Gamma < 0$ region (for example, the upstream of shock at point A and downstream at point F in Figure 2.5), see Figure 2.6(b). The splitting-shock was also found in research by Argrow [99] analysing the Reimann problem in a shock tube. Cramer [100] and Kluwick [101] studied the density distribution in the throat area of an quasi-one-dimensional Laval nozzle with BZT fluids, and they found both positive and negative shocks can theoretically exist together. See Figure 2.6(c), three possible shocks exist together in the Laval nozzle. Kluwick [101] also studied the flow over an airfoil and proposed that lower drag can be achieved in BZT fluids because shock waves are avoided. Monaca [102] studied supersonic flow over a 2D cascade and found that no compression shock occurs at the leading edge and therefore the supersonic flow is completely isentropic. Cinnella [103] studied viscous flows over airfoils and proposed that the BZT effect can reduce the frictional heating in the turbulence boundary layer. Cramer [104] studied shock-induced separation in BZT fluids and concluded that the separation can be suppressed and the boundary layer can remain attached.

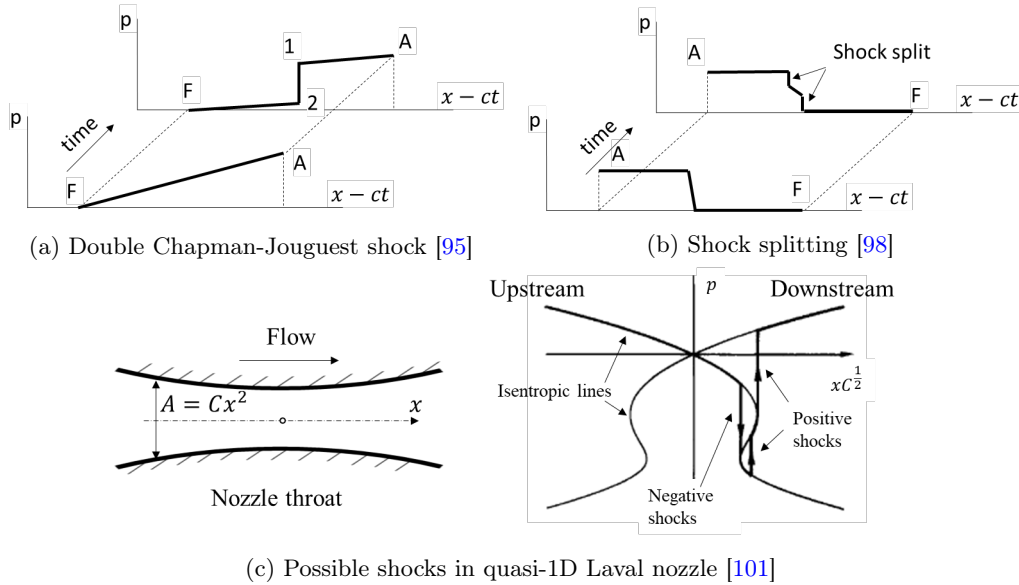


Figure 2.6: Non-classical gasdynamic behaviour in BZT fluids.

Pursuit for Experimental Evidence of Non-Classical Gasdynamic Behaviours

Although these non-classical phenomena have been found and analysed in theoretical analysis, it is difficult to provide experimental evidence for them. The first difficulty is the accuracy of the EoS,

since it has a strong influence on the simulation of non-classical phenomena [105, 87]. Even though some fluids are reported as BZT fluids when their minimum Γ is calculated with a less accurate EoS (such as the VDW EoS) [106], they may not actually be true BZT fluids. More accurate experimental data on the thermodynamic properties of fluids, especially near the saturation line and the critical point, are required to establish a more accurate EoS and to calculate Γ correctly. The second difficulty is the thermal and chemical stability of potential BZT fluids due to their complex molecular structure [107]. Cramer [6] and Guardone [108] suggested that BZT fluids can be found in the alkanes and perfluorocarbons with heavy molecular weight, while their $\Gamma < 0$ region is close to their molecular stable temperature limits.

Colonna [107] suggested that the experimental evidence for non-classical phenomena can be found in a new group of gas: Siloxanes (e.g., D_6), which have better stability. The other difficulty is the misleading by two-phase effects, since the range $\Gamma < 0$ is very close to the saturation line of fluids. Borisov [109] supposedly observed a rarefaction shock wave in a shock tube containing Freon-13, but Fergason [110] refuted this and showed that Borisov's experiment is affected by critical-point phenomena and two-phase effects, so it cannot be experimental evidence for a BTZ fluid. Nannan [111, 112] also proposed that these non-classical behaviours can also be seen in the near-critical vapour-liquid equilibrium region and not in the pure vapour region. Because of these difficulties, experimental evidence remains a challenge to this day. Colonna [113] and Casati [114] designed and built a Flexible Asymmetric Shock Tube (FAST) to measure the velocity and intensity of the waves. They have validated the test rig [115], but detection of rarefaction shock waves is still awaited.

Studies of Classical Non-ideal Gasdynamic Behaviours

In most (or say all) fluids in ORC applications, Γ is always greater than zero but can be lower than unity, so classical non-ideal gasdynamic behaviours are important to understand. According to Equation 2.32, if the Mach number is high enough to reach a positive j ($Ma > 1/(1 - \Gamma)$), the Mach number in the isentropic expansion process will decrease [96]. An increase in Mach number after an oblique shock wave can occur when $0 < \Gamma < 1$ [116, 117, 28], which is also called a 'non-ideal oblique shock wave'. Ahmadabadi [118] simulated supersonic flows over a cascade of wedge-shaped straight plates in air and a dense gas, R245fa. They showed that an oblique shock occurs at the leading edge instead of a bow shock and the separation point is later in the dense gas. The non-ideal effects also should be paid more attention. Vimercati [119] studied the cascade flows with a dense vapour and found that the upstream thermodynamic state of the gas determines the variation of the relevant properties across the cascades.

2.3.2 Wall-Bounded Turbulent Behaviours

The understanding of wall-bounded turbulent flows is the theoretical basis for the development of simulation methods based on turbulence models (e.g. RANS and LES simulation method). Even these methods have already been widely applied in industrial and scientific research of dense vapours, there are still doubts in the theoretical basis of directly applying the experiences from ideal gases to non-ideal gases. In this section, the research of ideal-gas turbulent boundary layers is reviewed at beginning, and then recent studies on the turbulent boundary layers in dense vapours are reviewed.

Ideal-Gas Compressible Wall-Bounded Turbulent Behaviours

The ideal-gas wall-bounded turbulent flows are studied by considering the compressibility effects based on the understanding of incompressible turbulent boundary layers. The theories of incompressible turbulent boundary layers can be seen in Kovaszny [120], Pope [9] and Cebeci [121]. Pope [9] sketched the structure of turbulent channel flows at high Reynolds number in Figure 2.7, where y is the wall distance, θ is the channel half height, and y^+ is the wall distance normalised by the wall viscous length scale. In the inner layer, the flow is nearly independent on the mainstream flows, so behaviour in the inner layer for channel flows is essentially the same as that for boundary layers on a flat plane [9]. It is found that the Reynolds number mainly influences the range of log-law region, but does not affect the flows in viscous wall region [10, 122], see the comparison of mean velocity profiles between turbulent channel flows under different Reynolds number in Figure 2.8.

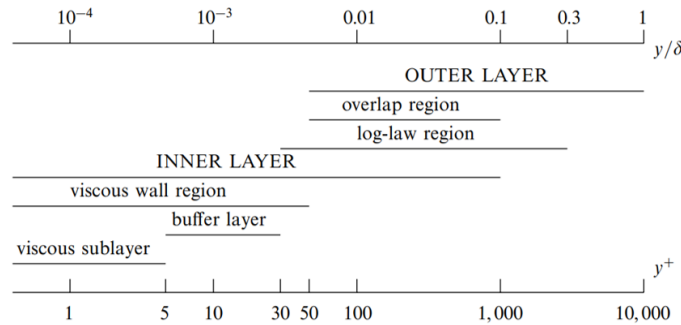


Figure 2.7: A sketch showing the various wall regions and terminology for a turbulent channel flow at $Re = 10,000$ [9].

Most studies of compressible turbulent boundary layers have focused only on ideal gases, and Fernholz [123], Bradshaw [124], Lele [125], and Smits [126] have reviewed early experimental and numerical investigations of this. The inconstant density, the compressibility and the strong viscous dissipation distinguish the turbulence behaviour of compressible boundary layers from incompressible flows. To understand the mean flow field, Morkovin [127] first proposed a hypothesis, in which

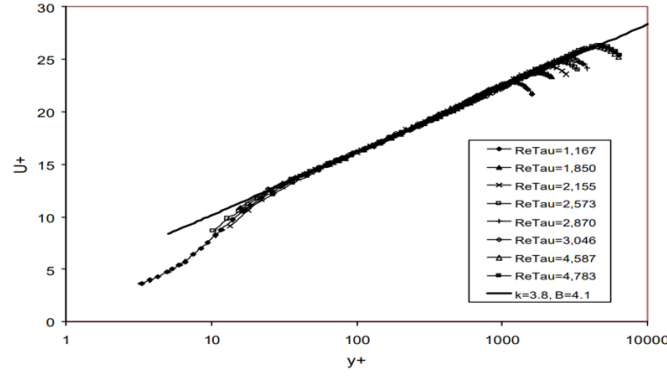


Figure 2.8: Mean velocity profiles of turbulent channel flows under different Reynolds number and the comparison with log-law [10].

the effects of density fluctuations are assumed to be relatively small compared to those of the mean density variation. Based on the Morkovin's hypothesis, Van Derist [128] proposed a density-weighted transformation to match the velocity profile in a compressible boundary layer to that in an equivalent incompressible flow, and it works in the log-law region. The Van Driest (VD) transformation [128] is given as follows:

$$\bar{u}_{VD} = \int_0^{\tilde{u}} \left(\frac{\bar{\rho}}{\bar{\rho}_w} \right)^{\frac{1}{2}} d\tilde{u}, \quad (2.34)$$

where $\tilde{u}$ is the Favre-averaged velocity. Recently, Trettel & Larsson [11] proposed a new transformation (called TL transformation) that takes into account not only the mean density variation but also the mean viscosity variation:

$$\bar{u}_{TL} = \int_0^{\tilde{u}} \left(\frac{\bar{\rho}}{\bar{\rho}_w} \right)^{\frac{1}{2}} \left(1 + \frac{1}{2} \frac{1}{\bar{\rho}} \frac{d\bar{\rho}}{dy} y - \frac{1}{\bar{\mu}} \frac{d\bar{\mu}}{dy} y \right) d\tilde{u}. \quad (2.35)$$

They applied VD transformation and TL transformation on three compressible cases with different Mach number, and they compared the velocity profile with an incompressible case. In Figure 2.9(a) and (b) [11], it showed that TL transformation makes the match of velocity profile in compressible boundary layers to that in incompressible boundary layers better than VD transformation. Here, y^+ is the wall viscous length scale, y^* is the semi-local viscous length, U_{VD}^+ and U_{TL}^+ are the values of $\bar{u}_{VD}$ and $\bar{u}_{TL}$ normalised by the wall friction velocity u_τ (definition of these parameters see the discussion in Chapter 5). Modesti [129] proved that the TL transformation significantly improves the model accuracy in the viscous sublayer compared to the Van-Driest transformation. Moreover, the mean temperature profile has a relation with the mean velocity profile in ideal-gas flows, according to the Reynolds analogy. This relation was derived by Walz [130] and is well

known as Walz's equation or Crocco's relation. Walz's equation was validated by the experimental work of Voisinnet [131] at Mach 4.9 with three different wall temperatures. Duan [132, 133] found that the Mach number has limited effect on the accuracy of the Walz's equation, but a lower wall temperature can lead to a noticeable uncertainty (up to 10%) in the Walz's equation.

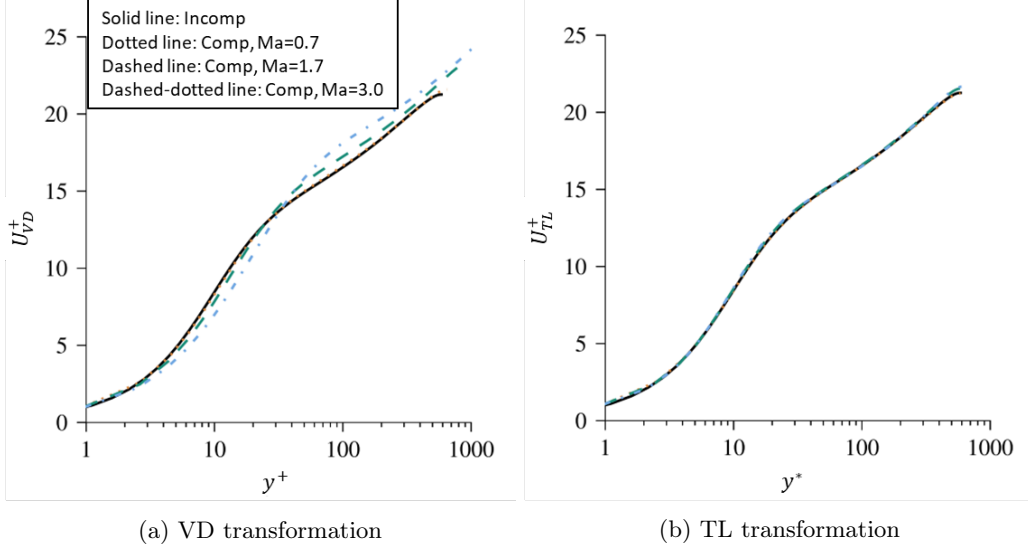


Figure 2.9: Comparison of the mean velocity profile in compressible boundary layers after transformed with that in incompressible boundary layers [11].

For fluctuation flow fields, more detailed studies on turbulence statistics and turbulence structures are performed using direct numerical simulation (DNS). As for turbulence statistics, Huang [134] found that the compressibility effects in air flows lead to only a small difference between Reynolds and Favre averages for the streamwise velocity, Reynolds shear stress, and turbulent heat flux. Meanwhile, the dilatation term in kinetic energy budget was found to be very small at moderate Mach numbers. Pirozzoli [135] studied the statistics of the velocity fluctuation at different Reynolds numbers. They found that velocity fluctuation statistics in compressible boundary layers, even up to the fourth order, is analogous to that in equivalent incompressible boundary layers when the mean density variation is properly accounted for. The validation of the strong Reynolds analogy (SRA) has also been studied recently. It was first proposed by Morkovin [127] to relate the statistics of the temperature fluctuation to that of the velocity. Considering the 'mixing length' assumption, Gaviffio [136] and Huang [134] modified the SRA and proposed new models separately. These modified models are validated in the work of Duan [132, 133] in compressible air flows under different wall temperatures and Mach numbers. According to these current research results, the turbulence statistics in compressible air flows are similar to those in incompressible cases.

For turbulent coherence structures, Coleman [12] studied near-wall streaks and found that the

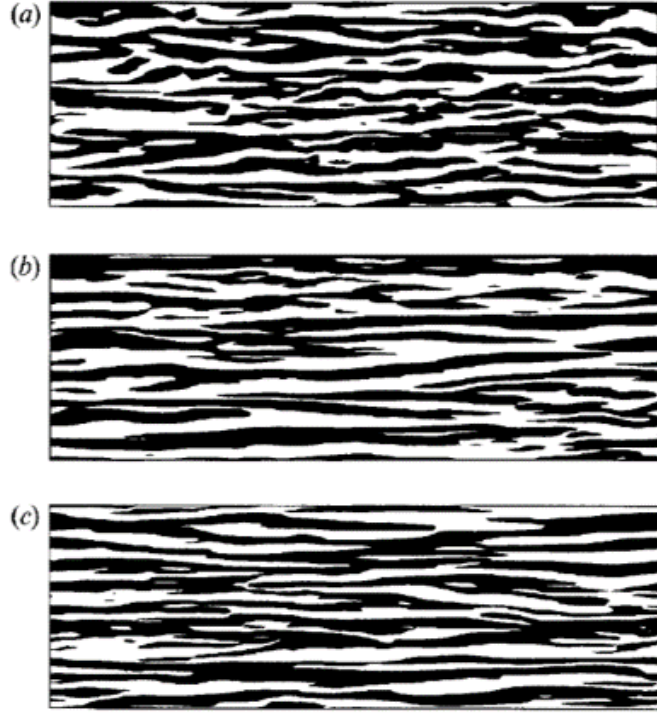


Figure 2.10: Contour of near-wall "streaks" for (a) incompressible case (b) Case $Ma = 1.5$ and (c) Case $Ma = 3.0$. Black region refers to negative wall-normal vorticity and white region refers to positive vorticity. (Figure 6 in reference [12])

streamwise coherence is enhanced in isothermal compressible boundary layers. In Figure 2.10 [12], Coleman compared the near-wall "streaks" at different Mach number and found the "streaks" are less "wiggly" when Mach number increases. Morinishi [137] and Duan [132] also studied this phenomenon and found that a lower wall temperature can decrease spanwise coherence but increase streamwise coherence. Duan [132] explained this by the change of anisotropy ratio (root-mean-square ratios of velocity fluctuations between different directions, v'_{rms}/u'_{rms} and w'_{rms}/u'_{rms}), and they concluded that the lower meandering and mixing in spanwise and wall-normal directions result in the 'longer' streaks. Adrian [138] studied the dynamics of the hairpin vortex in incompressible boundary layers and found that hairpin packets 'ride' on low-speed streaks. Pirozzoli [135] found that this phenomenon is also observed in compressible boundary layers. They showed that the integral longitudinal length scales and orientation of these vortices match those in incompressible flows. Duan [132] studied the effects of wall temperature on these vortices and found that lower wall temperature makes the vortex structures fatter and less chaotic.

These research of compressible wall-bounded turbulent behaviours are the basis of the development of RANS simulation method in compressible flows. For example, the studies of mean velocity transform and Walz's equation are the theoretical basis for setting wall boundary conditions in RANS. The theories of compressible wall-bounded turbulent behaviours in dense gases should be

developed further, since molecular-complexity effects and non-ideal effects have to be considered.

Dense-Vapour Compressible Wall-Bounded Turbulent Behaviours

Sciacovelli [139, 140, 141] has studied the dense-gas effects on detailed turbulent behaviour in boundary layers. They focus on a particular gas: PP11 (perfluoro-perhydrophenanthrene, $C_{14}F_{24}$), which has very high molecular weight and molecular complexity. They simulated fully-developed turbulent channel flows of PP11 at one thermodynamic state close to its critical point using the DNS method. In their case, extremely strong dense-gas effects make the friction heating effects insignificant, because the heat capacity of PP11 is very high. As a result, the boundary layers resemble 'incompressible flow' even at high Mach numbers. They explained that an extremely low characteristic Eckert number ($Ec = u^2/c_p T$) of PP11 leads to this phenomenon, and the Eckert number of PP11 is more than three orders of magnitude lower than that of air. However, the boundary layers for gases with moderate molecular-complexity effects are still unclear. In their cases, a liquid-like behaviour of mean viscosity profile (viscosity is lower in channel central than at wall) is observed, which is different from ideal-gas flows. However, it is not known whether this phenomenon also occurs when non-ideal effects are moderate. This will be discussed in this dissertation.

There are some other studies of wall-bounded turbulent behaviours considering the influence of fluid thermodynamic characteristics. Patal and Pecnik [142, 143] studied the influence of variable property in channel flows. They considered the density as constant or proportional to T^{-1} , and the dynamic viscosity proportional to $T^{-0.5}$, $T^{0.7}$, T^{-1} or $T^{1.2}$ in different cases, and they supported that using semi-local scaling, which proposed by Huang[134], can make a good collapse of profiles of $\bar{u}_{VD}$ and second-order turbulent statistics between different cases. A group of studies [144, 145, 146, 147, 148, 149, 150, 151] focus on the impact of strong non-ideal effects on the wall-bounded turbulent behaviours in fluids with simple molecules (like CO_2 and N_2) within low Mach numbers ($Ma < 0.3$), which is less related to the dense vapour studied in this dissertation, so they are not reviewed here in details.

2.3.3 Laminar-Turbulent Transition in Boundary Layers

The laminar-turbulent transition phenomenon is important for the internal flows of turbines, especially at the blade leading edge, while it has been studied only to a limited extent in real gases. There are two main types of transition in boundary layers: the natural transition and the bypass-type transition [13]. The natural transition happens when environmental disturbances are small, while the bypass transition occurs when the environmental perturbations are strong.

In natural transition, the process consists of three stages: Receptivity, Linear Stability, and Nonlinear Breakdown (see Figure 2.11), while in the bypass-type transition the nonlinear breakdown occurs directly without the first two stages [13]. In the receptivity stage, instability waves are generated by perturbations, including acoustic, vortical, temperature, and vibrational fluctuations. These instability waves are also called Tollmien-Schlichting (T-S) waves, which are the unstable eigen-mode of the Orr–Sommerfeld equations. The linear stability stage is the process of amplification of the instability waves. It is described by the linear hydrodynamic stability theory (see the book by Drazin [152]). In the nonlinear breakdown stage, the instability waves reach significant amplitudes and then break up into turbulent flows. This process is associated with resonant phenomena and coherent structures, and this is the focus of Chapter 6.

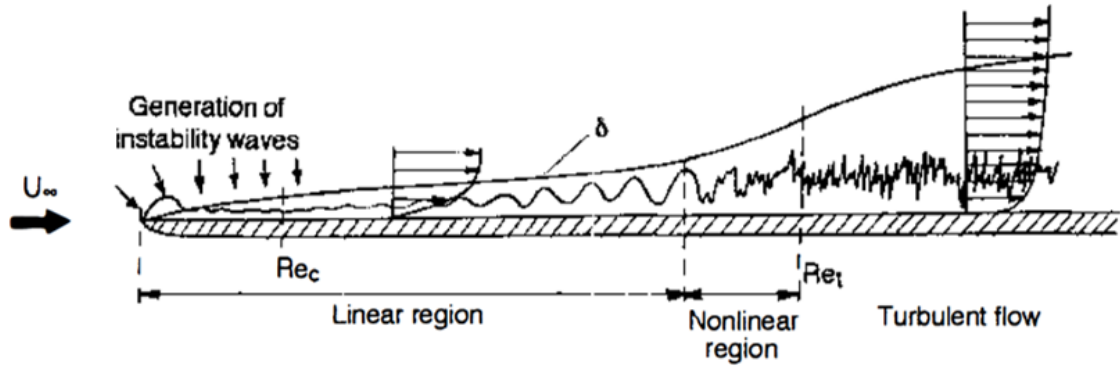


Figure 2.11: The sketch of natural transition process. [13].

There are three main types of breakdown process: K-breakdown, N-breakdown and O-breakdown [13, 153]. K-breakdown is named after Klebanov [154]. It is characterised by aligned Λ -vortices and occurs mainly when the fundamental-wave amplitude of the instability waves is relatively large. The N-breakdown is named after Novosibirsk, the institution where Kachanov [155], Herbert [156], and Craik [157] worked in. It is characterised by a staggered order of Λ -vortices and occurs mainly when the fundamental-wave amplitude of the instability waves is relatively small. The resonant amplification of the subharmonic modes is the main reason for the N-breakdown. The O-breakdown is discovered by Golstein [158] and Schmid [159], which also form staggered Λ -vortices. These staggered structures are caused by a pair of oblique waves at the fundamental frequency (instead of half the fundamental frequency in N-breakdown). Although the formation mechanisms of these breakdowns are different in the instability theory, the features of the developing vortex structures in the late stage are similar [160, 161].

Bake [162] divided the transition process of K-breakdown into 8 stages (shown in Figure 2.12). The first two stages correspond to primary and secondary instability theory, and these two stages are usually very short in the bypass transition. The resonant interaction of 3D and 2D modes

of the frequency-wavenumber spectrum is the reason of the rapid growth of spanwise modulation [157, 163, 164]. Then vortex structure generated from this modulation and ‘spikes’ (high-frequency, flash-like oscilloscope traces) appears at the top of a Λ -vortex (the centre of the hairpin vortex) [165, 166]. This is also where the first random fluctuations are observed. After the first Ω -vortex is formed, a series of Ω -vortices form from it according to the vortex dynamics, leading to a packet of vortices [167], and having a strong effect on the surrounding fluid through a velocity gradient and a pressure gradient [168, 162]. Finally, the vortex structures and high-shear layers interact and lead to more small vortices and high-shear layers, and these processes are very sensitive to background disturbances [169]. The randomness is caused by the amplification of the random background disturbance by a large local velocity gradient generated by the complex interaction of countless vortex structures [162].

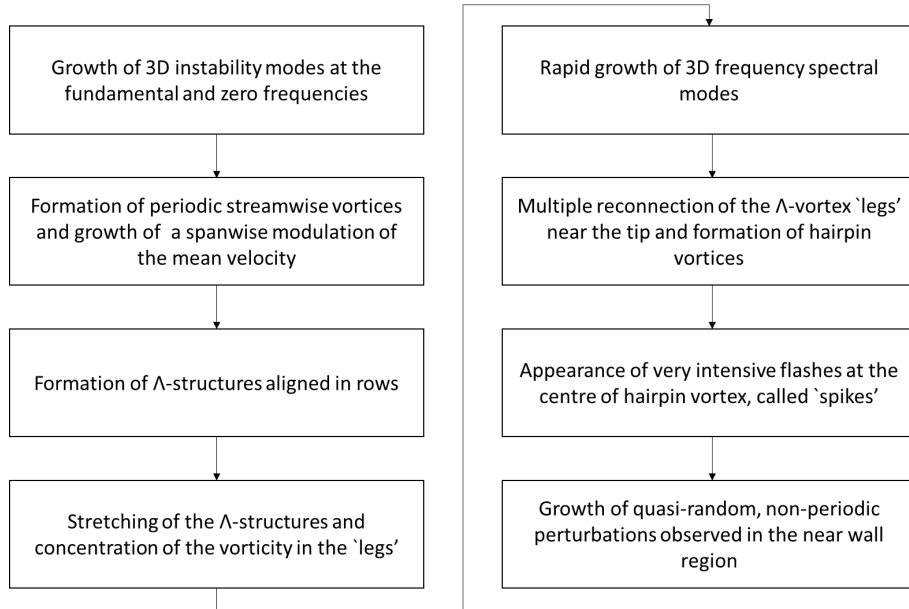


Figure 2.12: Transition process of K-breakdown.

Lee [170, 171] proposed that solitonlike coherent structures (SCSs) form earlier than the Λ -vortex, which is the low-speed streak in the transition process. They argue that SCS directly leads to the second closed vortex, and the interaction between the Λ -vortex and the second closed vortex results in the high-frequency vortices (called the chain of ring vortices). Guo [172] found that the sweep and ejection events caused by the Λ -vortex and the Ω -vortex lead to a ‘dark spot’ where all hydrogen bubbles (tracer particles) disappear. Lu [173, 174] studied the mechanism of the generation of the chain of Ω -vortices and proposed that the strong sweeps caused by the leading vortex lead to strong positive spikes and a high shear layer that is not stable, therefore generating small length scales near the wall. Bernard [175] analysed both one-leg and two-leg hairpin

vortices in transition and found that these two types of vortices represent the rotation of tilted and symmetric vortex furrows, respectively. They believed that the vortex furrows ("elongated, streamwise-oriented, raised folds in the surface vorticity layer") is better for describing the rotational signature of structure than the traditional way. Liu et al [176, 177, 178, 179] proposed that the Λ -vortex legs and the vortex rings (Ω -vortex) are formed separately and independently, which is different from traditional understanding. They found that the Λ -vortex is always open on head which is not a 'vortex tube'; meanwhile, they found that the ring structure is generated by shear layer instability caused by the ejection events of the rotation effect of the Λ -vortex legs, and not by Λ -vortex breakdown. Based on their research, Dong [180, 181] compared the vorticity lines with vortex structure and found that vorticity lines in a Λ -vortex start from the side boundary and end there, while vorticity lines in a vortex ring are mainly self-closed. They also found that the volume vorticity is strongly correlated with the vortex strength, implying that the flow fluctuations are mainly caused by the vortex. Zhao [182] found that vortex reconnection is the main reason for the rapid increase of skin friction coefficients, because it can induce a opposite velocity to the mean flow, blocking the flow above the wall and thus accelerating the near-wall flows. Following this concept, Zheng [183] proposed an image-based modelling of skin friction coefficient in the transition, which is more accurate than current models.

In contrast to the 'ordered' regime breakdown, normal bypass transition is caused by free-stream turbulence which is non-modal perturbations (also known as "Klebanoff modes", "breathing modes" or "streaks") [184, 185, 186]. Another way to understand the bypass transition is that it is the continuous mode of the Orr-Sommerfeld equation, which is different from the T-S wave (discrete mode) [187, 186]. These streaks are caused by jets in the perturbation field, and the streaks are only seen in the streamwise component of the velocity. The formation of streaks can be explained by linear distortion theory (or rapid distortion theory) [188, 185]. At the start of transition, a turbulent spot is observed (see Figure 2.13). Jacobs [14] simulated a bypass transition with free-stream turbulence and found that the long streak is observed in the fluctuating u -velocity field, and the turbulent spot (a patch of irregular motion) is observed in the fluctuating v -velocity field (see Figure 2.13). A Kelvin-Helmholtz instability is observed at the leading of the spot, and then the spot spreads downstream and merges into turbulent boundary layer. The bypass transition induced by passing wakes is also seen in the reference works [189, 190].

The interaction of "Klebanoff modes" and T-S waves has also been researched recently. When the T-S wave is strong, Λ -vortices forms but neither K- nor N-type, and the pattern of Λ -vortices depends on the frequency and spanwise width of the Klebanoff streak; when "Klebanoff modes" are strong, the bypass transition dominates and the influence of the T-S wave is small [191, 192, 193].

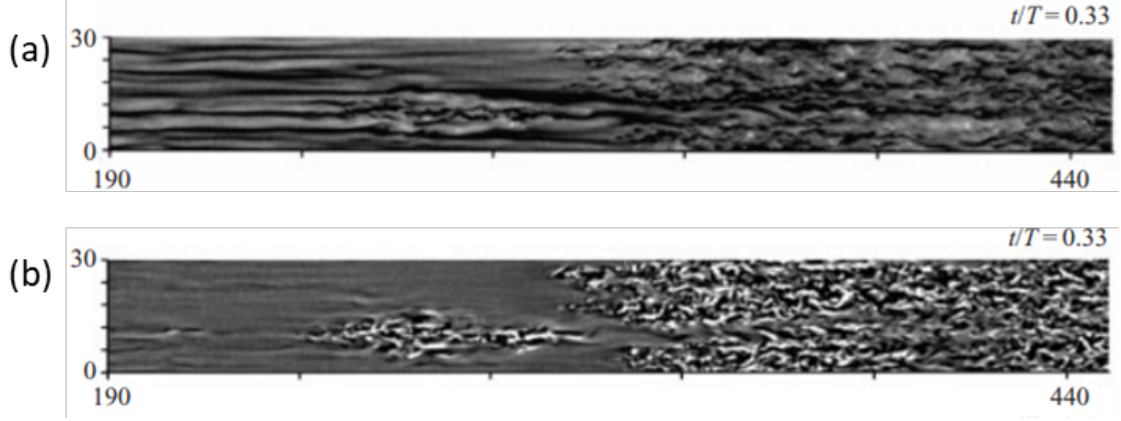


Figure 2.13: (a) Streak and (b) turbulent spot images. (a) is u' and (b) is v' counters on a near-wall X-Z plane from DNS results [14].

Although the transition in incompressible flows and compressible air flows has been studied for decades, research on the transition in compressible dense-vapour flows has only recently begun. Gloerfelt [194] studied the linear stability theory in dense vapours. However, the breakdown stage of the transition in dense vapours has not been studied, and this is the focus of Chapter 6.

2.4 ORC Turbines

The studies of ORC turbine, especially, the supersonic stator and the experimental research of dense vapour supersonic flows are review.

2.4.1 Design and Analysis of ORC Turbines

ORC Turbine Characteristics

The thermodynamic characteristics of dense vapours lead to special requirements of the design of ORC turbines. Persico & Pini [195] pointed out that the high molecular complexity of dense vapours reduces the specific enthalpy drop in the turbine, therefore making the compact configurations (only a single stage or a few stages) possible for the ORC turbines. These compact configurations can simplify turbine structures and save costs.

However, if a single stage is used, the expansion ratio will be high enough to lead to highly supersonic flows. Meanwhile, the low speed of sound in these dense vapour also enhance the Mach number in ORC turbine. It means the supersonic nozzle with the converging-diverging shape should be used in these applications, which is usually used when Mach number at nozzle exit is over 1.4 [195]. The threshold working conditions of the need of the converging-diverging nozzle are calculated for different organic fluids. For example, in a single-stage turbine designed for an

ORC system with the condensing temperature at 35°C or 85°C, if the turbine reaction degree is zero, the loss in the nozzle is ignored, and the overheating temperature at turbine inlet is 10°C, the threshold turbine inlet temperature $T_{tur,in}$ and the nozzle total-static pressure ratio $PR_{ts,n}$ are shown in Table 2.5. If turbine working conditions is higher than the values in Table 2.5 for an organic fluid, the nozzle-exit Mach number will exceed 1.4, and the converging-diverging nozzle is needed for reducing the shock loss.

Fluid	R134a	R1234yf	R1233zd(E)	R245fa	MM	MDM	Pentane	Toluene
Condensing temperature is 35°C								
$T_{tur,in}$	85.7	87.4	79.3	78.0	68.2	62.7	77.8	68.3
$PR_{ts,n}$	2.70	2.67	2.74	2.73	2.70	2.70	2.73	2.77
Condensing temperature is 85°C								
$T_{tur,in}$	-	-	142.1	140.7	128.9	121.6	140.8	128.6
$PR_{ts,n}$	-	-	2.68	2.66	2.68	2.69	2.69	2.74

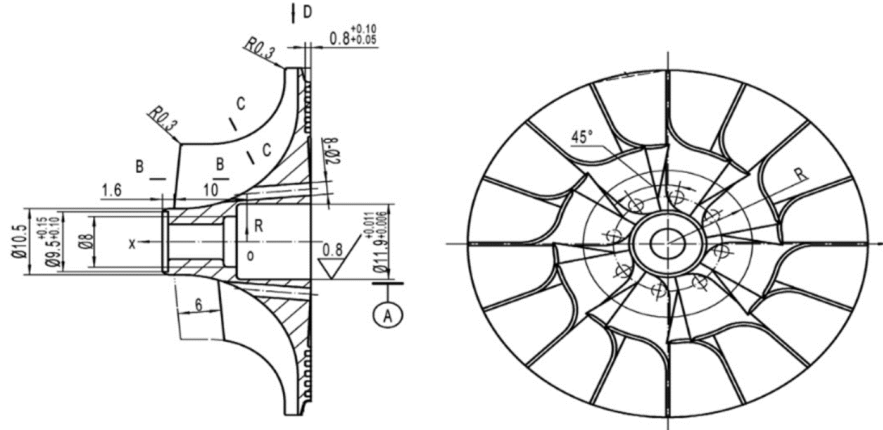
Table 2.5: Threshold working conditions requiring the converging-diverging nozzle for different organic fluids. Overheating temperature at turbine inlet is assumed at 10 °C.

ORC Turbine Architectures

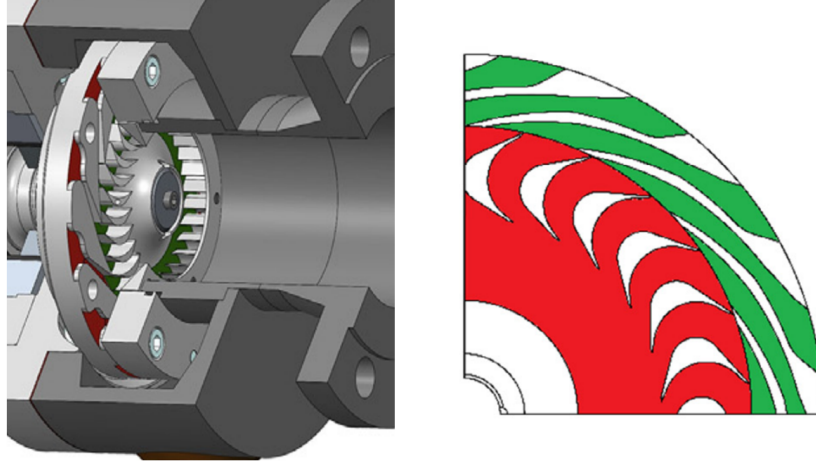
Three main types of turbines are studied and used in ORC systems: radial inflow turbines, axial turbines, and multistage radial outflow turbines (centrifugal turbines).

Radial inflow turbines have the advantage of high power density, high peak efficiency, and small size [196], and they are usually used at low power output (tens to hundreds of kW, and also some applications in a few MW) [195]. The conventional 90° radial-inflow rotors are used in some applications [15, 197, 198, 199, 200, 201] (see the meridional scheme and front view in Figure 2.14(a)); while the radial-inflow cantilever rotors are also used in high-expansion ratio ORC turbines [202, 16] (see the meridional scheme and front view in Figure 2.14(b)). One advantage of the radial-inflow cantilever rotors is that nearly zero reaction can be designed (zero pressure drop in rotors), so it is suitable for working with a partial-admission nozzle ring (a portion of nozzle channels are blocked off)[16]. This nozzle ring has the advantages of a higher blade height (for small flow rate) and a flexible control strategy for partial-load working conditions (blocking partial nozzle channels)[203]. Weiß [16] compared a radial-inflow cantilever impulse turbine with an axial turbine, which are designed for the same output power (about 12-13kW), and the tested efficiency of this radial turbine (76.8%) is slightly higher than that of the axial turbine (73.4%). These mentioned experimental studies of radial turbine are listed in Table 2.6, where the pressure

ratio, turbine efficiency and output power are also shown.



(a) Meridional scheme and front view of 90° radial inflow rotors[15]



(b) 3D sketch and front view of radial-inflow cantilever rotors [16, 17]

Figure 2.14: Sketch of (a) 90° radial-inflow rotors [15] and (b) radial-inflow cantilever rotors[16, 17].

Axial turbine is usually used when the mass flow rate is large and the output power is high (hundreds of kW to a few MW) [195]. Multi-stage axial turbines are applied in the some systems with large power output[204], and compact single-stage turbines are applied to simply turbine structures. Reaction rotors are used in some applications [205, 206, 207, 208, 209]; while for avoiding high supersonic flows in the rotor, small-reaction rotors or impulse rotors are also studied[16]. Partial admission nozzles are also applied in axial ORC turbines for enlarging the blade height when mass flow rate is very low [215, 210, 211, 212]. These experimental studies are also listed in Table 2.6.

Radial-outflow (centrifugal) turbines have the advantage of a large volumetric flow ratio, which is suitable for ORC applications, so it can be used in both large and small ORC systems[195]. Besides, by applying multi stages on one rotor disk, the high supersonic flows can be reduced within a relative compact structure. Pini [213] designed a six-stage ORC centrifugal turbine,

Reference	Type of turbine	Fluid	Method	Expansion ratio	Maximum efficiency	Power
					%	kW
Pei [15]	Radial inflow	R123	Experimental	7.1	65	1
Kang [197]	Radial inflow	R245fa	Experimental	2.62 - 2.72	78.7	24.5 - 31.2
Shao [198]	Radial inflow	R123	Experimental	<2.3	75.2	~1.2
Han [199]	Radial inflow (two stages)	R245fa	Experimental	2.8 & 3.17	72.4	205.4
Alshammari [200]	Radial inflow	not report	Experimental	<10	<35	<6.3
Demierre [201]	Radial inflow	R134a	Experimental	3.1-4.5	62-74	~3
Bülten[202]	Radial-inflow cantilever rotor	Methylcyclohexane	Experimental	~50	79	68
Weiß [16]	Radial-inflow cantilever rotor	MM	Experimental	12 - 24	76.8	5.1 - 16.0
Yang [204]	Axial flow (four stages)	R245fa	Experimental	3.74 (overall)	78.52	~650
Yue [205] & Pu [206]	Axial flow	R245fa	Experimental	~3.5	60	<2
Moroz [207] & Fu [208, 209]	Axial flow	R245fa	Experimental	5.74 & 7.22	63.7 & 62.2	~250
Klonowicz [210]	Axial flow (partial admission)	R227ea	Experimental	~2.8	58	13.2
Li [211]	Axial flow (two stages, partial admission)	R123	Experimental	6.6	53	~6.5
Weiß [16]	Axial flow	MM	Experimental	12.6 - 19.4	73.4	5.6 - 14.1
Seume[212]	Axial flow (partial admission)	Ethonal	Experimental	50	57	8.0
Pini [213]	Radial outflow (six stages)	MDM	3D simulated	~4	86.92	1,272
Kim [214]	Radial outflow (single stage)	R143a	3D simulated	1.47	85	400

Table 2.6: Review of some ORC turbine research.

whose efficiency is 86.92% (by CFD simulation). Several studies [216, 217, 214] on the preliminary design and performance analysis of centrifugal turbines by CFD simulation method are carried out following Pini's work, but the published experimental studies on centrifugal turbines are limited up till now. The simulated performance of the centrifugal turbines designed by Pini [213] and Kim [214] is listed in Table 2.6 for compared with other turbine architectures.

To claim, Table 2.6 does not include the test of commercial ORC turbines, and the summary of commercial ORC turbines can be seen in reference [218].

Design Process

The conventional design process of a turbine stage is shown in Figure 2.15 [195]. After the turbine architecture, the working fluid, and the turbine inlet and outlet states are determined, the preliminary design starts to decide the critical parameters: the flow coefficient ϕ , the load coefficient Ψ , the degree of reaction χ , Reynolds number Re , Mach number Ma , and dimensionless geometrical characteristics vector σ [219]; Then the 3D blade geometry is designed (sometimes with the help of CFD simulation); Finally, the 3D blade geometry is optimized with the help of both CFD and experimental method.

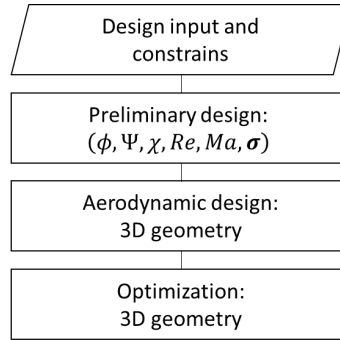


Figure 2.15: Design process of turbines.

The influence of thermodynamic characteristics of dense vapours on the preliminary design is studied recently. Giuffrè & Pini [219] proposed that the volumetric flow ratio $\alpha_\rho = \rho_{in}/\rho_{out}$ can be dramatically increased when increase the enthalpy drop slightly in a stage, so α_ρ should be considered in the preliminary design. They [219] also proposed that the isentropic pressure–volume exponent γ^* , which is defined in the relation p/ρ^{γ^*} , does not only depend on working fluids but also on the local thermodynamic states, and it is also should be considered. Based on these, they proposed a non-ideal similarity equation: $\eta = f(\phi, \Psi, \chi, Re, \alpha_\rho, \gamma^* \sigma)$ for the preliminary design of ORC turbines. Then, the loss models (including boundary layer loss, mixing loss, shock loss, endwall loss and tip-leakage loss) are applied to predict turbine efficiency, so as to optimize the

preliminary design. In the study of Costall[220] (a preliminary design of radial ORC turbine), loss models of incidence loss, nozzle loss, rotor loss, windage loss, shock loss, and tip-leakage loss are considered to predict the turbine loss. CFD-based throughflow method is a more reliable preliminary method (zFlow, developed and used by Persico[195] and Pini [213]), especially in the design of unconventional ORC turbines (e.g. radial-outflow turbines).

The aerodynamic design of 3D blade shapes follows the results of preliminary design, and the camber line, pressure and suction surfaces, and leading and trailing edges are designed[195]. However, when a supersonic nozzle is applied, the blade shape should be designed focusing on the nozzle channel shape for reducing the shock loss [195]. This is very important for ORC turbine design, so it is specially reviewed later in Section 2.4.2.

After the blade shape is designed and parameterized, the turbine performance should be analysed by either CFD or experimental method, which is the basis of the optimization. To claimed that CFD-based automatic blade-optimization method is a powerful design tool in industrial applications, including adjoint-based gradient optimization and evolutionary algorithms method (see details in reference [195, 43, 221]).

Analysing Methods

The experimental method and the numerical method (CFD simulation method) and are the two main analysing methods to analyse ORC turbine performance and internal flows. For the experimental method, a part of research focus on the test of the entire turbine performance, which has been summarised in Table 2.6; while the other part focus on the measurement of detailed flow features in turbines. The latter is more helpful for understanding the ORC turbine internal flows, and it is highly related to the work of this dissertation, so it is reviewed in detailed later in the Section 2.4.3.

The investment cost and time cost of the numerical method are much lower than the experimental method, and it can provide more detailed information of internal flow fields, so it is also widely used to analyse the ORC turbines. The non-ideal effect should be considered in the development of numerical algorithm, since the relation between thermodynamic properties is more complex. For example, the energy does not only depend on the temperature, but also on another thermodynamic property (e.g. density or pressure). Up till now, some commercial, open-source and in-house solvers are available for the simulation of non-ideal gases, e.g. ANSYS Fluent[222], ANASYS CFX[222], OpenFOAM[18], zFlow[85], SU2[223, 224] and in-house solvers [225, 139].

For the studies of the algorithm for non-ideal gas CFD, jarczyk and Pfitzner [18] modified the PISO (Pressure Implicit with Splitting of Operators) algorithm by considering the non-ideal

effects. They proposed that the PISO loop should not only calculate the pressure equation but also take the energy equation into the iteration loop, see the comparison between Figure 2.16 (a) and (b). Colonna and Rebay [226] developed a numerical method for non-ideal gases on unstructured grids, and they proposed the form of Jacobian matrix for non-ideal gases. Guardone [227] studied the Roe linearization of the convection term in conservation equations and found that the Roe matrix is no longer a strict Jacobian matrix but a quasi-Jacobian matrix which is augmented by additional pressure derivatives. The Roe linearization applied in real gases is also seen in the work of Glaister [228]. Rinaldi [229] studied the exact Jacobian matrices of convective terms and proposed the method to apply different finite-volume schemes (including Roe, AUSM⁺, HLLC, KT schemes) into the simulation of non-ideal-gas flows.

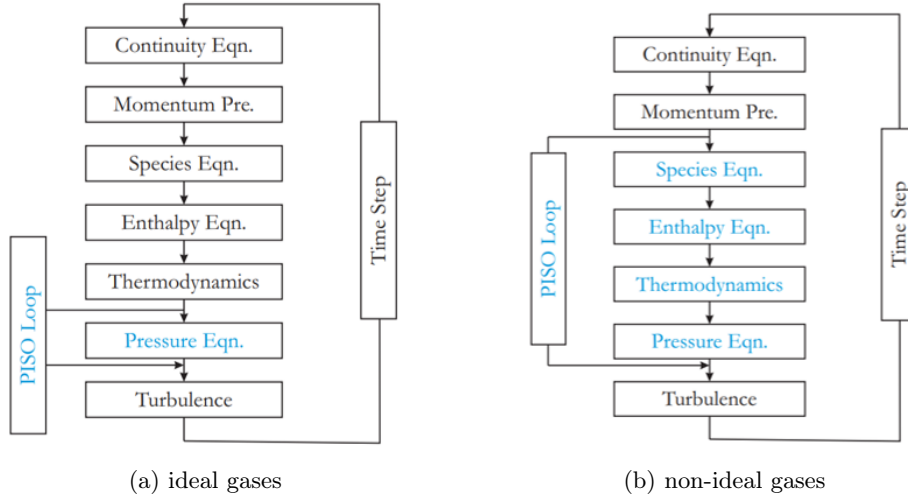


Figure 2.16: Modification of PISO algorithm for non-ideal gases [18].

Besides the CFD algorithm, the selecting and applying the non-ideal EOS are also important in the numerical method. A non-ideal EOS is necessary for the CFD simulation, but the highly accurate EOS (e.g. SW EOS[1]) is not always the best choice, since it leads to a complicated calculation process and a longer calculating time. Some studies compared different non-ideal EoSs in CFD simulations. Colonna[85] and Harinck [230] compared ideal-gas EOS, Peng-Robinson-Stryjek-Vera (PRSV) EOS and Span-Wagner (SW) EOS (the-state-of-art EOS) applied on the two dimensional supersonic nozzle flows with toluene and R245fa as working fluids. They found the derivation of PRSV EOS is <2% in all flow parameters (except the total pressure loss) when compared to SW EOS, while the derivation of ideal-gas EOS can be up to 18–25%. By using PRSV EOS instead of SW EOS, the computing time can be reduced by about 1/3. Robertson [231] compared the ideal-gas EOS, Peng-Robinson (PR) EOS and SW EOS (using NIST REFPROP) in the simulation of a converging-diverging nozzle flow using R1233zd(E) as the working fluid.

According to their results, the simulated pressure ratio by PR EOS is 1.7-2.2% higher than that by SW EOS, while the overestimation by ideal-gas EOS is 10.1-15.4%. To reduce the extra computing time caused by using non-ideal EOS instead of ideal-gas EOS, a lookup table interpolation is considered in some CFD methods [232, 233]. Pini [232] studied the accuracy and computational cost of using a look-up table (5,000 cells), and found that the computing time for a supersonic nozzle flow can be reduced by 65%, while the Mach number distribution perfectly overlap the CFD results from SW EOS. Rinaldi [229] also studied the time cost, consistency and accuracy of the look-up table method, and they compared three interpolation methods: bilinear, least-squares gradient and 3rd order Lagrange polynomial interpolation schemes. It was found that in the same table edge note, the bilinear scheme has the smallest computational cost but the polynomial scheme has the highest accuracy.

Flow Features and Loss Generations

Some research studied the ORC turbines whose expansion ratio are not too high to require a converging-diverging nozzle. Congedo [234] studied the non-ideal effects in an axial turbine, in which the rotor blade uses the von-Karman Institute LS-59 plane cascade (VKI LS-59). They found that the isentropic efficiency can be increased if the turbine inlet condition is selected in the region with lower Γ , because the Mach number after expansion is decreased and the shock loss is therefore reduced. This finding is consistent with a later research of Sciacovelli [235], in which the flows in multistage conventional axial turbines with different working fluids are studied. Tosto [236] studied the impact of cascade solidity on loss generation and found that the optimal solidity in the ORC turbine cascade is higher when exit Mach number is higher, regardless of the working fluid.

Wheeler [19] studied a radial turbine (90° radial-inflow rotor) by both steady and unsteady CFD. The working fluid is pentane, and the stator exit Mach number is about 1.35. They found that the rapidly increasing Mach number in the inducer leads to a separation on the rotor suction surface (see Figure 2.17(a)). Then an optimization of the endwall shape was proposed to avoid this separation, see the endwall shape before (ROTOR1) and after (ROTOR1) the optimization in Figure 2.17i(b). They also compared the steady and unsteady CFD results and found that the unsteadiness reduces the efficiency by about 1.25-1.5 percentage points. De Servi [237] studied the same type ORC turbine, but the stator exit Mach number is about 2. Both steady and unsteady CFD results predict a similar total-to-static efficiency at 84%. From the analysis of loss generation, they found that the stator loss is more significant compared to conventional turbines whose Mach number is lower, and it is due to the viscous dissipation and mixing.

Rinaldi [20, 238] studied a high expansion ratio (>100), single stage, radial turbine (with a can-

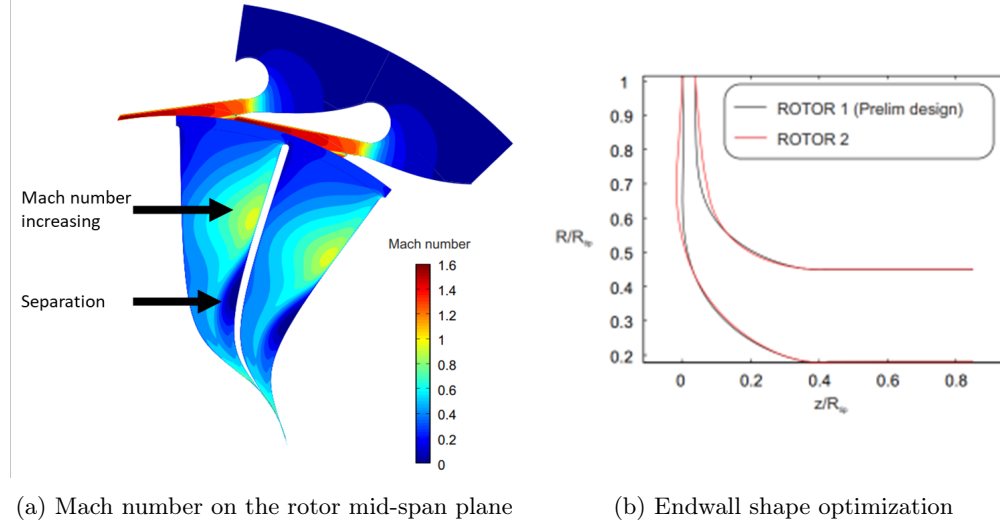


Figure 2.17: The boundary layer separation in rotor and the optimization of endwall shape [19].

tilever rotor) by quasi-3D unsteady simulation, and the simulation domain is shown in Figure 2.18 (a). The Mach number at nozzle exit is about 2.8, so supersonic flow features are observed in the domain, see the contour of transient pressure gradient in Figure 2.18 (b). Two strong oblique shocks (ST1, ST2) are originated from the stator trailing edge, and one of them is reflected on the stator surface(R); a bow shock (BS) locates in front of the rotor leading edge; a oblique shock (OS) is on the suction surface of rotor blade; two oblique shocks (RT1, RT2) are originated from the rotor trailing edge. The interaction between the stator trailing shocks and the rotor front shocks lead to highly fluctuated blade loading (30-60% of the time-averaged value). The loss generation is found mainly in boundary layers: on the stator trailing edge and, especially, the rotor suction surface (where a separation is induced by OS). Obert [239] simulated the first stage of a three-stage axial turbine by both unsteady and steady RANS CFD. In the unsteady simulation result, they found a similar flow characteristics to Rinaldi's Work [20]. By comparing the steady to unsteady simulation result, it is found that the difference of the total-to-total efficiency is less than 0.2% for the studied turbine. It should be noted that the gap between stator and rotor is large in Obert's turbine.

2.4.2 Research of Supersonic Stator

Design Method

The blade channel shape, especially the diverging part, instead of the blade shape itself is critical for the nozzle loss [195], so the design of supersonic converging-diverging nozzles usually starts from the design of the diverging part of the blade channel. The method of characteristics (MOC)

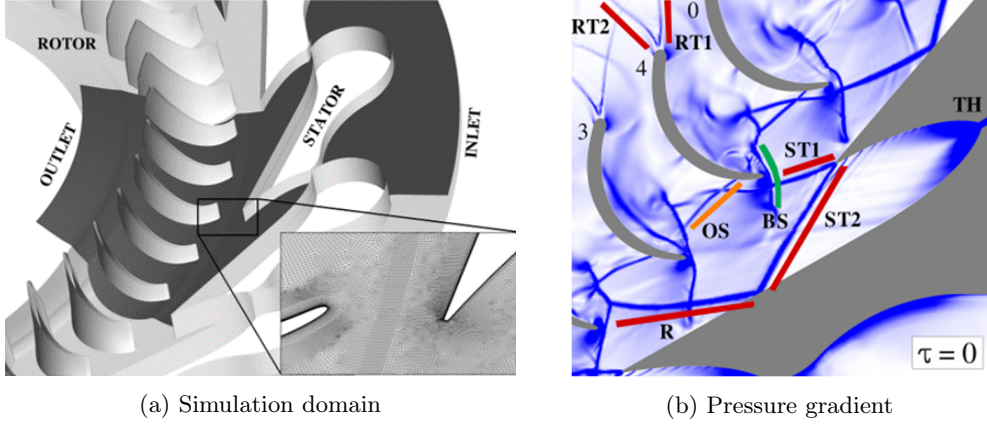


Figure 2.18: Quasi-3D unsteady simulation of a radial turbine [20].

is a widely-used method to design the diverging channel shape. In the MOC, the specific total enthalpy and entropy are assumed uniform, and the flow is assumed as an irrotational 2D flow. Therefore the continuity and momentum conservation equation can be simplified to the equation of velocity potential ϕ [240]:

$$(\phi_x^2 - c^2) \phi_{xx} + 2\phi_x \phi_y \phi_{xy} + (\phi_y^2 - c^2) \phi_{yy} = 0 \quad (2.36)$$

where $\nabla\phi = \mathbf{v} = (u, v)$, and the subscripts indicate partial derivatives in two directions. The solution of Equation 2.36 gives the conserved relations along a pair of characteristic lines:

- Along characteristic line C^+ , $(\theta - \nu)$ is constant, and the slope is $\left(\frac{dy}{dx}\right)_{C^+} = \tan(\theta + \mu)$;
- Along characteristic line C^- , $(\theta + \nu)$ is constant, and the slope is $\left(\frac{dy}{dx}\right)_{C^-} = \tan(\theta - \mu)$.

Here θ is the flow angle, μ is the Mach angle $\sin(\mu) = 1/Ma$, and Prantdl-Meyer function is used to solve ν :

$$\nu(Ma_2) - \nu(Ma_1) = \int_{Ma_1}^{Ma_2} \sqrt{Ma^2 - 1} \frac{dU}{U}, \quad (2.37)$$

where $U = \sqrt{u^2 + v^2}$. The sketch of a pair of characteristic lines through a point is shown in Figure 2.19. Both Aldo [241] and Guardone [242] derived the solution of the Prantdl-Meyer function in non-ideal gases and applied the MOC in the design of diverging channel shape for non-ideal gases. Then, Guardone [243] compared the nozzle sizes of different fluids designed by MOC, and they found that nozzle length and exit height are reduced by molecular complexity due to a smaller value of Γ . Colonna [85] studied the real-gas effects on the design of ORC turbine nozzle. They found that a larger exit-to-throat ratio is required to achieve equivalent expansion at supercritical conditions than at subcritical conditions. Wheeler [21] proposed a simplified method for approximating $\nu(Ma)$, in which the isentropic exponent γ_k is considered as a constant ($\gamma_k < 1$

can exist in dense vapours). They compared the Mach number distribution predicted by simplified MOC with that from RANS simulation, and the difference is shown below 0.5%. The designed blade shape can be seen in Figure 2.20 (a), where the black lines are a symmetric diverging channel, blue and red lines are the inducing part, and green lines are the post-expansion part.

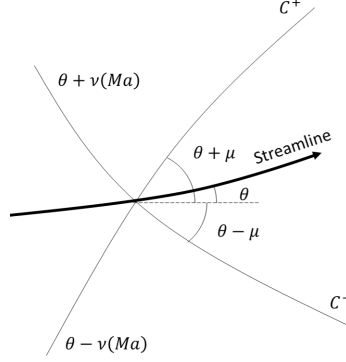


Figure 2.19: Sketch of characteristic lines.

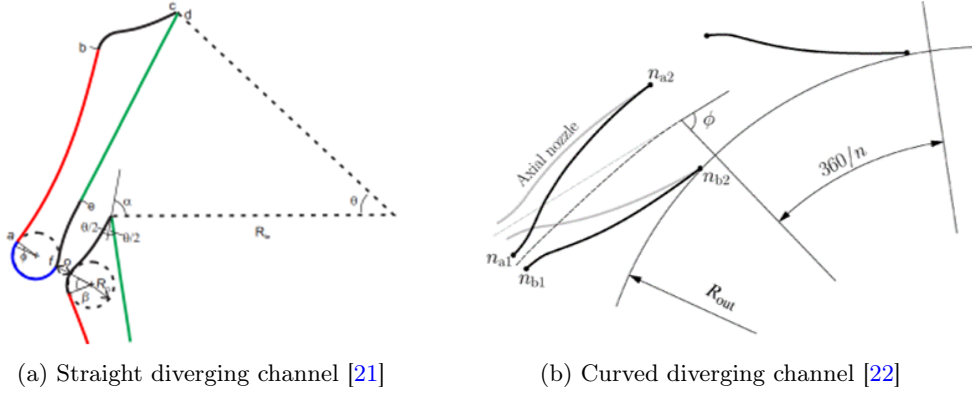


Figure 2.20: MOC-based design of supersonic nozzle blades [21, 22].

Annand [22] proposed a MOC-based preliminary design method for a radial nozzle vane, in which a curved diverging channel is achieved by conformal mapping from a straight nozzle (see changing from thin lines to bold lines in Figure 2.20(b)). By CFD analysis of designed nozzles, they pointed out that the post-expansion ratio is a critical parameter for nozzle efficiency. Subsequently, Annand [244] found that the blade metal angle mostly influences the optimum post-expansion ratio compared to other design variables, e.g. the solidity and the total-to-static pressure ratio. Zocca [23] developed a design method for a planar asymmetric nozzle with a curved mean line based on MOC, see Figure 2.21.

The CFD-based optimization method is also able to help achieve a supersonic nozzle design. Pasquale [245] proposed a method to optimize the design by parameterizing the blade to minimize the loss in the nozzle. Pini [221] proposed an adjoint-based shape optimization method for su-

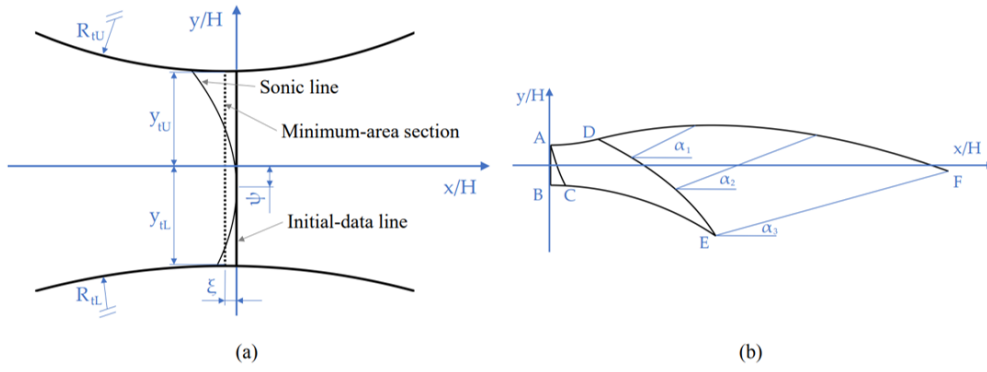


Figure 2.21: Design of diverging channel with a curved mean line. (a) Throat area, (b) channel shape. [23]

personic nozzle cascades to reduce the total pressure loss coefficient from 11.78 to 3.6. Bufl [246] proposed a robust optimization strategy, which improves the nozzle isentropic efficiency from 0.879 to 0.962.

Analysis

Romei [24] studied supersonic linear cascades with MM as working fluids, and focus on the influence of non-ideal effects. The flow features are shown in Figure 2.22, where the fish-tail shocks and trailing-edge wake can be seen in the pressure contour and Mach number contour. They studied the influence of non-ideal effects. By compared two cascaded designed at different inlet thermal states, they found that exit-to-throat ratio is smaller for a similar exit Mach number when the inlet thermal state is in the region with strong non-ideal effects. Meanwhile, they found the cascade performance is highly sensitive to the inlet thermal states.

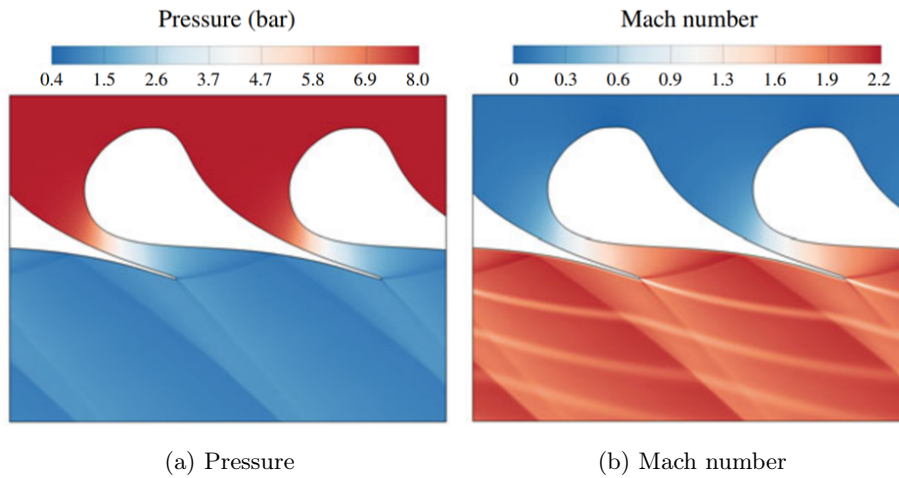


Figure 2.22: An example of the flow field in a supersonic linear cascade studied by Romei [24].

Galiana [25, 30] studied the loss generation at the nozzle trailing-edge by both CFD and ex-

perimental method. They compared the flow around the trailing-edge of a plane in air, CO_2 and SF_6 . The Mach number distributions are shown in Figure 2.23, where a strong over expansion can be seen in the Case SF_6 and the shock wake after it induce a strong separation bubble on tube wall. They also found that the shapes of trailing edge nearly do not influence the loss generation. Baumgärtner [31, 247] studied the loss generation of cascade flows with different fluids by both CFD and experimental methods, considering their different isentropic exponents. They proposed a correlation between the isentropic exponent and the loss based on their analysis.

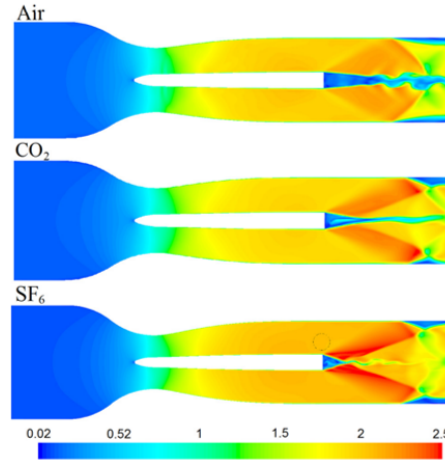


Figure 2.23: Mach number distribution simulated by LES in different fluids [25].

2.4.3 Experimental Research of Supersonic Nozzle Flows with Dense Vapours

The experimental research of the gasdynamic behaviours in transonic flows in organic fluids has made a good progress in the last decades. Two types of experimental facilities are used: Shock tube and Blowdown tunnel.

Spinelli [26] designed the Test-Rig for Organic Vapours (TROVA) at the Politecnico di Milano, and its layout is shown in Figure 2.24. Organic fluids are heated to the required temperature and pressure in the high pressure vessel (HPV) and blow down into the test section when the controlled valve is suddenly opened. A Schlieren visualisation system and a Laser Doppler Velocimetry (LDV) system were also developed and applied on TROVA [248, 249]. A siloxane, MDM, is selected as the gas studied in this serious work. Two converging-diverging nozzles with $Ma = 2.0$ and 1.5 , respectively, are tested on TROVA [27, 250]. The pressure along the centerline of the channel is measured and Schlieren images are displayed (see Figure 2.25). The measured pressure along the centerline is compared with the results from CFD based on the polytropic ideal-gas EoS, and it was found that the deviation between them is within 7.6%, since the total compressibility factor

is not very small (≈ 0.8). The Mach lines are identified in the Schlieren images. Zocca [28] tested the supersonic flow over a diamond airfoil and observed oblique shock waves on it (see Figure 2.26). Gallarini [251] tests the velocity of MM using LDV at three Mach numbers $Ma = 0.7, 1.7$ and 1.4 . Titanium dioxide (TiO_2), a solid particle with the dimension of 200nm , was selected as the seeding particle for LDV. The difference between the velocities from LDV and CFD is less than $\pm 6.6\%$.

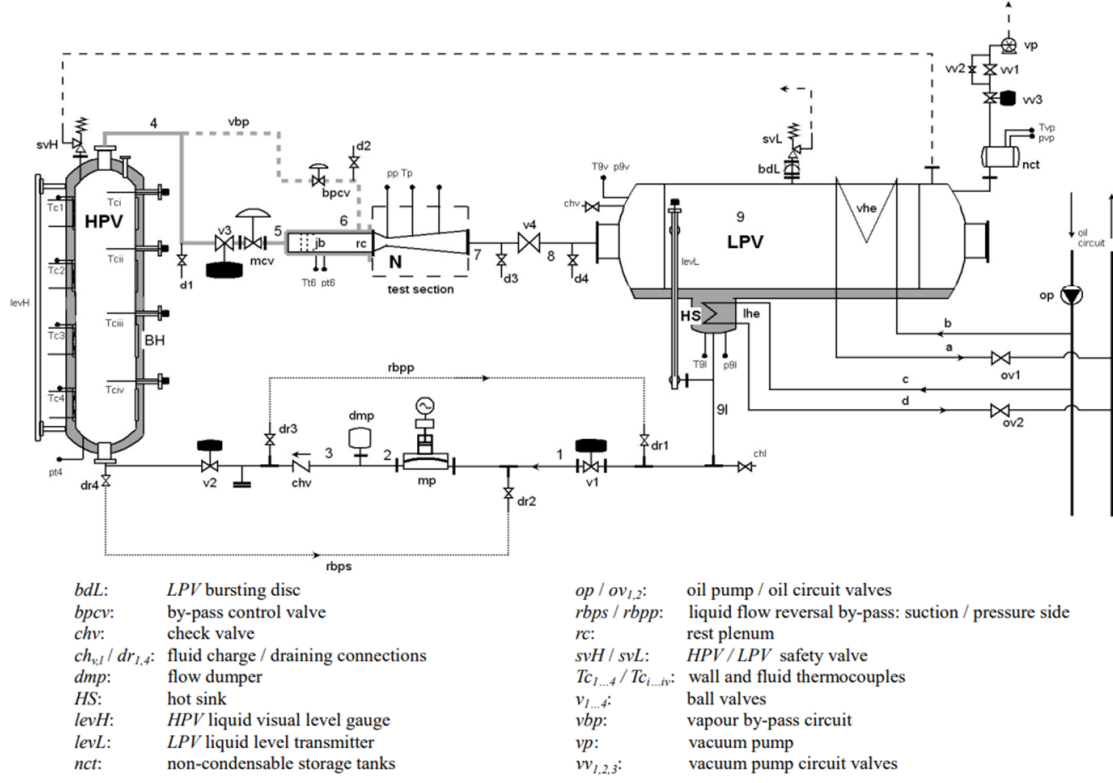


Figure 2.24: Test rig layout of TROVA [26].

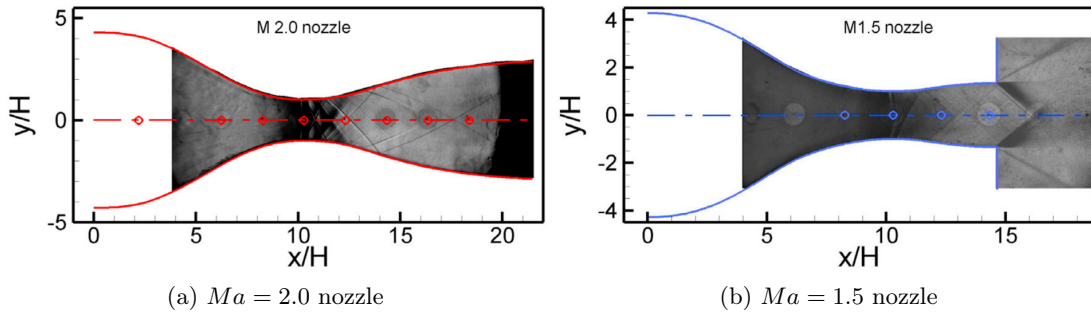
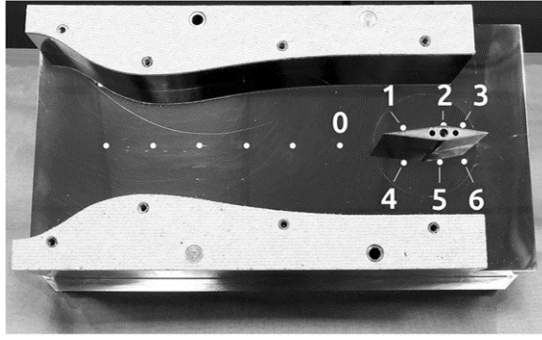
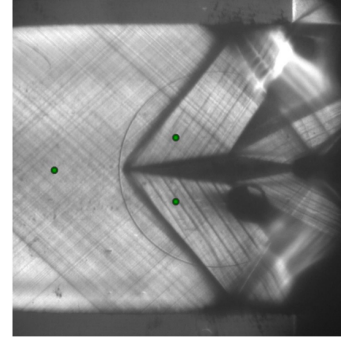


Figure 2.25: Schlieren images of transonic nozzle tested on TROVA [27].

Head [252, 29] designed and constructed the Organic Rankine Cycle Hybrid Integrated Device (ORCHID) at Delft University of Technology, which can be used to test both an organic turbine and just the nozzle flow (see Figure 2.27). The pressure distribution along the wall of a converging-diverging nozzle is tested when MM is used as the working fluid, and the flow field is observed



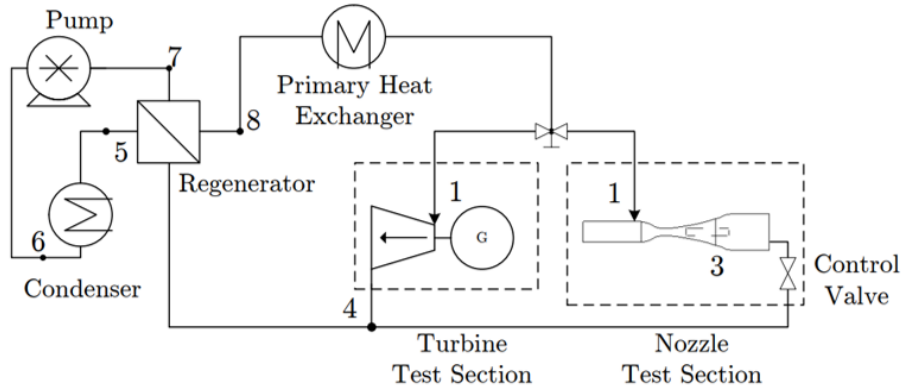
(a) Test section structure



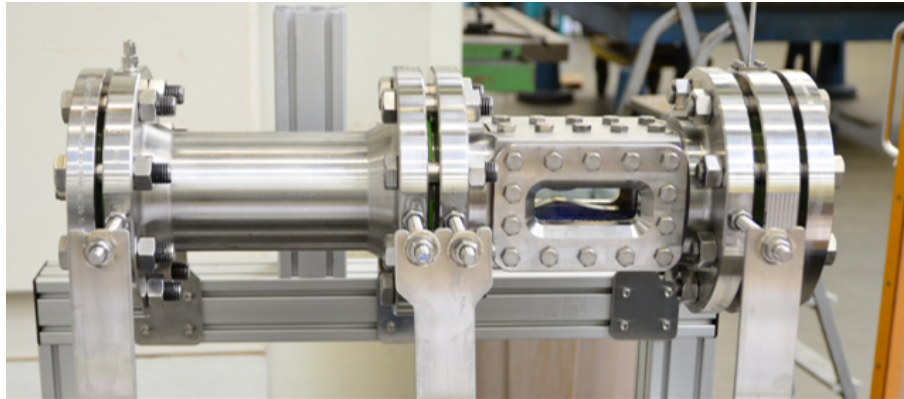
(b) Schlieren image

Figure 2.26: Schlieren image of oblique shock waves [28].

by Schlieren imaging system [253, 29]. The local Mach number can be measured directly from the Mach line in the Schlieren image. A Particle Image Velocimetry (PIV) system has also been developed and will be installed on this test rig in the future [254].



(a) Test rig layout



(b) Nozzle structure

Figure 2.27: Structure of ORCHID [29].

Galiana [249, 255] has established a Ludwig tube at the University of Southampton to measure the trailing-edge wake of nozzle blades. The structure of this rig is shown in Figure 2.28 (a), and the pressure distribution downstream of the flat plate is measured using air, CO_2 and SF_6 . The

pressure profile on a transverse surface downstream of the flat plate agrees well with the simulation results from LES. Recently, Baumgärtner [31, 247] used the same facility to test annual cascade flows with argon, air, CO₂, and R134a, see Figure 2.28 (b). A rotating casing is designed for the pressure measurement at different annual angle, and it is rotated by 2° in each running.

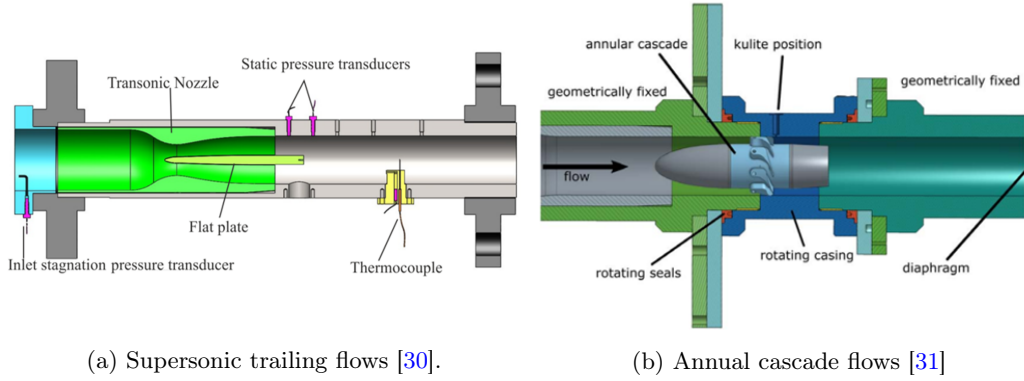


Figure 2.28: Research on a Ludwig tube [30, 31]

The closed Loop Organic Wind Tunnel (CLOWT) is designed for continuous operation at Muenster University of Applied Sciences [256, 257, 258, 259]. Their goal was to test the nozzle flow of NovecTM 649 at $p = 0.5\text{MPa}$ and $T = 382\text{K}$. The construction and preliminary operation of the rig has already been reported, but the experimental data of the nozzle flow has not been reported yet.

In the turbo group of Imperial College London, a ORC blowdown facility has been built up to test the transonic nozzle flow of R1233zd(E). The layout of this rig is shown in Figure 2.29. A convergent-divergent nozzle is tested and the pressure along the centerline is measured and compared to the results from CFD [260, 231]. The disagreement between test pressure and CFD simulated pressure is 9.59%.

2.5 Gaps and Knowledge

From the literature presented the following gaps of knowledge are identified:

1. The study of supersonic stators is critical for improving the performance of high-expansion-ratio ORC turbines, and the experimental studies are important in this field.
2. The viscous loss in the boundary layer of the supersonic stators takes a large proportion of the ORC loss, but the fundamental understanding of the wall-bounded turbulent behaviours in dense vapours is still not well studied.
3. Even the RANS simulation method has been widely used in both industrial and academic studies of ORC turbines, the scientific question is still need to be answered: whether the modelling

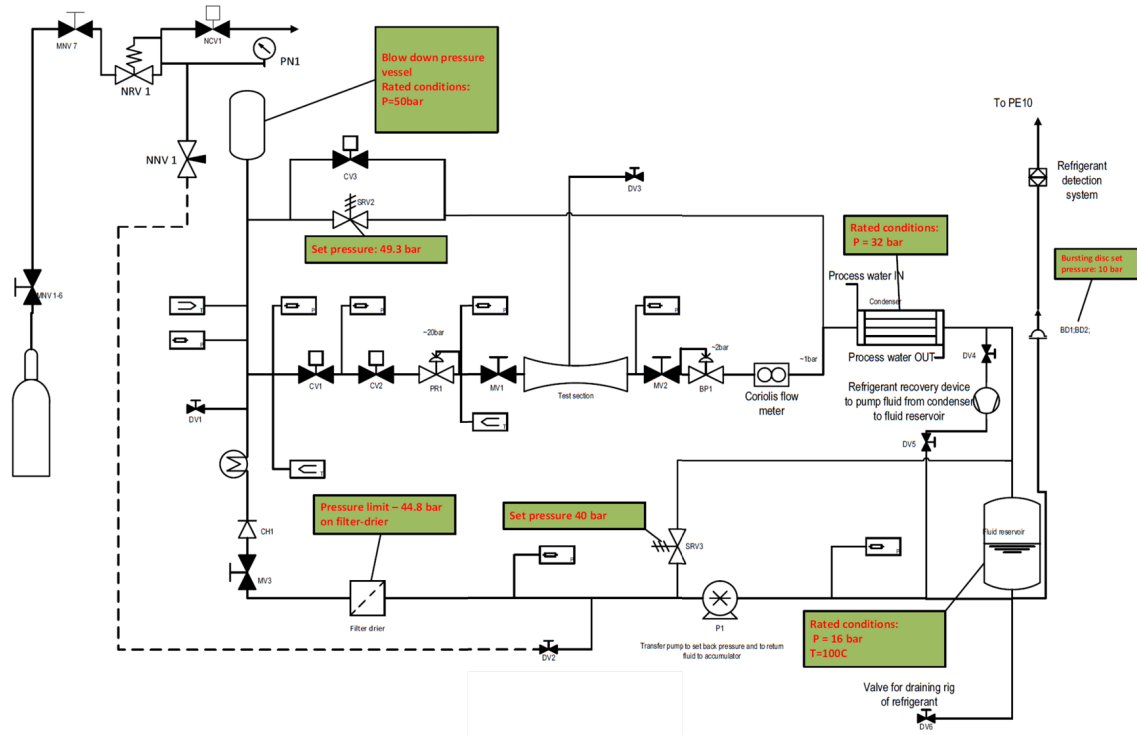


Figure 2.29: Layout of ORC blowdown facility [32].

assumptions is valid in dense vapours.

Chapter 3

Methodology

3.1 Numerical methods

3.1.1 Direct Numerical Simulation (DNS) Method

A DNS solver for non-ideal-gas flows is established, which is based on an ideal-gas compressible DNS solver developed by Li [261]. The non-ideal-gas solver is used in the study of turbulent channel flows and flat-plate flows.

The compressible Navier-Stokes equations are the governing equations of the simulated flows, since Sciacovelli [139] has confirmed that the Stokes' assumption is still acceptable in real-gas flows. The equations are shown as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0, \quad (3.1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{i,j}}{\partial x_j} + S_{m,i}, \quad (3.2)$$

$$\frac{\partial \rho(e + \frac{1}{2}u_i^2)}{\partial t} + \frac{\partial \rho u_j(e + \frac{1}{2}u_i^2)}{\partial x_j} = -\frac{\partial u_j p}{\partial x_j} + \frac{\partial u_i \tau_{i,j}}{\partial x_j} - \frac{\partial q_j}{\partial x_j} + S_{e,i}, \quad (3.3)$$

where ρ is density, p is pressure, e is specific inner energy and u_i is the velocity vector. $S_{m,i}$ and $S_{e,i}$ are source terms in momentum equation and energy equation, which is non-zero in the channel flow cases. This is discussed in Chapter 5. The viscous stress tensor τ_{ij} and the heat flux q_i are defined by

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right), \quad (3.4)$$

$$q_i = -\lambda \frac{\partial T}{\partial x_i}, \quad (3.5)$$

where μ is the dynamic viscosity, T is the temperature, and λ is the thermal conductivity. For

perfect gases, the ideal-gas law holds, and h , μ and λ depend only on temperature. Equations 2.1 - 2.7 are used to close the NS equations. For real gases, the Span-Wagner EoS [1] (see Equation 2.19 - 2.21) is used, and Equations 2.22 - 2.28 are used for closure. For simplicity, the governing equations are rewritten as follows:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_j}{\partial x_j} = \frac{\partial \mathbf{V}_j}{\partial x_j} + \mathbf{S}. \quad (3.6)$$

$\mathbf{U}$, $\mathbf{F}_j$, $\mathbf{V}_j$ and $\mathbf{S}$ are column vectors of NS equations, given by

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{pmatrix}, \quad \mathbf{F}_j = \begin{pmatrix} \rho u_j \\ \rho u_j u_1 + \delta_{j1} p \\ \rho u_j u_2 + \delta_{j2} p \\ \rho u_j u_3 + \delta_{j3} p \\ u_j (E + p) \end{pmatrix}, \quad \mathbf{V}_j = \begin{pmatrix} 0 \\ \tau_{j,1} \\ \tau_{j,2} \\ \tau_{j,3} \\ \lambda \frac{\partial T}{\partial x_j} + u_j \tau_{i,j} \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} 0 \\ S_{m,1} \\ S_{m,2} \\ S_{m,3} \\ S_{e,i} \end{pmatrix}, \quad (3.7)$$

where

$$E = \rho \left(e + \frac{u_i^2}{2} \right). \quad (3.8)$$

$\mathbf{U}$ is the conservative solution vector, $\mathbf{F}_j$ is the convective flux vector, $\mathbf{V}_j$ is the dissipative flux vector, and $\mathbf{S}$ is the source vector.

Finite difference method is used for the spatial discretization, and the approximation of convective terms and dissipative terms are introduced as follows. For ideal gas, the convective flux derivatives are approximated by the Steger-Warming splitting method [262]. By local linearization, the Jacobian matrix $\mathbf{A}_j \equiv \partial \mathbf{F}_j(\mathbf{U}) / \partial \mathbf{U}$ is a constant matrix at local, and the convective term is given as follows:

$$\frac{\partial \mathbf{F}_j}{\partial x_j} = \frac{\partial \mathbf{F}_j}{\partial \mathbf{U}} \frac{\partial \mathbf{U}}{\partial x_j} = \mathbf{A}_j \frac{\partial \mathbf{U}}{\partial x_j} \quad (3.9)$$

If the pressure has the functional form $p = \rho f(e)$, $\mathbf{F}_j(\mathbf{U})$ is a homogeneous function of degree one in $\mathbf{U}$:

$$\mathbf{F}_j(\mathbf{U}) = \mathbf{A}_j \mathbf{U}. \quad (3.10)$$

The eigenvalues (characteristic velocity) of $\mathbf{A}_j$ are u_j , u_j , u_j , $u_j + c$ and $u_j - c$. Here, a diagonal matrix $\mathbf{\Lambda}_j$ is defined as follows:

$$\mathbf{\Lambda}_j = \text{diag}(\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5), \quad (3.11)$$

where $\lambda_1 = \lambda_u = u_j$, $\lambda_5 = \lambda_{u-c} = u_j - c$, $\lambda_{1+j} = \lambda_{u+c} = u_j + c$, and the remaining eigenvalues

are equal to $\lambda_u = u_j$. Then $\mathbf{\Lambda}_j$ can be split into a positive matrix and a negative matrix:

$$\mathbf{\Lambda}_j = \mathbf{\Lambda}_j^+ + \mathbf{\Lambda}_j^-, \quad (3.12)$$

where

$$\mathbf{\Lambda}_j^+ = \frac{\mathbf{\Lambda}_j + |\mathbf{\Lambda}_j|}{2}, \quad \mathbf{\Lambda}_j^- = \frac{\mathbf{\Lambda}_j - |\mathbf{\Lambda}_j|}{2}. \quad (3.13)$$

Then Equation 3.10 can be divided as follows:

$$\mathbf{F}_j = \mathbf{A}_j \mathbf{U} = \mathbf{R}_j \mathbf{\Lambda}_j \mathbf{L}_j \mathbf{U} = \mathbf{R}_j \mathbf{\Lambda}_j^+ \mathbf{L}_j \mathbf{U} + \mathbf{R}_j \mathbf{\Lambda}_j^- \mathbf{L}_j \mathbf{U} = \mathbf{F}_j^+ + \mathbf{F}_j^-, \quad (3.14)$$

where $\mathbf{F}_j^+$ and $\mathbf{F}_j^-$ can be derived and represented as follows:

$$\mathbf{F}_j^\pm = \frac{\rho}{2\gamma} \begin{pmatrix} 2(\gamma-1)\lambda_u^\pm + \lambda_{u+c}^\pm + \lambda_{u-c}^\pm \\ 2(\gamma-1)u_1\lambda_u^\pm + (u_1 + c\delta_{j1})\lambda_{u+c}^\pm + (u_1 - c\delta_{j1})\lambda_{u-c}^\pm \\ 2(\gamma-1)u_2\lambda_u^\pm + (u_2 + c\delta_{j2})\lambda_{u+c}^\pm + (u_2 - c\delta_{j2})\lambda_{u-c}^\pm \\ 2(\gamma-1)u_3\lambda_u^\pm + (u_3 + c\delta_{j3})\lambda_{u+c}^\pm + (u_3 - c\delta_{j3})\lambda_{u-c}^\pm \\ (\gamma-1)u_i^2\lambda_u^\pm + \left(\frac{c^2}{\gamma-1} + \frac{1}{2}u_i^2 + u_i c\right)\lambda_{u+c}^\pm + \left(\frac{c^2}{\gamma-1} + \frac{1}{2}u_i^2 - u_i c\right)\lambda_{u-c}^\pm \end{pmatrix} \quad (3.15)$$

Then $\frac{\partial \mathbf{F}_j^+}{\partial x_j}$ and $\frac{\partial \mathbf{F}_j^-}{\partial x_j}$ are discretized by the upwind scheme.

For non-ideal gases, the pressure does not follow the form: $p = \rho f(e)$, so $\mathbf{F}_j(\mathbf{U})$ is no longer a homogeneous function of degree one in $\mathbf{U}$. Therefore, the Steger-Warming splitting method should be modified in real gases. In this work, an inhomogeneous part is defined as below:

$$\mathbf{F}_j = \mathbf{F}_{j,inh} + \mathbf{A}_j \mathbf{U}, \quad (3.16)$$

For real gases, the Jacobian matrix $\mathbf{A}_j$ is shown here:

$$\mathbf{A}_1 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ c^2 - u^2 - \frac{p_e}{\rho}(H - u_i^2) & 2u - \frac{p_e}{\rho}u & -\frac{p_e}{\rho}v & -\frac{p_e}{\rho}w & \frac{p_e}{\rho} \\ -uv & v & u & 0 & 0 \\ -uw & w & 0 & u & 0 \\ u(c^2 - H) - \frac{p_e}{\rho}u(H - u_i^2) & H - \frac{p_e}{\rho}u^2 & -\frac{p_e}{\rho}uv & -\frac{p_e}{\rho}uw & u + \frac{p_e}{\rho}u \end{pmatrix}, \quad (3.17)$$

$$\mathbf{A}_2 = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ -uv & v & u & 0 & 0 \\ c^2 - v^2 - \frac{p_e}{\rho} (H - u_i^2) & -\frac{p_e}{\rho} u & 2v - \frac{p_e}{\rho} v & -\frac{p_e}{\rho} w & \frac{p_e}{\rho} \\ -vw & 0 & w & v & 0 \\ v(c^2 - H) - \frac{p_e}{\rho} v (H - u_i^2) & -\frac{p_e}{\rho} uv & H - \frac{p_e}{\rho} v^2 & -\frac{p_e}{\rho} vw & v + \frac{p_e}{\rho} v \end{pmatrix}, \quad (3.18)$$

$$\mathbf{A}_3 = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ -uw & w & 0 & u & 0 \\ -vw & 0 & w & v & 0 \\ c^2 - w^2 - \frac{p_e}{\rho} (H - u_i^2) & -\frac{p_e}{\rho} u & -\frac{p_e}{\rho} v & 2w - \frac{p_e}{\rho} w & \frac{p_e}{\rho} \\ w(c^2 - H) - \frac{p_e}{\rho} w (H - u_i^2) & -\frac{p_e}{\rho} uw & -\frac{p_e}{\rho} vw & H - \frac{p_e}{\rho} w^2 & w + \frac{p_e}{\rho} w \end{pmatrix}, \quad (3.19)$$

where

$$H = p + \rho e + \frac{1}{2} \rho u_i^2, \quad (3.20)$$

$$p_\rho \equiv \left(\frac{\partial p}{\partial \rho} \right)_e, \quad p_e \equiv \left(\frac{\partial p}{\partial e} \right)_\rho. \quad (3.21)$$

The eigenvalues (characteristic velocity) of $\mathbf{A}_j$ in real gases are still u_j , u_j , u_j , $u_j + c$ and $u_j - c$, and $\mathbf{A}_j \mathbf{U}$ can still be split into a positive part and a negative part following the concept of Steger-Warming splitting, $\mathbf{A}_j \mathbf{U} = \mathbf{A}_j^+ \mathbf{U} + \mathbf{A}_j^- \mathbf{U}$. Skip intermediate steps in the derivation, the final expression is given as follows:

$$\mathbf{A}_j^\pm \mathbf{U} = \begin{pmatrix} \left(\rho - \frac{\rho p_\rho}{c^2} \right) \lambda_u^\pm + \frac{\rho p_\rho}{2c^2} (\lambda_{u+c}^\pm + \lambda_{u-c}^\pm) \\ \left(\rho - \frac{\rho p_\rho}{c^2} \right) u_1 \lambda_u^\pm + \frac{\rho p_\rho}{2c^2} (u_1 + c \delta_{j1}) \lambda_{u+c}^\pm + \frac{\rho p_\rho}{2c^2} (u_1 - c \delta_{j1}) \lambda_{u-c}^\pm \\ \left(\rho - \frac{\rho p_\rho}{c^2} \right) u_2 \lambda_u^\pm + \frac{\rho p_\rho}{2c^2} (u_2 + c \delta_{j2}) \lambda_{u+c}^\pm + \frac{\rho p_\rho}{2c^2} (u_2 - c \delta_{j2}) \lambda_{u-c}^\pm \\ \left(\rho - \frac{\rho p_\rho}{c^2} \right) u_3 \lambda_u^\pm + \frac{\rho p_\rho}{2c^2} (u_3 + c \delta_{j3}) \lambda_{u+c}^\pm + \frac{\rho p_\rho}{2c^2} (u_3 - c \delta_{j3}) \lambda_{u-c}^\pm \\ \left(\frac{H}{\rho} - \frac{\rho c^2}{p_e} \right) \left(\rho - \frac{\rho p_\rho}{c^2} \right) \lambda_u^\pm + \frac{\rho p_\rho}{2c^2} \left(\frac{H}{\rho} + u_j c \right) \lambda_{u+c}^\pm + \frac{\rho p_\rho}{2c^2} \left(\frac{H}{\rho} - u_j c \right) \lambda_{u-c}^\pm \end{pmatrix}. \quad (3.22)$$

In this vector, H are calculated by taking Equations 2.22 and 2.23 into Equation 3.20, and c are calculated by Equation 2.24. p_e and p_ρ are calculated by the following relations:

$$p_e = \left(\frac{\partial p}{\partial T} \right)_V / c_v, \quad (3.23)$$

$$p_\rho = c^2 - \frac{p p_e}{\rho^2}, \quad (3.24)$$

where $\left(\frac{\partial p}{\partial T}\right)_V$ and c_v are calculated from Helmholtz energy Equation 2.21 [1]:

$$\left(\frac{\partial p}{\partial T}\right)_V = R\rho \left[1 + \delta \left(\frac{\partial \alpha^r}{\partial \delta}\right)_\tau - \delta \tau \left(\frac{\partial^2 \alpha^r}{\partial \delta \partial \tau}\right)\right], \quad (3.25)$$

$$c_v = -R\tau^2 \left[\left(\frac{\partial^2 \alpha^o}{\partial \tau^2}\right)_\delta + \left(\frac{\partial^2 \alpha^r}{\partial \tau^2}\right)_\delta\right]. \quad (3.26)$$

Then the inhomogeneous part $\mathbf{F}_{j,inh}$ can be obtained by Equation 3.16, and $\mathbf{F}_{j,inh}$ is related to $p - \rho p_\rho$:

$$\mathbf{F}_{j,inh} = (p - \rho p_\rho) (0, \delta_{j1}, \delta_{j2}, \delta_{j3}, u_j)^T \quad (3.27)$$

$\frac{\partial \mathbf{A}_j^\pm \mathbf{U}}{\partial x_j}$ are approximated by upwind scheme according to the sign of eigenvalues, and $\frac{\partial \mathbf{F}_{j,inh}}{\partial x_j}$ is approximated by simple upwind scheme. To achieve high accuracy, the seventh-order upwind difference scheme is used in this solver [261]. For example, (see the structured Cartesian grid in Figure 3.6) the derivative in x direction can be given in the following expression:

$$\begin{aligned} \frac{\partial f}{\partial x} \approx \frac{1}{420\Delta x} & (3f_{i-4,j,k} - 28f_{i-3,j,k} + 126f_{i-2,j,k} \\ & - 420f_{i-1,j,k} + 105f_{i,j,k} + 250f_{i+1,j,k} - 42f_{i+2,j,k} + 4f_{i+3,j,k}). \end{aligned} \quad (3.28)$$

The dissipative derivatives are approximated by sixth-order central scheme:

$$\frac{\partial f}{\partial x} \approx \frac{1}{60\Delta x} [45(f_{i+1,j,k} - f_{i-1,j,k}) - 9(f_{i+2,j,k} - f_{i-2,j,k}) + (f_{i+3,j,k} - f_{i-3,j,k})]. \quad (3.29)$$

It is claimed that in first three grids on domain boundaries (except periodic boundaries), the lower order of discretized scheme is used, and it is reduced to second-order in the cases of this work. To speed up the computational speed of dissipative terms, a 2D look-up table of viscosity and thermal conductivity is created at the beginning of the computation, which is generated from the ECS model. The derivation of viscosity and thermal conductivity obtained by the bilinear interpretation of look-up tables from by the ECS model remains within 10^{-4} , which is lower than the accuracy of ECS model.

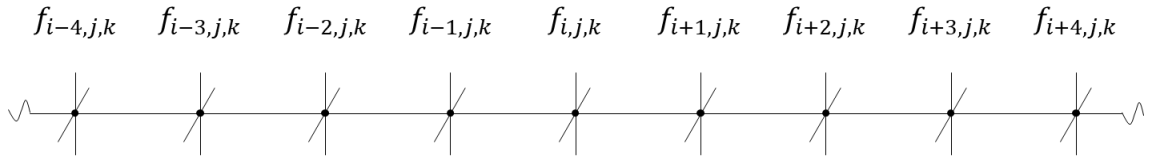


Figure 3.1: Structured Cartesian grid in x direction.

The third-order Runge-Kutta method is used for the temporal discretization in this solver [261].

The solving process in each Runge-Kutta step is summarised and shown in Figure 3.2.

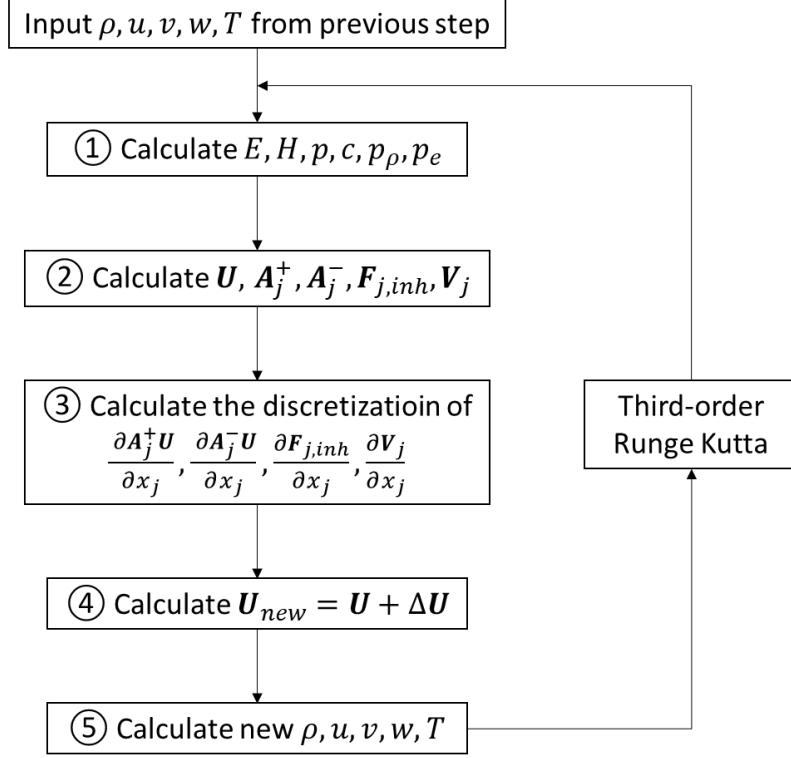


Figure 3.2: Solving process in each Runge-Kutta step.

Discussion on $\mathbf{F}_{j,inh}$

To clarify the importance of the inhomogeneous term $\mathbf{F}_{j,inh}$ in this finite difference method for non-ideal fluids, $\mathbf{F}_{j,inh}$ and the convective flux vector $\mathbf{F}_j$ are compared in the following example. The example is a fully-developed turbulent supersonic channel flow on cold walls with R1233zd(E) as working fluid. A plane vertical to spanwise direction in this channel flow is selected as the discussed region, see the blue plane in Figure 3.3. The main flow direction is along the 'x' axis, the channel walls are a pair of infinite flat plane, and the channel height is $2l$. Three cases with different working conditions are considered, which are named Cases R1, R2 and R3. The non-ideal effects in Case R1 are weakest, in Case R2 are moderate, and in Case R3 are strongest. These cases are the same as Chapter 5.

According to Equation 3.27, the $(j+1)$ th and fifth terms of $\mathbf{F}_{j,inh}$ are not equal to zero in non-ideal fluids. Here, the 2nd term in $\mathbf{F}_{1,inh}$ is discussed and compared with the corresponding term in $\mathbf{F}_1$, and the ratio is given as follows:

$$\frac{F_{1,2,inh}}{F_{1,2}} = \frac{p - \rho p_\rho}{\rho u^2 + p}. \quad (3.30)$$

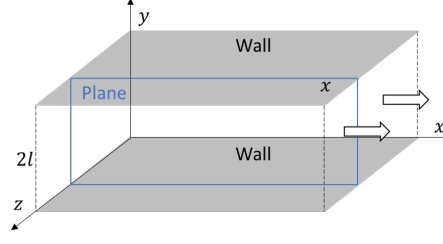


Figure 3.3: Sketch of a plane in channel flows

The distribution of $\frac{F_{1,2,inh}}{F_{1,2}}$ in the region near wall ($0 < y_{wall}/l < 0.2$) is shown in Figure 3.4 (a)-(c) for three cases. Figure 3.4 (a) shows that $\frac{F_{1,2,inh}}{F_{1,2}}$ is almost larger than 0.005 in the region $y_{wall}/l < 0.1$ in Case R1, and it can reach about 0.035 on the channel wall; Figure 3.4 (b) shows that $\frac{F_{1,2,inh}}{F_{1,2}}$ in Case R2 is nearly one order of magnitude higher than that in Case R1; while in Case R3 (Figure 3.4 (c)), $\frac{F_{1,2,inh}}{F_{1,2}}$ is negative near the wall, and its absolute value can reach 2. This means that $\frac{F_{1,2,inh}}{F_{1,2}}$ can not be ignored in non-ideal flows especially in the near-wall region.

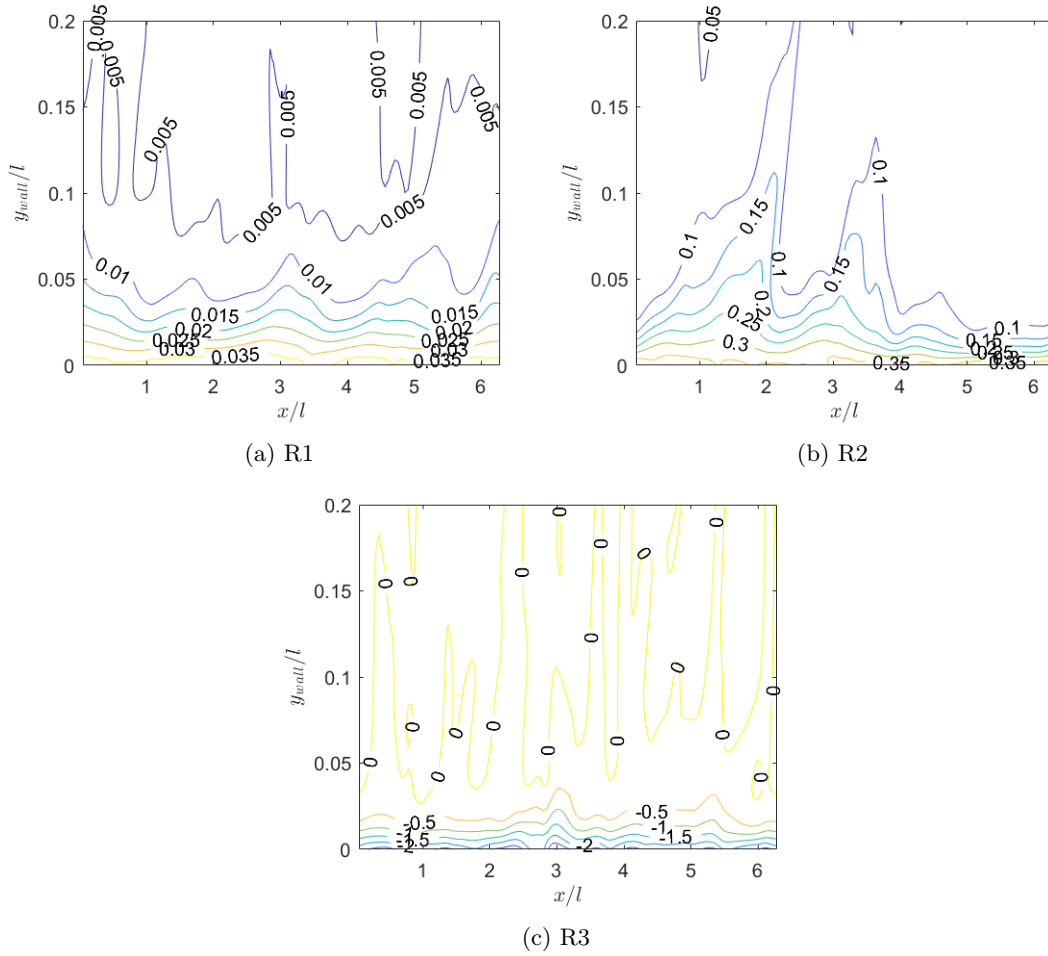


Figure 3.4: Distribution of $\frac{F_{1,2,inh}}{F_{1,2}}$ in the near wall region on the selected plane for three cases.

This ratio is influenced by a thermodynamic property $(p - \rho p_\rho)/p$ and the momentum ρu^2 .

If ρu^2 is relative small to p (in the near-wall region), this term is approximately equal to the thermodynamic property $(p - \rho p_\rho)/p$, but if ρu^2 is relative large to p (far from channel wall), this term approaches to zero. The contour of $(p - \rho p_\rho)/p$ for R1233zd(E) is shown in T-S diagram, see Figure 3.5. It has the maximum value on the saturation line close to critical point, and it has negative values in the region with low entropy and high temperature (top-left in T-S diagram). The thermodynamic states of all points on the XY plane for each case are also shown in Figure 3.5. The groups of blue, green and red dots refer to the points in Case R1, R2 and R3 respectively. In turbulent flows, the thermal states fluctuate around the mean thermal state, so these states locate in a region instead of a line in Figure 3.5. In each group of dots, the dots with lower temperature refer to the points close to channel wall, and the dots with higher temperature refer to the points in the central region of the channel. $(p - \rho p_\rho)/p$ in Case R1 is much lower than 0.1, but its value in Case R2 is between 0.2 and 0.4, so it can explain that $\frac{F_{1,2,inh}}{F_{1,2}}$ is nearly one order of magnitude higher in Case R2 than in Case R1. $(p - \rho p_\rho)/p$ in Case R3 is almost in the negative region, so $\frac{F_{1,2,inh}}{F_{1,2}}$ is negative near the wall.

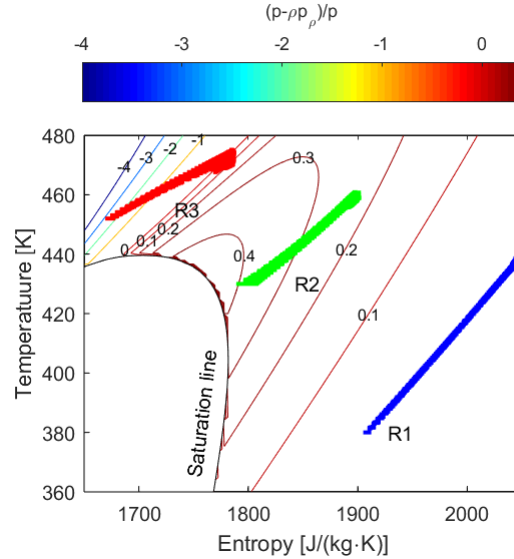


Figure 3.5: Distribution of $(p - \rho p_\rho)/p$ for R1233zd(E) in T-S diagram. Blue dots for points on the plane in Case R1, green dots for Case R2, and Red dots for Case R3.

As it is mentioned above, the $(j + 1)$ th and fifth terms of $\mathbf{F}_{j,inh}$ are not equal to zero. The comparison of other non-zero terms of $\mathbf{F}_{j,inh}$ with $\mathbf{F}_j$ shows a similar conclusion, so it is not mentioned here.

In summary, $\mathbf{F}_{j,inh}$ is necessary to be considered in the finite difference method for non-ideal flows, and it takes a significant proportion of the convective flux vector $\mathbf{F}_j$. If it is not considered, the DNS cannot converge, to author's experience.

3.1.2 Reynolds-Averaged Navier–Stokes (RANS) Simulation Method

The RANS simulation method is used in Chapter 4 for simulating the cascade flows, where the Reynolds numbers are very large. ANSYS CFX solver are used here [222]. The governing equations of the RANS method are obtained by applying Reynolds averaging to Equations 3.1-3.3 (ignoring source terms):

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0, \quad (3.31)$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial (\bar{\tau}_{i,j} - \widetilde{\bar{\rho} u_i'' u_j''})}{\partial x_j}, \quad (3.32)$$

$$\frac{\partial (\bar{\rho} h_{tot} - \bar{p})}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j h_{tot}}{\partial x_j} = -\frac{\partial \bar{\rho} \widetilde{h'' u_j''}}{\partial x_j} - \frac{\partial \bar{\rho} \tilde{u}_i \widetilde{u_i'' u_j''}}{\partial x_j} - \frac{\partial (\frac{1}{2} \bar{\rho} \widetilde{u_i'' u_i'' u_j'' u_j''})}{\partial x_j} + \frac{\partial \overline{u_i \tau_{i,j}}}{\partial x_j} - \frac{\partial \bar{q}_j}{\partial x_j}, \quad (3.33)$$

where

$$h_{tot} = \tilde{h} + K_m + k_t, \quad \tilde{h} = \tilde{e} + \bar{p}/\bar{\rho}, \quad K_m = \frac{1}{2} \tilde{u}_i^2, \quad k_t = \frac{1}{2} \widetilde{u_i''^2}. \quad (3.34)$$

This method focuses only on the mean flow, and all fluctuation terms are calculated by models. The influence of the fluctuations of viscosity and thermal conductivity (μ' and λ') is ignored in the solver, so the averaged shear stress and heat conduction terms are given as follows:

$$\bar{\tau}_{ij} = \bar{\mu} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right), \quad (3.35)$$

$$\bar{q}_i = -\bar{\lambda} \frac{\partial \bar{T}}{\partial x_i}. \quad (3.36)$$

$k - \varepsilon$ two-equation closure model is used to calculate the turbulent shear stress in RANS. Following the eddy viscosity assumption [263], this term is modelled:

$$-\bar{\rho} \widetilde{u_i'' u_j''} = \mu_t \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \bar{\rho} k_t, \quad (3.37)$$

where

$$\mu_t = C_\mu \bar{\rho} \frac{k_t^2}{\varepsilon}. \quad (3.38)$$

Two additional modelling equations, the k equation and ε equation, are used to calculate the local k_t and ε :

$$\frac{\partial \bar{\rho} k_t}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j k_t}{\partial x_j} = -\bar{\rho} \widetilde{u_i'' u_j''} \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_k} \frac{\partial k_t}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\bar{\mu} \frac{\partial k_t}{\partial x_j} \right) - \bar{\rho} \varepsilon. \quad (3.39)$$

$$\frac{\partial \bar{\rho} \varepsilon}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \varepsilon}{\partial x_j} = -C_{1\varepsilon} \frac{\varepsilon}{k_t} \bar{\rho} \widetilde{u_i'' u_j''} \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\bar{\mu} \frac{\partial \varepsilon}{\partial x_j} \right) - C_{2\varepsilon} \bar{\rho} \frac{\varepsilon^2}{k_t}. \quad (3.40)$$

The constant coefficients are $C_{1\varepsilon} = 1.44$, $C_{2\varepsilon} = 1.92$, $C_\mu = 0.09$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$. The turbulent heat transfer term is modelled with a relation to the turbulent shear stress by the turbulent Prandtl number:

$$Pr_t \equiv \frac{\widetilde{u_i'' u_j''}(\partial \widetilde{h}/\partial x_j)}{\widetilde{h'' u_j''}(\partial \widetilde{u_i}/\partial x_j)}, \quad (3.41)$$

In the RANS simulation in this thesis, Pr_t is assumed constant $Pr_t = 0.9$.

The PR EoS (Equation 2.14 - 2.18) is used in this simulation method, together with a fourth-order polynomial expression of heat capacity (Equation 2.25). The required coefficients for R1233zd(E) in these equations are list in Table 3.1.

T_{cr}	p_{cr}	V_{cr}	ω	
K	kPa	cm ³ /mol	-	
438.75	3772.1	271.7391	0.3025	
A_1	A_2	A_3	A_4	A_5
-	K ⁻¹	K ⁻²	K ⁻³	K ⁻⁴
3.1494	0.0377	-1.4950e-5	-1.7512e-5	1.3018e-11

Table 3.1: Coefficients used in PR EoS model in Fluent CFX solver.

3.2 Data Analysing Method of DNS Results

3.2.1 Averaging Methods

The DNS simulation result provides the flow information at all grid nodes of the simulation domain within a long time. Two averaging methods are applied: Reynolds averaging and Favre averaging. The Reynolds averaging of a parameter f is defined as:

$$\bar{f} = \sum_{t, x_p}^{t, x_p} f(t, x_i), \quad (3.42)$$

where x_p is the periodic direction. The Favre averaging is defined as:

$$\tilde{f} = \frac{\overline{\rho f}}{\bar{\rho}}. \quad (3.43)$$

The fluctuation part in the Reynolds and Favre averages is given respectively as follows:

$$f' = f - \bar{f}, \quad (3.44)$$

$$f'' = f - \tilde{f}. \quad (3.45)$$

3.2.2 Vortex Visualization Method

The Q criterion [264] is used to identify vortex in the instantaneous flow field. Q is defined as follows:

$$Q = \frac{1}{2} \left(\|\vec{\Omega}\|^2 - \|\vec{S}\|^2 \right), \quad (3.46)$$

where $\vec{\Omega}$ is the vorticity tensor (anti-symmetric part of the velocity gradient) and $\vec{S}$ is the rate of strain (symmetric part of the velocity gradient):

$$\vec{\Omega} = \frac{1}{2} (\nabla \vec{u} - \nabla \vec{u}^T), \quad \vec{S} = \frac{1}{2} (\nabla \vec{u} + \nabla \vec{u}^T), \quad (3.47)$$

$Q > 0$ represents the region where the magnitude of the vorticity is greater than the magnitude of the strain.

3.2.3 Proper Orthogonal Decomposition (POD) Method

POD is used for the modal decomposition of the flow field, which helps to capture the dominant components (the ‘modes’) of an infinite-dimensional process [265]. The POD of a k -dimensional vector $\mathbf{Y} \in \mathbb{R}^k$ consists in choosing the n -dimensional orthogonal basis $\boldsymbol{\varphi}$ to minimize the error between $\mathbf{Y}$ and its projection on $\boldsymbol{\varphi}$:

$$\min \frac{1}{n} \sum_{j=1}^n \|\mathbf{Y} - (\mathbf{Y}, \boldsymbol{\varphi}) \boldsymbol{\varphi}\|^2. \quad (3.48)$$

$(\cdot, \cdot)$ is the inner production between two vectors, $\|\cdot\|^2$ is the self inner production of a vector, and $\|\boldsymbol{\varphi}\|^2 = 1$. Therefore, $\mathbf{Y}$ can be restructured to $\boldsymbol{\varphi}$ from the leading n modes:

$$\mathbf{Y} \approx \mathbf{Y}_r \equiv \sum_{j=1}^n a_j \boldsymbol{\varphi}_j. \quad (3.49)$$

The DNS results are interpolated into a uniform grid ($N_x \times N_y \times N_z$), and then the flow parameters at the nodes of the grid ($f(x, y, z)$) are decomposed by the method of snapshot [266]. The element number of this grid is N , and the snapshot number is M . An $N \times M$ data matrix is created:

$$\mathbf{P} = \begin{bmatrix} \mathbf{f}_{1,1} & \cdots & \mathbf{f}_{1,M} \\ \vdots & \vdots & \vdots \\ \mathbf{f}_{N,1} & \cdots & \mathbf{f}_{N,M} \end{bmatrix}_{N \times M} = [\mathbf{Y}_1, \cdots, \mathbf{Y}_M], \quad (3.50)$$

where $\mathbf{f}$ is an aggregate of flow parameters, $\mathbf{f} = \{\rho, u, v, w, T, p\}$, and $\mathbf{Y}_j$ is the flow field at snapshot j (at one time). In this thesis, the inner product between two flow parameter aggregates is defined as follows:

$$(\mathbf{f}_1, \mathbf{f}_2) \equiv \frac{1}{2} (\rho_1^{0.5} u_1 \times \rho_2^{0.5} u_2 + \rho_1^{0.5} v_1 \times \rho_2^{0.5} v_2 + \rho_1^{0.5} w_1 \times \rho_2^{0.5} w_2), \quad (3.51)$$

and the inner product between two vectors is defined as:

$$(\mathbf{Y}_1, \mathbf{Y}_2) \equiv \sum_{i=1}^N (\mathbf{f}_{i,1}, \mathbf{f}_{i,2}) \quad (3.52)$$

The $N \times N$ eigenvalue problem is given as:

$$\mathbf{P}\mathbf{P}^T \boldsymbol{\varphi} = \lambda \boldsymbol{\varphi}. \quad (3.53)$$

This problem is solved by the singular value decomposition of $\mathbf{P}$:

$$\mathbf{P} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \sum_{j=1}^r \sigma_j \boldsymbol{\varphi}_j \mathbf{v}_j^T, \quad (3.54)$$

where $\boldsymbol{\varphi}_j$ is the eigenvector. The eigenvalue λ_j is given by $\lambda_j = \sigma_j^2$, and the POD basis (function of POD mode) is given by:

$$\mathbf{v}_i = \frac{1}{\sqrt{\lambda_i}} \mathbf{P} \boldsymbol{\varphi}_i \quad (3.55)$$

Therefore, flow field ($\mathbf{Y}_j$) can be reconstructed by the first r POD modes, and it is given as follows:

$$\mathbf{Y}_j \approx \mathbf{Y}_{r,j} = \sum_{i=1}^d a_i(j) \mathbf{v}_i, \quad (3.56)$$

where $a_i(j) = (\mathbf{v}_i, \mathbf{X}_j)$ is the time coefficient of the POD basis $\mathbf{v}_i$, and d is the number of modes used for the reconstruction.

3.3 Experimental Methods

Supersonic flows in a transonic nozzle are tested on the **ORC Blowdown Facility at Imperial College London**. The pressure along nozzle surface is measured, and Schlieren images are taken by a Schlieren imaging system designed and established by author. This blowdown facility is designed by Peter Newton and Miles Robertson, and the flows of both R1233zd(E) and Nitrogen in a convergent-divergent nozzle have been tested on this facility, see reference [32, 260, 231]. The basic information of this facility is shown in Section 3.3.1. Then, the design of the test section of a

blade-shaped transonic nozzle is shown in Section 3.3.2. After that, the Schlieren imaging system is described in Section 3.3.3.

3.3.1 Introduction of the Blowdown Facility

The concept of the blowdown facility is shown in Figure 3.6. This facility is a closed system that is charged with a specific organic gas and has liquid fluid stored in its reservoir ('6'). The fluid tested in this work is R1233zd(E), which is an environmentally friendly substitute for the widely-used organic fluid R245fa.

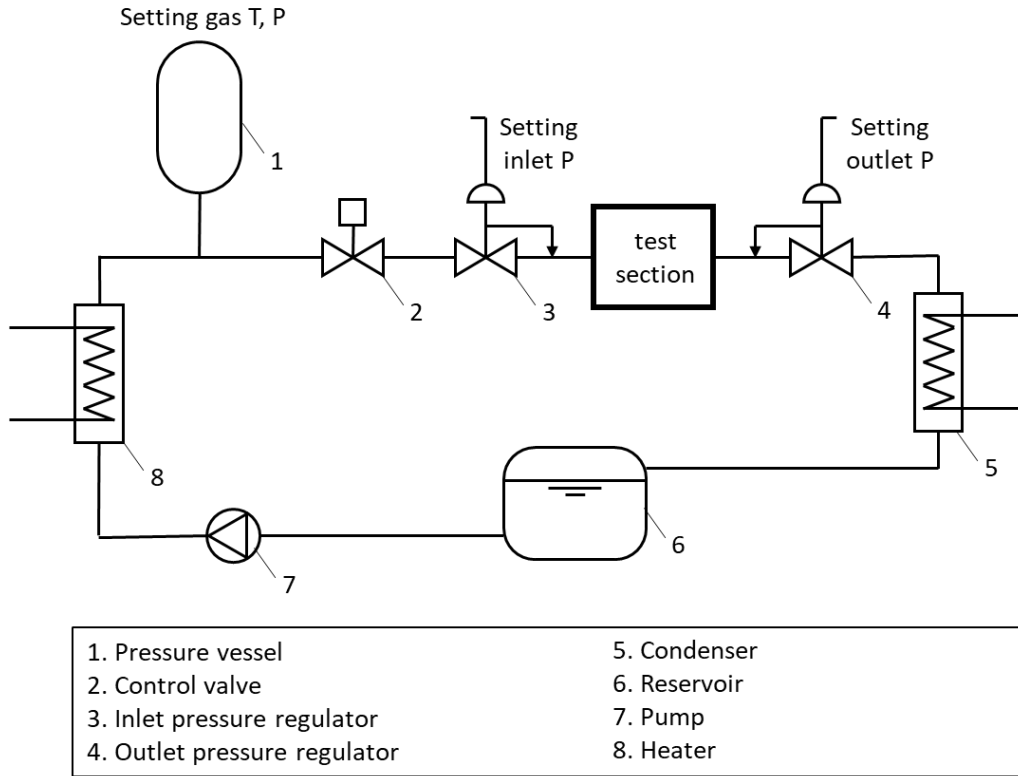


Figure 3.6: Concept of the ORC blowdown facility at Imperial College London.

During the preparation process, the control valve ('2') is closed. Liquid fluids are pumped by the pump ('7') and pressurized. Then the fluids are heated as they flow through the heater ('8'), and they evaporate into the vapor phase before entering the pressure vessel ('1'). The pressure and temperature are measured at the bottom of the pressure vessel to monitor the thermodynamic states of the fluid. This state is controlled by the mass flow rate of the pump and the setting temperature of the heater.

During the test process, the pump is off to prevent backflow. The inlet and outlet static pressure of the test section is set by a pressure regulator at the inlet ('3') and a pressure regulator at the outlet ('4'), respectively. Blowdown is initiated by rapidly opening the control valve ('2') and the

high-pressure, high-temperature organic gases blows downstream through the test section. The stable supersonic flow is achieved within a certain period of time ($>1s$) when the measurement of the test section takes place. After the stable flow is completed, the control valve is closed. The low-pressure gases condense to liquid in the condenser ('5'), and then flow (or are pumped by an auxiliary pump) back to the reservoir.

The frontal view of this blowdown facility is shown in Figure 3.7. The basic information is listed in Table 3.2. The pressure vessel consists of three stainless steel vessels, each with a volume of 3.785L. The safety temperature is the thermal stable temperature of R1233zd(E) - $220^{\circ}C$ [267]. More detailed information on the operational safety and individual component can be found in our previous published work [260, 231, 32]. This facility is operated by LABVIEW, and all data are recorded through it.

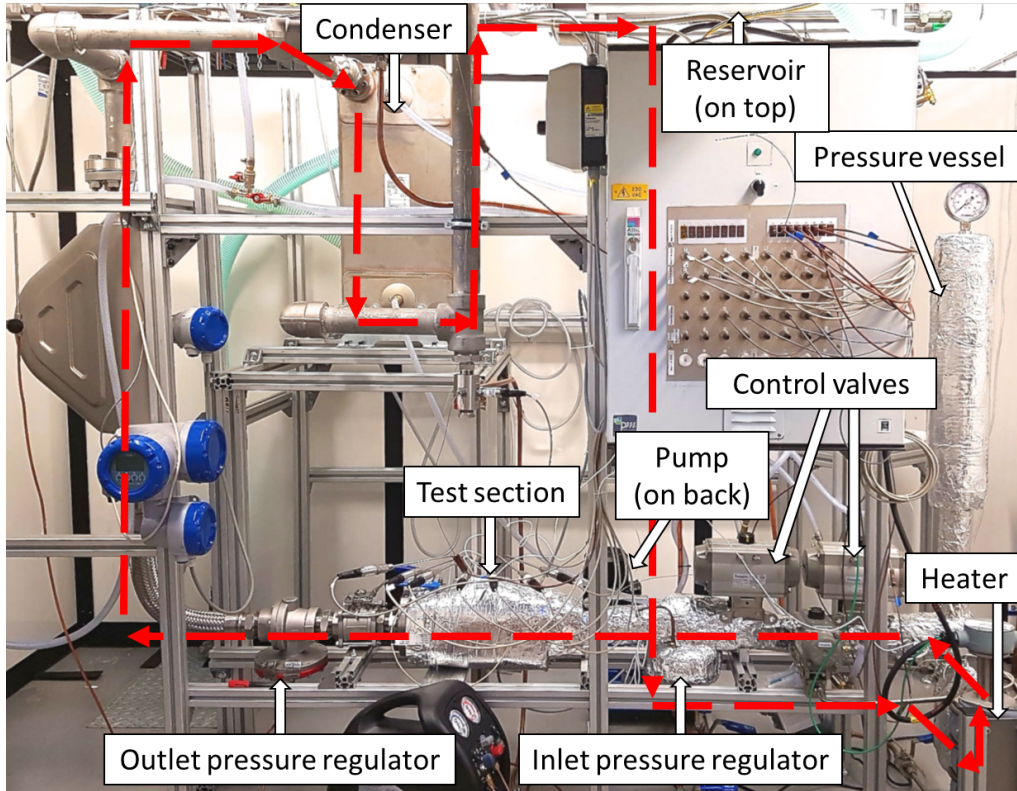


Figure 3.7: Frontal view of the ORC blowdown facility at Imperial College London.

3.3.2 Test Section

The test section for a blade-shaped transonic nozzle is manufactured from stainless steel. The design of the nozzle geometry will be presented later in Chapter 4. The measurement of pressure along blade surface and the Schlieren image of the nozzle flow are the two experimental require-

Parameter	Value	Unit
Working fluid	R1233zd(E)	-
Pressure vessel volume	3.785×3	L
Vessel safety pressure	500	kPa
Vessel safety temperature	220	K
Designed mass flow rate	0.3	kg/s

Table 3.2: Basic information of the ORC blowdown facility.

ments in this work. To fulfill these requirements, a ‘sandwich’ structure is used in this test section (see Figure 3.8). Figure 3.8(a) and (b) show the sectional and exploded views of the test section, respectively. The nozzle plates (green part) is clamped by a lid (yellow part) and a base (red part), and these three parts are assembled together before mounted onto the block (grey). The structures of three parts are described in the following.

The nozzle is shaped by a pair of flat plates, whose top view and sectional view at half of the blade height are shown in Figure 3.9 (a) and (b) respectively. The shape of the pressure surface and suction surface of a blade are cut on each plate. Eleven holes are drilled on blade surfaces for the pressure measurement, with a distance of 4mm between the centerline of adjacent holes (see a series of horizontal pressure holes in Figure 3.9 (b)). These horizontal pressure holes have the diameter of $<0.5\text{mm}$ on the blade-shape side and have the diameter of 2mm on the other side. These horizontal holes are blocked on the wider ends after manufacturing. Eleven vertical blind holes are drilled on the top of each plate to connect with the horizontal holes one by one. Therefore, the pressure along blade surfaces can be measured through these pressure holes. The photo of the real nozzle plates are shown in Figure 3.10.

Figure 3.11(a) and (b) shows the top view and sectional view of the base part, respectively. The nozzle plates are mounted on the base with screws, and four dowels are used to hold the relative position between the nozzle plates and the base so that the shape of the nozzle can be maintained. In the base, there is a first-surface mirror that reflects the light on the top surface of the mirror. This mirror is pressed onto the back of the nozzle plates with screws, and there is a flat plate between the screws and the mirror to prevent stress concentration. The assembly of the nozzle plates and the base is shown in Figure 3.12.

Figure 3.13(a) and (b) show the bottom view and top view of the lid part, respectively. In the bottom view (Figure 3.13(a)), there are two sets of through holes that connect to the vertical holes on the nozzle plates, and an O-ring groove is machined around each hole. The base with the nozzle plates is mounted to this lid with the help of two dowels for fixing the relative position between

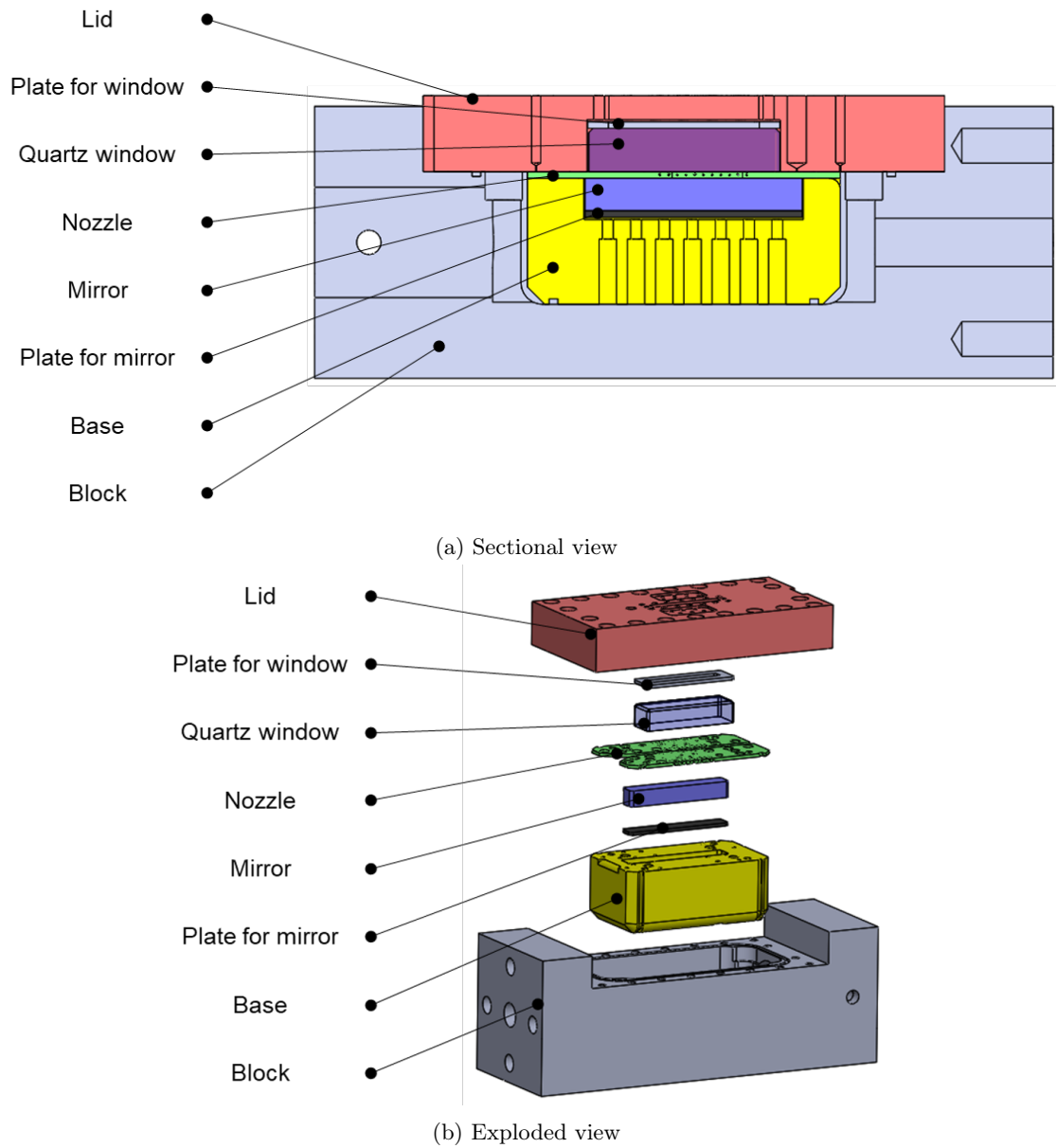


Figure 3.8: Structure of the test section.

them. A piece of quartz window is inserted into the lid and pressed to the nozzle plates with screws on the back. To avoid stress concentrations, a metal flat plate is set between the screws and the quartz window. Figure 3.13(b) shows the top view of the lid, and O-rings grooves are also machined around the through holes on this side for sealing requirement. Then, these through holes are connected to pressure pipes (see Figure 3.14(a)), and these pipes are connected to the pressure transducer on the top side. It is noted that these pressure pipes are connected to a metal block by silver soldering, which simplifies the assembly of the lid and pressure pipes. Photo of the lid on the bottom view is also shown in Figure 3.14(b).

Seven Omega pressure transducers with high accuracy (0.08%) are used to measure the surface

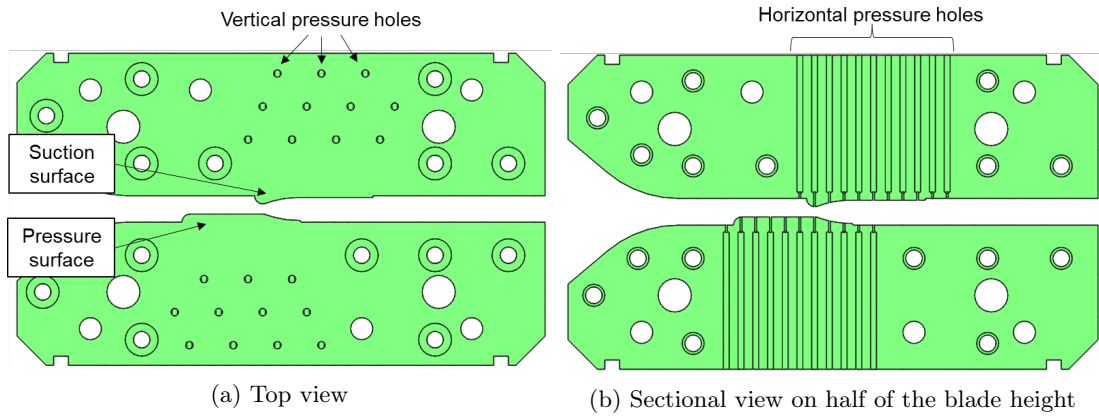


Figure 3.9: Structure of nozzle plates pair.

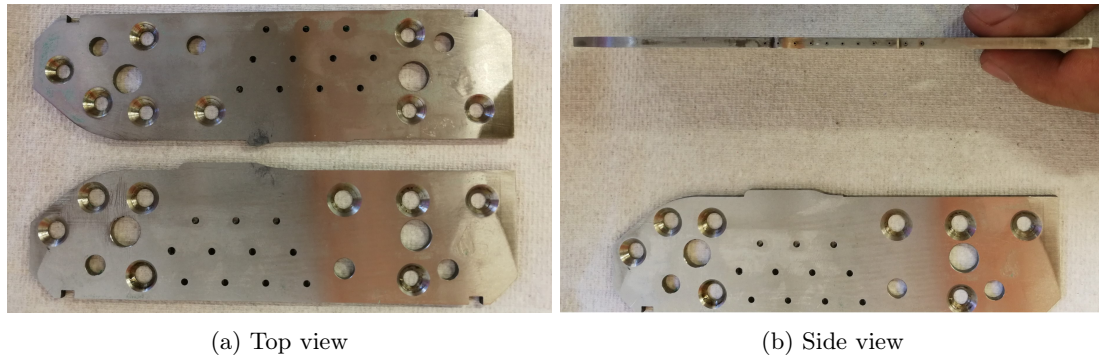


Figure 3.10: Photo of the real nozzle plates.

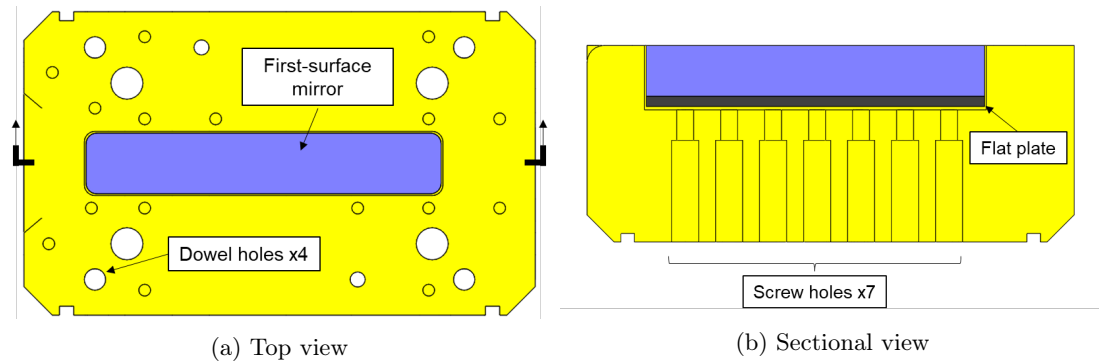


Figure 3.11: Structure of the base.

pressure via pressure pipes. These transducers can work up to 200bar and the sampling frequency can be ($<1\text{ms}$). Twenty-two pressure pipes need to be tested, which is more than the number of current pressure transducers. To finish the pressure test of all pipes, four test runs should be performed under one certain experiment condition. Two Kulite XTEH-10L-190 (M) Series high temperature, high frequency transducers are used and connected directly to the lid to validate the performance of Omega transducers. They are also used to measure the inlet and outlet static pressure of the nozzle channel. The assembly of all test section on the test rig is shown in Figure 3.15.

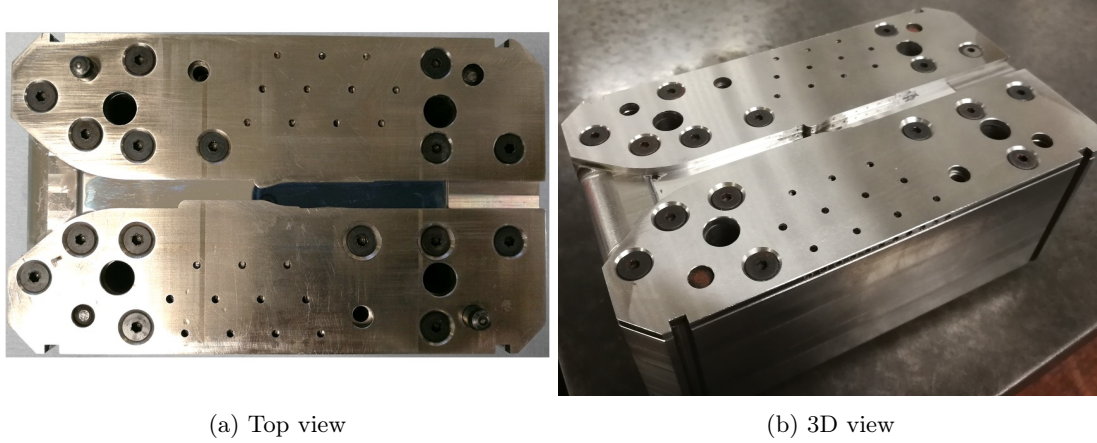


Figure 3.12: Assembly of nozzle plates with the base.

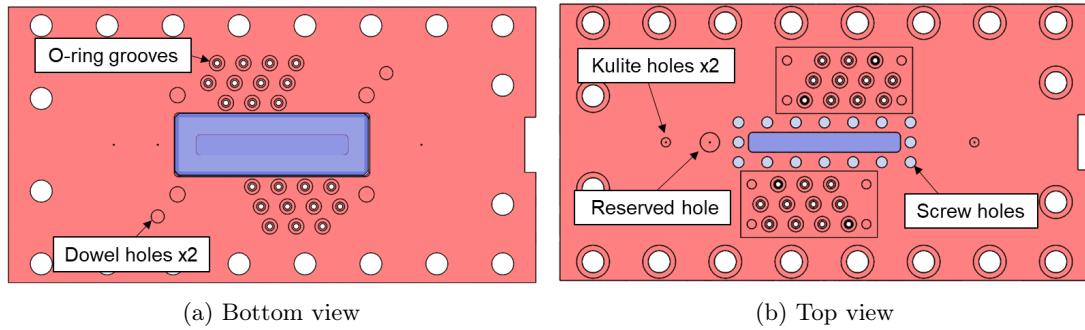


Figure 3.13: Structure of the lid.

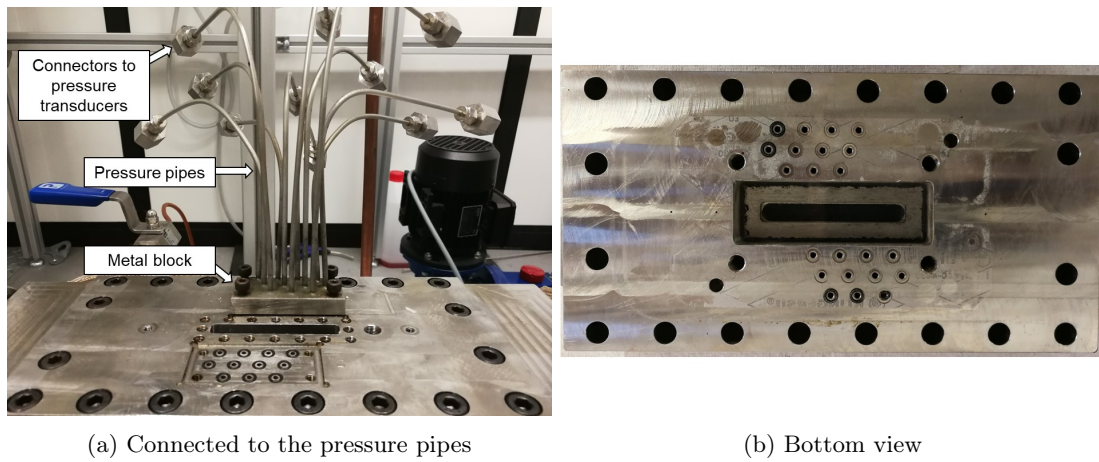


Figure 3.14: Photo of the lid.

The uncertainty of the pressure transducers is tested by Robertson [32] and the author. The data fit between electrical and physical values in LABVIEW is created through a calibration process. Seven points from zero pressure to maximum working pressure are calibrated with values measured by a pressure calibration unit, and a linear fit is made based on these seven points. The standard error between the calibration data and the calculated fit is given according to the



Figure 3.15: Assembly of all parts of the test section.

equation [268]:

$$\sigma = \sqrt{\frac{1}{n - \nu} \sum_{i=1}^n [y_i - f(x_i)]^2} \quad (3.57)$$

$\pm 2\sigma$ are taken as the uncertainty range. The uncertainty of the Omega transducer is $\pm 861 \sim 2,167\text{Pa}$, and the uncertainty of Kulite probe is $\pm 774 \sim 1,413\text{Pa}$.

The same Kulite probes are also installed upstream of the test section and in the pressure vessel, and two T-Type thermocouples are placed in the same location. The temperature range is within $0\text{-}400^\circ\text{C}$, and the uncertainty of the thermocouple is $\pm 2.2\text{K}$ or $\pm 0.75\%$.

3.3.3 Schlieren Imaging Method

A Schlieren system is developed for observing the waves in the nozzle flows. The layout of this system is shown in Figure 3.16.

The light beam from the light source is focused on the light source cut-off and made into a ‘square’ shape ($2 \times 2\text{mm} \times \text{mm}$). Then the divergent light beam passes through the 50% beam splitter and is converted into a collimated beam by a parabolic mirror. This collimated beam passes through the test field and is reflected by the flat mirror on the back-wall of tested nozzle, then returns along the input path. The returning beam is partially reflected at the 50% beam splitter and focused on the schlieren cut-off. Half of the beam is blocked at the knife edge of the schlieren cut-off, and the unblocked light beam is projected onto the camera sensor.

The Schlieren method can bring out the information about the density gradient of the flow field. The refraction is defined as $n = c_0/c$, where c_0 is the speed of light in vacuum, and c is the local speed of light. n depends on the local density. The light path is deflected by the gradient of

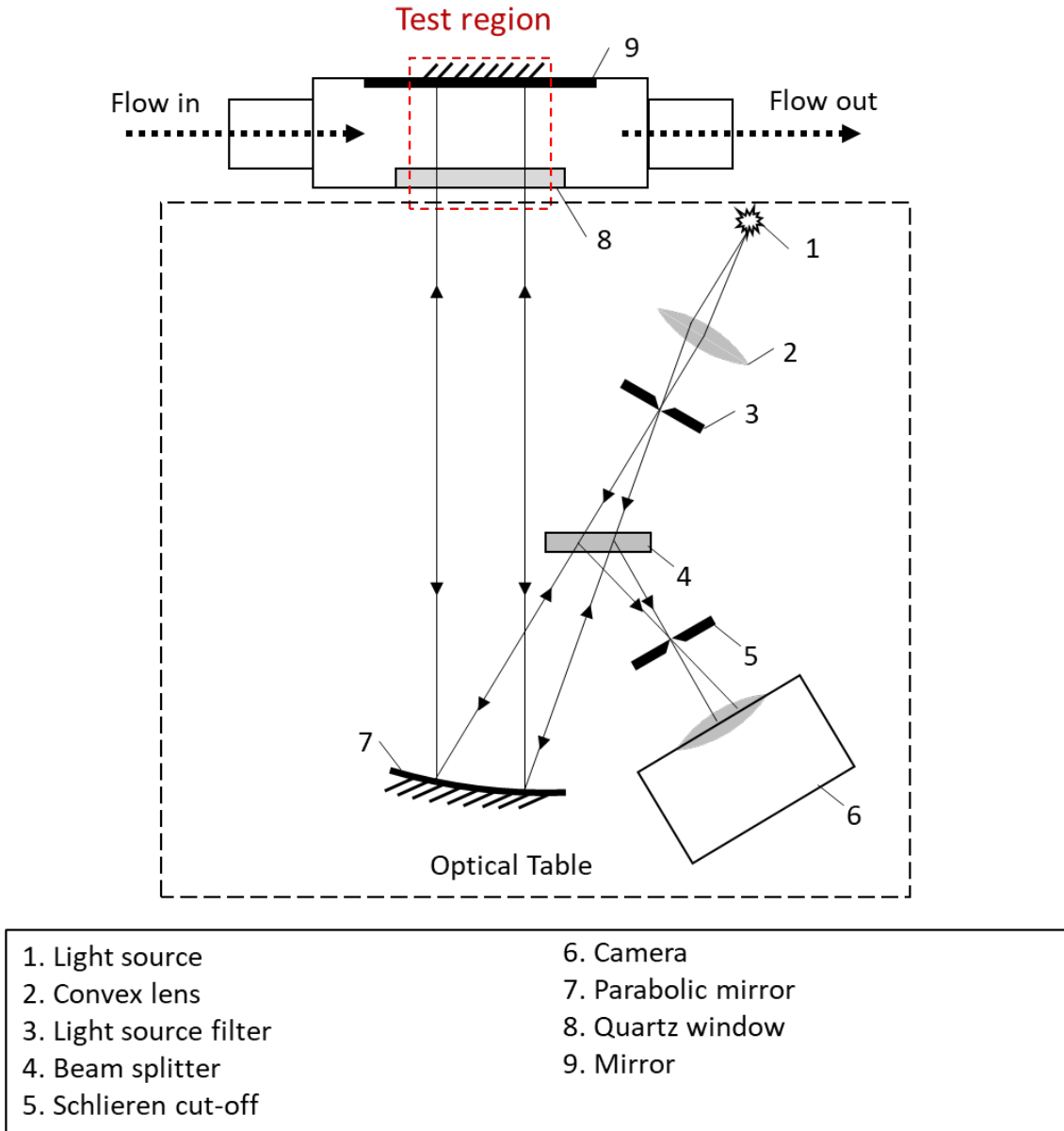


Figure 3.16: Layout of the Schlieren imaging system.

refraction (see Figure 3.17), and the light path follows the relation [269]:

$$\frac{\partial^2 x}{\partial z^2} = \frac{1}{n} \frac{\partial n}{\partial x}, \quad \frac{\partial^2 y}{\partial z^2} = \frac{1}{n} \frac{\partial n}{\partial y}. \quad (3.58)$$

The angle of deviation in these two directions are called ε_x and ε_y . The theory of Schlieren method is shown in Figure 3.18. The light beam with no deviation is focused on the focal point of the parabolic mirror and maps the shape of the light source (a ‘square’ shape in this work), while the light beam with a deviation angle ε_x maps another ‘square’ shape with a distance of Δx from the previous square. In this focal plane there is a Schlieren cut-off blocking a part of the light beam.

For the light beam without deflection, $1/2$ of the light beam is blocked, while for the light beam after deflection $(\Delta x + 1/2 l_s)/l_s$ of the light beam is blocked. The relation between the deflection angle ε_x and the distance Δx is:

$$\Delta x = \varepsilon_x(l + f_{pm}). \quad (3.59)$$

Therefore, the region with a positive ε_x is brighter than one with a negative ε_x . When ε_x is extremely high, the light beam is deflected far from the axis of the parabolic mirror, which also results in a dark region. This is the reason why the shock wave is always dark in Schlieren images.

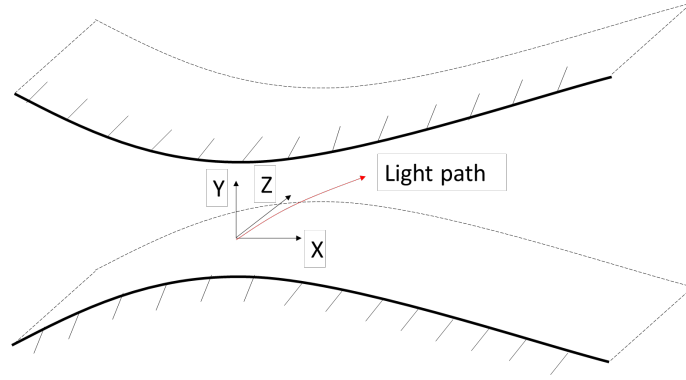


Figure 3.17: Light path under refraction gradient.

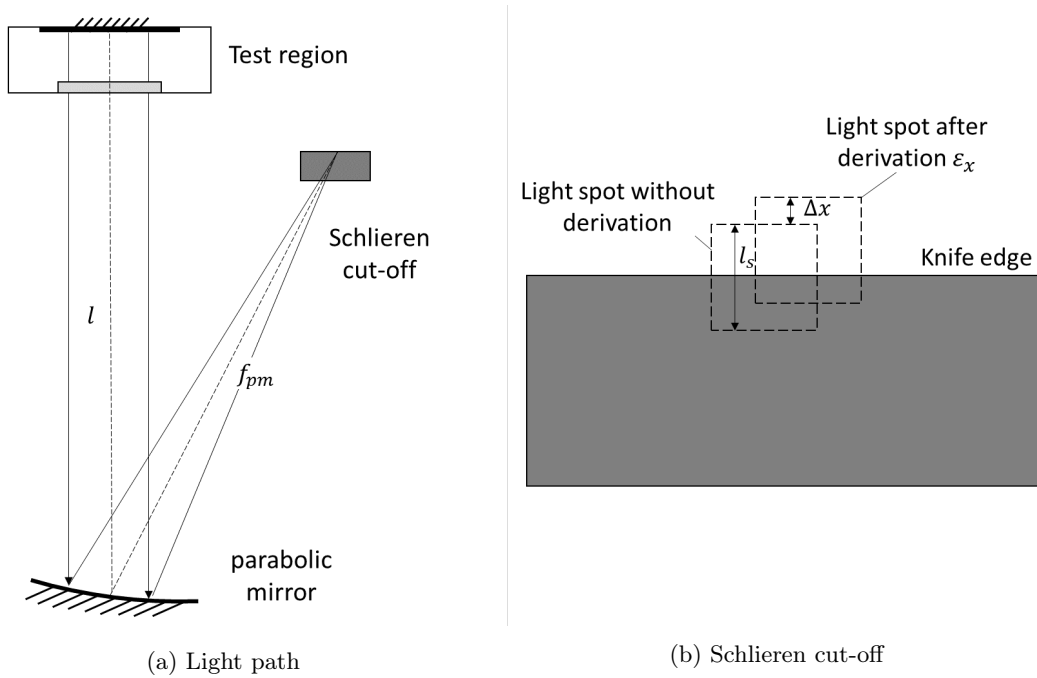


Figure 3.18: Theory of Schlieren method.

The established Schlieren imaging system is shown in Figure 3.19. The light source is a LED light with 3000Lu white light. The parabolic mirror used in this thesis is a 30' off-axis parabolic

mirror manufactured by Edmund Optics. It has the diameter of 101.6mm and the effective focal length is $f_{pm} = 326.7\text{mm}$. The distance between the test section and the parabolic mirror is $\approx 2300\text{mm}$. A flat mirror is placed above the test section to help rotate the direction of the light beam direction from horizontal to vertical. In this system, a 50% beam splitter is used to reflect half of the input light. After the Schlieren cut-off, the convex lens B and the camera lens work together to produce the image on the camera sensor at a suitable size. The camera used here is a Ximea MC050CG-SY camera, which has a CMOS RGB Bayer Matrix 2/3 " sensor. The resolution is 2464×2056 pixels, and the frame rate is 76fps. All optical components are installed on an optical table.

3.4 Chapter Summary

Numerical simulation methods used in this work have been introduced in this chapter. A DNS simulation solver for non-ideal-gas flows is established, which is used in Chapter 5 and 6. The RANS simulation method is also presented; the analysis is presented in Chapter 5 and applied in Chapter 4. The post CFD methods for analysing the DNS results are also mentioned here, including a POD method which will be used in Chapter 6.

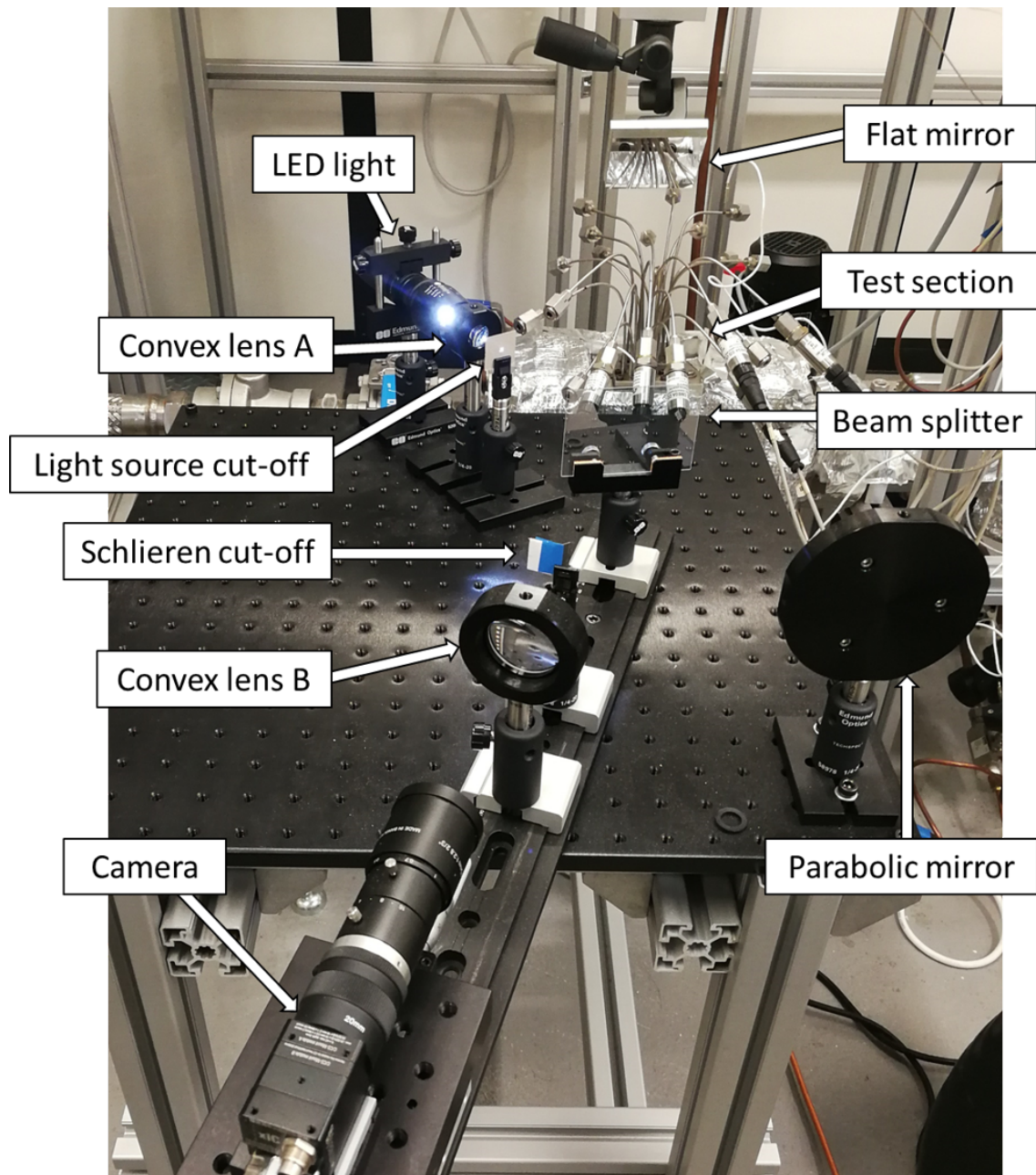


Figure 3.19: Photo of the Schlieren system.

Chapter 4

Design of a Supersonic Cascade and Preliminary Test of a Blade-Shaped Nozzle using the Designed Geometry

4.1 Overview

A linear supersonic cascade is designed based on the method of characteristics (MOC) which uses R1233zd(E) as working fluids. This fluid is an environmental-friendly substitute of the widely-used organic fluid, R245fa. The performance of the nozzle on the design condition is analysed by RANS simulation method. Due to the limitation in the flow capacity of current test facility, multi-passage cascade is not able to be tested even after scaling, so a blade-shaped nozzle, which uses the blade geometry of the designed cascade, is tested. To claim that the flow in this blade-shaped nozzle is not the same as the cascade flow, but it is still helpful to understand the supersonic flow of dense vapours, and it is also a preparation for the test of cascade flow in the future. The pressure distributions along both pressure and suction surfaces of the nozzle are measured by transducers and the flow features are observed by the Schlieren imaging. The preliminary test results are provided in this chapter, even the schlieren images are disturbed by the recondensation of the fluid. This chapter organised as follows: in Chapter 4.2, the design and analysis of the supersonic cascade is introduced; the results of a preliminary test of the blade-shaped nozzle are shown in Chapter 4.3.

4.2 Design and Analysis of a Supersonic Cascade

4.2.1 Design of the Blade Shape by the Method of Characteristics

A sketch of a typical supersonic linear cascade for illustration is shown in Figure 4.1. θ_{in} and θ_{out} represent the inlet and outlet flow angles, respectively, and S_c is the blade pitch. These three parameters together with inlet total thermal state, outlet pressure (or Mach number), blade height and mass flow rate per passage are inputs of the cascade design. The details are shown in Table 4.1. The isentropic expansion process of the supersonic cascade is shown in Figure 4.2, which is closed to the saturation line of the fluid R1233zd(E).

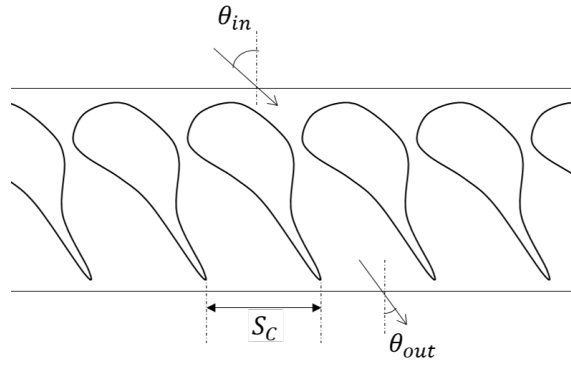


Figure 4.1: Sketch of a supersonic linear cascade.

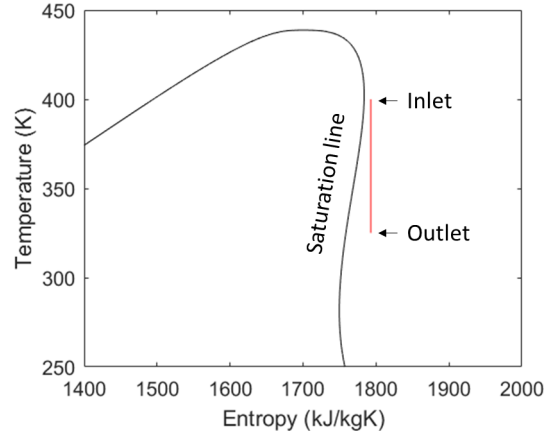


Figure 4.2: Isentropic expansion process of the designed cascade in a T-S diagram.

The design of the cascade blade is performed in two steps. In the first step, the diverging part is designed by the method of characteristics (MOC), see the blue part in Figure 4.3. Here, the simplified MOC for non-ideal gases proposed by Wheeler [21] is used, in which the isentropic exponent is assumed as constant. A straight mean line of the diverging channel is considered here, instead of a curved one. In the second step, the design of the converging and trailing-edge parts of

Parameters	Unit	Value
Inlet flow angle θ_{in}	$^\circ$	70
Outlet flow angle θ_{out}	$^\circ$	70
Blade pitch S_c	mm	39.23
Blade height	mm	5
Inlet total temperature	K	400
Inlet total pressure	kPa	1,700
Outlet Mach number	-	2.0
Mass flow rate per passage	kg/s	0.2
Theoretical outlet static pressure	kPa	210.53
Theoretical pressure ratio	-	8.07

Table 4.1: Design inputs.

the blade are determined based on the diverging part, see the red and brown parts in Figure 4.3. The simplest geometry is used for both leading and the trailing edges, namely a straight line followed by a semi-circle. The main parameters of the designed cascade are listed in Table 4.2.

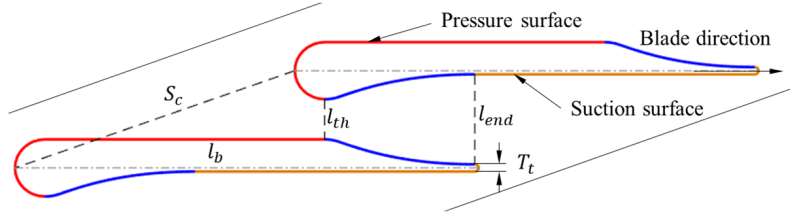


Figure 4.3: Designed nozzle.

Parameters	Unit	Value
Throat width l_{th}	mm	5.56
Width at the end of divergent section l_{end}	mm	12.42
Trailing-edge thickness T_t	mm	1
Blade length l_b	mm	60.07

Table 4.2: Geometrical parameters of the designed cascade.

4.2.2 Analysis of the Designed Supersonic cascade

Simulation Set-up

The designed linear cascade is simulated in ANSYS CFX [222] using the steady RANS simulation with the $k - \varepsilon$ turbulence model (shown in Chapter 3.1.2). The simulation domain is shown in Figure 4.4. The total temperature and pressure of the inlet boundary and the static pressure of the outlet boundary are given as boundary conditions, and the inlet flow angle is give the same as design condition. Non-slip wall boundary conditions are set at the spanwise boundaries and the surface of the blade. The upper and lower boundaries are periodic boundaries. The simulation domain includes two chord lengths upstream of the nozzle and seven chord lengths downstream.

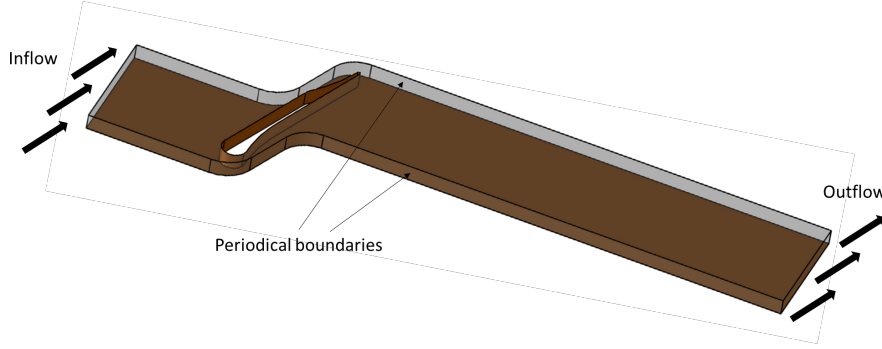


Figure 4.4: Simulation domain of the linear cascade.

The hexahedral mesh is generated by ANSYS ICEM, and the grid independence is checked in seven grids by comparing the volume integral of the entropy generation rate (σ) (see Figure 4.5), which is defined as the irreversible entropy production rate per unit volume [270]:

$$m \frac{ds_{irr}}{dt} = \iiint_{V_{system}} \sigma dV, \quad (4.1)$$

where m is the mass flow rate. y^+ is larger than 30 in all grids. The results show that the grid is almost independent of the cells number when the element number is greater than two million. As a result, the cells number per passage of the grid used in this simulation is 4,464,852.

The Peng-Robinson equation of state (PR-EoS) is used, and the zero-pressure specific heat capacity is fitted by a fourth order polynomial, which is already introduced in Chapter 3.1.2. The dynamic viscosity and the thermal conductivity of R1233zd(E) are simulated by the model based on the elementary kinetic theory which is provided in ANSYS CFX [222].

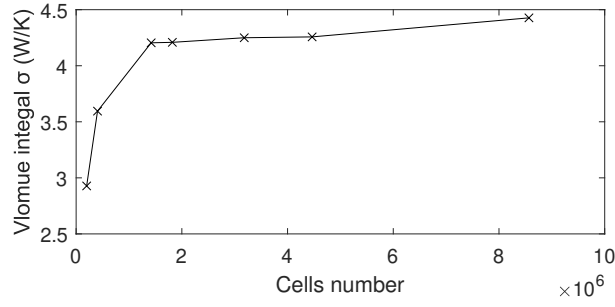


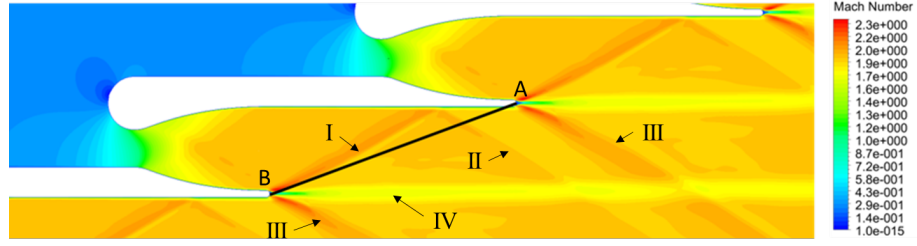
Figure 4.5: Grid Independence study by comparing the volume integral of the entropy generation rate (σ).

Performance of the Designed Cascade

Figure 4.6 (a) shows the Mach number distribution in the cascade on the midspan plane. The Mach number increases through the channel and gets to about 2.0. A pair of trailing-edge 'fish tail' waves (I, III) are identified, of which the upper wave (I) is then reflected on the suction surface to form a reflected wave (II). The trailing-edge wake (IV) is identified by the low-speed region originated from the trailing edge. Each trailing-edge wave consists of an expansion fan in the front and a shock at the back, so the Mach number firstly increases and then decreases across the trailing-edge wave. A nearly uniform Mach number distribution is achieved at the trailing-edge plane (see Figure 4.6 (b)). The Mach number profile on the central line of the plane is shown in Figure 4.6 (c)), which shows the Mach number is within the range 2.0 ± 0.2 (except the trailing-edge wake). These results show that the designed cascade nearly meets the design requirement (Mach number about 2.0).

Figure 4.7 shows the sonic line at the throat. On the suction surface, the sonic line moves slightly forward from the throat area, which leads to an under-expansion in the upper-right region of the nozzle. The growing boundary layer is also a reason of this under-expansion at the nozzle outlet, since it reduces the exact cross-sectional area. It means that this design method can be improved by considering the sonic line curve and the boundary layer thickness.

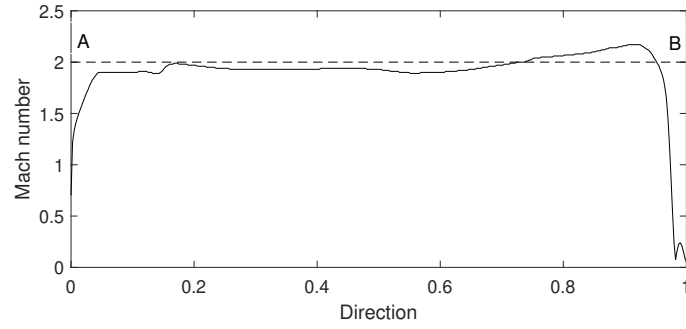
The loss generation is identified by the entropy generation rate (σ). The distribution of σ on the mid-plane and the 15% span plane are shown in Figure 4.8 (a) and (b), where three white lines refer to different distances from blade trailing edge ($0.5 S_c$, S_c and $1.5 S_c$). On the midspan plane (Figure 4.8 (a)), the blade surface boundary layer loss, trailing-edge wake loss (mixing loss) and shock loss are identified. The mixing loss is found mainly generated within the region from the trailing edge to $0.5 S_c$ downstream the trailing edge, while it become much weaker in the region further downstream. On the 15% span plane (Figure 4.8 (b)), leading-edge loss and the endwall boundary layer loss are identified. The leading-edge loss is a secondary flow loss due to the leading-edge vortex near endwall, and the region of leading-edge loss stretches into the throat area



(a) On 50% span plane



(b) On the trailing edge plane



(c) Along central line of the trailing-edge plane

Figure 4.6: Mach number distribution.

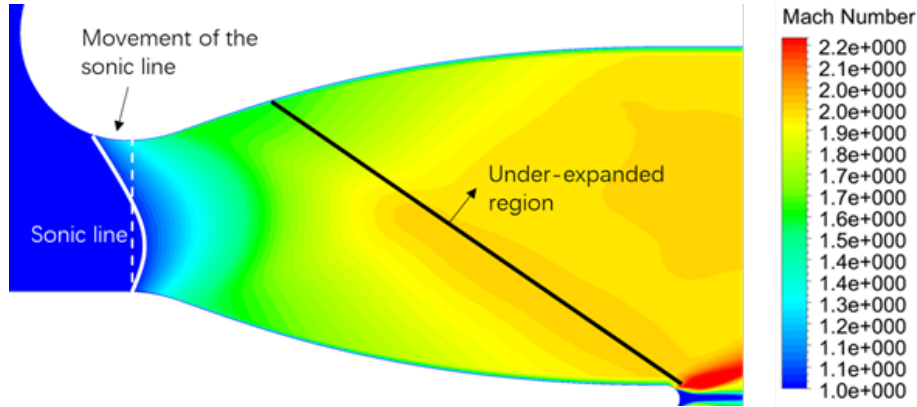


Figure 4.7: Sonic line at the throat.

in this design. The endwall boundary loss region is observed downstream of trailing-edge shocks on the 15% span plane (see the red region in Figure 4.8 (b)), it means that the boundary layer thickness on the endwall increases after the shock. The peak of this thickness increase (red region) is observed starting from $0.5 S_c$ downstream of the trailing edge, and it locates in the middle region

of a passage instead of closed to blade surfaces.

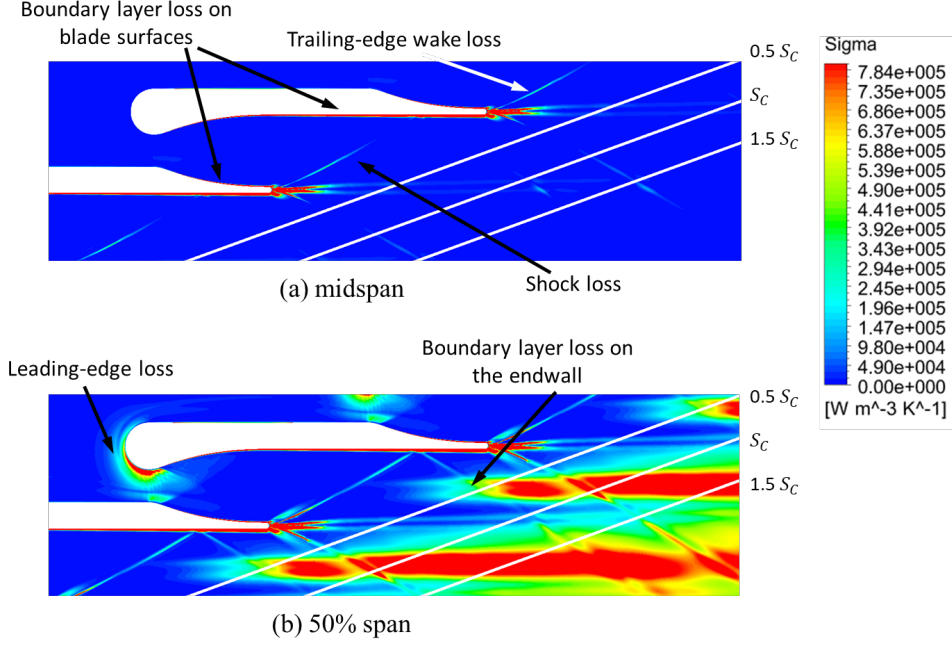


Figure 4.8: σ distribution on different span planes.

To quantitatively analyse the loss distribution, an entropy loss coefficient ε^s is defined:

$$\varepsilon^s = \frac{\bar{s}^M - \bar{s}_\infty^M}{R}. \quad (4.2)$$

The passage is divided by a series of planes which are shown in Figure 4.9(a), and the entropy is averaged on each plane by the mass-flow-averaging. The entropy loss coefficient ε^s from cascade inlet to the position of each plane is calculated and shown in Figure 4.9(b). The overall entropy loss coefficient (from the inlet to $1.5 S_c$ downstream of the trailing edge) is 0.252. Only 2.04% of the loss generated in the converging part (upstream of the throat) where the velocity is relative low. After the throat, the entropy loss significantly increases due to the acceleration, and the loss generated in the diverging part (from the throat to the end of the expansion region) accounts for 26.13% of the overall loss. The remained 71.83% loss is generated in the post-expansion region (from the end of the expansion region to $1.5 S_c$ downstream the trailing edge) where the shock loss and the mixing loss contribute.

In summary, the CFD results show that designed cascade geometry is able to achieve a nearly uniform distribution of Mach number. The overall entropy loss coefficient of this cascade is 0.252, among which most loss (71.83%) is generated in the post-expansion region, and 25.13% is generated in the diverging part. The loss in the converging part is only 2.04% which is nearly negligible.

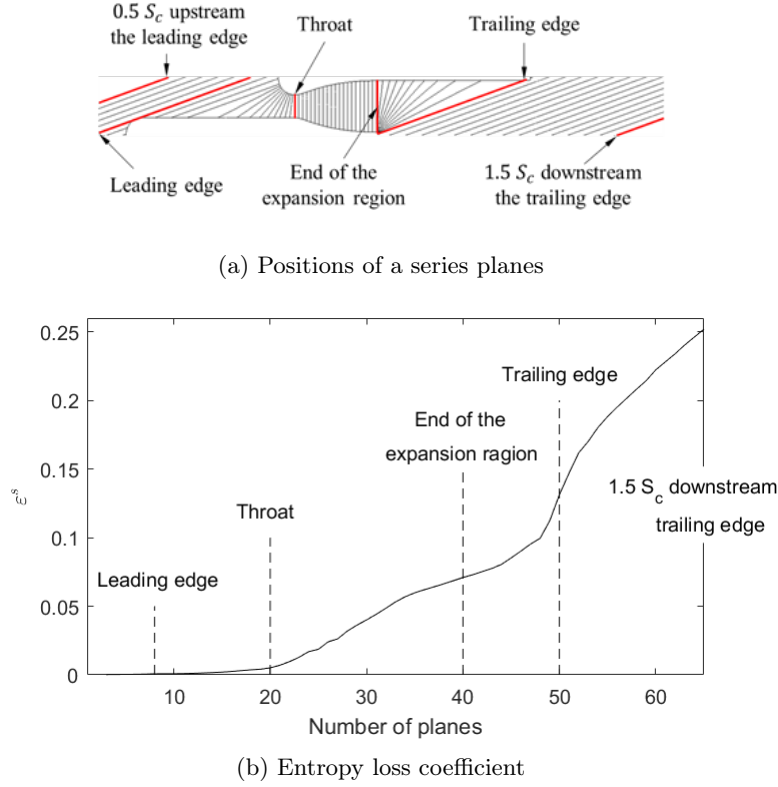


Figure 4.9: Entropy loss coefficient distribution along the main stream.

4.3 A Preliminary Test of a Blade-Shaped Nozzle

4.3.1 Geometry of the Nozzle

The geometry of the blade-shaped nozzle is achieved from the designed cascade blade by scaling due to the flow capacity limitation of current test rig. It is shown in Figure 4.10, and the parameters are listed in Table 4.3. The blade length is $l_b = 32.41\text{mm}$, the length of the subsonic part (from leading-edge to the throat) is $l_{sub} = 22.03\text{mm}$, the length of supersonic expansion (from the throat to the end of the divergent part) is $l_{sup} = 9.88\text{mm}$, the leading-edge thickness is $T_l = 4.44\text{mm}$, and the trailing-edge thickness is $T_t = 1.00\text{mm}$. Upstream of the blades is a convergent-straight channel with the total length of $l_{up} = 44.97\text{mm}$ and the width of $l_{ch} = 7.21\text{mm}$, and downstream of the blades is a straight channel with the length of $l_{down} = 46.81\text{mm}$ and the same width of $l_{ch} = 7.21\text{mm}$. The throat width is $l_{th} = 2.77\text{mm}$, and the blade height is $h_b = 3.00\text{mm}$.

4.3.2 Testing Process

By the experimental method introduced in Chapter 3.3, this nozzle is tested in two fluids: nitrogen and R1233zd(E), and one test is for nitrogen and two tests are for R1233zd(E). Nitrogen at room temperature can be almost considered as an ideal gas, which is tested for compared with

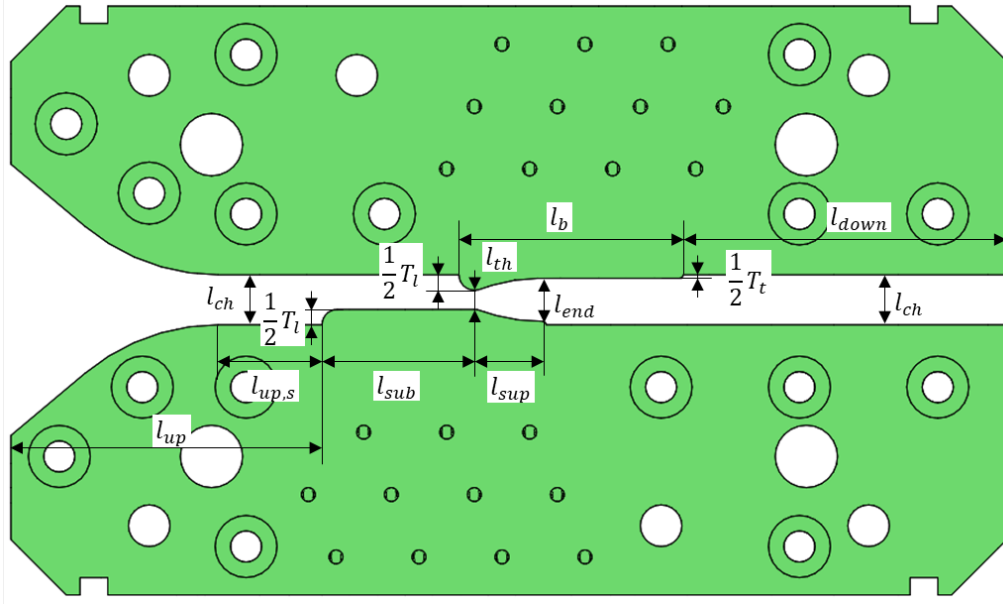


Figure 4.10: Geometry of the tested single-passage nozzle.

Parameters	Value	Parameters	Value	Parameters	Value
T_l	4.44	T_t	1.00	l_{ch}	7.21
l_{th}	2.77	l_{end}	6.21	l_b	32.41
l_{sub}	22.03	l_{sup}	9.88	l_{up}	44.97
$l_{up,s}$	15.00	l_{down}	46.81	h_b	3.00

Table 4.3: Parameters of the single-passage nozzle (unit is mm).

R1233zd(E). The working conditions for each test is shown in Table 4.4, including inlet total pressure, inlet total temperature and outlet static pressure.

In each test, four runs are taken at the same inlet and outlet conditions so as to measure the pressure at all pressure holes on the nozzle surface. These four repeating runs are due to the limit on the number of transducers. There are twenty two pressure holes need to be measured but only seven transducers available currently. The exact working conditions of the four runs cannot be same, and the maximum derivation from the set value is the uncertainty of the working condition (also shown in Table 4.4). The uncertainties of all parameters are below 1% in Test N, but they are slightly larger in Test R8 and R10. This is because the flow control of real gas is more difficult, since phase changing may happen inside. All these uncertainties are lower than 3%, which shows the agreement of four runs in each test is acceptable.

The thermodynamic states of R1233zd(E) at total inlet conditions for Test R8 and R10 are shown in T-S diagram, see Figure 4.11. These two points are close to the vapour saturation line,

Parameters	Unit	Test N	Test R8	Test R10
Inlet total pressure	kPa	1,336.59	753.02	1,000.78
Uncertainty of inlet total pressure	%	<0.1	1.04	2.17
Inlet total temperature	K	286.09	369.03	373.24
Uncertainty of inlet total temperature	%	0.33	1.45	0.47
Outlet static pressure	kPa	399.15	384.42	551.98
Uncertainty of outlet pressure	%	<0.1	1.97	2.67

Table 4.4: Working conditions of experimental tests.

where non-ideal effects are strong. These two preliminary tests do not reach the design inlet condition of the blade (1,700 kPa, 400 K), because of the limitation in the heating and pumping system of the current blowdown rig. In the preparation process of the test, the pressure vessel upstream of the test section should be pumped into high-pressure overheated organic vapours; Meanwhile, the pressure in the vessel should be much higher than the total inlet pressure of test section for providing a long running time. Otherwise, a nearly stable flow cannot be achieved. The current pumping and heating system can provide vapours with the thermal state at about 3,000 kPa and 450 K, which is not able to support a run with higher inlet total pressure and temperature than those of Test R10. The back pressure for these preliminary tests are set for a smaller expansion ratio than the designed value. This is because the back pressure control system is suffering from leakage. More tests with higher inlet total pressure and higher expansion ratio will be taken in the future, after these problems are solved.

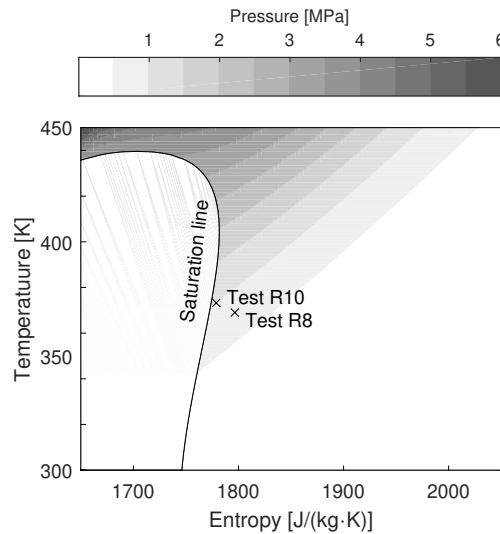


Figure 4.11: Inlet total thermal states of R1233zd(E) tests shown in T-S diagram.

In one test, Figure 4.12 (a) shows the arrangement for the connection between pressure holes and pressure transducers in each run. For example in the first run, pressure holes S1 - S7 are connected to pressure transducers A - G. In one run, the measurement and recording of transient pressure starts at about one second before the opening of the upstream controlling valve and ends after the steady flow. For example, the pressure measurement in the first run of Test P8 is show in Figure 4.12 (b). At the beginning, the pressure remains at a low level, which means the upstream controlling valve is closed. Once the controlled valve is opened, the pressure suddenly increases at all measured positions. Then, it takes about three seconds to achieve a nearly steady flow. This period time between the open of controlling valve and the start of a steady flow is mainly due to the lag effect of the pressure regulator. The steady flow can maintain a period of time before the inlet pressure becomes lower than the required working condition. In the post treatment of each run, the pressure within the period of steady flow is averaged and recorded as the measured steady pressure.

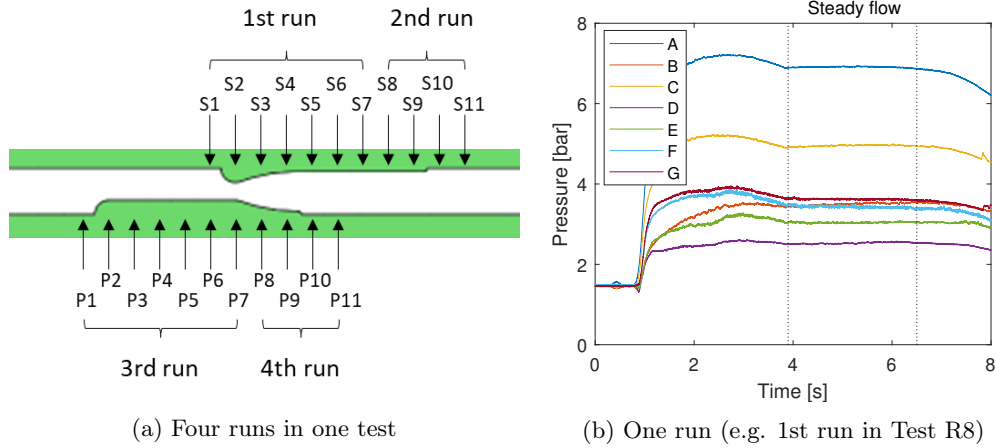


Figure 4.12: Pressure test process.

The Schlieren system starts to work before the opening of the controlling valve, for recording the flow features within each run. The camera framework frequency in these tests is about 16 Hz, which is enough to catch the moment of steady flow. The timings of pressure measurement system and the Schlieren system should be matched in post treatment, since these two systems are controlled separately. The first Schlieren image after the opening of the controlling valve is not difficult to be identified, and it helps to match the timings between two systems.

4.3.3 Test Results and Discussion

The measured steady pressure distributions along two surfaces of the blade-shaped nozzle for Test N are shown in Figure 4.15. The black vertical lines refer to leading edge and trailing edge of

the pressure surface, and the red vertical lines refer to the range of the suction surface. On the pressure surface, the pressure drops a little at the leading edge and then maintains at a high level; From the point before throat (at $x = 17.9$ mm), the pressure significantly drops, and the lowest pressure is seen at the point downstream of the throat (at $x = 25.9$); Then, the pressure rises again. On the other nozzle surface, the pressure drops significantly at the leading edge, since the throat is close to the leading edge; the pressure at the throat ($x = 21.9$) is lower on the suction surface than on the pressure surface, and this asymmetric pressure drop on two sides of nozzle is due to the asymmetric geometry upstream of the throat; This asymmetric is also seen at positions downstream of the throat, where the pressure on the suction surface is slightly lower than that on the pressure surface; A pressure rise is also seen on the suction surface, and it starts from the same point as that on the pressure surface; Around the trailing edge of the suction surface, the pressure nearly maintains at a platform.

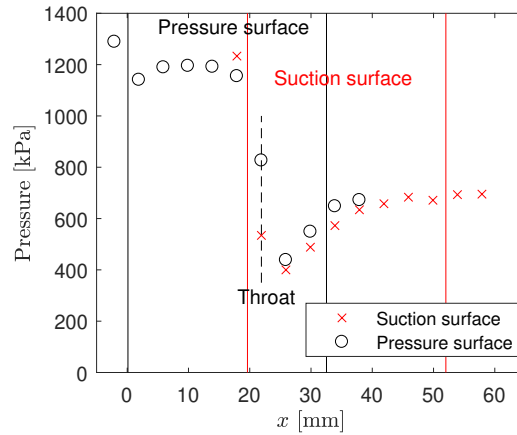


Figure 4.13: Pressure distributions on nozzle surfaces in Test N.

The significant pressure rise downstream the throat indicates a shock there. Figure 4.14 shows the transient Schlieren images in Test N, of which (a) - (d) are taken at the beginning of the test run and (f) is taken at the nearly steady flow period. Here, $t = 0$ approximately refers to the moment that the controlling valve opens, so Figure 4.14 (a) does not show any flows. In Figure 4.14 (b), a series of oblique shocklets can be seen in the region downstream of the throat, which indicates a supersonic flow in the nozzle. At the end of window region, some 'X' shape shadows can be seen, and it means that the adverse pressure gradient exists in this region. In Figure 4.14 (c), two strong normal shocks are observed in the diverging region, following by a series of weak shocks, and it means that the shock train has already formed at this moment. The two normal shocks indistinctly show γ -shape foots in the near-wall region. This shock train could form from the accumulation and development of the adverse pressure gradient effects. In Figure 4.14 (d), the leading of the shock

train slightly moves upstream, and the shape of the shock becomes similar to 'X' shape instead of a straight line. After $t = 187$ ms, the position and shape of shocks do not change significantly but slightly vibrate until the end of the test run. Figure 4.14 (e) is the Schlieren image within the period of nearly steady flow, and the shock train is also observed in the diverging part of nozzle. It can explain the pressure rise downstream of the throat on both nozzle pressure and suction surfaces in Figure 4.15.

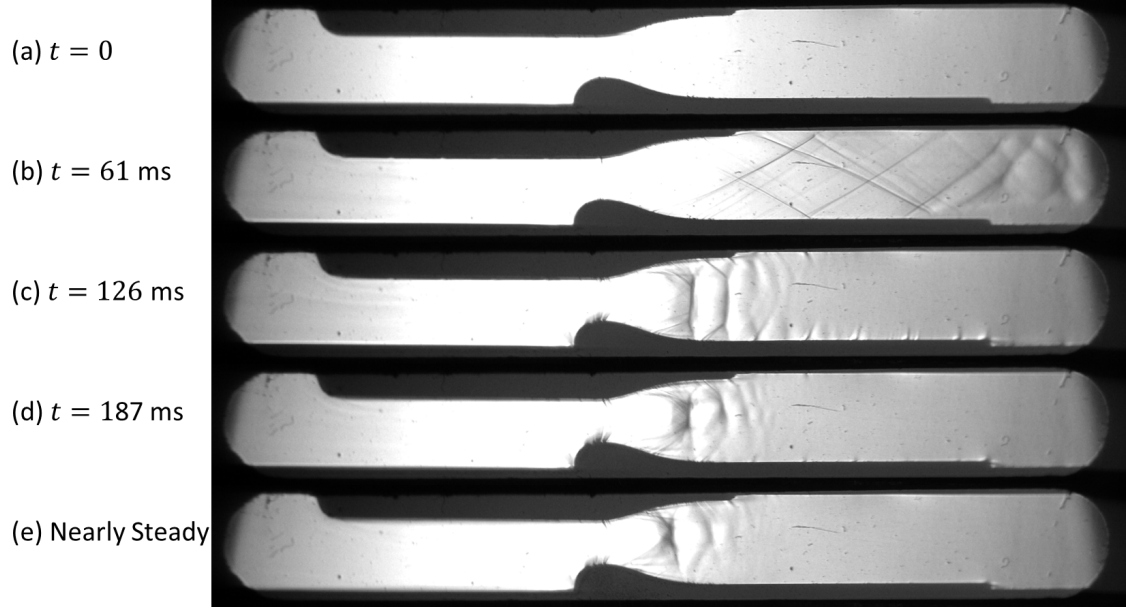


Figure 4.14: Transient Schlieren images of Test N.

The measured steady pressure distribution for two R1233zd(E) tests are shown in Figure 4.15 (a) and (b). The pressure distributions show a similar trend in both Test R8 and R10 as that in Test N, where the pressure decreases significantly around the throat ($x = 21.9$ mm) and then rises. In both R1233zd(E) tests, the pressure on the suction surface is also found lower than on the pressure surface for the same position, and the pressure difference shows the maximum at the throat. The pressure on two nozzle surfaces are also directly compared with Test N in Figure 4.16 (a) and (b), after normalised by the inlet total pressure. In Figure 4.16 (a), the normalised pressure distributions in three tests nearly coincide before the throat, but they become different after that. The difference of pressure distribution is also found on the suction surface. This difference is due to the complex two-phase flows in R1233zd(E), and the evidence of two-phase flows is shown in the following paragraph.

Figure 4.17 shows the Schlieren images at the steady flow period for all three tests. Here, Figure 4.17 (a) is the duplication of Figure 4.14 (e) for the convenience of comparison. The background in Figure 4.17 (a) is 'clean', but those in Figure 4.17 (b) and (c) are not. There are

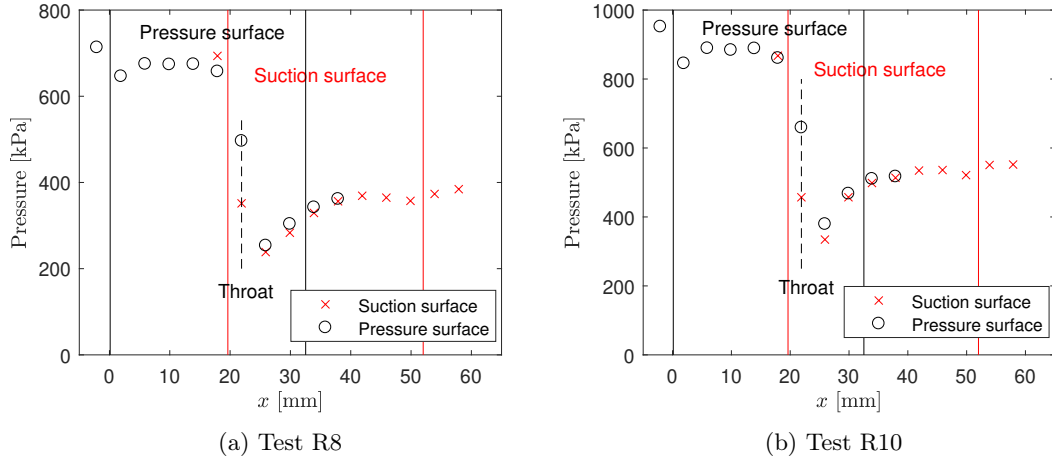


Figure 4.15: Pressure distributions on nozzle surfaces in R1233zd(E) tests.

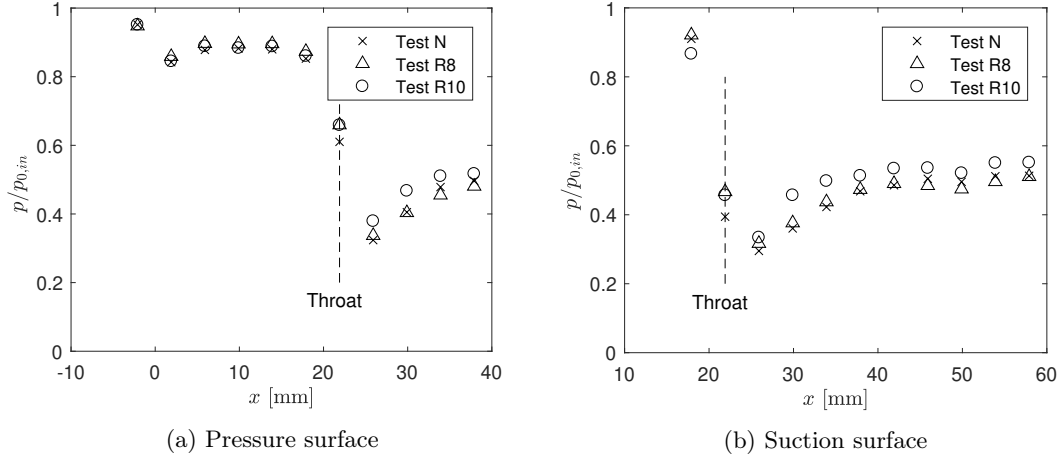


Figure 4.16: Comparison of normalised pressure distribution on two nozzle surfaces.

long dark lines in both Figure 4.17 (b) and (c), which are the traces of droplets, and disorderly background can be seen upstream of the throat in Figure 4.17 (b), which indicates liquid on the nozzle endwall. These droplet and liquid partially come from the pressure vessel and partially form by recondensation. They not only changes the flow features of nozzle but also make the Schlieren images obscure. The shock train structure can not be clearly identified in Figure 4.17 (b) and (c), since they cannot be fully distinguished from the traces of droplets and recondensed liquid.

The current experimental results show that the two-phase flow is a serious problem for the test of fluids whose thermal state is close to the saturation line. The pipework should be designed carefully to avoid the influence of the condensed liquid on pipe walls. It also should be make sure that there is no liquid in the test section in the preparation stage.

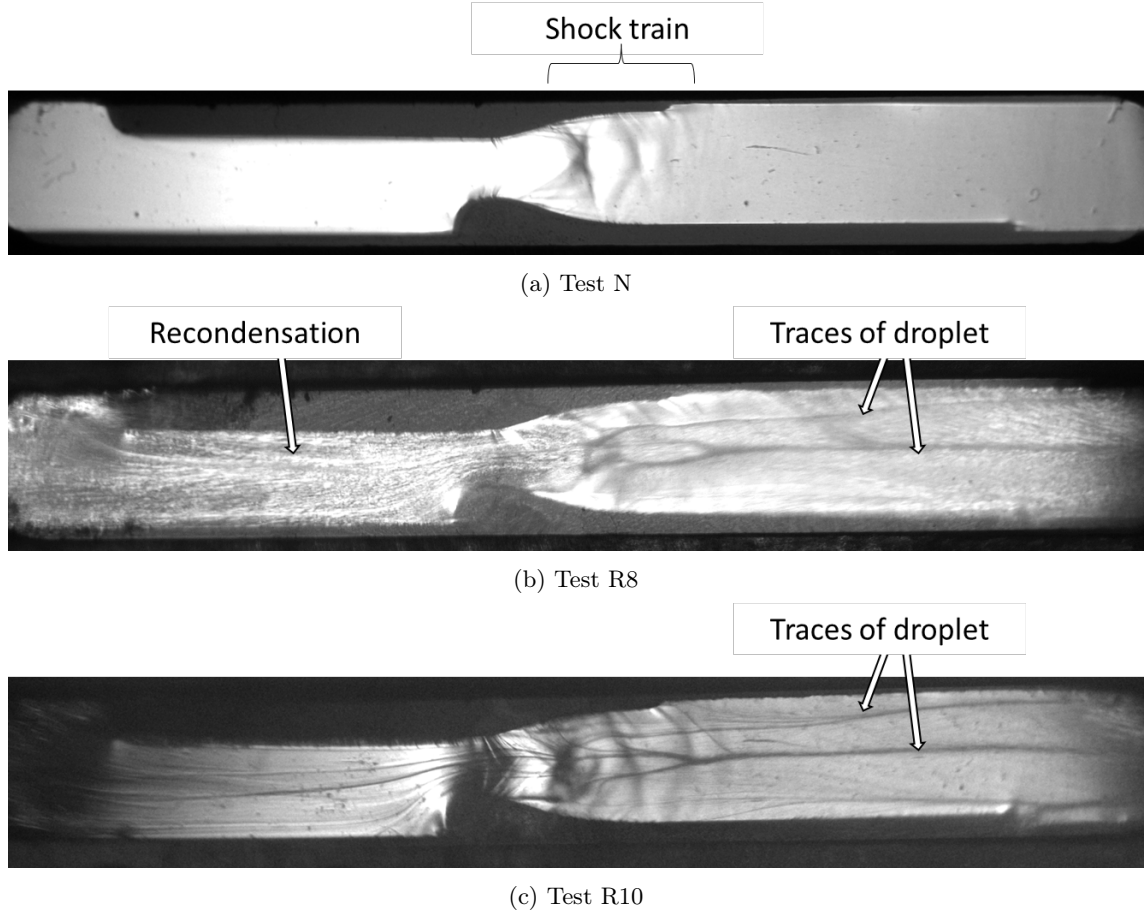


Figure 4.17: Schlieren images at the steady flow period for Test N, R8 and R10.

4.4 Chapter Summary

A supersonic cascade for the gas R1233zd(E) is designed by a MOC-based method, whose designed outlet Mach number is 2.0. Steady RANS simulation method is used to validate the design geometry and analyse the performance of the supersonic cascade. The simulation results show that the Mach number at the trailing-edge plane is in the range 2.0 ± 0.2 , which means the designed cascade nearly meets the requirement. The overall entropy loss coefficient is 0.252, when $1.5 S_c$ downstream of the trailing edge is considered as the cascade outlet. Among the loss, only 2.04% generated in the converging part, 26.13% is generated in the diverging part, and 71.83% is generated in the post-expansion region.

The blade shaped of this supersonic nozzle is used to build up a blade-shaped nozzle, and the preliminary test results of this nozzle is discussed. One test with nitrogen and two tests with R1233zd(E) are taken, and the vapour works close to its saturation line in two R1233zd(E) tests. The experimental results of nitrogen test show that the pressure drops around the nozzle throat but rise in the downstream. This is explained by a shock train in the nozzle, which is observed

in the Schlieren images. The pressure distribution follow a similar trend in R1233zd(E) tests as that in the nitrogen test, but the Schlieren images for these two tests are disturbed by two-phase flows. The reason for the existence of two-phase flows is discussed, and the method could be able to avoid the problem is also provided.

Chapter 5

Study of Supersonic Fully-Developed Turbulent Channel Flows of Dense Vapours using DNS Method

5.1 Overview

This chapter studies the influence of molecular-complexity effects and non-ideal effects on the wall-bounded turbulent behaviours. The study of near-wall turbulent behaviours is the fundamental basis for understanding the boundary-layer loss generation and the heat transfer features. It is normally studied in simplified flows [12, 132], like the flows over a flat plate and the channel flows. The behaviours in the inner layer of these two types of flows are essentially the same [9]. This chapter studied the turbulent behaviours in the fully-developed turbulent channel flows, which focus on the inner-layer region of boundary layers. The fundamental turbulent behaviours in non-ideal gases is discussed.

The studied Reynolds number is $Re_G = \rho_B u_G l / \mu_B = 4880$, where ρ_B is the bulk averaged density $\rho_B \equiv \frac{1}{l} \int_0^l \bar{\rho} dy$, u_B is the bulk velocity $u_B \equiv m_B / (\rho_B l)$, m_B is the bulk mass flow rate $m_B \equiv \int_0^l \bar{\rho} u dy$, l is the half channel height, μ_G is global viscosity $\mu_G \equiv \mu(\rho_B, T_w)$, and T_w is the wall temperature. This Reynolds number is suitable for the study of the structure of inner-layer and log-law region [12], and it is the basic for understanding the boundary layer at a larger Reynolds number, where the log-law region is longer but the inner-layer is nearly the same [271]. This studied Reynolds number is also convenient for comparing with current studies of ideal-gas flows. The studied Mach number is $Ma_G = u_B / c_G = 2.25$, where c_G is the global speed of sound

Gas name	Type	$\mathcal{M}$	T_{cr}	p_{cr}	ρ_{cr}	Z_{cr}	$c_{v,\infty}^{cr}/R$	Γ_{min}
		g/mol	K	MPa	kg/m ³	-	-	-
Air	ideal gas	28.9	-	-	-	1	2.5	1.2
R1233zd(E)	non-ideal gas	130.5	439.6	3.62	480.2	0.269	17.48	0.746
MDM	non-ideal gas	236.5	564.1	1.42	256.7	0.278	61.77	0.116

Table 5.1: Basic information of researched gases.

$c_G = c(\rho_B, T_w)$. The compressibility of dense vapour can be studied at a high Mach number, and the Mach number in applicants is not commonly higher than 2.25, so the studied Mach number is selected at 2.25.

Two organic gases: R1233zd(E) and MDM are simulated and analysed. The basic information of these gases are list in Table 5.1. In the table, $\mathcal{M}$ is molecular weight; T_{cr} , p_{cr} , ρ_{cr} and Z_{cr} are critical temperature, pressure density and compressibility factor respectively; $c_{v,\infty}^{cr}/R$ is the dimensionless heat capacity; Γ_{min} is the minimum fundamental derivative of gasdynamics in vapour phase. R1233zd(E) is a low global warming potential (GWP) refrigerant with moderate molecular weight, and MDM is a high molecular weight siloxane. By comparing the turbulent boundary layers in R1233zd(E) and MDM with those in air, the influence of molecular-complexity effects is analysed. At the same time, three different thermodynamic states of each organic gas are also studied to analyse the influence of non-ideal effects. Thermodynamic states of these three cases are in the dilute-gas region, near the saturation line, and in the supercritical region, whose non-ideal effects are weak, moderate and strong respectively.

This chapter is structured as follows. In Chapter 5.2, the mathematical methodology and calculated cases are introduced. The mean flow field of is discussed in Chapter 5.3, and behaviour of turbulence is discussed in Chapter 5.4. Based on this analysis, turbulence modelling issues in dense vapours are discussed in Chapter 5.5. Finally, the main conclusions are summarised in Chapter 5.6.

5.2 Methodology and cases set-up

5.2.1 Simulation method

The DNS method introduced in Chapter 3.1.1 is used to simulate the 3D NS equations in compressible channel flows. Sciacovelli [139] confirmed that Stokes' assumption is still acceptable in

dense-vapour flows. The flows between two infinite flat planes are simulated, and the simulation domain is shown in Figure 5.1. Its size is $L_x \times L_y \times L_z = 2\pi l \times 2l \times \pi l$, where l is the half channel height (characteristic length scale of channel flows), L_x , L_y and L_z are domain length in mean streamwise direction, wall-normal direction and spanwise direction respectively. The periodic boundary condition is applied at the streamwise and spanwise domain edges, so as to approximate the flows between infinite flat planes. The isothermal non-slip boundary condition is applied at the channel walls. For maintaining a stable mass flow rate, a uniform body force instead of streamwise pressure gradient is added, following the concept of Coleman's work [12]. Therefore the source terms in Equations 3.2 and 3.3 is given as follows:

$$S_{m,i} = \rho f_{b,i}, \quad S_{e,i} = \rho u_i f_i, \quad (5.1)$$

$$f_1 \neq 0, \quad f_2 = 0, \quad f_3 = 0. \quad (5.2)$$

The uniform body force f_i is non-zero only in the streamwise direction, and its value is calculated ever time step for maintaining a constant channel mass flow rate. The coefficients of Span-Wagner EoS for R1233zd(E) and MDM are obtained from the work of Mondejar [86] and Colonna [87].

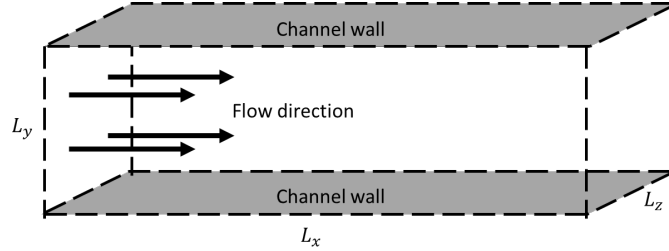


Figure 5.1: The simulation domain of channel flows.

The governing equations are solved by the finite difference method, where convective flux derivatives and viscous flux derivatives are approximated by the seventh-order upwind difference scheme and the sixth-order central scheme respectively. Time advance is solved by the third-order Runge-Kutta method. Due to the periodic boundary conditions in streamwise and spanwise directions, there are no traditional inlet and outlet boundaries, but the bulk averaged density ρ_B and bulk mass flow rate m_B are explicitly constrained after each Runge-Kutta step [12, 272, 139]. After convergence of the simulation, the statistic is taken every $\hat{t} \equiv tu_B/l = 2$ within a time range $\hat{t} = 1000$.

There is no experimental data for dense-vapour boundary layers up till now, so this DNS method can only be validated in ideal-gas flows. This method is applied to a compressible turbulent channel flow of air and is compared with the result of Coleman [12]. This case is at $Re_B = 4880$ and

$Ma_B = 3$. Figure 5.2 shows the profiles of the mean velocity (after Van Driest transformation), root mean square of velocity fluctuations, and Reynolds shear stress. Comparison of DNS results in this chapter with those of Coleman [12] shows that the accuracy of this DNS method is acceptable.

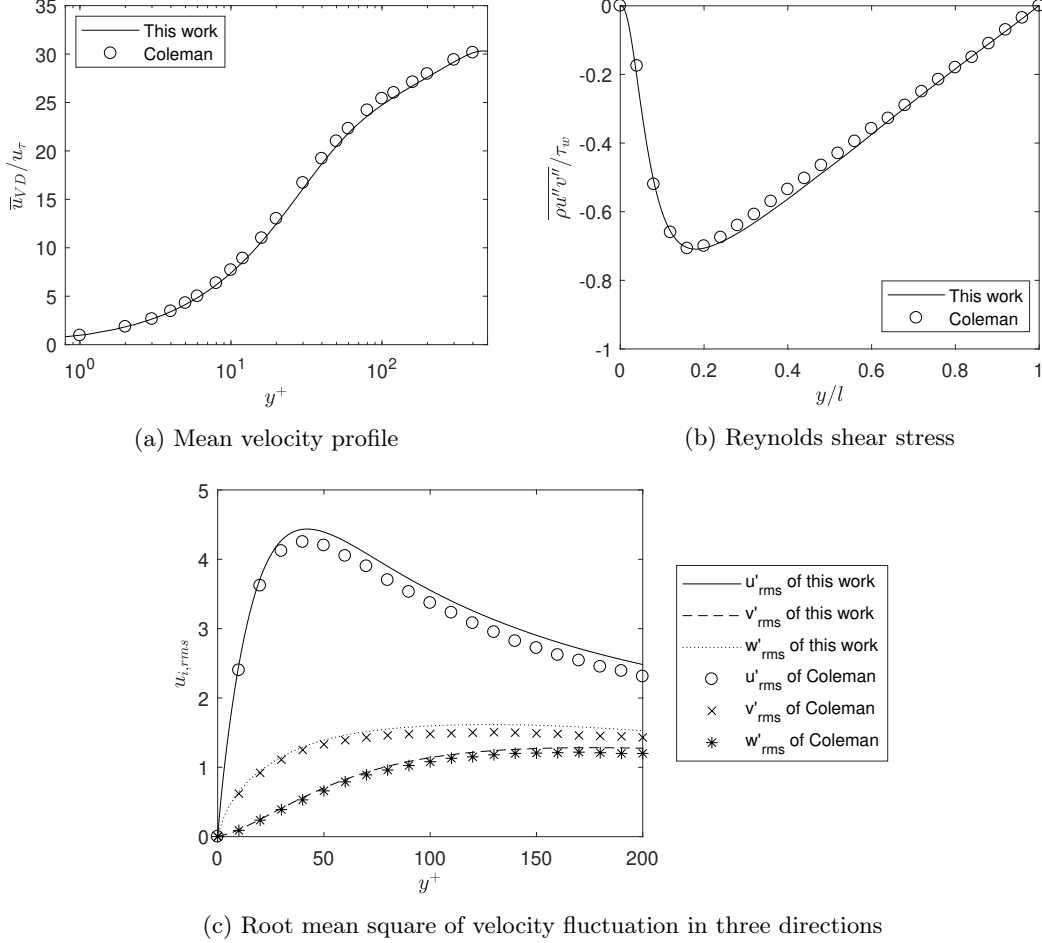


Figure 5.2: Comparison of DNS results of this thesis with the data from Coleman [12].

5.2.2 Cases set up

Three cases of each organic gas (R1233zd(E) and MDM) and one case of air are simulated, the information of which is present in Table 5.2. For R1233zd(E), Cases R1, R2, and R3 are located in the dilute-gas region, near the saturation line, and in the supercritical region respectively (see figure 5.3(a)). The relative temperature and density (T_w/T_{cr} and ρ_B/ρ_{cr}) of cases increase from Case R1 to R3 (shown in Table 5.2). The thermodynamic state (T_w, ρ_B) is defined as the characteristic thermodynamic state of a channel flow, and the point in Figure 5.3 refers to this state. Moreover, in this chapter, the subscript 'G' refers to this state. Cases of MDM are set in the same way (see Figure 5.3(b)), and their T_w/T_{cr} and ρ_B/ρ_{cr} are equal to those of the R1233zd(E) cases

(see table 5.2). Cases R1 and M1 are in the dilute-gas region with $Z_G \approx 1$ (see Table 5.2), so the non-ideal effects are very weak here. Cases R3 and M3 are in the supercritical region with the smallest Z_G , so the non-ideal effects are strongest here. Cases R2 and M2 are set between the other cases with moderate ideal-effects while having the smallest Γ_G . The heat capacity $c_{v,G}/R$ differs significantly between the different gases, which is enhanced by gas molecular weight; while it changes insignificantly between the cases of each organic gas.

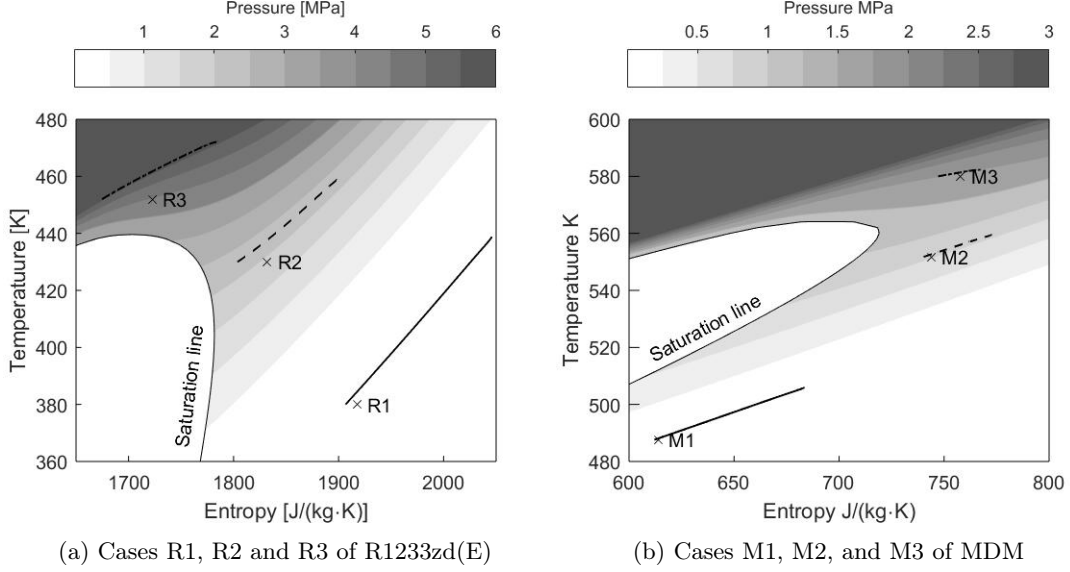


Figure 5.3: Characteristic thermodynamic state of each organic-gas channel flow case in temperature-entropy (T-S) diagram.

The global Reynolds number and Mach number ($Re_G = \rho_B u_B l / \mu_G$ and $Ma_G = u_B / c_G$) are set at 4880 and 2.25 for all cases (see Table 5.2). The distinction between the global Reynolds number and the bulk Reynolds number is discussed here. The bulk Reynolds number ($Re_B = \rho_B u_B l / \tilde{\mu}_w$), which is commonly used in the analysis of ideal-gas flows, is different from Re_G , and the difference between them is magnified by non-ideal effects (see Table 5.2). The bulk Mach number ($Ma_B \equiv u_B / c_w$) is also different from Ma_G , and the difference is enhanced by a lower Γ_G . Other Reynolds numbers and Mach numbers are discussed in Chapter 5.3.2.

The node grid resolutions is $N_x \times N_y \times N_z = 128 \times 257 \times 128$ for all cases. The spatial resolutions in three directions ($(\Delta x / \eta)_{max}$, $(\Delta y / \eta)_{max}$ and $(\Delta z / \eta)_{max}$) are shown in Table 5.2, where Δx , Δy and Δz are the distance between neighbour grid nodes in three directions. η is the smallest length scale equal to the Kolmogorov length scale ($\eta_k \equiv \bar{\rho}^{-3/4} \cdot \bar{\mu}^{3/4} \cdot \varepsilon^{-1/4}$) if $Pr < 1$, and equal to $\eta \approx \eta_k / \sqrt{Pr}$ if $Pr > 1$ [273]. In all cases, spatial resolutions are at the same level as in the works of Zonta [274], Lee [275] and Sciacovelli [139], which means that the spatial resolution is small enough. The grid spacing in wall-normal direction is reduced near channel wall to achieve good

Case	AIR	R1	R2	R3	M1	M2	M3
Gas	Air	R1233zd(E)			MDM		
T_w/T_{cr}	-	0.86	0.98	1.03	0.86	0.98	1.03
ρ_B/ρ_{cr}	-	0.02	0.27	1.00	0.02	0.27	1.00
Z_G	1	0.96	0.67	0.32	0.96	0.68	0.33
Γ_G	1.2	1.01	0.82	1.90	0.97	0.59	1.62
$c_{v,G}/R$	2.5	13.4	15.7	17.3	53.1	58.3	61.9
Re_G	4880	4880	4880	4880	4880	4880	4880
Ma_G	2.25	2.25	2.25	2.25	2.25	2.25	2.25
Re_B	4880	4881	4530	2683	4881	4836	4175
Ma_B	2.25	2.26	2.52	1.26	2.25	2.32	2.09
$(\Delta x/\eta)_{max}$	12.6	9.9	11.1	14.3	9.4	9.4	10.6
$(\Delta y/\eta)_{max}$	0.8	1.0	1.1	1.9	1.1	1.1	1.3
$(\Delta z/\eta)_{max}$	6.3	5.0	5.6	7.1	4.7	4.7	5.3
y_w^+	0.46	0.36	0.36	0.24	0.33	0.34	0.31
$N_{y^+ < 10}$	16	20	20	27	21	21	23

Table 5.2: Set-up information for DNS cases.

resolution. y^+ of the first grid layer from the wall is less than 1 (see Table 5.2), and the number of grid layers within $y^+ < 10$ is greater than 16 for all cases (see Table 5.2). Here $y^+ \equiv \bar{\rho}_w u_\tau y_{wall} / \bar{\mu}_w$ is the distance from wall y_{wall} normalised by the mean density $\bar{\rho}_w$, mean viscosity $\bar{\mu}_w$ and wall friction velocity $u_\tau \equiv \sqrt{\tau_w / \bar{\rho}_w}$, where wall shear stress τ_w is defined as $\tau_w \equiv [\mu(\partial u / \partial y)]_w$.

The number of nodes in the grid has a great impact on the computation time, which makes it difficult to check the grid independence in DNS method. In this chapter, the grid independence is checked in the following way: If no significant change is found after doubling the element number in streamwise (X-) or spanwise (Z-) direction, the simulation result is considered as independent of the grid. The grid independence in Y- direction is not necessary to be checked, since the y^+ on the first grid is small enough and the grid numbers within $y^+ < 10$ is large enough. Table 5.3 shows the grid information of original grid together with refined grids. The distributions of the mean streamwise velocity and Reynolds shear stress is compared between the grids, and the comparison result in Case AIR, R3 and M3 are shown in Figure 5.4. To note, $\bar{u}_{TL}$ refers to the mean velocity after Trettel & Larsson transformation [11], which will be introduced later in Chapter 5.3.3. The

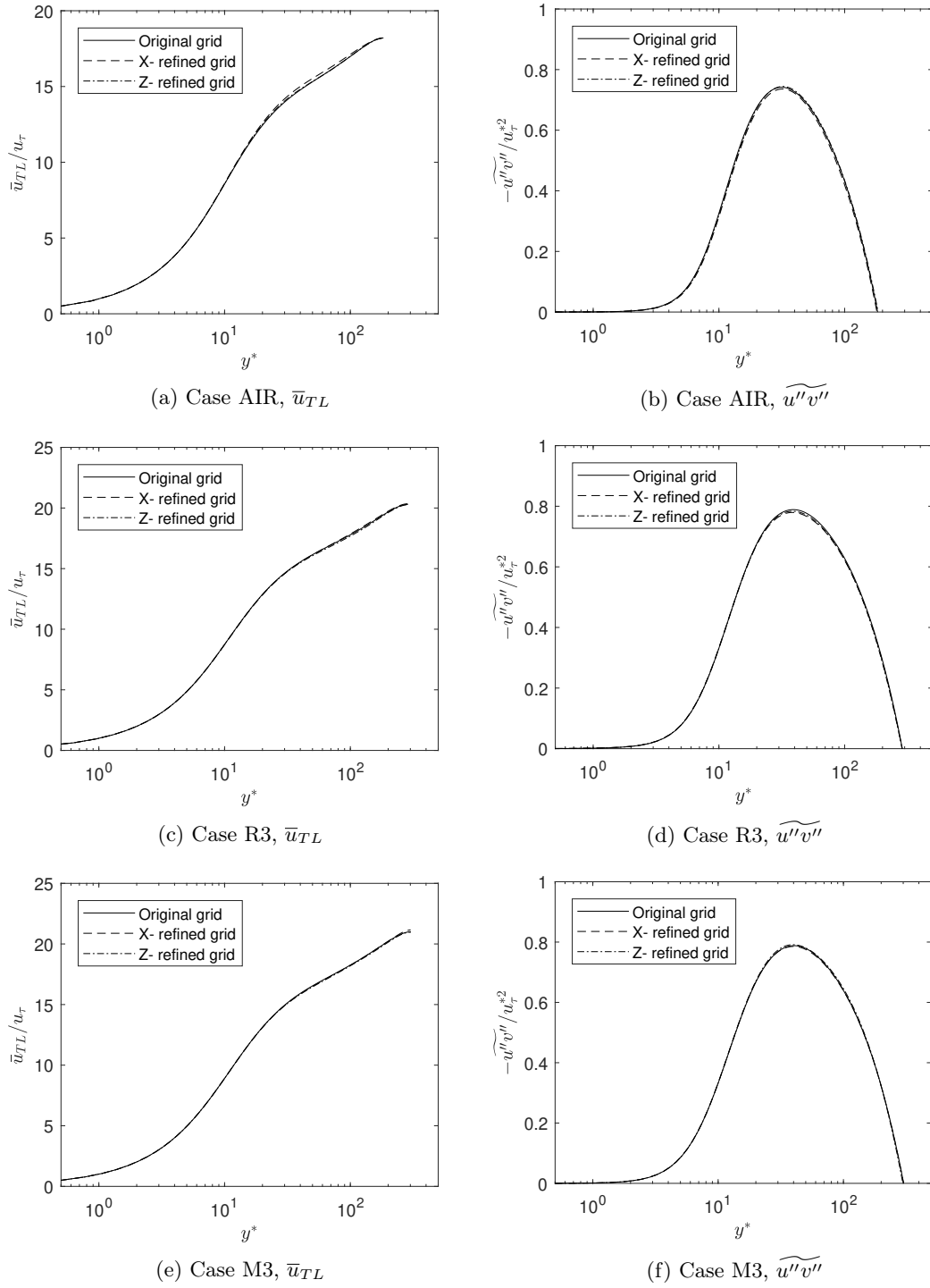


Figure 5.4: Comparison of simulation results using different grids.

impact of grid on the mean streamwise velocity is less than 1% for all cases, and on peak value of Reynolds shear stress is less than 2%. This supports that the original grid is fine enough, and the DNS result is independent of grid size.

In this chapter, the line styles for each DNS case in following figures are shown in Table 5.4.

Grid	X-	Y-	Z-
Original grid	128	257	128
X- refined grid	256	257	128
Z- refined grid	128	257	256

Table 5.3: Information of grid size for grid independence.

The black line refers to air, red lines refer to R1233zd(E) and blue lines refer to MDM; solid lines refers to weak non-ideal effects, dash lines refers to moderate non-ideal effects, and dash-dotted lines refer to strong non-ideal effects.

Case	AIR	R1	R2	R3	M1	M2	M3
Line style	————	————	- - - -	- . - . -	————	- - - -	- . - . -
	(black)	(red)	(red)	(red)	(blue)	(blue)	(blue)

Table 5.4: Line styles for each DNS channel flow case.

The two-point self-correlations of u is defined as follows:

$$R_{uu}(\Delta r) = \frac{\overline{u'_r u'_{r+\Delta r}}}{\overline{u'^2}}, \quad (5.3)$$

where Δr is the distance between the two points. Figure 5.5 shows the R_{uu} on a near-wall plane ($y_{wall}/l = 0.04$) and the channel central plane ($y_{wall}/l = 1$). Figure 5.5 (a) and (b) show that R_{uu} reduced to a low level as the distance between two points increases (on both two planes), which shows that u at two points is nearly uncorrelated. It means the length of the simulation domain in X- direction is long enough [12, 276]. For the same reason, Figure 5.5 (c) and (d) show that the length of the simulation domain in Z- direction is long enough.

The Fourier spectra of streamwise velocity u is given as follows:

$$E_{uu}(k_r \Delta r) = 1 + 2 \sum_{k_r=1}^{N_r/2} R_{uu}(k_r \Delta r) \cos\left(\frac{2\pi n k_r}{N_r}\right), \quad n = 0, 1, \dots, N_r/2. \quad (5.4)$$

It is calculated from the profile of R_{uu} . Figure 5.6 shows E_{uu} on the two planes ($y_{wall}/l = 0.04$ and 1), where k_1 and k_3 are the wavenumbers in X- and Z- directions. Figure 5.6 (a) and (b) show that E_{uu} in X-direction decrease by at least four orders from the largest wavenumber to the smallest wavenumber. This reduction in the Fourier spectra is comparable to that in the DNS cases of Coleman [12] and Morinishi [276], suggesting that the grid resolution in X- direction is

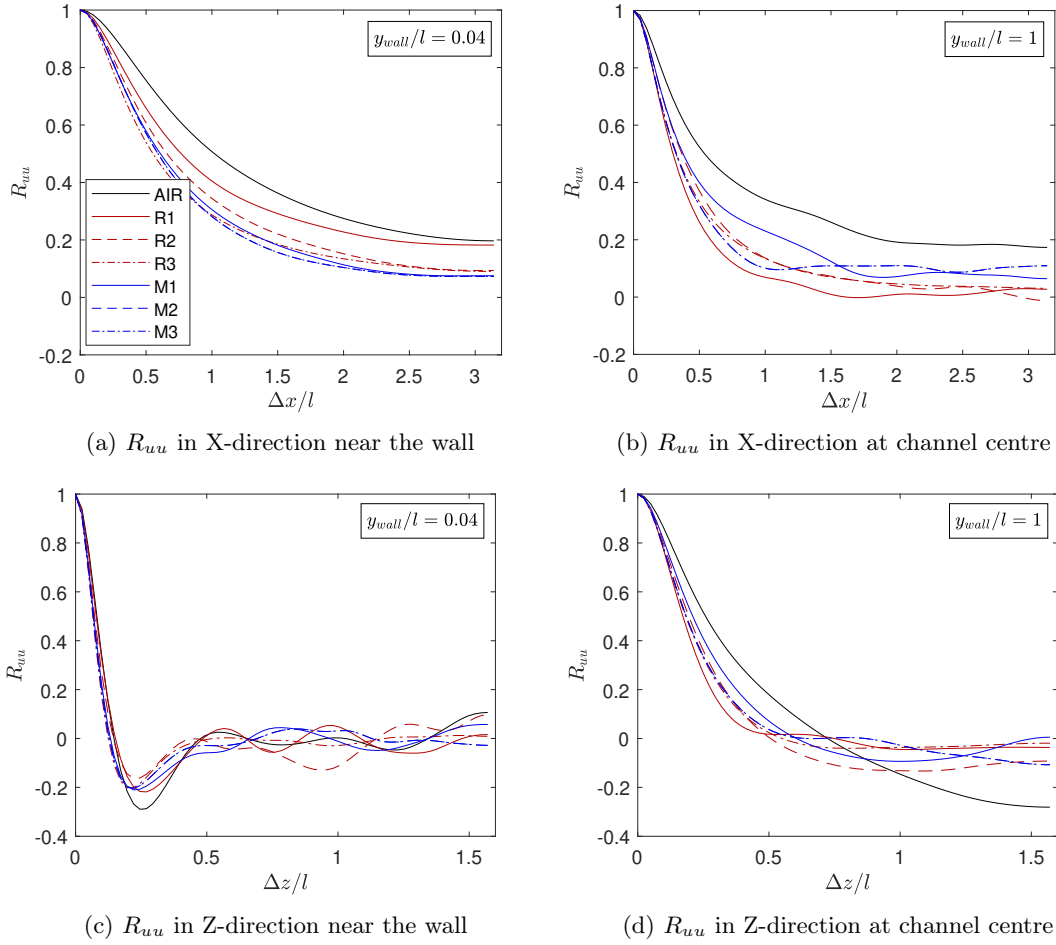


Figure 5.5: Two-point self-correlations of streamwise velocity in two directions on two X-Z planes. The meanings of line styles, see Table 5.4

sufficient to catch the details in turbulent flows. The grid resolution in Z- direction can also be concluded from Figure 5.6 (c) and (d) for the same reason.

5.3 Behaviour of mean flow field

5.3.1 Distributions of mean thermodynamic properties

Figure 5.7 shows the distributions of mean temperature, density, and pressure normalised by their values on the wall. In Figure 5.7(a), the mean temperature increases from the wall to the channel centre in all cases, but the ranges of increase are different. To compare the temperature rises quantitatively, the values of $\tilde{T}_c/T_w$ are listed in Table 5.5. $\tilde{T}_c/T_w$ is smallest in the gas with more complex molecules, MDM (blue lines), and smallest in the case with the strongest non-ideal effects in each gas (dash-dotted lines). This means both the molecular-complexity effects and non-ideal effects reduce the temperature rise. This temperature rise is found related to Ecker number

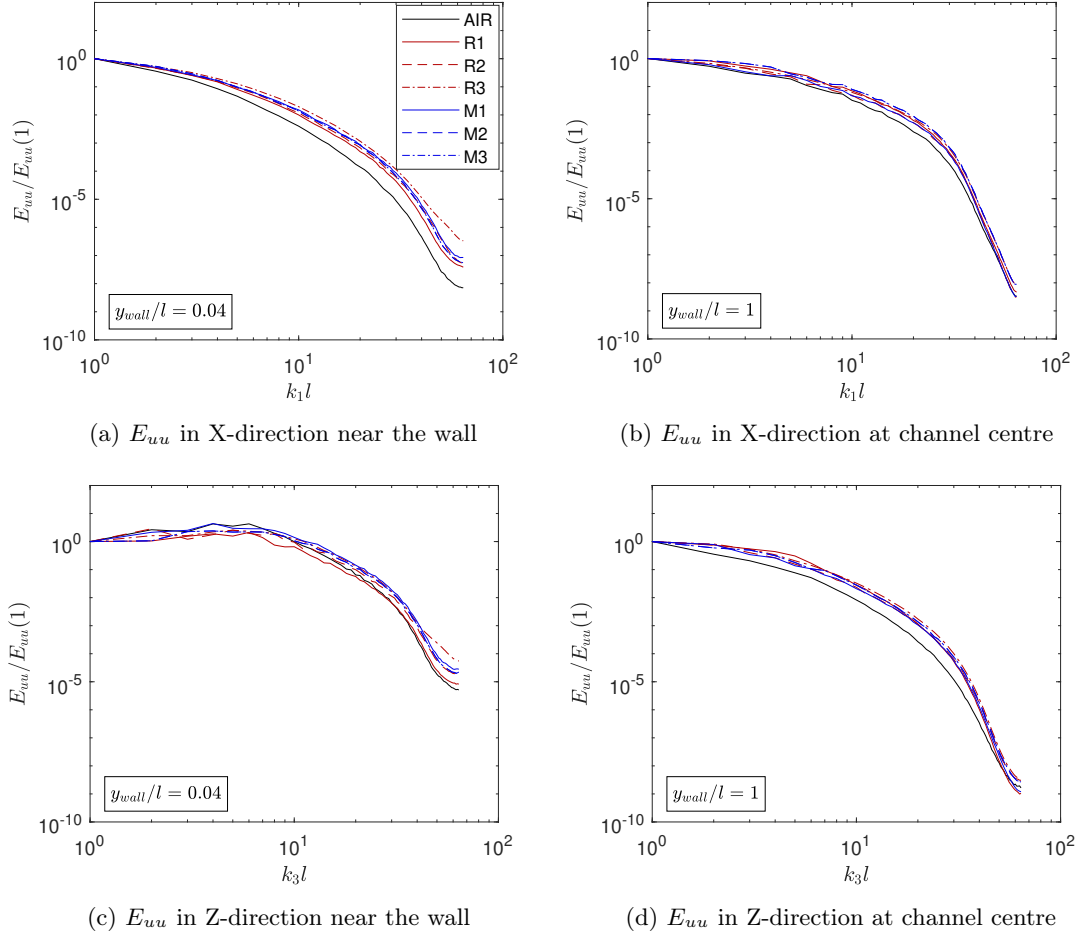


Figure 5.6: One-dimensional Fourier spectra of streamwise velocity, E_{uu} , in two directions on two X-Z planes.

$Ec \equiv a^2/c_p T$ by Sciacovelli [139], while in this chapter it is also found related to Prandtl number.

To explain this, the following explanation is given.

The total thermal conduction rate consists of two parts, molecular thermal conduction and turbulent thermal conduction:

$$q_{tot}(y_{wall}) = q_\lambda + q_t, \quad (5.5)$$

where $q_\lambda \equiv \overline{\lambda \frac{\partial T}{\partial y}}$. Huang [134] found that the total thermal conduction rate has a nearly linear relationship with wall distance,

$$q_{tot}(y_{wall}) = q_w + \frac{\tau_w}{\rho_B l} \int_0^y \tilde{\rho} \tilde{u} dy \approx q_w \left(1 - \frac{y_{wall}}{l}\right). \quad (5.6)$$

If a ratio is defined as $f_q \equiv q_\lambda/q_{tot}$, the mean temperature gradient can be derived to:

$$\frac{d\tilde{T}}{dy} \approx \frac{1}{\lambda} \overline{\lambda \frac{\partial T}{\partial y}} = \frac{1}{\lambda} f_q q_w \left(1 - \frac{y_{wall}}{l}\right). \quad (5.7)$$

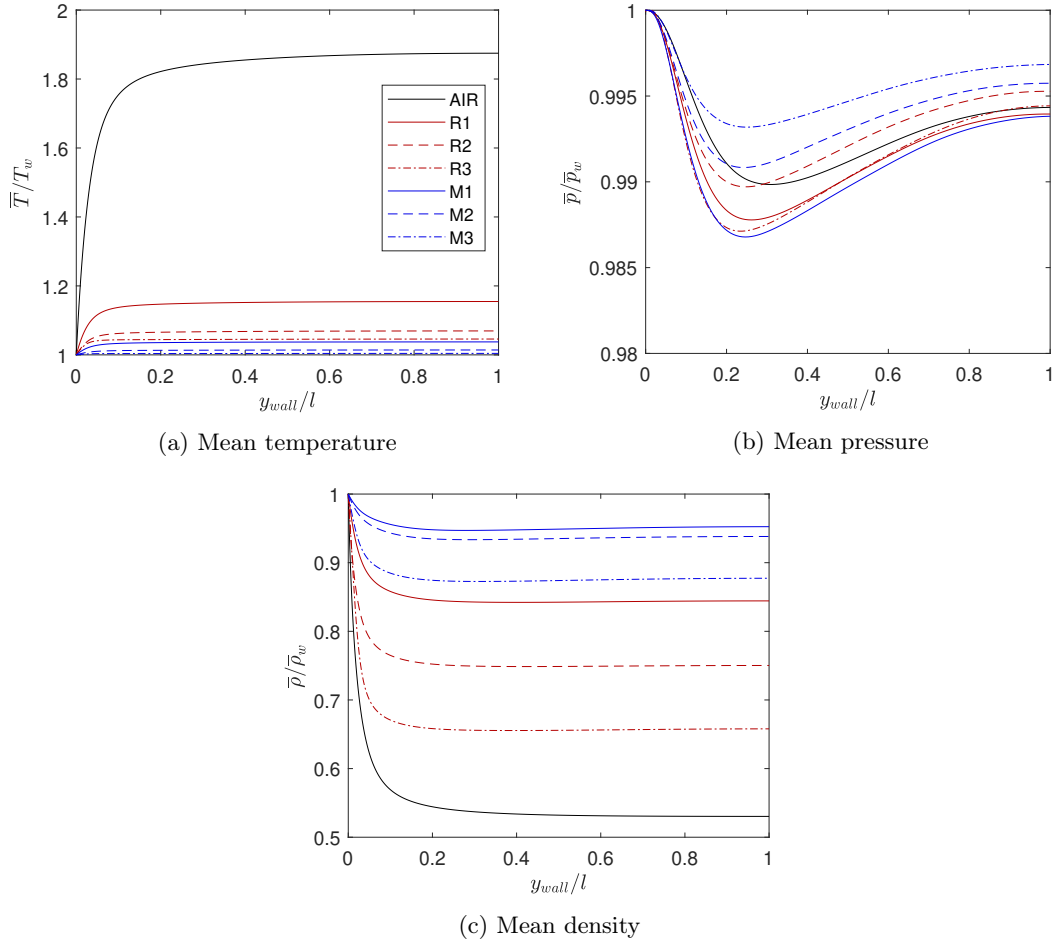


Figure 5.7: Distribution of mean temperature, pressure and density normalised by their values on the wall. The meanings of line styles, see Table 5.4

Then the normalised temperature gradient $\widehat{\frac{dT}{dy}} \equiv \frac{d\tilde{T}}{dy} / \frac{T_w}{l}$ can be derived as:

$$\widehat{\frac{dT}{dy}} \approx \frac{\rho_B u_B^3}{\frac{\lambda T_w}{l}} f_q \left(1 - \frac{y_{wall}}{l}\right) = Re_G M_G^2 Pr_G Ec_G \frac{\lambda_G}{\lambda} f_q \left(1 - \frac{y_{wall}}{l}\right). \quad (5.8)$$

Assuming that the profile of the thermal conduction ratio $f_q(y_{wall})$ is the same in all cases and $\frac{\lambda_G}{\lambda}$ is approximately equal to 1, the central-to-wall temperature ratio, T_c/T_w , can be obtained by integrating Equation 5.8 and represented as follows:

$$T_c/T_w = 1 + \int_0^1 \frac{d\widehat{T}}{d(y/l)} d(y/l) \propto Re_G M_G^2 Pr_G Ec_G. \quad (5.9)$$

In this chapter, Re_G and Ma_G is the same in all cases, so T_c/T_w is proportional to $Pr_G Ec_G$ as indicated above. If only the impact of Ec_G is considered, it can not explain that $\widehat{T}/T_w$ is lower in Case M1 than in Case R3. The values of Pr_G and Ec_G are listed in Table 5.5, where the case with

smaller $Pr_G Ec_G$ always has a smaller T_c/T_w . Pr_G is largest in the cases with strong non-ideal effects (Cases R3 and M3), and Ec_G is smallest in the gas with more complex molecules (MDM) and in the cases with the strongest non-ideal effects.

Case	AIR	R1	R2	R3	M1	M2	M3
Gas	Air	R1233zd(E)			MDM		
$\tilde{T}_c/T_w$	1.875	1.155	1.069	1.045	1.038	1.014	1.004
$Pr_G Ec_G$	0.28	0.055	0.025	0.018	0.013	0.005	0.002
Pr_G	0.7	0.81	1.02	4.77	0.73	0.67	1.41
Ec_G	0.4	0.069	0.025	0.004	0.017	0.007	0.001
$\bar{\rho}_c/\bar{\rho}_w$	0.53	0.85	0.75	0.66	0.95	0.93	0.88
$-\widehat{\left(\frac{\partial \rho}{\partial T}\right)}_{p,G}$	1	1.1	3.9	31.4	1.1	3.9	33.3

Table 5.5: Important parameters of channel flows.

Figure 5.7(b) shows that the mean pressure decreases and then increases from the wall to channel centre, and the maximum pressure drop is less than 1.5% in all cases. Therefore, it can be considered as nearly constant in the analysis of the mean flow field.

The mean density decreases from the wall in all cases (see Figure 5.7(c)). This density drop is smallest in the gas with more complex molecules, MDM (blue lines), and largest when non-ideal effects are strong (Cases R3 and M3, dash-dotted lines). In other words, molecular-complexity effects increase the density ratio, $\bar{\rho}_c/\bar{\rho}_w$, and non-ideal effects decrease it (see Table 5.5). To explain this change, the relationship between the temperature rise and the density drop is analysed as follows. Based on the assumption of constant mean pressure, the density gradient has a relationship with the temperature gradient:

$$\frac{\partial \bar{\rho}}{\partial y} \approx \left(\frac{\partial \rho}{\partial T} \right)_p \frac{\partial \bar{T}}{\partial y}. \quad (5.10)$$

The derivative $\left(\frac{\partial \rho}{\partial T} \right)_p$ is always negative, so the distribution of the mean density is opposite to that of the mean temperature. After normalisation, the normalised derivative is shown as $\widehat{\left(\frac{\partial \rho}{\partial T} \right)}_p = \left(\frac{\partial \rho}{\partial T} \right)_p / \left(\frac{\rho}{T} \right)$, and its absolute value is equal to 1 under the ideal-gas law, so a smaller density drop is always found in the case with a smaller temperature rise. This is the truth for Case AIR, R1 and M1. However, when non-ideal effects become stronger, the absolute value of $\widehat{\left(\frac{\partial \rho}{\partial T} \right)}_p$ increases significantly (see Table 5.5). Therefore even the temperature increase is smaller, the density drop can be larger. For example, in Case R3, the temperature rise is smaller than in Case R1, but the density drop is larger (see the red solid line and red dash-dotted line in

Figure 5.7(a) and (c)).

As for the other gas properties, the speed of sound $\bar{c}$ is proportional to the square root of temperature in Case AIR, R1 and M1, where non-ideal effects are insignificant. Therefore, $\bar{c}$ increases from the wall (see solid lines in Figure 5.8(a)), and this increase is smaller in the gas with more complex molecules, just like the temperature rise. However, when non-ideal effects become stronger, this relationship is no longer maintained, so the $\bar{c}$ distribution is different from the temperature distribution. For any organic gas, the increase in $\bar{c}$ is larger in cases with moderate non-ideal effects (Case R2 and M2, see red and blue dash lines in Figure 5.8(a)), but $\bar{c}$ decreases from the wall in cases with strong non-ideal effects (Case R3 and M3, see red and blue dash-dotted lines in Figure 5.8(a)). This impact of non-ideal effects on $\bar{c}$ distribution is more evident in a gas with moderate molecular complexity, R1233zd(E).

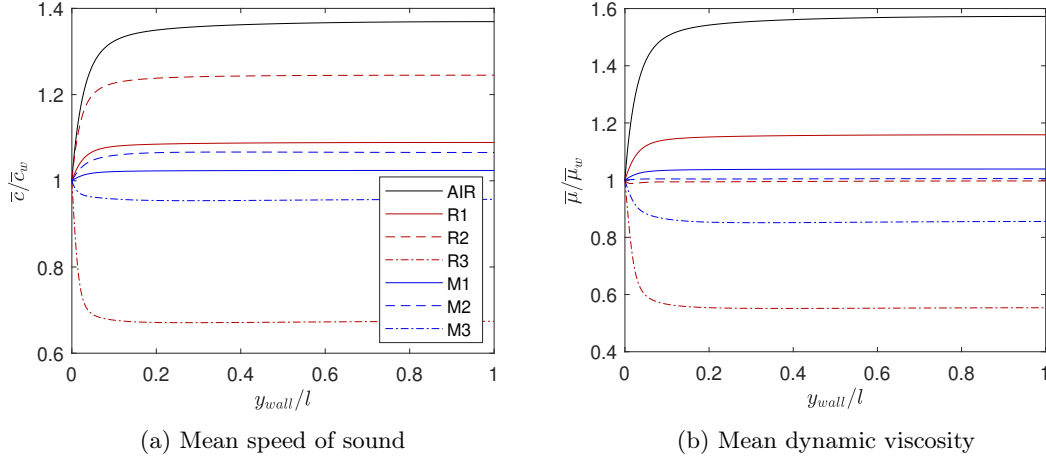


Figure 5.8: Distribution of the mean speed of sound and mean dynamic viscosity, normalised by their values on the wall.

Figure 5.8(b) shows that profiles of $\bar{\mu}$ follows the same trend as those of temperature when non-ideal effects are weak (in Case AIR, R1 and M1, see solid lines). As non-ideal effects increase in each gas, the viscosity rise is reduced and even reversed (see Case R3 and M3, dash-dotted lines in Figure 5.8(b)). The feature that the viscosity decreases from channel wall to centre was also found by Sciacovelli [139] in channel flows of another organic gas, PP11, in the supercritical region. This feature is considered as a ‘liquid-like’ behaviour [139], since it is normally observed in liquid channel flows. By contrast, the reversed feature is considered as a ‘gas-like’ behaviour. The results of this chapter suggest that the non-ideal effects rather than molecular-complexity effects reverse the viscosity distribution from a ‘gas-like’ behaviour to a ‘liquid-like’ behaviour.

In summary, the mean temperature rise (from the wall to channel centre) is smaller in gases with stronger molecular-complexity effects and also smaller in the cases with strong non-ideal

effects, which is due to a smaller product of Prandtl number and Eckert number $Pr_G Ec_G$; the mean density drop is smaller in gases with stronger molecular-complexity effects but larger in the cases with weak non-ideal effects, which is associated with a larger thermal derivative $-\left(\frac{\partial \rho}{\partial T}\right)_p$. The trends of $\bar{c}$ and $\bar{\mu}$ distributions are the same as that of the temperature distribution when non-ideal effects are weak, and they reverse when non-ideal effects are strong, resulting in a ‘liquid-like’ behaviour. The impact of non-ideal effects on all the properties discussed is more significant in R1233zd(E) (moderate molecular-complexity effects) than in MDM (strong molecular-complexity).

5.3.2 Reynolds numbers and Mach numbers

Although the global Reynolds number and Mach number are the same for all cases, other Reynolds and Mach numbers for analysing boundary layers can differ between different cases due to the variable density, viscosity and the speed of sound. Here two commonly-used Reynolds numbers and two Mach numbers are discussed.

The distributions of semi-local Reynolds number ($Re_G^* = \rho_B u_B l / \bar{\mu}$) and semi-local viscous Reynolds number ($Re_\tau^* \equiv l / \delta_v^* = \bar{\rho} u_\tau^* l / \bar{\mu}$) are shown in Figure 5.9(a) and (b), where $u_\tau^* \equiv \sqrt{\tau_w / \bar{\rho}}$ is the semi-local wall friction velocity. In air flow, both Reynolds numbers drop significantly from the wall, while this is not always the case in non-ideal-gas flows. Molecular-complexity effects make the profiles of two Reynolds numbers ‘flatter’ (see Case M1, solid blue line in Figure 5.9(a) and (b)), and non-ideal effects can reverse their distributions from decreasing to increasing (see Cases R3 and M3, dash-dotted lines in in Figure 5.9(a) and (b)). This feature is due to the ‘liquid-like’ behaviour of the $\bar{\mu}$ distribution caused by strong non-ideal effects.

Figure 5.9(c) and (d) show the distributions of semi-local Mach number ($Ma_G^* \equiv u_B / \bar{c}$) and mean Mach number ($\overline{Ma} \equiv \overline{u/c}$). Near the channel centre ($y_{wall}/l = 1$), Ma_G^* differs significantly between cases, even Ma_G is the same in all cases at 2.25 (see Figure 5.9(c)). The difference of Ma_G^* from 2.25 is smaller in the gas with stronger molecular-complexity effects (MDM cases, blue lines) and larger when non-ideal effects are strong (Case R3 and M3, dash-dotted lines). This difference is also evident in the distribution of local mean Mach number, $\overline{Ma} \equiv \overline{u/c}$, near the channel centre (see Figure 5.9(d)), while in all cases $\overline{Ma}$ rapidly increases to 1 within the region $y_{wall}/l < 0.1$.

To summarise, despite the same global Reynolds number and Mach number of all cases, both molecular-complexity effects and non-ideal effects quantitatively affect the distributions of these four dimensionless numbers (Re_G^* , Re_τ^* , Ma_G^* and $\overline{Ma}$), while non-ideal effects can even reverse the trends of the distributions of Re_G^* , Re_τ^* and Ma_G^* .

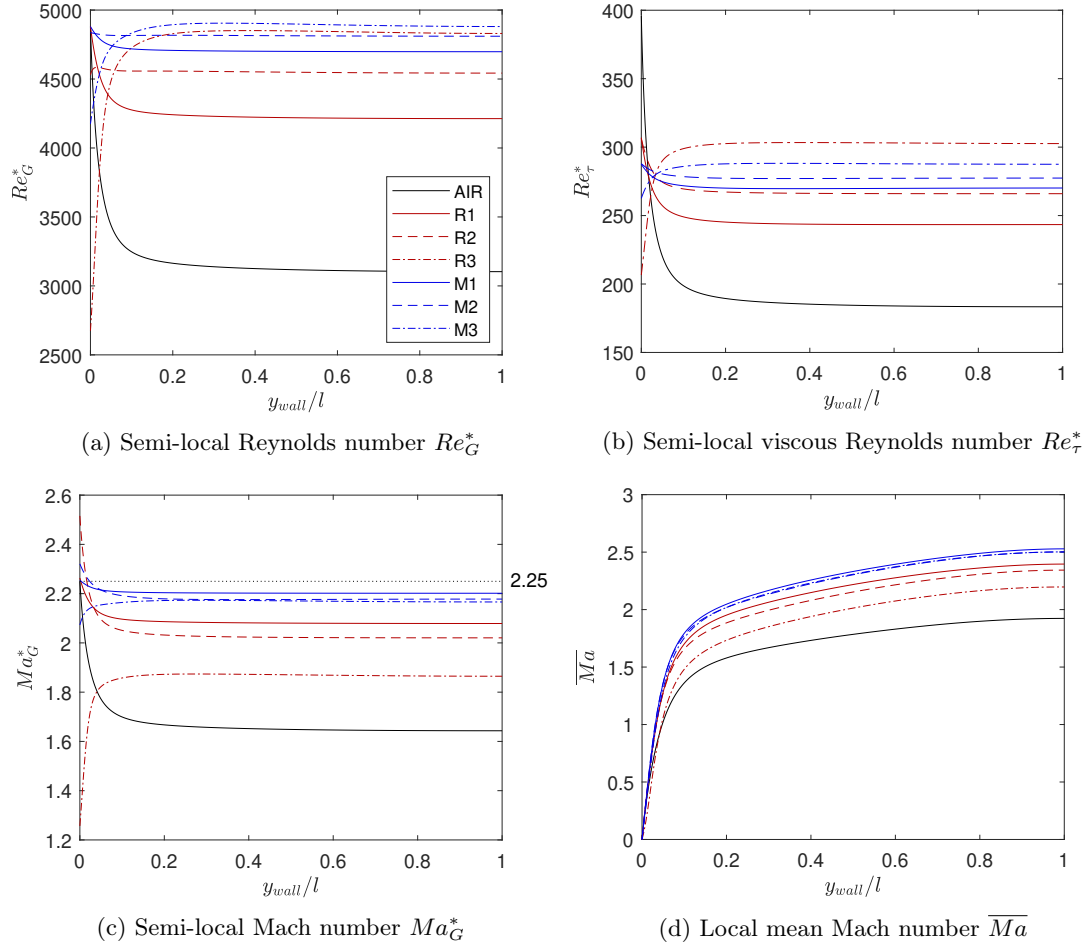


Figure 5.9: Distribution of Reynolds numbers and Mach numbers.

5.3.3 Mean streamwise velocity distribution

Van Driest [128] proposed a velocity transformation,

$$\bar{u}_{VD} = \int_0^{\tilde{u}} \left(\frac{\bar{\rho}}{\bar{\rho}_w} \right)^{\frac{1}{2}} d\tilde{u}, \quad (5.11)$$

which makes the log law still valid in compressible boundary layers. The mean streamwise velocity distributions after the Van Driest (VD) transformation are shown in Figure 5.10(a), where the abscissa is the wall distance normalised by the wall viscous length scale: $y^+ = y_{wall}/\delta_{v,w} = \bar{\rho}_w u_\tau y_{wall}/\bar{\mu}_w$. Figure 5.10(a) shows that the log law is still evident in dense vapours, but the velocity profile in the buffer region is different between cases, so the log-law region starts at different y^+ . For example, the log-law region starts early in Case R3 (at $y^+ \approx 30$) and late in Case AIR (at $y^+ \approx 80$). This difference is due to the different viscosity distributions mentioned in Chapter 5.3.1, that $\bar{\mu}$ decreases from the wall in Case R3 but increases from the wall in Case AIR

(see Figure 5.8(b) in Chapter 5.3.1). The difference in the $\bar{\mu}$ distribution cannot be considered in the VD transformation.

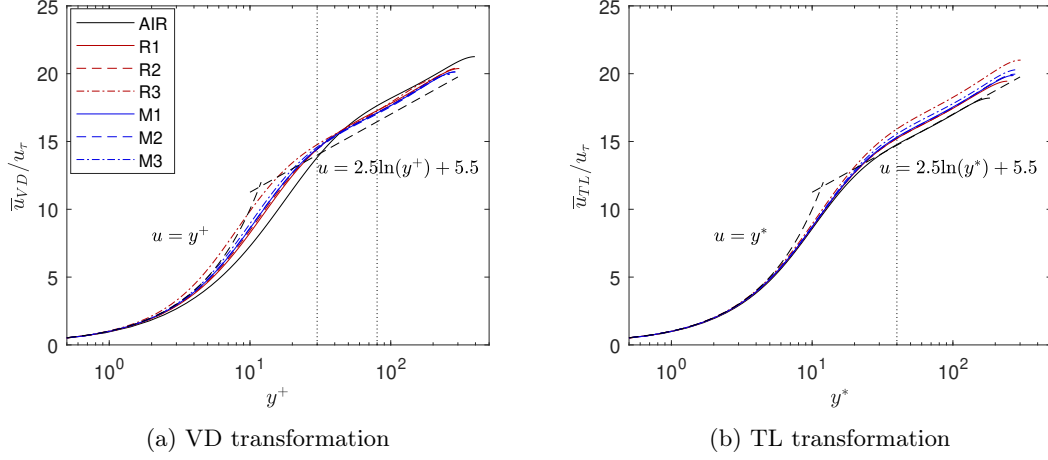


Figure 5.10: Velocity profile in channel flow after transformation.

The wall distance normalised by the semi-local viscous length scale, $y^* = y_{wall}/\delta_v^* = \bar{\rho}u_\tau^*y_{wall}/\bar{\mu}$, and Trettel & Larsson (TL) transformation [11],

$$\bar{u}_{TL} = \int_0^{\tilde{u}} \left(\frac{\bar{\rho}}{\bar{\rho}_w} \right)^{\frac{1}{2}} \left(1 + \frac{1}{2} \frac{1}{\bar{\rho}} \frac{d\bar{\rho}}{dy} y - \frac{1}{\bar{\mu}} \frac{d\bar{\mu}}{dy} y \right) d\tilde{u}, \quad (5.12)$$

are used to account for the impact of variable viscosity. Figure 5.10(b) shows that the profiles of the mean velocity after the TL transformation are almost the same for all cases in the viscous sublayer and buffer region, and they are slightly different in the log-law region. In this way, the log-law region starts at nearly the same wall distance $y^* \approx 40$ in all cases. This means that the influence of molecular-complexity effects and non-ideal effects on the mean streamwise velocity distribution is insignificant when the variations in both mean density and viscosity are considered by TL transformation and y^* . It suggests that a wall function based on y^* instead of y^+ and the TL transformation instead of VD transformation is more appropriate in RANS simulations for wall-bounded turbulent flows with dense vapours, and that the value of y^* instead of y^+ on the first grid layer should be considered in RANS simulations.

5.3.4 Walz's equation

Walz's equation [130] is usually known as the relation between mean velocity and mean temperature:

$$\frac{\tilde{T}}{\tilde{T}_\delta} = 1 + \frac{\tilde{T}_r - \tilde{T}_w}{\tilde{T}_\delta} \left(\frac{\tilde{u}}{\tilde{u}_\delta} - 1 \right) + r \frac{\gamma - 1}{2} \overline{Ma}_\delta^2 \left[1 - \left(\frac{\tilde{u}}{\tilde{u}_\delta} \right)^2 \right], \quad (5.13)$$

where subscript δ refers to the boundary layer edge, $\tilde{T}_r$ is the recovery temperature, and r is the recovery factor. Voisinet [131] have validated Walz's equation in air by comparing it with experimental data of flat-plate flows under conditions $Ma = 4.9$ and $T_w/T_r = 1.0, 0.8$, and 0.25 . The recovery factor used in their work is $r = 0.89$. While this equation is based on the assumption of an ideal gas, $dh = c_p dT$, and it is not applicable to non-ideal gases. In non-ideal gases, the differential of enthalpy dh depends not only on the differential of temperature dT but also on the differential of pressure dp :

$$dh = c_p dT + \left(\frac{\partial h}{\partial p} \right)_T dp. \quad (5.14)$$

The second term on the right-hand side of Equation 5.14 is a non-ideal term, where $\left(\frac{\partial h}{\partial p} \right)_T$ is not zero in non-ideal gases (see Figure 5.11(a)). This non-ideal term makes that $\frac{\partial \tilde{h}}{\partial y}$ can not be represent by $\bar{c}_p \frac{\partial \tilde{T}}{\partial y}$, since the ratio $\bar{c}_p \frac{\partial \tilde{T}}{\partial y} / \frac{\partial \tilde{h}}{\partial y}$ is far from 1 (see Case R3 and M3 in Figure 5.11(b)). Consequently, the expression of Walz's equation in terms of enthalpy [130] should be used in non-ideal-gas flows, as shown here:

$$\frac{\tilde{h}}{\tilde{h}_\delta} = 1 + \frac{\tilde{h}_r - \tilde{h}_w}{\tilde{h}_\delta} \left(\frac{\tilde{u}}{\tilde{u}_\delta} - 1 \right) + r \frac{\tilde{u}_\delta^2}{2\tilde{h}_\delta} \left[1 - \left(\frac{\tilde{u}}{\tilde{u}_\delta} \right)^2 \right], \quad (5.15)$$

where $\tilde{h}_r \equiv \tilde{h}_\delta + r \frac{\tilde{u}_\delta^2}{2}$ is the recovery enthalpy.

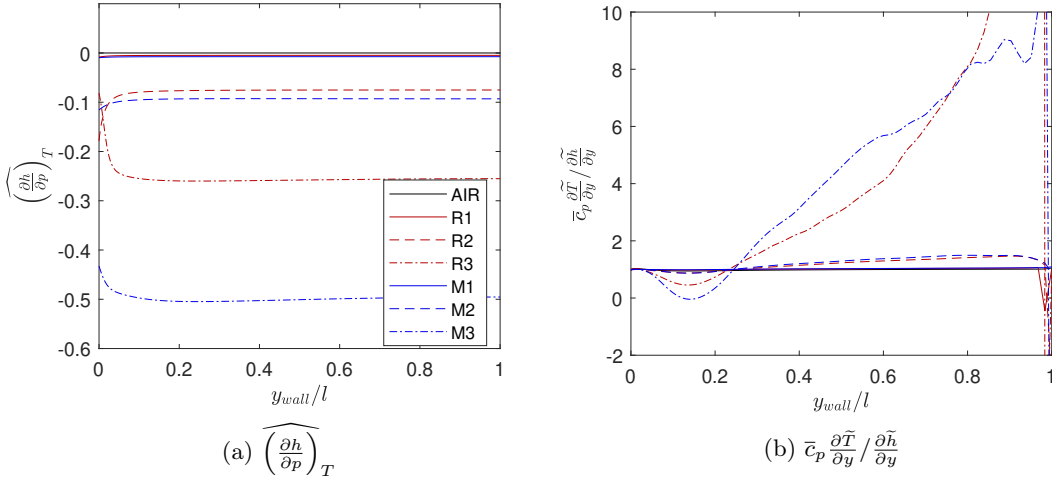


Figure 5.11: (a) Normalised thermal derivative $\left(\frac{\partial h}{\partial p} \right)_T \equiv \left(\frac{\partial h}{\partial p} \right)_T / \frac{\tilde{h}}{p}$ and (b) the comparison between the mean temperature gradient and enthalpy gradient $\bar{c}_p \frac{\partial \tilde{T}}{\partial y} / \frac{\partial \tilde{h}}{\partial y}$.

In this chapter, Walz's equation 5.15 is studied in dense vapours, and the deviation of this equation from DNS results is shown in Figure 5.12. To note, the variables at the edge of boundary layers (with subscript δ) in Equation 5.15 are replaced by the variables at channel center (with

subscript c). Figure 5.12 shows that Walz's equation overestimates the enthalpy in Case AIR by about 8%, which agrees with the result of the cold-wall case in the work of Duan [132]. For cases of dense vapours, the overestimation of Walz's equation decreases and even reverses to an underestimation (e.g. in Case R3), and the deviation is within about $\pm 3\%$. It means Walz's equation (written in enthalpy expression) is valid in the dense vapours studied in this chapter, and it can still be used to set boundary conditions in RANS simulations for dense vapours.

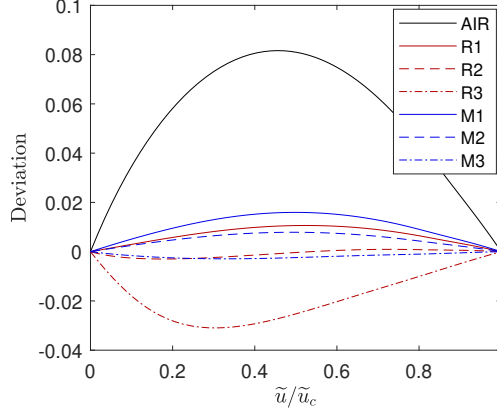


Figure 5.12: Deviation of the Walz's equation 5.15 from DNS results, which is defined as $(\tilde{h}_{Walz} - \tilde{h})/\tilde{h}$.

5.4 Behaviour of turbulent fluctuations

5.4.1 Reynolds shear stress and velocity fluctuation intensities

The distribution of Reynolds shear stress is given in Figure 5.13, where $\widetilde{u''v''}$ is normalised by the square of the semi-local friction velocity, u_τ^{*2} . The abscissa is the semi-local wall distance (y^*) in Figure 5.13(a) and is the wall distance normalised by half channel height (y_{wall}/l) in Figure 5.13(b). The profiles of $\widetilde{u''v''}/u_\tau^{*2}$ almost coincide in the near-wall region ($y^* < 20$) in Figure 5.13(a) and coincide in the outer layer ($y_{wall}/l > 0.3$) in Figure 5.13(b). However, the peak value of $\widetilde{u''v''}/u_\tau^{*2}$ is different in these cases and the location of the peak is also different. It shows that the peak value is larger in the case with a larger maximum y^* (in Figure 5.13(a)), which is the y^* at channel centre. This maximum y^* is also equal to the semi-local viscous Reynolds number at the channel centre, $Re_{\tau,c}^*$, so this difference can be considered as a Reynolds number effect which due to the variation of the mean properties.

Figure 5.14 shows the normalised turbulence fluctuation intensities of three velocity components, where subscript rms refers to root mean square $(\cdot)_{rms} \equiv \sqrt{(\cdot)^2}$, and they are normalised

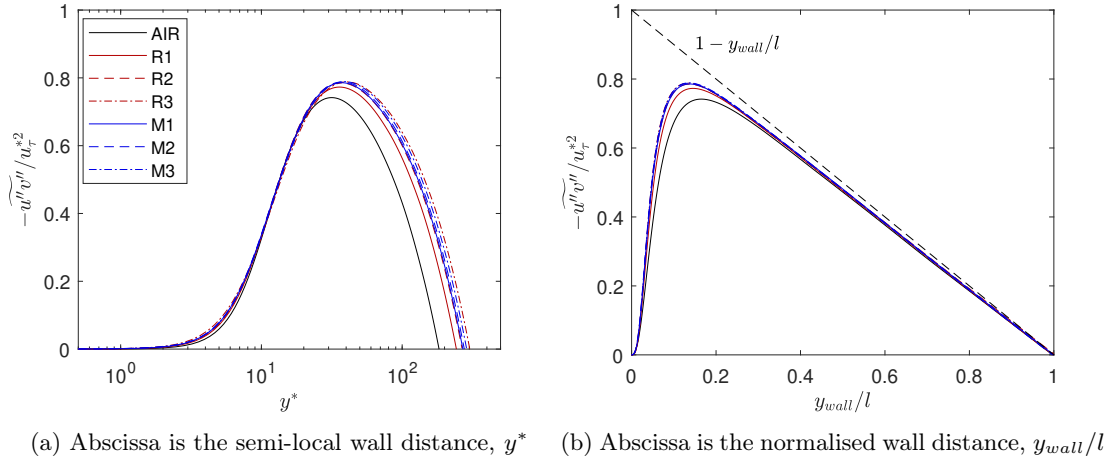


Figure 5.13: The distribution of Reynolds shear stress $\widetilde{u''v''}$ normalised by the square of the semi-local friction velocity u_τ^{*2} . The meanings of line styles, see table 5.4

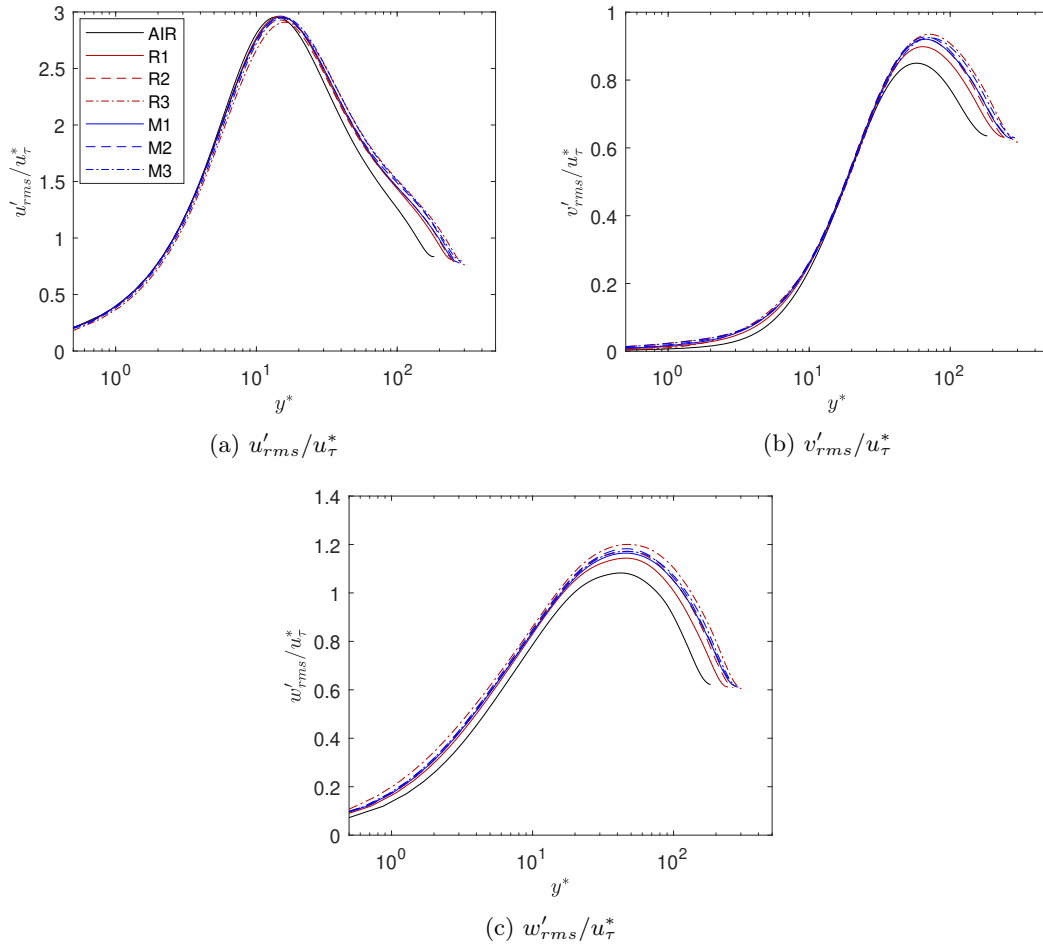


Figure 5.14: Normalised turbulence fluctuation intensity (root mean square) of velocity in three directions.

by u_τ^* . In streamwise direction, u'_{rms}/u_τ^* has nearly the same trend and value in all cases, and the Reynolds effects only slightly differ u'_{rms}/u_τ^* in the channel centre region. While in the other two directions, the peak values of v'_{rms}/u_τ^* and w'_{rms}/u_τ^* are larger in dense-vapour cases, and the locations (y^*) of the peaks are also larger, which is due to the Reynolds effects. To summarise, the profiles of Reynolds shear stress and the root mean square of velocity fluctuations in three directions show the same trend in all cases, but the peak values and their location (y^*), except u'_{rms}/u_τ^* , are affected by the Reynolds number effect which is caused by the variation of the mean properties.

5.4.2 Temperature, pressure and density fluctuation intensities

The fluctuation intensities (the root mean square) of temperature, pressure and density are shown in Figure 5.15(a-c), where are normalised by they local mean value. Gerolymos [272] found that they are of the same order of magnitude in air flows under any Mach number or Reynolds number, but in this chapter this relationship is found not to hold in non-ideal-gas flows. In Figure 5.15(a), the temperature intensity has a peak at about $y^* \approx 10$ in all cases, while the peak value is lower in dense-vapour cases. Both molecular-complexity effects and non-ideal effects reduce $T'_{rms}/\tilde{T}$ significantly, so that $T'_{rms}/\tilde{T}$ is no longer of the same order as $p'_{rms}/\bar{p}$ and $\rho'_{rms}/\bar{\rho}$. Figure 5.15(d) shows the ratio of temperature intensity to pressure intensity $\frac{T'_{rms}}{\tilde{T}}/\frac{p'_{rms}}{\bar{p}}$, which is smaller than 10^{-1} in all MDM cases (blue lines).

Figure 5.15(b) shows that $p'_{rms}/\bar{p}$ has the same trend but different values in all cases. $p'_{rms}/\bar{p}$ remains on a plateau in the inner layer, then it drops after. Even the values of $p'_{rms}/\bar{p}$ vary from case to case, they are of the same order of magnitude.

The distributions of $\rho'_{rms}/\bar{\rho}$ differ significantly between the cases (see Figure 5.15(c)). In Case AIR, the profile has the shape of a ‘bell’ which is similar to the $T'_{rms}/\tilde{T}$ distribution, but this shape can be changed in dense vapours. For MDM cases (blue lines in Figure 5.15(c)), the $\rho'_{rms}/\bar{\rho}$ distribution is no long a ‘bell-shaped’ but resembles the $p'_{rms}/\bar{p}$ profile. For R1233zd(E) cases, the ‘bell shape’ is still present in Case R3, but not in Cases R1 and R2. This means that the relationship between density, pressure and temperature fluctuations in dense vapours is different from that in air. Sciacovelli [139] proposed a relation between T'_{rms} , p'_{rms} and ρ'_{rms} for an organic gas, PP11, shown as follows:

$$\frac{\rho'_{rms}}{\bar{\rho}} \approx \frac{1}{\bar{\rho}} \left[p'_{rms} - \left(\frac{\partial p}{\partial T} \right)_\rho T'_{rms} \right] / \left(\frac{\partial p}{\partial \rho} \right)_T, \quad (5.16)$$

which is validated in their channel flow cases. However, even this equation cannot be applied to

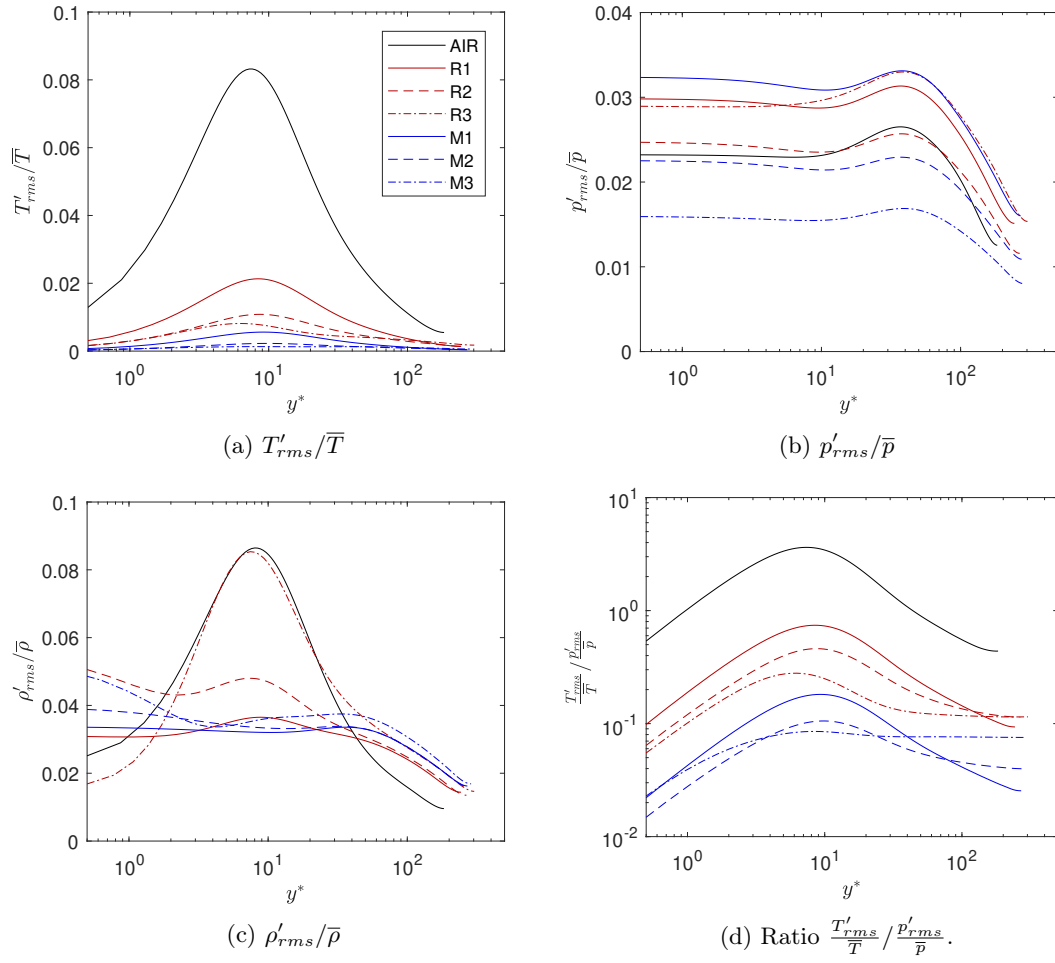


Figure 5.15: Normalised intensities of temperature, pressure and density.

all cases in this chapter (see below). To fill this gap, a new relation is derived.

For non-ideal gases, the relationship between differential pressure, temperature, and density is $dp = \left(\frac{\partial p}{\partial \rho}\right)_T d\rho + \left(\frac{\partial p}{\partial T}\right)_\rho dT$. If the fluctuation of the derivatives $\left(\frac{\partial p}{\partial \rho}\right)_T$ and $\left(\frac{\partial p}{\partial T}\right)_\rho$ are insignificant (assuming a linear relationship), it is able to state the following relation:

$$\frac{p'}{\bar{p}} \approx \left(\widehat{\frac{\partial p}{\partial \rho}}\right)_T \frac{\rho'}{\bar{\rho}} + \left(\widehat{\frac{\partial p}{\partial T}}\right)_\rho \frac{T'}{\bar{T}}, \quad (5.17)$$

where $\left(\widehat{\frac{\partial p}{\partial \rho}}\right)_T \equiv \overline{\left(\frac{\partial p}{\partial \rho}\right)_T} / \left(\frac{\bar{p}}{\bar{\rho}}\right)$ and $\left(\widehat{\frac{\partial p}{\partial T}}\right)_\rho \equiv \overline{\left(\frac{\partial p}{\partial T}\right)_\rho} / \left(\frac{\bar{p}}{\bar{T}}\right)$. Figure 5.16(a) and (b) show the profile of $\left(\widehat{\frac{\partial p}{\partial \rho}}\right)_T$ and $\left(\widehat{\frac{\partial p}{\partial T}}\right)_\rho$. With insignificant non-ideal effects (in Case AIR, R1 and M1) they are almost equal to 1, but in other dense-vapour cases they are far from 1.

Then, a general relationship between T'_{rms} , p'_{rms} and ρ'_{rms} can be established by taking the

root mean square of both sides of Equation 5.17:

$$\frac{p'_{rms}}{\bar{p}} \approx \sqrt{\left[\left(\widehat{\left(\frac{\partial p}{\partial \rho}\right)}_T \frac{\rho'_{rms}}{\bar{\rho}}\right)^2 + \left[\left(\widehat{\left(\frac{\partial p}{\partial T}\right)}_\rho \frac{T'_{rms}}{\bar{T}}\right)^2 + 2\left(\widehat{\left(\frac{\partial p}{\partial \rho}\right)}_T \left(\widehat{\left(\frac{\partial p}{\partial T}\right)}_\rho R_{\rho T} \frac{\rho'_{rms} T'_{rms}}{\bar{\rho} \bar{T}}\right)\right]} \quad (5.18)$$

where $R_{\rho T} \equiv \frac{\overline{\rho' T'}}{\sqrt{\rho'^2} \sqrt{T'^2}}$ is the correlation coefficient between ρ' and T' . The error of this equation is calculated by comparing the term on the right hand side to the term on the left hand side, $(RHS - LHS)/LHS$. Figure 5.17(a) shows that the error is within $\pm 2\%$ for all dense-vapour cases and has a maximum value up to 7.5% in Case AIR. It is considered that the source of error in this relation comes from the assumption of a linear relation between T' , p' and ρ' in Equation 5.17. This error is much smaller than the error in Equation 5.16 (see Figure 5.17(b)), which is larger than 100% in R1233zd(E) cases (red lines).

This new relation 5.18 can be simplified under certain conditions. For example, if $R_{\rho T} \approx 1$, it can be simplified to

$$\frac{p'_{rms}}{\bar{p}} \approx \left(\widehat{\left(\frac{\partial p}{\partial \rho}\right)}_T \frac{\rho'_{rms}}{\bar{\rho}} + \left(\widehat{\left(\frac{\partial p}{\partial T}\right)}_\rho \frac{T'_{rms}}{\bar{T}}\right), \quad (5.19)$$

which is equivalent to the Relation 5.16. This relation can also be obtained if $R_{\rho p} \approx 1$ and $\frac{p'_{rms}}{\bar{p}} > \left(\widehat{\left(\frac{\partial p}{\partial \rho}\right)}_T \frac{\rho'_{rms}}{\bar{\rho}}\right)$ are applied. This simplified relation 5.19 is acceptable in a gas with more complex molecules, MDM (see blue lines in Figure 5.17(b)), but not in a gas with less complex molecules, R1233zd(E). In R1233zd(E) cases, the invalidity is caused by the derivation of $R_{\rho T}$ from 1 (or $R_{\rho p}$ from 1), which will be shown in Chapter 5.4.3.

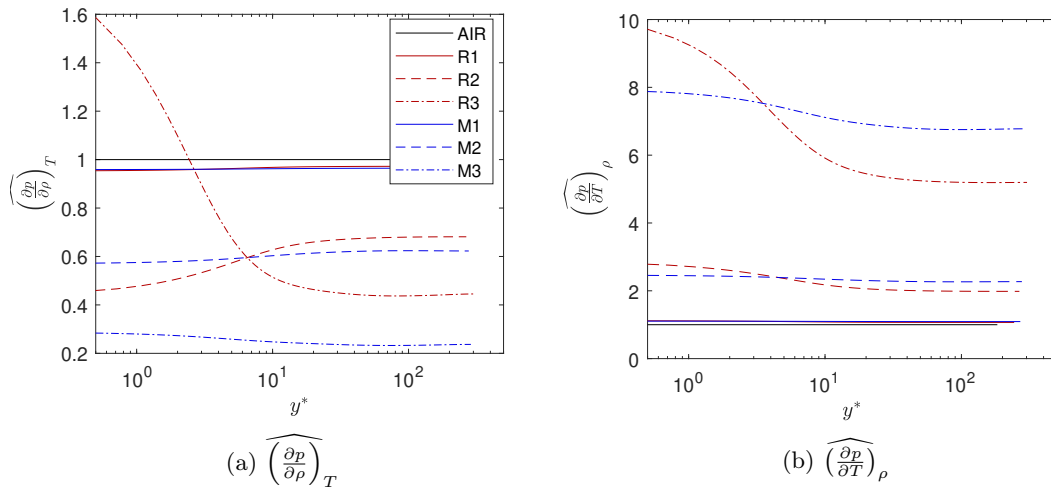


Figure 5.16: Distribution of normalised thermodynamic derivatives.

Similarly, if the condition $R_{\rho T} \approx -1$ is applied, then another simplified relation can be obtained

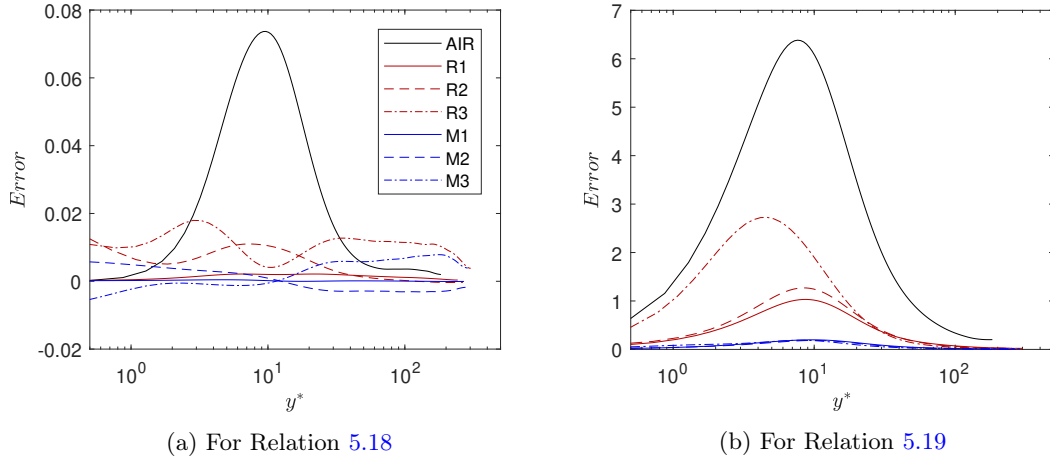


Figure 5.17: Error of the relations between p'_{rms} , ρ'_{rms} and T'_{rms} .

from Equation 5.18:

$$\frac{p'_{rms}}{\bar{p}} \approx \left| \left(\frac{\partial p}{\partial \rho} \right)_T \frac{\rho'_{rms}}{\bar{\rho}} - \left(\frac{\partial p}{\partial T} \right)_\rho \frac{T'_{rms}}{\bar{T}} \right|. \quad (5.20)$$

This condition is more acceptable in Case AIR and R3 (will be shown in Chapter 5.4.3).

To summarise, $T'_{rms}/\bar{T}$, $p'_{rms}/\bar{p}$ and $\rho'_{rms}/\bar{\rho}$ in dense vapours are no longer of the same order of magnitude, because both molecular-complexity effects and non-ideal effects significantly reduce $T'_{rms}/\bar{T}$. The profile of $\rho'_{rms}/\bar{\rho}$ in dense vapours (except Case R3) no longer has the shape of a ‘bell’ and is more similar to the profile of $p'_{rms}/\bar{p}$ than to that of $T'_{rms}/\bar{T}$. A new equation 5.18 is proposed to relate $T'_{rms}/\bar{T}$, $p'_{rms}/\bar{p}$ and $\rho'_{rms}/\bar{\rho}$, which includes a correlation coefficient $R_{\rho T}$. The error of this equation is within 7.5% for all cases and within 2% for all dense-vapour cases. Two simplified relations of Equation 5.18 are also proposed, which can be applied under certain conditions.

5.4.3 Correlation coefficients between temperature, pressure and density

The correlation coefficient between two parameters is defined by

$$R_{\alpha\beta} = \frac{\overline{\alpha'\beta'}}{\sqrt{\overline{\alpha'^2}}\sqrt{\overline{\beta'^2}}}. \quad (5.21)$$

Figure 5.18(a-c) shows the distributions of $R_{\rho p}$, R_{pT} and $R_{\rho T}$. In Figure 5.18(a), density and pressure show a positive correlation in all cases. It decreases from 1 to the minimum value in the region $y^* < 10$ and then approaches 1 at the channel centre. Near the wall, $R_{\rho p} \approx 1$ is due to the isothermal-wall boundary conditions. $R_{\rho p, min}$ is close to 0 in the Case AIR and is identical to the

result of Gerolymos [272]. While $R_{pp,min}$ is larger in the gas with more complex molecules (MDM, blue lines), and R_{pp} remains close to 1 throughout the boundary layer. This behaviour, $R_{pp} \approx 1$, is also reported for the boundary of another organic gas, PP11, by Sciacovelli [139]. However, for a gas with less complex molecules (R1233zd(E)), $R_{pp,min}$ differs significantly from case to case, and it is reduced by non-ideal effects (see red lines in Figure 5.18(a)). This is the reason for the invalidity of Equation 5.19 in R1233zd(E) mentioned above in Chapter 5.4.2.

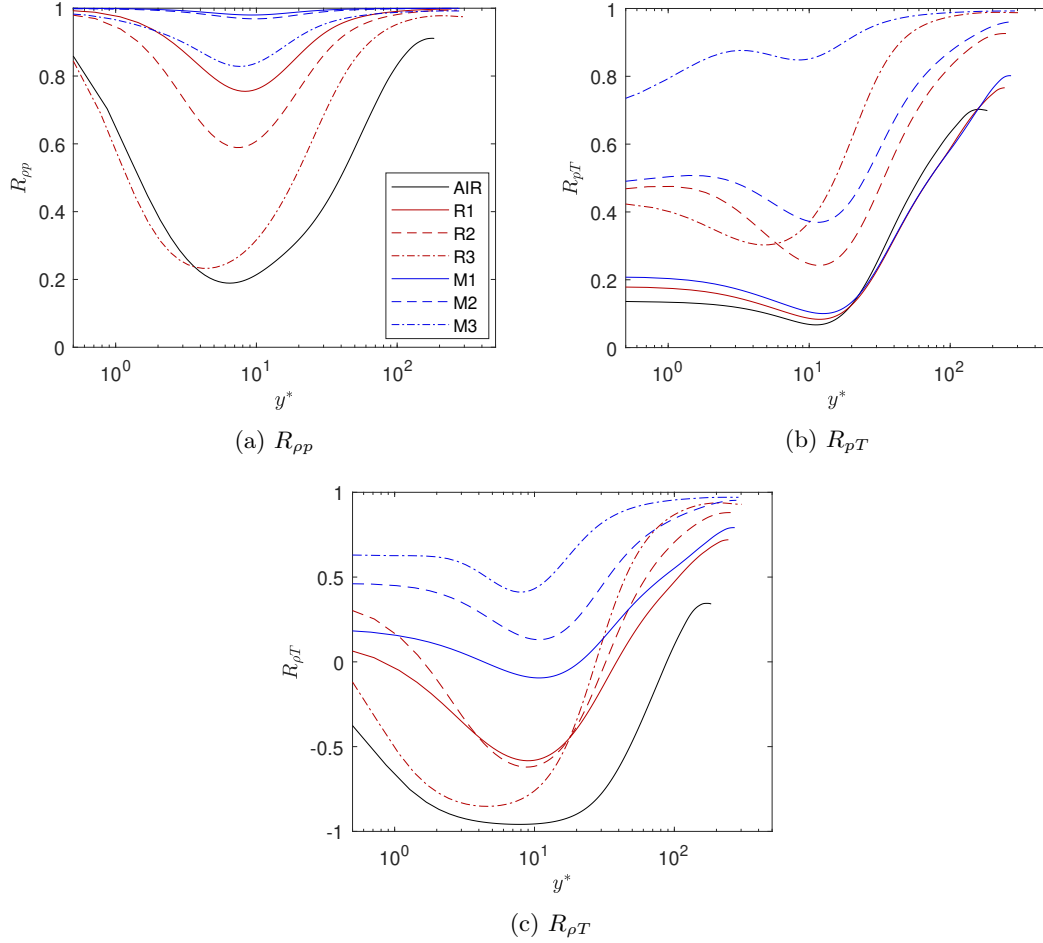


Figure 5.18: Correlation coefficients between temperature, pressure and density.

Figure 5.18(b) shows the distribution of R_{pT} . In Case AIR, R1, and M1, where non-ideal effects are weak, R_{pT} remains close to 0 within the viscous sublayer ($y^* < 15$) and then it increases. The distribution of R_{pT} is the same in these three cases, implying that molecular-complexity effects do not significantly affect R_{pT} . While non-ideal effects increase R_{pT} throughout the boundary layer, therefore R_{pT} is almost equal to 1 in Case M3 (blue dash-dotted line). It is worth noting that R_{pT} is smaller in Case R3 than in Case R2 near the wall, which is due to the variation of a thermodynamic derivative discussed later in this chapter.

Figure 5.18(c) shows the distribution of $R_{\rho T}$. Gerolymos [272] found that $R_{\rho T}$ is about -1 in the buffer region of air flows, which is also the fact in this chapter (see Case AIR, black solid line). To note, $R_{\rho T}$ approaching 0 near wall is due to the isothermal-wall condition. However, $R_{\rho T}$ is no longer negative in the inner layer in some dense-vapour cases (see Case M2 and M3). By comparing Cases AIR, R1, and M1, it can be seen that molecular-complexity effects increase $R_{\rho T}$ and make $R_{\rho T}$ in the inner layer $y^* < 30$ closer to zero. While the impact of non-ideal effects is different in the two organic gases: Non-ideal effects increase $R_{\rho T}$ in the whole boundary layer region in MDM (blue lines); but increase $R_{\rho T}$ only in the outer layer in R1233zd(E) (red lines).

To summarise, the stronger molecular-complexity effects change the density in the inner layer from a strong negative correlation to temperature to a strong positive correlation to pressure, except for the very near-wall region due to the isothermal wall conditions. The strong non-ideal effects cause the temperature to correlate strongly positively with pressure in a gas with more complex molecules (see Case M3, blue dash-dotted line in Figure 5.18), but to correlate strongly negatively with density in a gas with less complex molecules (see Case R3, red dash-dotted line).

To explain the change in these correlation coefficients in dense vapours, the mechanism of thermodynamic property fluctuation generation is analysed. Kovaszny [120] analysed the disturbance fields of compressible flows and proposed that disturbance can be caused by three modes: vorticity mode, sound-wave mode, and entropy mode. The vorticity mode is associated with vortex transport, the sound-wave mode is associated with the pressure perturbation, and the entropy mode is associated with the heat transfer. It should be noted that the heat transfer process is not affected by molecular-complexity effects and non-ideal effects, so it is not discussed here.

In the vorticity mode, the fluctuation of thermodynamic properties is mainly caused by vortex transport, and the pressure fluctuation is almost ignored, so Equation 5.17 can be reduced to:

$$0 = \left(\widehat{\frac{\partial p}{\partial \rho}} \right)_T \frac{\rho'}{\bar{\rho}} + \left(\widehat{\frac{\partial p}{\partial T}} \right)_\rho \frac{T'}{\bar{T}}. \quad (5.22)$$

According to this relation, density and temperature are negatively correlated, and pressure has a lower correlation with density and temperature, so $R_{\rho p} \approx 0$, $R_{pT} \approx 0$ and $R_{\rho T} \approx -1$. This is the fact for the buffer region in Case AIR (see Figure 5.18). While in the sound-wave mode the density and temperature fluctuations are caused by the local pressure disturbance (an isentropic process), so their relation can be shown as follows:

$$\frac{p'}{\bar{p}} \approx \left(\widehat{\frac{\partial p}{\partial \rho}} \right)_s \frac{\rho'}{\bar{\rho}} \approx \left(\widehat{\frac{\partial p}{\partial T}} \right)_s \frac{T'}{\bar{T}}, \quad (5.23)$$

where $\widehat{\left(\frac{\partial p}{\partial \rho}\right)}_s \equiv \overline{\left(\frac{\partial p}{\partial \rho}\right)}_s / \left(\frac{\bar{p}}{\bar{\rho}}\right)$ and $\widehat{\left(\frac{\partial p}{\partial T}\right)}_s \equiv \overline{\left(\frac{\partial p}{\partial T}\right)}_s / \left(\frac{\bar{p}}{\bar{T}}\right)$. Figure 5.19(a) and (b) shows the values of $\widehat{\left(\frac{\partial p}{\partial \rho}\right)}_s$ and $\widehat{\left(\frac{\partial p}{\partial T}\right)}_s$ at different wall distances for mean flow, and the derivatives are always positive, so $R_{\rho p} \approx 1$, $R_{pT} \approx 1$ and $R_{\rho T} \approx 1$. This is the fact for Case M3 (see Figure 5.18). The distributions of $R_{\rho p}$, R_{pT} and $R_{\rho T}$ in dense vapours depend on whether vorticity mode or sound-wave mode dominates the generation mechanisms of the density and temperature fluctuations. These two modes are compared quantitatively below.

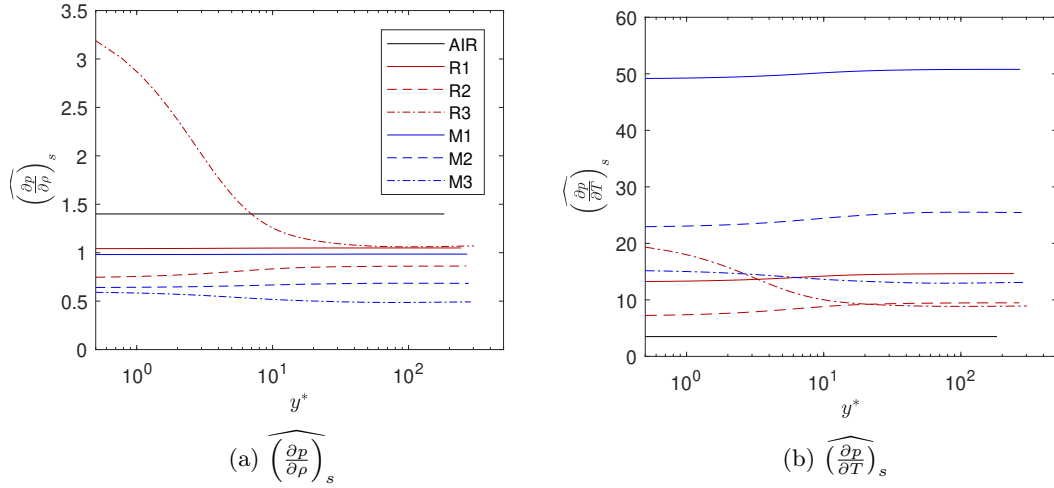


Figure 5.19: Distribution of normalised thermodynamic derivatives.

Despite the complicated non-linear combined effects of the two modes, the density and temperature fluctuations caused by vorticity mode and sound-wave mode are calculated separately. The strength of ρ and T fluctuation caused by the vorticity mode is defined as the fluctuation caused by a vortex with the length scale of y_{wall} under the mixing length hypothesis:

$$\Delta\rho_{vor} \equiv \left| \frac{\partial \bar{\rho}}{\partial y} \right| y_{wall}, \quad (5.24)$$

$$\Delta T_{vor} \equiv \left| \frac{\partial \bar{h}}{\partial y} \right| y_{wall} / \bar{c}_p. \quad (5.25)$$

The strength of density and temperature fluctuation caused by sound-wave mode is defined as their changing in an isentropic process within a pressure change of p'_{rms} :

$$\Delta\rho_{sw} \equiv \rho(\bar{p} + p'_{rms}, \bar{s}) - \rho(\bar{p}, \bar{s}), \quad (5.26)$$

$$\Delta T_{sw} \equiv T(\bar{p} + p'_{rms}, \bar{s}) - T(\bar{p}, \bar{s}). \quad (5.27)$$

The ratios of fluctuations caused by the two modes ($\Delta\rho_{sw}/\Delta\rho_{vor}$ and $\Delta T_{sw}/\Delta T_{vor}$) are shown in

Figure 5.20.

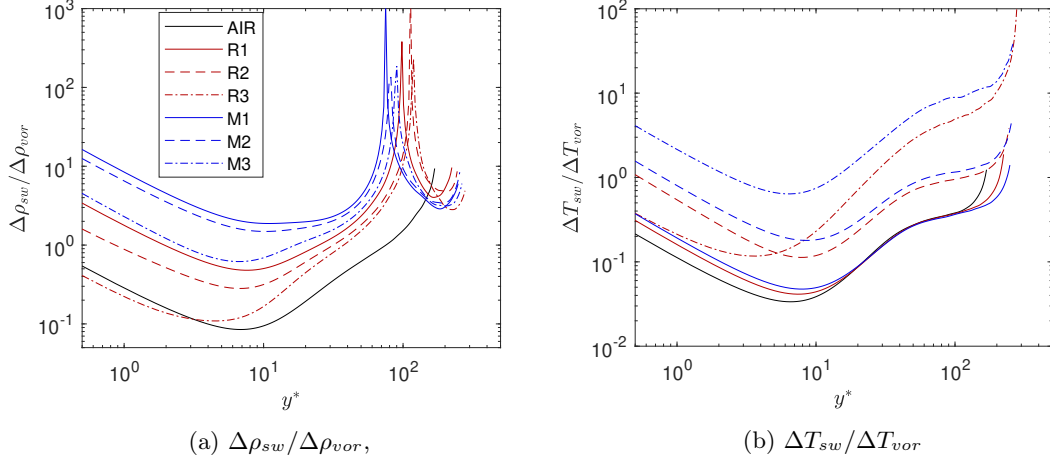


Figure 5.20: Density and temperature scale ratios.

Figure 5.20(a) shows $\Delta\rho_{sw}/\Delta\rho_{vor} \ll 1$ at $y^* = 10$ in Case AIR. This means that the impact of sound-wave mode on the density fluctuation is relatively weaker than that of the vorticity mode, so that density and pressure are less related, $R_{\rho p} \approx 0$ (already seen in Case AIR of Figure 5.18(a)). $\Delta\rho_{sw}/\Delta\rho_{vor}$ is larger than 1 at $y^* = 10$ in Case M1 and M2 (shown in Figure 5.20(a)), where sound-wave mode has larger influence, so that $R_{\rho p}$ is close to 1 (already seen in Figure 5.18(a)). The case with larger $\Delta\rho_{sw}/\Delta\rho_{vor}$ in Figure 5.20(a) always has a larger $R_{\rho p}$ in Figure 5.18(a), so it can successfully explain the change in $R_{\rho p}$.

Figure 5.20(b) shows $\Delta T_{sw}/\Delta T_{vor} \ll 1$ at $y^* < 10$ in Case AIR, R1 and M1, which means that the sound-wave mode has an insignificant impact on the generation of temperature fluctuation, so temperature and pressure are less correlated, $R_{pT} \approx 0$ (already shown in Figure 5.18(b)). As the non-ideal effects become stronger, the impact of sound-wave mode on the temperature fluctuation increases (see Cases R3 and M3, dash-dotted lines). In R1233zd(E) cases, the ratio $\Delta T_{sw}/\Delta T_{vor}$ of Case R3 near the wall turns out to be lower than that of Case R2 (see red dash line and dash-dotted line in Figure 5.20(b)), which is different from that of the MDM cases. This is because the derivative $\left(\frac{\partial p}{\partial T}\right)_s$ increases significantly in the R3 case near the wall (see Figure 5.19(b)), reducing the strength of the temperature fluctuation caused by the sound-wave mode according to Equation 5.23. The case with larger $\Delta T_{sw}/\Delta T_{vor}$ in Figure 5.20(b) always has a larger R_{pT} in Figure 5.18(b), so it can successfully explain the change in R_{pT} .

To summarise, the change of $R_{\rho p}$ and R_{pT} can be explained by the generation of ρ and T fluctuations in the vorticity mode and sound-wave mode. In air flows, vorticity mode dominates the generation of both ρ and T fluctuations in the inner layer, so $R_{\rho p} \approx 0$, $R_{pT} \approx 0$ and $R_{\rho T} \approx -1$ are seen. In dense-vapour flows, molecular-complexity effects enhance ρ fluctuation generated

in sound-wave mode, leading to $R_{\rho p}$ closer to 1; while non-ideal effects enhance T fluctuation generated in sound-wave mode and lead to R_{pT} closer to 1. The variation of derivatives $\widehat{\left(\frac{\partial p}{\partial \rho}\right)}_s$ and $\widehat{\left(\frac{\partial p}{\partial T}\right)}_s$ can also influence the distribution of the correlation coefficients. We will show more evidence for our conclusions in Chapter 5.4.4.

5.4.4 Near-wall turbulence structure

Slices of the instantaneous flow field in the layer $y^* = 10$ are analysed for Cases AIR, R1, R3, M1 and M3, and the fluctuations of streamwise velocity and pressure are plotted in Figures 5.21 and 5.22. The fluctuations are normalised by their local root-mean-squared values and are plotted within semi-local coordinates $(x^*, z^*) \in (0 \sim 1200, 0 \sim 600)$.

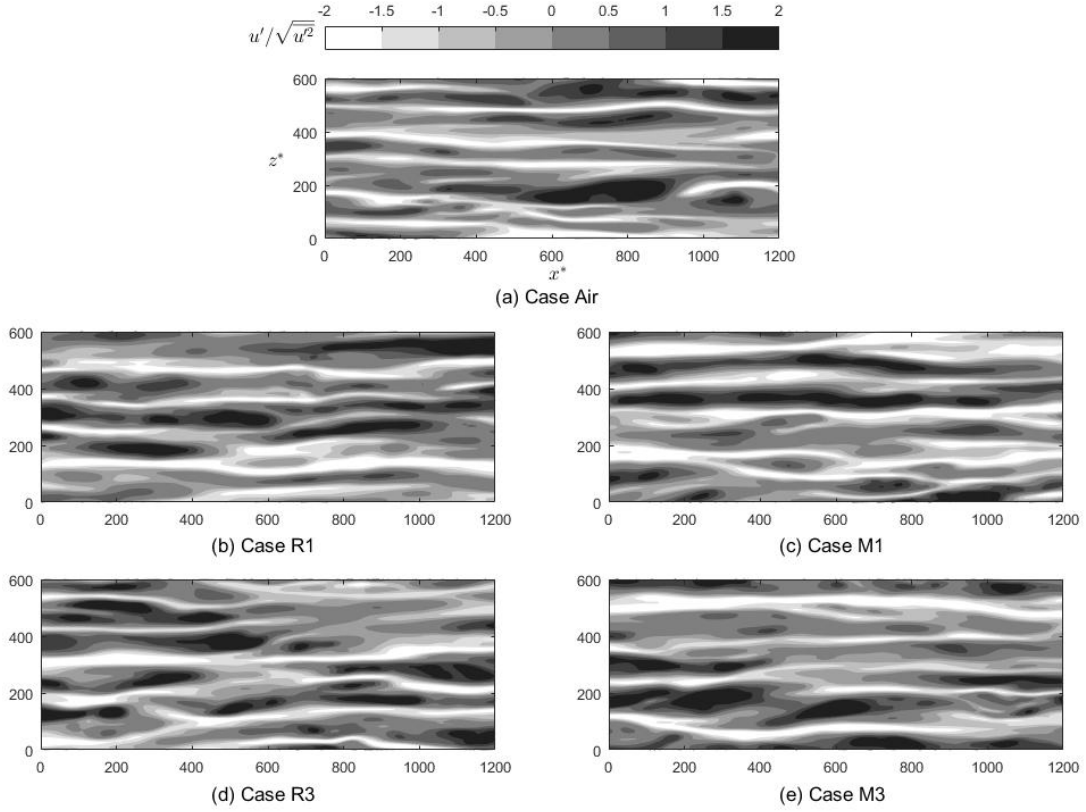


Figure 5.21: Instantaneous flow field of streamwise velocity fluctuation on x-z plane at $y^* = 10$.

Figures 5.21 show that low-speed streaks can be observed in all cases and there is little difference in the shape of streaks between cases. Smith [277] and Kim [278] have experimentally and numerically reported that the spanwise spacing of near-wall low-speed streaks in incompressible boundary layers is about 100 wall units ($\lambda_z^+ \approx 100$), and Morinishi [137] showed that the spacing is about 100 semi-local wall units, ($\lambda_z^* \approx 100$) in the compressible boundary layer. In this chapter,

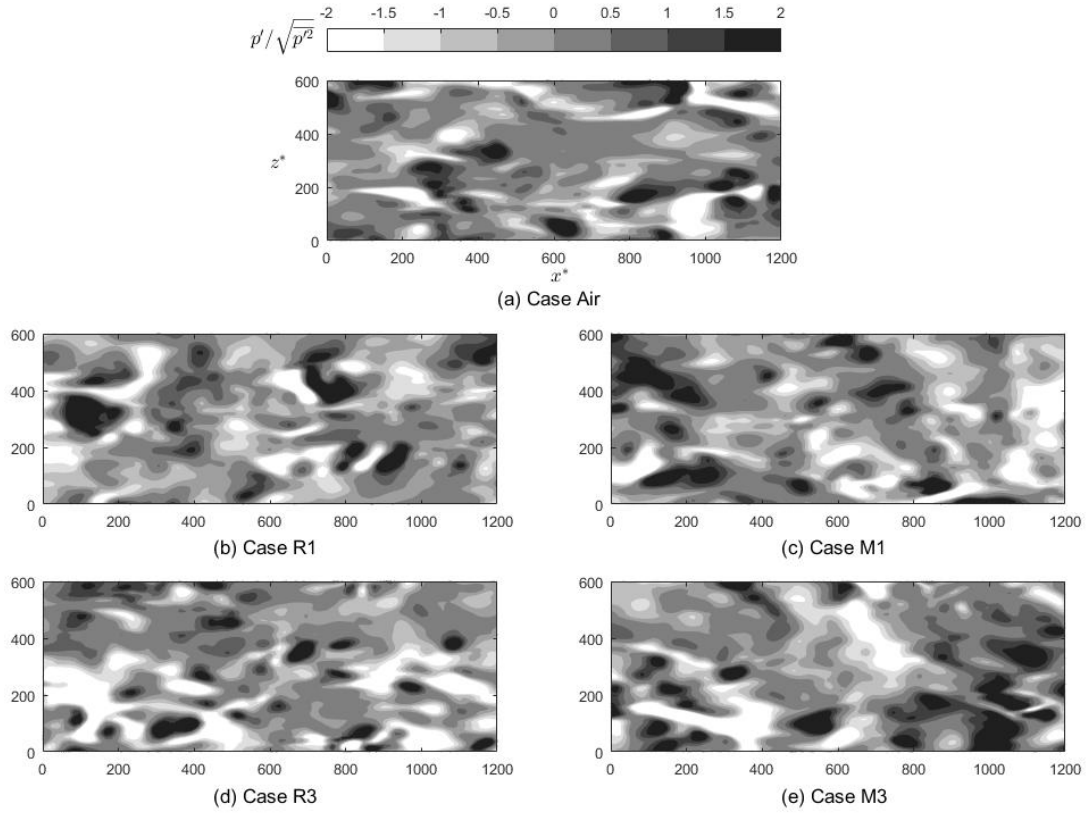


Figure 5.22: Instantaneous flow field of pressure fluctuation on x-z plane at $y^* = 10$.

the spanwise spacing in dense-vapour flows is analysed using the method proposed by Ringuette [279]. In this method, the location of the low-speed streak is identified by considering u' smaller than a threshold ($-0.4u'_{rms}$ here), and the spacing is defined as the length between the centres of adjacent streaks. The probability-density function (PDF) of the low-speed streak spanwise spacing $P(\lambda_z)$ is shown in Figure 5.23, and the peak of the PDF is at about $\lambda_z^* \approx 85$ in all cases. This means that molecular-complexity effects and non-ideal effects have an insignificant influence on near-wall spanwise spacing of low-speed streaks.

Figure 5.22 shows the the field of instantaneous pressure fluctuations near the wall. It is more homogeneous than the field of streamwise velocity fluctuations, and the ‘streak’ structure disappears in the pressure flow field. The pressure wavelengths in the streamwise and spanwise directions are analysed, and their PDF distributions are shown in Figure 5.24(a) and (b). It shows the wavelengths on these two directions are not significantly different in all cases, so the ‘streak’ structure does not exist here. The peak of wavelength PDF distribution does not obviously differ from case to case, which means the molecular-complexity effects and non-ideal effects do not influence the pressure fluctuation significantly.

Instantaneous near-wall flow fields of temperature and density on x-z plane at $y^* = 10$ are

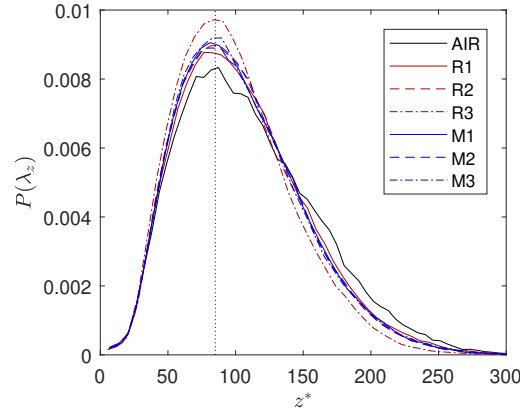


Figure 5.23: Probability-density function of the spanwise spacing of near-wall low-speed streaks at $y^* = 10$. The meanings of line styles, see table 5.4

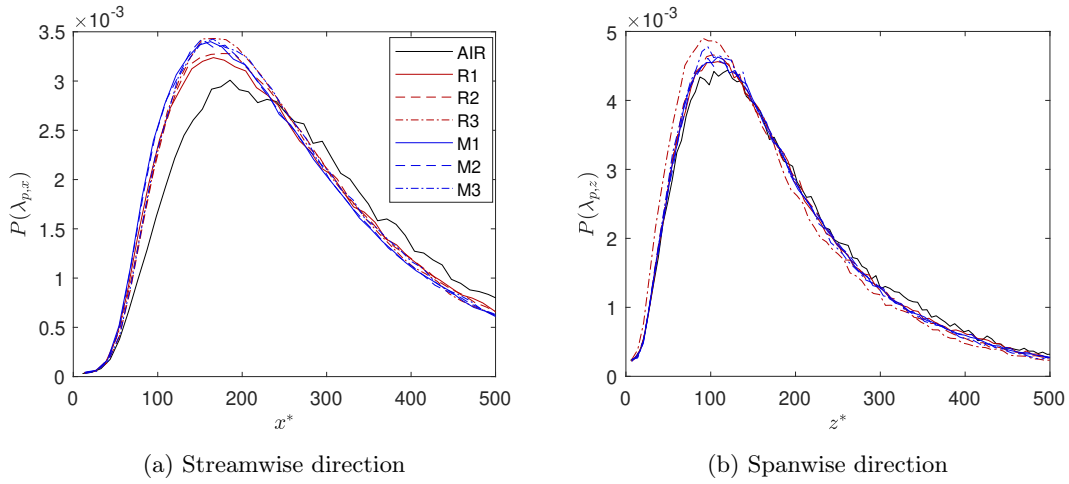


Figure 5.24: Probability-density function of pressure wavelength at $y^* = 10$.

shown in Figure 5.25 and 5.26. In Figure 5.25, the streaks of ‘large density’ in Case AIR and R3 (Figure 5.25(a) and (d)) are evident, and they are highly similar to the low-speed streaks of velocity flow field (figure 5.21(a) and (d)); while the ‘large density’ streaks are less clear in Case R1 and M3 (Figure 5.25(b) and (e)) and disappear in Case M1 (Figure 5.25(c)). The density fluctuation field in Case M1 (Figure 5.25(c)) is more similar to its pressure fluctuation field (Figure 5.22(c)). It supports our finding that molecular-complexity effects can enhance the ρ fluctuation generated by the sound-wave mode and make ρ and p more correlated. In Figure 5.26, the streaky structure is still evident in the temperature fluctuation field except in Case M3 (Figure 5.26(e)), and this field is more similar to the pressure field of this case (Figure 5.22(e)). It also supports our finding that non-ideal effects can amplify the T fluctuation generated by sound-wave mode, and make T and p more correlated.

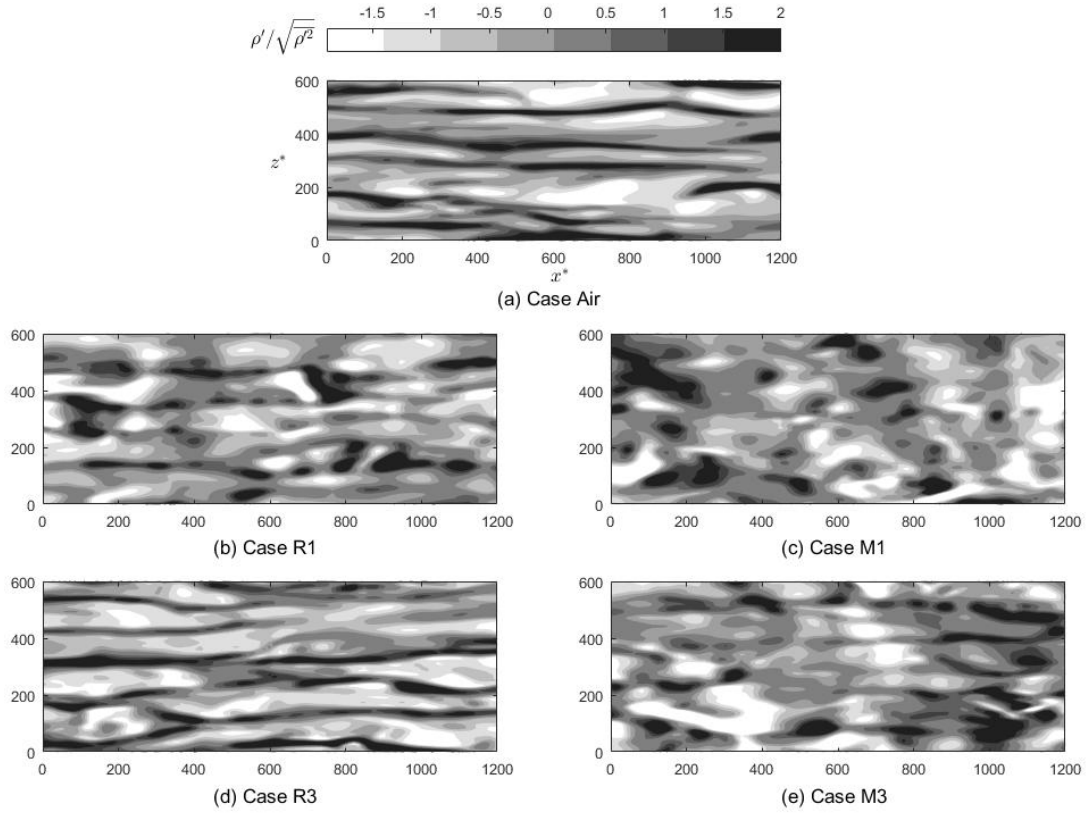


Figure 5.25: Instantaneous flow field of density fluctuation on x-z plane at $y^* = 10$.

5.4.5 Hairpin vortexes in channel flows

Hairpin vortexes are the main coherent structure in turbulent boundary layers, and these vortex in ideal air and dense vapours are compared here. The Q criterion [264] is used in this chapter to identify vortex. Figure 5.27 shows the three-dimensional vortex structure in Case AIR and Case M3, using half channel height (l) for scaling. The near-wall streamwise velocity fluctuation at $y^* = 10$ is also shown by the contour in the figure. The near-wall streamwise velocity fluctuation at $y^* = 10$ is also shown by contours in Figure 5.27. Asymmetric hairpins instead of complete ones are the main vortex structures in both cases, and this is also consistent with the experimental result of Adrian [138] and the numerical result of Ringuette [279]. The legs of the asymmetric hairpins form on the sides of each low-speed streak, and a group of similar vortexes (also called vortex packet) is also observed over the low-speed streaks, which is consistent with the dynamical mechanism of vortex development proposed by Zhou [167].

The main difference between Figure 5.27(a) and (b) is that the hairpins in Case M3 are smaller and more concentrated than in Case AIR. This is mainly due to the different distribution of the mean properties (e.g., density and viscosity). To consider this difference, the semi-local length

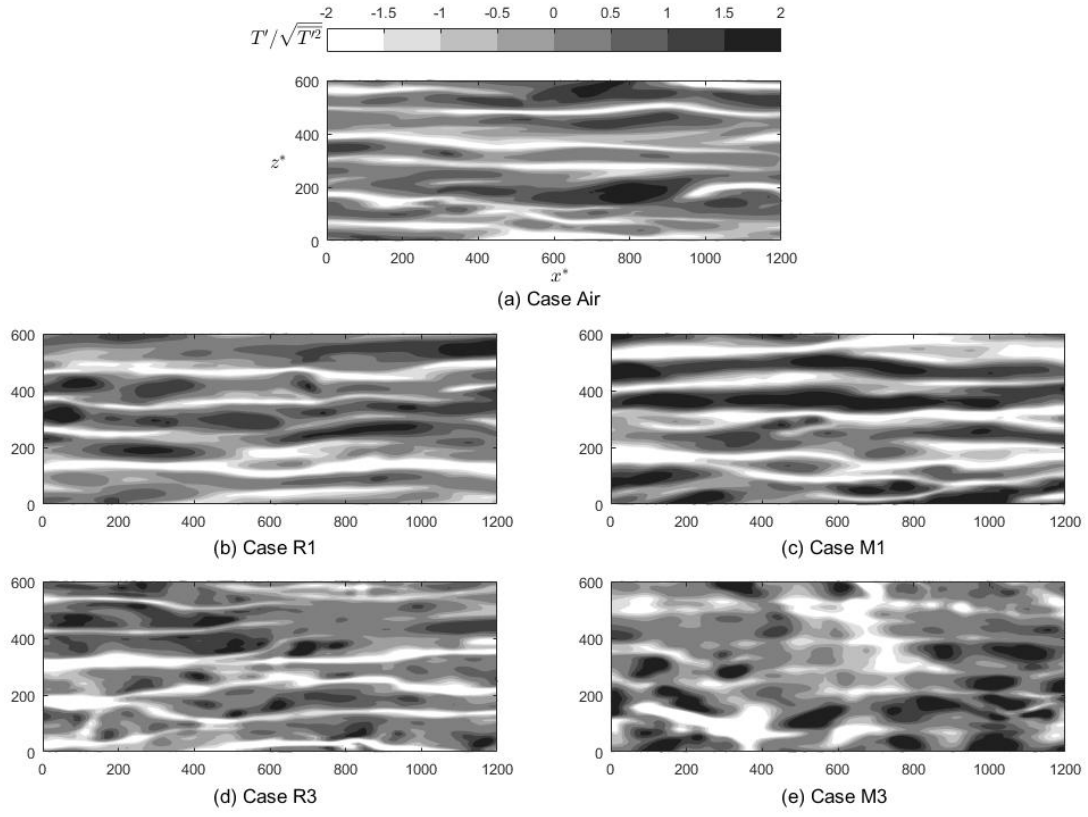


Figure 5.26: Instantaneous flow field of temperature fluctuation on x-z plane at $y^* = 10$.

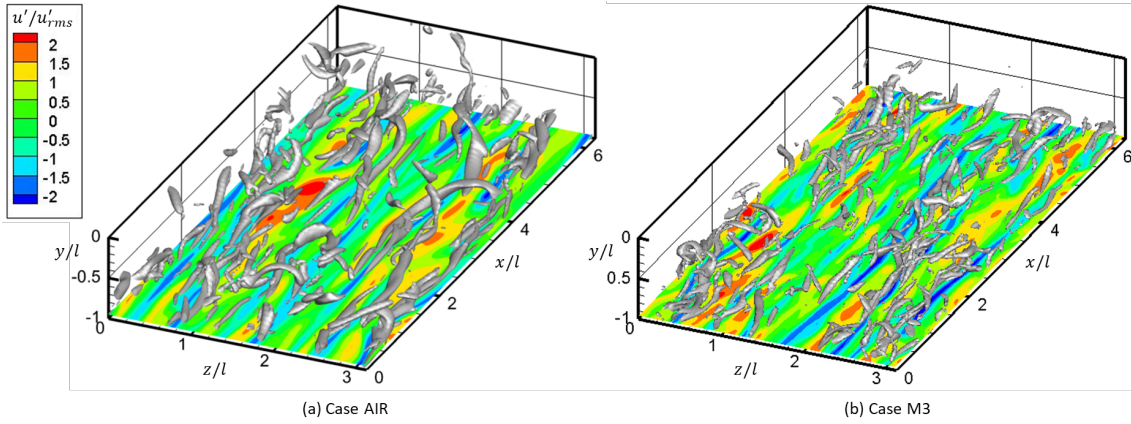


Figure 5.27: Three-dimensional vortex structure scaled by half channel height l in Case AIR and M3.

scale at the channel centre, $\delta_{v,c}^* = \bar{\mu}_c / \bar{\rho}_c u_\tau^*$, is applied, and the entire channel flow fields scaled by $\delta_{v,c}^*$ are shown in Figure 5.28(a) and (b). It should be clarified that although the mean properties in the channel are variable, they are relatively stable in the log-law region where hairpins are mainly observed. Therefore, $\delta_{v,c}^*$ is suitable to scale the entire channel field. By using this scaling method, the difference in the hairpin size and concentration between cases become insignificantly

(see Figure 5.28(a) and (b)).

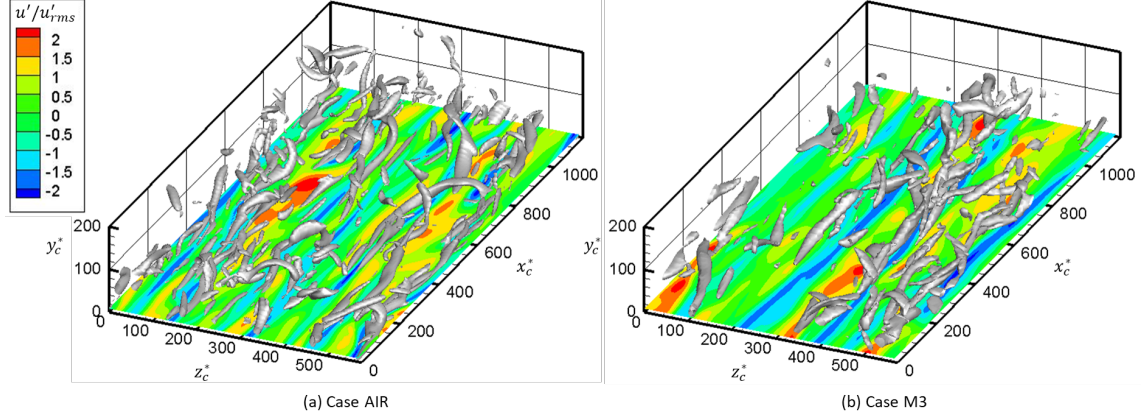


Figure 5.28: Three-dimensional vortex structure scaled by the semi-local viscous length scale at the channel centre $\delta_{v,c}^* = \bar{\mu}_c / \bar{\rho}_c u_\tau^*$ in Case AIR and M3.

In summary, asymmetric hairpins are still the main vortex structures in the boundary layer of dense vapours. The molecular-complexity effects and non-ideal effects change the scale and concentration of hairpins by varying the mean property, and this change is insignificant when using the semi-local viscous length scale at the channel centre $\delta_{v,c}^*$.

5.5 Analysis and suggestions for dense-vapour turbulence modelling issues

5.5.1 Favre and Reynolds averages

The use of the Favre average instead of Reynolds average helps to apply the turbulence knowledge found in incompressible flows directly to compressible flows. Huang [134] first compared the two averages in compressible turbulent flows. They found that the difference between them in air boundary layers is small when applied to the streamwise velocity, and the maximum difference is about 3% under $Ma = 3$ and is observed only near the wall. In this chapter, these two averages are discussed in dense vapours.

The differences between Favre and Reynolds averages applied to u and h are equal to the mean values of the fluctuation part after Favre averaging:

$$\bar{u} - \tilde{u} = \overline{\tilde{u} + u''} - \tilde{u} = \overline{u''}, \quad (5.28)$$

$$\bar{h} - \tilde{h} = \overline{\tilde{h} + h''} - \tilde{h} = \overline{h''}. \quad (5.29)$$

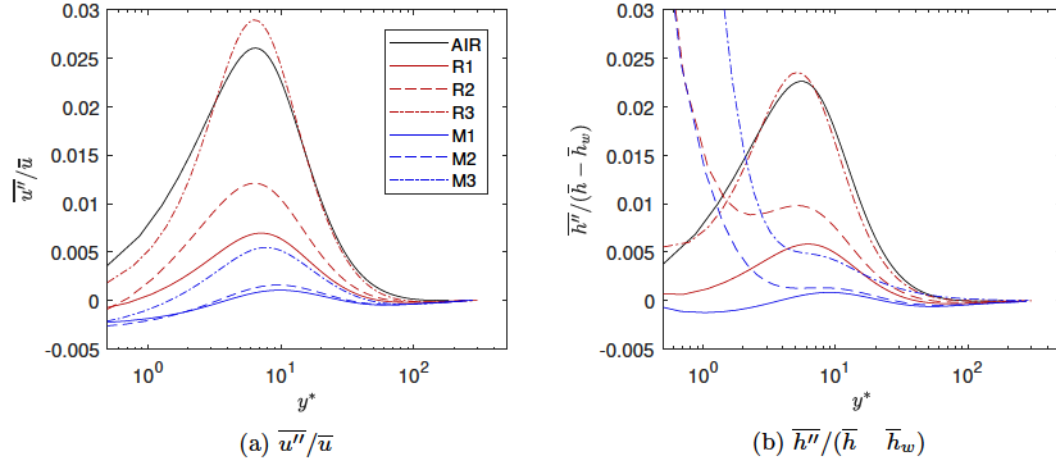


Figure 5.29: Mean value of the fluctuation part after Favre average when applied to streamwise velocity and enthalpy. The meanings of line styles, see table 5.4

These differences are normalised by $\bar{u}$ and $\bar{h} - \bar{h}_w$ respectively, and they are shown in Figure 5.29(a) and (b). $\overline{u''}/\bar{u}$ has the peak value near the wall ($y^* < 10$) in dense vapours, and this peak value is smaller in a gas with more complex molecules, MDM (blue lines in Figure 5.29(a)), and in the cases with weak non-ideal effects (solid lines there). In all cases, $\overline{u''}/\bar{u}$ is within $\pm 3\%$, which means that the difference between the two averages of u is still marginal in dense vapours. The same trend is also found in $\overline{h''}/(\bar{h} - \bar{h}_w)$ (see Figure 5.29(b)), except for the near-wall region ($y^* < 3$). Outside this region, $\overline{h''}/(\bar{h} - \bar{h}_w)$ is within $\pm 2.5\%$ in all cases. This rise near the wall is caused by the non-ideal effects on an isothermal wall: the enthalpy fluctuation does not approach zero due to the density fluctuation in non-ideal gases, while the mean enthalpy increase $\bar{h} - \bar{h}_w$ approaches zero. It means that two averages of h is still almost the same except the near-wall region.

Figure 5.30(a-c) shows the difference between Favre and Reynolds averages applied to second order fluctuation statistics: Reynolds shear stress, turbulent heat flux, and turbulence kinetic energy. It can be seen that the difference for all these statistics is reduced by molecular-complexity effects but increased by non-ideal effects. The maximum difference is in Case R3 (red solid line) in Figure 5.30(a-c), which is slightly larger than in Case AIR, so this difference should be paid attention in dense vapours. The difference is within $\pm 7.5\%$ for all these statistics in all gases.

To summarise, the molecular-complexity effects decrease the difference between the Favre and Reynolds averages, but non-ideal effect increase it. This difference can be larger in dense vapours than in air when non-ideal effects are strong in a gas with less complex molecules. The difference in all cases is within $\pm 3\%$ when applied to u and h except very close to the wall, and it is within $\pm 7.5\%$ when applied to the second-order fluctuation statistics.

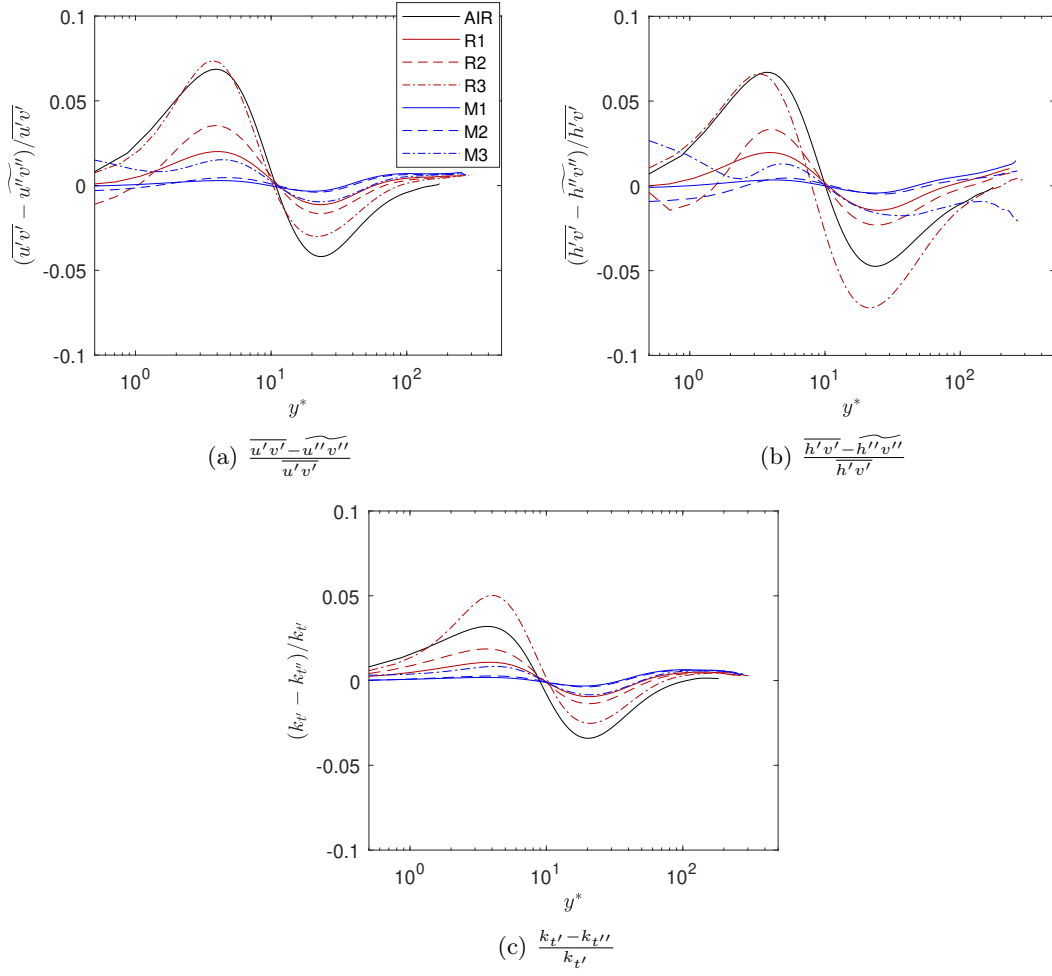


Figure 5.30: Difference between Farve and Reynolds averages applied to (a) Reynolds shear stress, (b) turbulent heat flux and (c) turbulent kinetic energy.

5.5.2 Strong Reynolds analogy

Morkovin [127] proposed the concept of strong Reynolds analogy (SRA) based on the assumption that the total energy fluctuation is zero:

$$c_p T'_{tot} = c_p T' + K' + k' = 0. \quad (5.30)$$

The SRA contains three important equations that show the relationship between temperature and velocity fluctuations:

$$R_{uT} \approx -1, \quad (5.31)$$

$$Pr_t \equiv \frac{\widetilde{u''v''}(\partial \tilde{T}/\partial y)}{\widetilde{T''v''}(\partial \tilde{u}/\partial y)} \approx 1, \quad (5.32)$$

$$\frac{\sqrt{T''^2}/\tilde{T}}{(\gamma - 1)Ma^2 \sqrt{u''^2}/\tilde{u}} \approx 1. \quad (5.33)$$

However, in dense-vapour flows, the heat capacity cannot be considered constant, so the SRA should be used in terms of enthalpy:

$$R_{uh} \approx -1, \quad (5.34)$$

$$Pr_t \equiv \frac{\widetilde{u''v''}(\partial\tilde{h}/\partial y)}{\widetilde{h''v''}(\partial\tilde{u}/\partial y)} \approx 1, \quad (5.35)$$

$$\frac{\sqrt{h''^2}}{\tilde{u}\sqrt{u''^2}} \approx 1, \quad (5.36)$$

which shows the relationship between enthalpy and velocity fluctuations. They are equivalent to Equations 5.31 - 5.33 in ideal gases. These equations will be discussed in this Chapter, except Pr_t (equation 5.35) discussed later in Chapter 5.5.4.

Figure 5.31 shows the R_{uh} distributions for all cases. Morinishi [137] and Brun [280] proposed that the SRA Equation 5.31 does not hold for boundary layers on cold walls. They found that R_{uT} is positive instead of negative, and R_{uT} decreases from the wall to channel centre. The R_{uh} distribution in Case AIR of this chapter (see Figure 5.31) agrees with their finding. In dense vapours the strong positive correlation between u and h persists near the wall, but R_{uh} decreases faster in cases with stronger non-ideal effects (see Case R3 and M3 in Figure 5.31).

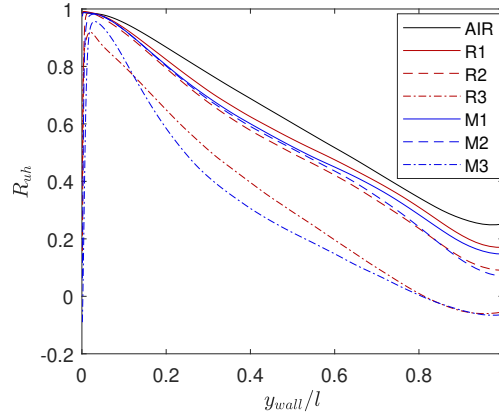


Figure 5.31: Correlation coefficients between streamwise velocity and enthalpy, R_{uh} .

Equation 5.33 was found invalid by Gaviglio [136], Guarini [281] and Maeder [282], because they found the assumption of negligible total energy fluctuation (Equation 5.30) is unacceptable. Some modifications of the right hand side of this equation were proposed, and Duan [132] evaluated four modified SRA models [121, 136, 283, 134] that apply to compressible boundary layers of air up to $Ma = 5$. They found that two models are more accurate which are proposed by Gaviglio [136],

$$\frac{\sqrt{h''^2}}{\tilde{u}\sqrt{u''^2}} = \frac{\sqrt{T''^2}/\tilde{T}}{(\gamma - 1)Ma^2\sqrt{u''^2}/\tilde{u}} \approx \frac{1}{1 - (\partial\tilde{h}_{tot}/\partial\tilde{h})}, \quad (5.37)$$

and Huang [134],

$$\frac{\sqrt{h''^2}}{\tilde{u}\sqrt{u''^2}} = \frac{\sqrt{T''^2}/\tilde{T}}{(\gamma-1)Ma^2\sqrt{u''^2}/\tilde{u}} \approx \frac{1}{Pr_t[1 - (\partial\tilde{h}_{tot}/\partial\tilde{h})]} \quad (5.38)$$

(shorten by GSRA and HSRA respectively in the following). These models are based on the assumption that the velocity mixing length scale $l_u \equiv \sqrt{u''^2}/(\partial\tilde{u}/\partial y)$ and the enthalpy mixing length scale $l_h \equiv \sqrt{h''^2}/(\partial\tilde{h}/\partial y)$ are comparable,

$$\frac{l_u}{l_h} = \frac{\sqrt{u''^2}/(\partial\tilde{u}/\partial y)}{\sqrt{h''^2}/(\partial\tilde{h}/\partial y)} = 1 \quad (\text{for GSRA}), \quad (5.39)$$

$$\frac{l_u}{l_h} = \frac{\sqrt{u''^2}/(\partial\tilde{u}/\partial y)}{\sqrt{h''^2}/(\partial\tilde{h}/\partial y)} = Pr_t \quad (\text{for HSRA}). \quad (5.40)$$

GSRA and HSRA (Equation 5.37 and 5.38) are checked in dense vapours, and the ratios of the left-hand-side term to right-hand-side term of two equations are calculated from DNS data and shown in Figure 5.32(a) and (b). It can be seen that the deviation from unity for the HSRA model is smaller than that for the GSRA model in all cases, which means HSRA model is more accurate. However, both two models are unacceptable in cases with strong non-ideal effects (Case R3 and M3 in Figure 5.32), where the models extremely overestimate the ratio $\frac{\sqrt{h''^2}}{\tilde{u}\sqrt{u''^2}}$. The reason for the failure is due the failure of the assumption that velocity mixing length scale l_u and enthalpy mixing length scale l_h are comparable. Figure 5.33 shows that the ratio $Pr_t l_h/l_u$ is not close to unity in Case R3 and M3, and this ratio increases significantly with increasing wall distance.

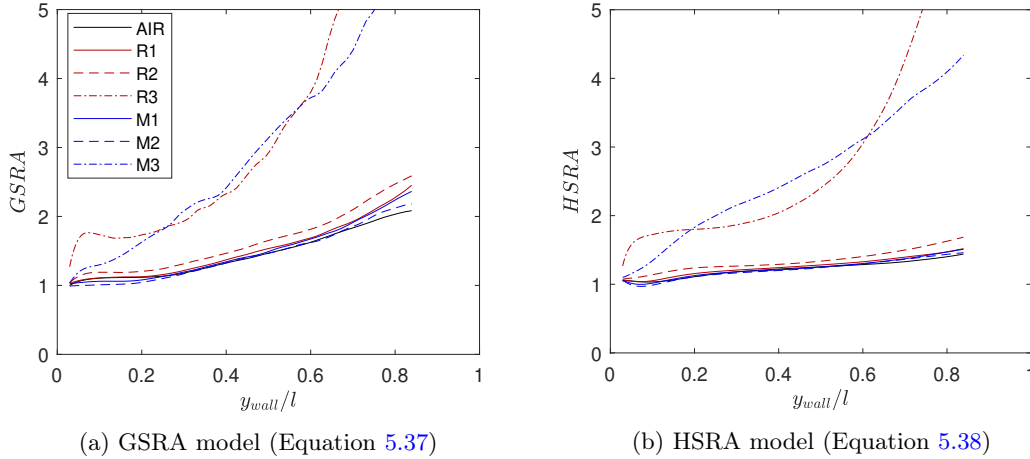


Figure 5.32: The ratio of left-hand-side value to right-hand-side value in modified SRA models.

To summarise, the distributions of R_{uh} in dense vapours shows the same trend as in air, but the decline of R_{uh} is faster in the cases with strong non-ideal effects. The modified SRA model (HSRA) of the relation between $\sqrt{h''^2}$ and $\sqrt{u''^2}$ is still acceptable in dense vapours except when

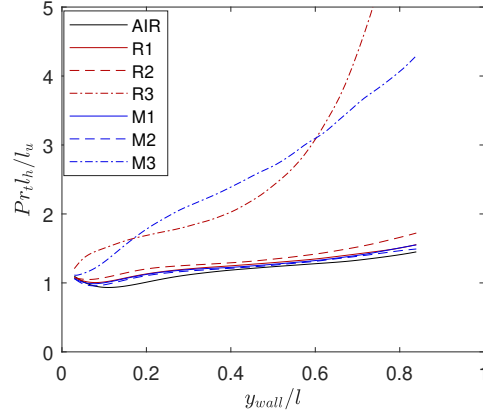


Figure 5.33: Comparison of the velocity mixing length scale with the enthalpy mixing length scale when considering Pr_t .

the non-ideal effects are very strong, and this deviation is due to the failure of the assumption that l_u and l_h are almost equal.

5.5.3 Turbulent kinetic energy budget

The transport equation of turbulent kinetic energy, $k_t = \frac{1}{2} \widetilde{u_i'^2}$, in dense vapours is analysed:

$$\frac{\partial \bar{\rho} k_t}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j k_t}{\partial x_j} = P_k + T_k + V_k - \bar{\rho} \varepsilon + \Pi_k + D_k. \quad (5.41)$$

Its left-hand side is zero in fully developed channel flows, and its right hand side consists of the production term P_k , turbulent transport term T_k , viscous transport term V_k , viscous dissipation term $\bar{\rho} \varepsilon$, velocity-pressure term Π_k and dilatation term D_k , where

$$P_k = -\bar{\rho} \widetilde{u_i'' u_j''} \frac{\partial \tilde{u}_i}{\partial x_j}, \quad (5.42)$$

$$T_k = -\frac{\partial (\frac{1}{2} \bar{\rho} \widetilde{u_i'' u_i'' u_j''})}{\partial x_j}, \quad (5.43)$$

$$V_k = \frac{\partial \overline{u_i' \tau_{i,j}'}}{\partial x_j}, \quad (5.44)$$

$$\bar{\rho} \varepsilon = \overline{\tau_{i,j}' \frac{\partial u_i'}{\partial x_j}}, \quad (5.45)$$

$$\Pi_k = -\frac{\partial \overline{u_j' p'}}{\partial x_j} + \overline{p' \frac{\partial u_i'}{\partial x_i}}, \quad (5.46)$$

$$D_k = \overline{u_i'' \frac{\partial \bar{p}}{\partial x_i}} + \overline{u_i'' \frac{\partial \bar{\tau}_{i,j}}{\partial x_j}}. \quad (5.47)$$

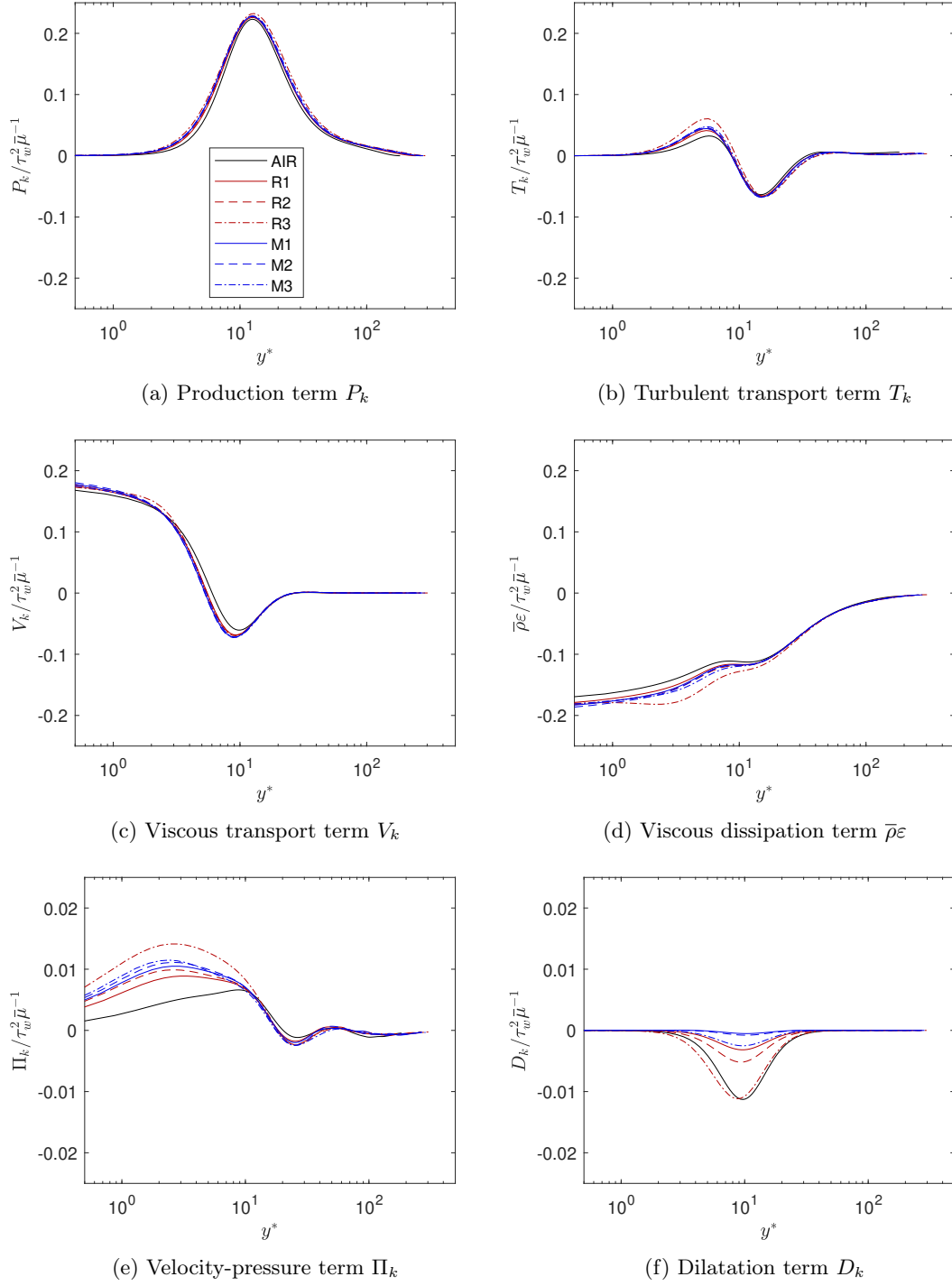


Figure 5.34: Turbulent kinetic energy budget. All terms are normalised by $\tau_w^2/\bar{\mu}$.

The profile of each term are shown in Figure 5.34(a-f), normalised by $\tau_w^2/\bar{\mu}$. y^* is used as abscissa to consider the variable mean properties. The profiles of P_k and V_k differ insignificantly from case to case (see Figure 5.34(a,c)), while the profile of the other four terms can be quantitatively affected by molecular-complexity effects and non-ideal effects (see Figure 5.34(b,d,e,f)). Figure 5.34(b) shows that T_k is larger in dense-vapour cases than in the air case within the region $y^* < 10$, and

the largest peak value is seen in Case R3, which is 87% larger than that in Case AIR. A similar influence is also seen in the profiles of $\bar{\rho}\varepsilon$ (see Figure 5.34(d)), that the largest absolute value of $\bar{\rho}\varepsilon$ is seen in Case R3. Although molecular-complexity effects and non-ideal effects affect the profile of Π_k and D_k (see Figure 5.34(e,f)), they are still of one order of magnitude lower than the other four terms. Huang [134] and Duan [132] proposed that the direct impact of pressure fluctuation effects and compressibility effects on the turbulent kinetic energy budget in air flows is marginal. This conclusion holds in dense vapours as well from the result of this chapter. In summary, when y^* is used to consider the variable mean properties, the terms of the energy budget have the same trend in dense vapours as in air, despite the value of T_k , $\bar{\rho}\varepsilon$, Π_k and D_k is quantitatively affected by molecular-complexity effects and non-ideal effects. Π_k and D_k are still small compared to other terms in dense vapours.

5.5.4 $k - \varepsilon$ Reynolds-averaged Navier-Stokes (RANS) modelling issues

Modelling assumptions for the $k - \varepsilon$ RANS model closure are discussed based on dense-vapour DNS results, including the eddy viscosity models and k equation term models. Models in the ε equation are not mentioned here because they are analogous to models in k equation, but the decomposition of the turbulent dissipation, $\bar{\rho}\varepsilon$, is discussed. To complete the modelling issues, models for the turbulent Prandtl number are also discussed.

Eddy viscosity models

For the closure of the Reynolds-averaged momentum equation, the Reynolds stress is usually modelled based on the eddy viscosity assumption [263],

$$-\widetilde{\bar{\rho}u_i''u_j''} = \mu_t \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \bar{\rho}k_t, \quad (5.48)$$

$$\mu_t = C_\mu \bar{\rho} \frac{k_t^2}{\varepsilon}. \quad (5.49)$$

The coefficient C_μ is constant and equal to 0.09 for high Reynolds number, but it is variable for low-Reynolds numbers. Patel [284] has summarised several models of C_μ at low-Reynolds numbers that can be used in further research. Sciacovelli [140] examined them and suggested that two models, those proposed by Lam & Bremhorst [285] (LB) and Chien [286] (CH) respectively, are more accurate than other models for an organic gas, PP11. In this chapter, these two models are discussed together with another model proposed by Shih [287] (SH).

In LB model, C_μ is calculated as follows:

$$C_\mu = 0.09 (1 + 20.5/R_t) [1 - \exp(-0.0165R_k)]^2, \quad (5.50)$$

where

$$R_k = \bar{\rho} \sqrt{k_t} y_{wall} / \bar{\mu}, \quad R_t = \bar{\rho} k^2 / \bar{\mu} \varepsilon. \quad (5.51)$$

In CH model, C_μ is calculated as follows:

$$C_\mu = 0.09 [1 - \exp(-0.0115y^+)]. \quad (5.52)$$

It should be noted that the damping term D in CH model is not considered in this chapter. This term is proposed to keep the dissipation close to zero, $\tilde{\varepsilon} \equiv \varepsilon - D \approx 0$ [286]; however, Sciacovelli [140] has suggested to ignore it in dense-vapour boundary layers since it can lead to negative values of $\tilde{\varepsilon}$. In the SH model, the wall distance y_{wall} is not included, where C_μ is modelled by

$$C_\mu = \frac{1}{A_0 + A_s U^{(*)} \frac{k_t}{\varepsilon}}, \quad (5.53)$$

where,

$$U^{(*)} = \sqrt{S_{ij} S_{ij} + \tilde{\Omega}_{ij}^* \tilde{\Omega}_{ij}^*}, \quad (5.54)$$

$$S_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right), \quad \tilde{\Omega}_{ij}^* = \Omega_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} - \frac{\partial \bar{u}_j}{\partial x_i} \right), \quad (5.55)$$

$$A_s = \sqrt{6} \cos \phi, \quad \phi = \frac{1}{3} \arccos(\sqrt{6}W), \quad W = \frac{S_{ij} S_{jk} S_{ki}}{\tilde{S}^3}, \quad \tilde{S} = \sqrt{S_{ij} S_{ij}}. \quad (5.56)$$

Near the channel centre, the mean velocity gradient is very small, causing the SH model extremely overestimate C_μ , so an upper bound $C_\mu \leq 0.1$ is added in the calculation here.

Figure 5.35(a-d) shows the exact value of the eddy viscosity μ_t from DNS results and the value calculated by the three models. A comparison of Figure 5.35(b) with (a) shows that the LB model overestimates μ_t in the buffer region for all cases, while it underestimates its peak value in the log-law region for Case AIR. Figure 5.35(c) shows that the CH model also has the overestimate in the buffer region, but it underestimates the peak value for all cases. Figure 5.35(d) shows that the SH model has a better estimate of μ_t in the log-law region for all cases, although it also does not perform well in the buffer region. In summary, all of these eddy viscosity models overestimate in the buffer region, while SH model has a better estimate in the log-law region for all dense-vapour cases.

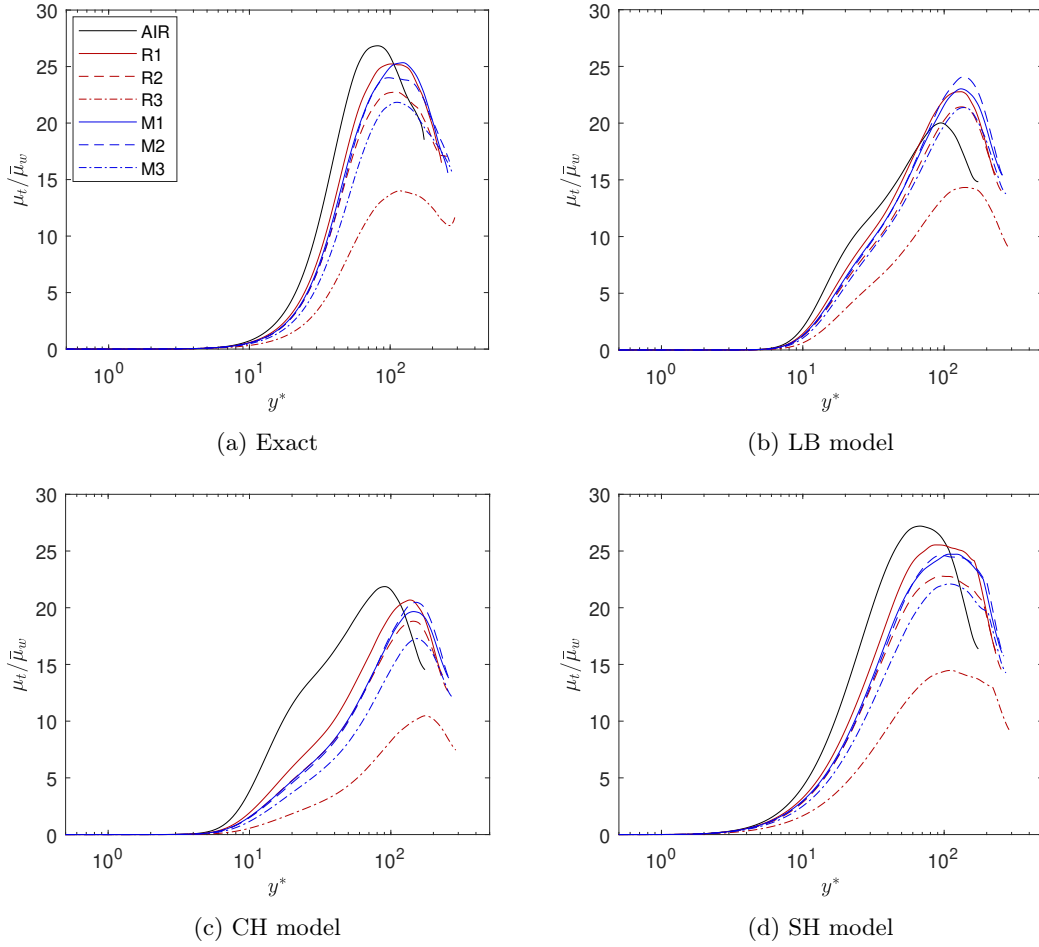


Figure 5.35: Eddy viscosity normalised by averaged wall molecular viscosity, $\mu_t/\bar{\mu}_w$, calculated directly from DNS results and by models.

Modelling issues in k equation

Standard k equation [285, 286, 287] can be directly applied to compressible flows by considering $\bar{\rho}$:

$$\frac{\partial \bar{\rho} k_t}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j k_t}{\partial x_j} = P_k + \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_k} \frac{\partial k_t}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\bar{\mu} \frac{\partial k_t}{\partial x_j} \right) - \bar{\rho} \varepsilon. \quad (5.57)$$

where coefficient σ_k is equal to 1, $\frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_k} \frac{\partial k_t}{\partial x_j} \right)$ is the model for T_k , and $\frac{\partial}{\partial x_j} \left(\bar{\mu} \frac{\partial k_t}{\partial x_j} \right)$ is the model for V_k . The terms Π_k and D_k are ignored in k equation, which is also acceptable for dense vapours based on our findings above.

The production term P_k depends only on the eddy viscosity models, so it is not discussed further here. The models for T_k and V_k are calculated and shown in Figure 5.36(a) and (b). By comparing $\frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_k} \frac{\partial k_t}{\partial x_j} \right)$ (Figure 5.36(a)) with T_k (Figure 5.34(b)), it can be seen that the model still follows the profile of the exact T_k in all cases, and the deviation of the model from T_k is within $\pm 35\%$ in boundary layers. $\frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_k} \frac{\partial k_t}{\partial x_j} \right)$ underestimates the peak and the lowest value of

T_k in dense-vapour cases; for example, in Case R3 it underestimates the peak by 20% and the lowest value by about 35%. Comparing $\frac{\partial}{\partial x_j} \left(\bar{\mu} \frac{\partial k_t}{\partial x_j} \right)$ (Figure 5.36(b)) with V_k (Figure 5.34(d)), it shows that $\frac{\partial}{\partial x_j} \left(\bar{\mu} \frac{\partial k_t}{\partial x_j} \right)$ also follows the profile of V_k except for Case R3 (red dash-dotted lines). In summary, the models of the turbulent transport term T_k and viscous transport term V_k still follow their exact profile in dense vapours, and the error of the models is still insignificant.

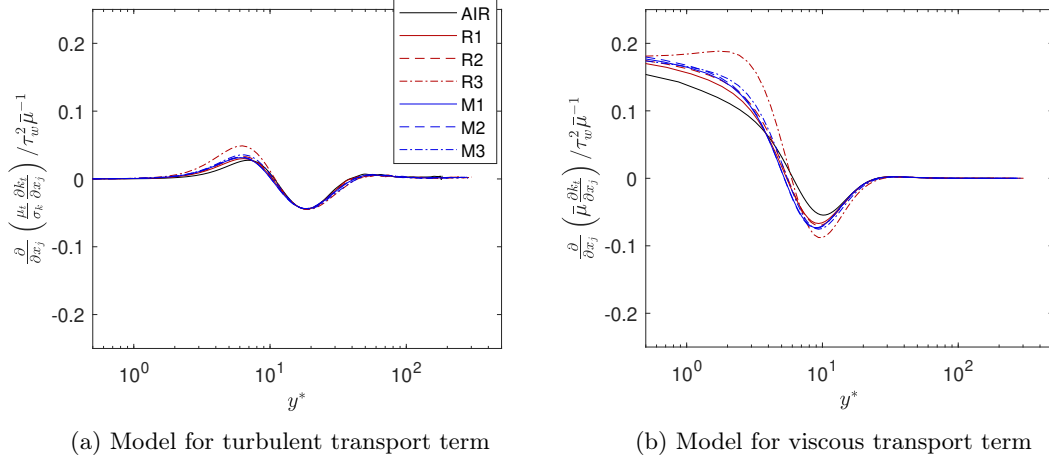


Figure 5.36: Modelled terms in k equation.

Decomposition of turbulent dissipation $\bar{\rho}\varepsilon$

Huang [134] first studied the decomposition of $\bar{\rho}\varepsilon$ and divided it into three parts:

$$\bar{\rho}\varepsilon = \overline{\tau'_{ij} \frac{\partial u'_i}{\partial x_j}} = \bar{\rho}\varepsilon_1 + \bar{\rho}\varepsilon_2 + \bar{\rho}\varepsilon_3, \quad (5.58)$$

where

$$\bar{\rho}\varepsilon_1 = \overline{\bar{\mu} \frac{\partial u'_i}{\partial x_j} \left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_k}{\partial x_k} \delta_{ij}}, \quad (5.59)$$

$$\bar{\rho}\varepsilon_2 = \overline{\mu' \left[\frac{\partial u'_i}{\partial x_j} \left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_k}{\partial x_k} \delta_{ij} \right]}, \quad (5.60)$$

$$\bar{\rho}\varepsilon_3 = \overline{\mu' \frac{\partial u'_i}{\partial x_j} \left[\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} \right]}. \quad (5.61)$$

The first part is the mean viscosity related term, and the last two parts are viscosity fluctuation related terms. Huang [134] found that the viscosity fluctuation related parts occupy a significant fraction (up to 16%) of $\bar{\rho}\varepsilon$ in the viscous sublayer. In this chapter, Figure 5.37(a) shows the ratio of $\bar{\rho}\varepsilon_1$ to the exact turbulent dissipation $\bar{\rho}\varepsilon$. The ratio for Case AIR is below 1 near the wall and slightly above 1 at $y^* > 10$, and the maximum deviation from unity is about 13%. This finding agrees with the result of Huang [134]. For dense-vapour cases, $\varepsilon_1/\varepsilon$ shows the same trend in the

cases with weak non-ideal effects (Case R1 and M1), but the opposite trend in the cases with strong non-ideal effects (Case R3 and M3). The largest deviation from unity is seen in Case R3 (about 25%), indicating that the viscosity fluctuation plays an important role in the decomposition of turbulent dissipation. The deviation from unity is smaller in MDM, which means the molecular-complexity effects can reduce the influence of viscosity fluctuation. This result shows that the influence of viscosity fluctuation cannot be ignored in the modeling of ε for dense vapours.

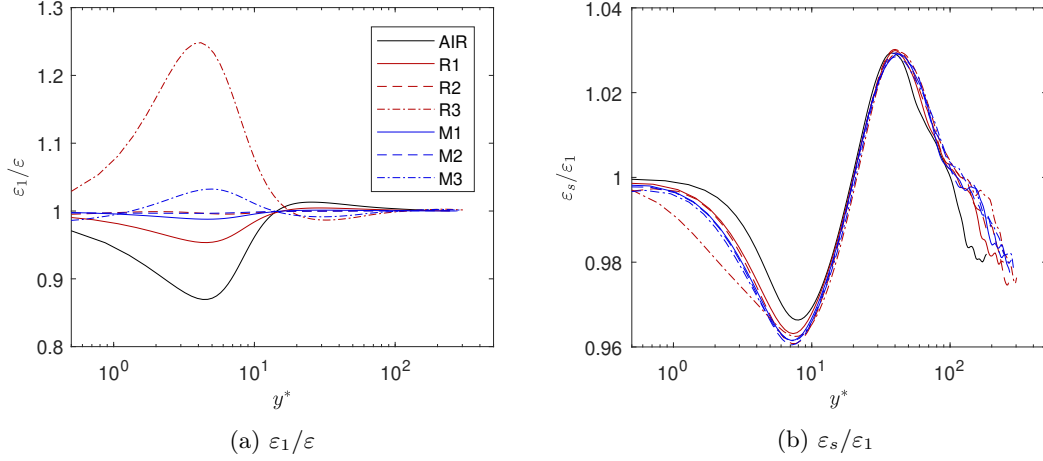


Figure 5.37: Decomposition of turbulent dissipation.

Then, $\bar{\rho}\varepsilon_1$ can be divided into solenoidal, dilatational and inhomogeneous parts:

$$\bar{\rho}\varepsilon_1 = \bar{\rho}\varepsilon_d + \bar{\rho}\varepsilon_s + \bar{\rho}\varepsilon_I, \quad (5.62)$$

where

$$\bar{\rho}\varepsilon_s = \frac{1}{2}\overline{\mu\omega'_i\omega'_i}, \quad (5.63)$$

$$\bar{\rho}\varepsilon_d = \frac{4}{3}\overline{\mu\frac{\partial u'_l}{\partial x_l}\frac{\partial u'_k}{\partial x_k}}, \quad (5.64)$$

$$\bar{\rho}\varepsilon_I = 2\bar{\mu}\left[\frac{\partial^2\overline{u'_i u'_j}}{\partial x_i\partial x_j} - 2\frac{\partial}{\partial x_i}\left(\overline{u'_i\frac{\partial u'_j}{\partial x_j}}\right)\right]. \quad (5.65)$$

Huang [134] proposed that the dilatational part and the inhomogeneous part occupy only a small proportion of $\bar{\rho}\varepsilon_1$ in air flows. In this chapter, Figure 5.37(b) shows the ratio between ε_s and ε_1 for dense vapours. The profile of it in all cases has a low point near the wall at $y^* \approx 8$ and a peak at $y^* \approx 40$. The maximum deviation from unity is smaller than $\pm 4\%$ and shows insignificant difference between air case and dense-vapour cases. This means that $\bar{\rho}\varepsilon_1$ still can be assumed to be almost solenoidal in dense vapours.

Turbulent Prandtl number models

Figure 5.38 shows the profile of the turbulent Prandtl number according to the definition (Equation 5.35). In Case AIR, Pr_t follows the same trend as in Huang [134], it has a peak value at $y_{wall}/l \approx 0.3$ and then decreases with increasing wall distance from about 1.0 to 0.6. In dense-vapour cases, it also follows the same trend, while the peak value of Pr_t is closer to the wall than in air. This peak value is larger in the case with strong molecular-complexity effects and non-ideal effects. For example, the maximum peak value is seen in Case M3, where $Pr_{t,peak} \approx 1.13$ (see blue dash-dotted line in Figure 5.38). In the region $y_{wall}/l > 0.3$, profiles of Pr_t is nearly coincided between the cases.

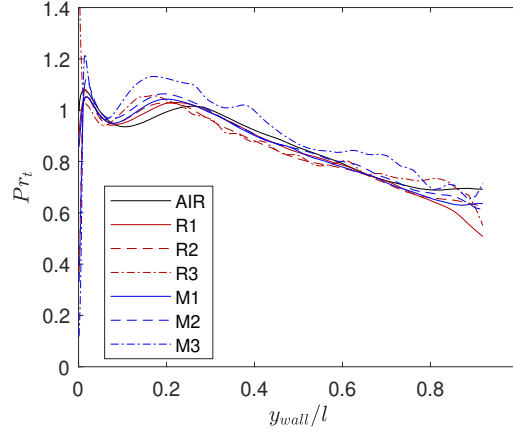


Figure 5.38: Turbulent Prandtl number Pr_t .

The simplest model of Pr_t is to assume that it is constant and equal to 0.9, and this model leads to an error of about $\pm 30\%$ for all gases. Another widely-used model is proposed by Cebeci [288] and validated by Na & Habib [289]:

$$Pr_t = \frac{k}{k_\theta} \frac{1 - \exp(-y^+/A)}{1 - \exp(-y^+ \sqrt{Pr}/B)}, \quad B = \sum_{i=1}^5 C_i (\log_{10} Pr)^{i-1} \quad (5.66)$$

with $k = 0.41$, $k_\theta = 0.46$, $A = 26$, $C_1 = 34.96$, $C_2 = 28.79$, $C_3 = 33.95$, $C_4 = 6.3$, $C_5 = -1.186$. The Pr_t calculated by Cebeci's model for all cases are shown in Figure 5.39(a). In this model, Pr_t decreases monotonically and approaches 0.9 as wall distance increases, and the difference between cases is not significant. Compared with the exact turbulent Prandtl number (in Figure 5.38), Cebeci's model fails to predict the local peak of Pr_t at $y_{wall}/l \approx 0.2$ and also overestimates Pr_t in channel central region.

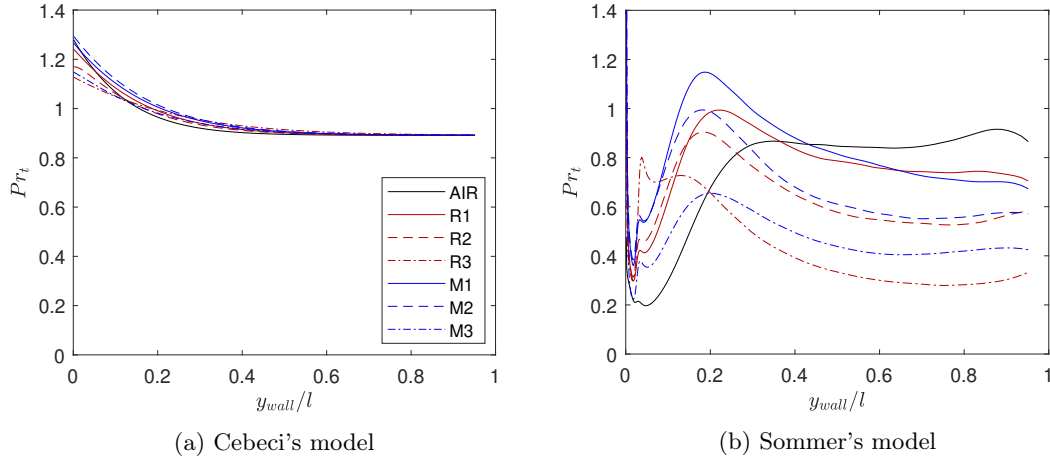


Figure 5.39: Turbulent Prandtl number calculated by models.

Another important model of Pr_t is proposed by Sommer [290],

$$Pr_t = \frac{\mu_t/\bar{\rho}}{\alpha_t}, \quad (5.67)$$

where α_t is turbulent thermal conductivity,

$$\alpha_t = 0.11 f_\lambda k_t \left[k_t \overline{T'^2} / \varepsilon \varepsilon_T \right]^{1/2}. \quad (5.68)$$

The damping function f_λ is given as

$$f_\lambda = \left[f_{w,\varepsilon_T} \frac{0.1}{\sqrt[4]{R_t}} \right] + [1 - \exp(-y^+/45)]^2, \quad (5.69)$$

where

$$f_{w,\varepsilon_T} = \exp \left[- (R_t/80)^2 \right]. \quad (5.70)$$

Dissipation rate ε_T is defined by

$$\varepsilon_T = \frac{\lambda}{\rho c_p} \frac{\partial T}{\partial x_k} \frac{\partial T}{\partial x_k}. \quad (5.71)$$

In Sommer's work, $\overline{T'^2}$ and ε_T are calculated by a two-equation model of $\overline{T'^2} - \varepsilon_T$ (with similar concept of $k - \varepsilon$ model). While in this chapter, the values of $\overline{T'^2}$ and ε_T are directly obtained from DNS results. Figure 5.39(b) shows the Pr_t calculated by Sommer's model. The local peak of Pr_t at $y_{wall}/l \approx 0.2$ can be predicted by this model, but Pr_t in the near-wall region is underestimated in all cases. Moreover, in the entire boundary layer, Pr_t in Case R3 and M3 are significantly underestimated (dash-dotted lines in Figure 5.39(b)), which means the strong non-ideal effects lead to a large error for this model. In summary, the two complicated models of Pr_t do not

perform better than the simplest model, $Pr_t = 0.09$, in dense vapours.

5.6 Chapter summary

In this chapter, the impact of molecular-complexity effects and non-ideal effects on the inner layer of turbulent boundary layers is studied using DNS, which is a fundamental study of wall-bounded turbulent behaviours with non-ideal gases. Two organic gases with different molecular weights are studied. They are R1233zd(E) and MDM, which can represent commonly-used organic fluids. Fully-developed turbulent channel flows over cold isothermal walls with these two gases are simulated and compared with air flows to analyse the molecular-complexity effects. For each organic gas, three DNS cases are simulated to analyse the non-ideal effects, whose thermodynamic states are in the dilute-gas region, near the saturation line, and in the supercritical region.

For mean flow fields, the mean temperature rise (from cold wall to channel centre) is shown to be lower in dense vapours than in air. This temperature rise is found to be proportional to $Pr_G Ec_G$, whose value is directly reduced by both molecular-complexity effects and non-ideal effects. The mean density decrease (from the wall to channel centre) is related to the mean temperature rise in ideal-gas flows due to the nearly constant pressure. In dense-vapour flows, non-ideal effects amplify this density drop, because the absolute value of the derivative $\left(\widehat{\frac{\partial \rho}{\partial T}}\right)_p$ is significantly higher. For other mean properties, the molecular-complexity effects reduce the rise (from the wall to centre) of the speed of sound ($\bar{c}$) and dynamic viscosity ($\bar{\mu}$); however, the non-ideal effects can reverse the $\bar{c}$ and $\bar{\mu}$ profiles from an increase to a decrease, therefore leading to a ‘liquid like’ behaviour. In addition, the impact of non-ideal effects is always stronger in the gas with less complex molecules, R1233zd(E), than in the gas with more complex molecules, MDM, suggesting that non-ideal effects should be paid more attention in the gases with moderate molecular weight.

The mean streamwise velocity profile as a function of the semi-local normalised wall distance y^* in dense vapour can coincide to that in air, if the Trettel & Larsson (TL) [11] velocity transformation is applied. The beginning position of log-law region is shown at $y^* \approx 40$ in all cases. This suggests that, in RANS simulation method, the current wall function for air flows is able to be used for dense-vapor flows, but the y^* and the TL transformation have to be considered. Walz’s equation, which relates the mean velocity and mean enthalpy to define the RANS wall function, is valid in dense vapours if the equation is used in terms of enthalpy instead of temperature. The error of Walz’s equation in dense-vapour cases is within $\pm 3\%$ (smaller than in air) when compared with DNS results.

For turbulent fluctuation fields, the molecular-complexity effects and non-ideal effects affects

the distributions of the root mean square of the velocity fluctuation (u'_{rms} , v'_{rms} and w'_{rms}) as well as the Reynolds shear stress ($\widetilde{u''v''}$) through a Reynolds number effect of $Re_{\tau,c}^*$. The intensities (root mean square values) of temperature, pressure and density fluctuations (T'_{rms} , p'_{rms} and ρ'_{rms}) are no longer of the same order of magnitude for dense vapours, because T'_{rms} is significantly reduced by both molecular-complexity effects and non-ideal effects. A new relationship between T'_{rms} , p'_{rms} and ρ'_{rms} is proposed in Equation 5.18, with a maximum deviation of 2% in dense vapours when compared with DNS results. The correlations between T' , p' and ρ' within the inner layer are important for turbulence boundary layers, and are found to be qualitatively influenced by molecular-complexity effects and non-ideal effects. Stronger molecular-complexity effects change the density from a strong negative correlation with temperature to a strong positive correlation with pressure, except for the very near wall region where isothermal effects are dominant. The strong non-ideal effects cause temperature to be highly positively correlated to pressure in the gas with more complex molecules, MDM, but highly negatively correlated to density in the gas with less complex molecules, R1233zd(E). To understand the change in these correlations, the impact of both the vorticity mode and the sound-wave mode on the generation of thermal property fluctuations are analysed. It is found that the sound-wave mode significantly increases density fluctuation through molecular-complexity effects, and this mode increases temperature fluctuation through non-ideal effects. Consequently, the sound-wave mode rather than the vorticity mode is the dominant mode for generation of thermodynamic property fluctuations in some dense-vapour cases.

Near-wall turbulence structure is analysed on the slice of the instantaneous flow field at $y^* \approx 10$. The low-speed ‘streak’ structure in dense vapours is similar to that in air, and the spanwise spacing for adjacent streak is still about 85 semi-local wall units. However, this ‘streak’ structure in some dense-vapour cases is broken in the fields of T' and ρ' , and these fields resemble the field of p' rather than the field of u' . This finding confirms our conclusion that the sound-wave mode can be dominant in some dense-vapour flows. For vortex structure within the entire boundary layer, when y^* is used to account for the variable gas properties affected by molecular-complexity effects and non-ideal effects, these effects have no significant influence on the vortex shape and concentration.

Turbulence modelling for dense-vapour flows is analysed by using DNS data. The difference between Farve and Reynolds averages is insignificant in dense vapours. However, when non-ideal effects are strong, the strong Reynolds analogy (SRA) is invalid: The correlation coefficient R_{uh} is significantly reduced by non-ideal effects; and the relationship between streamwise velocity and enthalpy fluctuation intensity (u'_{rms} and h'_{rms}) does not follow the state-of-the-art modified SRA models (proposed by Gaviglio [136] and Huang [134]). This is because the deviation between velocity mixing length scale and enthalpy mixing length scale becomes very large.

The energy budget in dense-vapour flows is compared with air flows. The production and viscous dissipation terms are only moderately affected by molecular-complexity effects and non-ideal effects, but the turbulent transport and viscous dissipation terms can be noticeably enhanced in the inner layer. The velocity-pressure and dilatation terms are still of one order of magnitude lower than other terms in dense-vapour flows. Important modelling issues for $k - \varepsilon$ RANS are investigated in dense vapours, by comparing the terms calculated from models with those directly from DNS results. Firstly, three eddy viscosity models, LB, CH and SH models (proposed by Lam & Bremhors [285], Chien [286], Shih [287] respectively), are analysed and show that the SH model has a better estimate in log-law region than the other two models in all dense-vapour cases. Secondly, the models of viscous transport term and turbulent transport term in the k equation still follow the trend of their exact profile, and the error of the models is not significantly increased by molecular-complexity effects and non-ideal effects. Thirdly, in the decomposition of the turbulent dissipation $\bar{\rho}\varepsilon$, the part associated with viscosity fluctuation can occupy 25% of $\bar{\rho}\varepsilon$ in some dense-vapour cases. In the decomposition of the part associated with mean viscosity, the dilatational and inhomogeneous parts still occupy only $\pm 4\%$ and are small compared to the solenoidal part in dense vapours. Finally, the turbulent Prandtl number in boundary layers of dense vapours is still within $0.6 < Pr_t < 1.1$ except in the very near-wall region, which means that it causes an uncertainty of $\pm 30\%$ if $Pr_t = 0.9$ is assumed. This uncertainty cannot be reduced by the two models proposed by Cebeci [288] and Sommer [290], suggesting that a more accurate turbulent Prandtl number model should be developed in the future.

Chapter 6

Study of Bypass Laminar-Turbulent Transition on a Flat Plate of Dense Vapours using DNS Method

6.1 Overview

To understand the boundary layer development in dense-vapour flows, it is meaningful to study the laminar-turbulent transition in fundamental flows. In this chapter, the bypass-type transition on flat plates at $Ma_\infty = 2.25$ in dense vapours is studied, and the uniform coming flows over a flat plate with zero incident angle are simulated using the DNS method. Two organic gases (R1233zd(E) and MDM) and air are studied, and three different thermodynamic states of each organic gas corresponding to those in Chapter 5 are considered. The basic information on these gases is already listed in Table 5.1 (see Chapter 5.1). The difference between laminar-turbulent transition in air flows and dense-vapour flows is compared and analysed in this chapter.

This chapter is organised as follows. In Chapter 6.2, the case setup information is introduced; the transition is analysed by turbulent statistics in Chapter 6.3. The coherent structures are discussed in Chapter 6.4 and analysed by using the POD method in Chapter 6.5.

6.2 Cases Setup

The simulation domain for the flow on a flat-plate is shown in Figure 6.1. The uniform incoming flows cause a laminar boundary layer at the leading-edge of the plate and the simulation domain

starts at the laminar boundary layer. A blowing and suction boundary is applied at the leading area of the simulation domain to induce the bypass-type transition, and then the fully-developed turbulent boundary layer is reached before the end of the domain. The DNS method of 3D compressible NS equations introduced in Chapter 3.1.1 is used to simulate the flow, and the source terms in the NS equations are zero here.

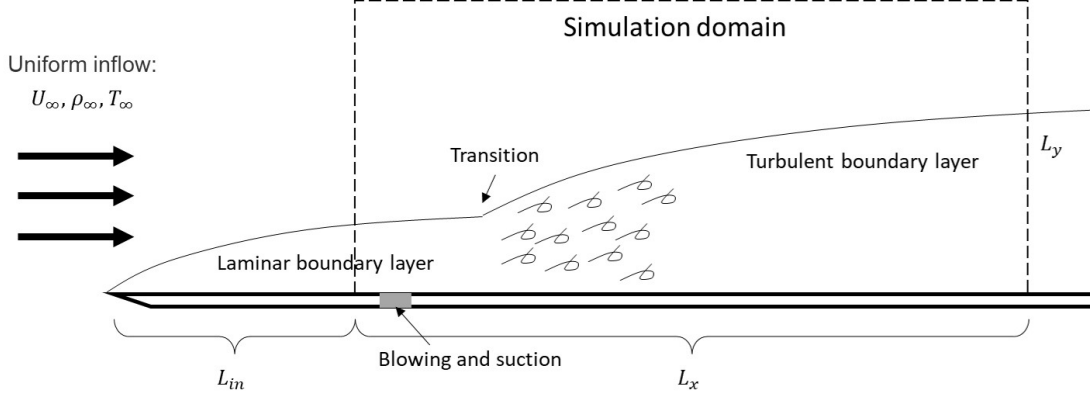


Figure 6.1: Simulation domain of flat-plate flows.

The inlet boundary is located at L_{in} downstream of the leading edge of the flat plate. The velocity and thermodynamic states at different wall distance at the inlet boundary are obtained from a pre-simulation of 2D steady laminar boundary layers (see Chapter 6.2.3). This boundary condition is time-independent and uniform at the same wall distance, and the spanwise velocity component is zero ($w = 0$). The wall boundary is non-slip adiabatic boundary represented as follows:

$$u_i = 0, \quad \frac{\partial T}{\partial y} = 0, \quad \frac{\partial p}{\partial y} = 0. \quad (6.1)$$

The outlet boundary and the upper boundary are set as non-reflect boundaries, and the spanwise boundary is the periodic boundary. The governing equations are solved by the finite difference method, where the convective flux derivatives and viscous flux derivatives are approximated by the seventh-order upwind difference scheme and the sixth-order central scheme respectively. The time advance is solved by the third-order Runge-Kutta method, which is the same as that in Chapter 5.

6.2.1 Air Cases

As a reference for comparison, an air case is simulated under the same conditions as Rai [291], Pirozzoli [292], and Li [293], which is close to the experimental condition of Shutts (reported by Fernholz [123]). The characteristic length of this case is one inch ($L_{char} = 1$ in.), and the characteristic velocity and thermodynamic state are their values of uniform inflows. Normalised

parameters are defined as:

$$\hat{x}_i \equiv \frac{x_i}{L_{char}}, \quad \hat{u}_i \equiv \frac{u_i}{U_\infty}, \quad \hat{t} \equiv \frac{tU_\infty}{L_{char}}, \quad \hat{T} \equiv \frac{T}{T_\infty}, \quad \hat{p} \equiv \frac{p}{\rho_\infty U_\infty^2}, \quad (6.2)$$

The Reynolds number ($Re_\infty \equiv \rho_\infty U_\infty L_{char}/\mu_\infty$) is equal to 635,000, and the Mach number ($Ma_\infty \equiv U_\infty/c_\infty$) is equal to 2.25. The simulation domain starts at $\hat{x} = 4$ and ends at $\hat{x} = 16.25$, and domain lengths in the wall-normal and spanwise directions are $\hat{L}_y = 0.22$ and $\hat{L}_z = 0.175$. The blowing and suction boundary condition is applied at the wall region $4.5 < \hat{x} < 5$, which is used to approximate the disturbance caused by wall roughness. The wall-normal velocity component in the blowing and suction boundary is given as follows: [291, 292, 293]:

$$v(\hat{x}, \hat{z}, \hat{t}) = A_{bs} U_\infty f(\hat{x}) g(\hat{z}) h(\hat{t}), \quad (6.3)$$

where

$$A_{bs} = 0.04, \quad (6.4)$$

$$f(\hat{x}) = 4 \sin \theta_{bs} (1 - \cos \theta_{bs}) / \sqrt{27}, \quad \theta_{bs} = 2\pi(\hat{x} - 4.5)/(5 - 4.5), \quad (6.5)$$

$$g(\hat{z}) = \sum_{l=1}^{10} Z_l \sin[2\pi l(z/L_z + \phi_l)], \quad \sum_{l=1}^{10} Z_l = 1, \quad Z_l = 1.25 Z_{l+1}, \quad (6.6)$$

$$h(\hat{t}) = \sum_{m=1}^5 T_m \sin(m\omega_{bs}\hat{t} + 2\pi\phi_m), \quad \sum_{m=1}^5 T_m = 1, \quad T_m = 1.25 T_{m+1}. \quad (6.7)$$

ϕ_l and ϕ_m are randomly generated between 0 and 1. ω_{bs} is the fundamental frequency of the blowing and suction boundary condition, it is equal to 2.5π which means that the period of the boundary condition is $\hat{t}_{p,bs} = 0.8$. The profile of $v(\hat{x}, \hat{z}, \hat{t})$ is shown in Figure 6.2.

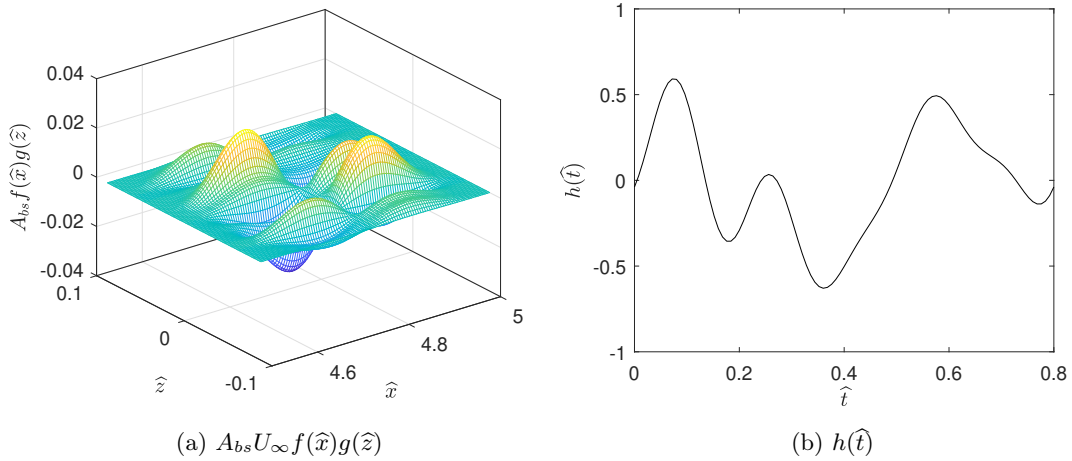


Figure 6.2: Blowing and suction boundary condition: $v(\hat{x}, \hat{z}, \hat{t}) = A_{bs} U_\infty f(\hat{x}) g(\hat{z}) h(\hat{t})$.

Grid independence of this case is checked on six different grids whose element numbers are given in Table 6.1. It should be clarified that all grids are gradually coarsened before outlet boundary to reduce the disturbance caused by the numerical treatment at the outlet boundary. The skin friction coefficient C_f distribution on streamwise direction and mean velocity profile (after Van Diredt transformation [128]) at $\hat{x} = 8.8$ calculated on these grids are compared and shown in Figure 6.3. The profile of C_f and δ_{99} are grid independent when the node numbers are greater than $2193 \times 81 \times 256$, so the 'fine grid' is sufficient for the simulation.

Grid	X-	Y-	Z-
Coarse grid A	1285	81	128
Coarse grid B	1660	81	192
Coarse grid C	2193	72	256
Fine grid	2193	81	256
X- refined grid	3032	81	256
Z- refined grid	2193	81	512

Table 6.1: Information of grid size for grid independence.

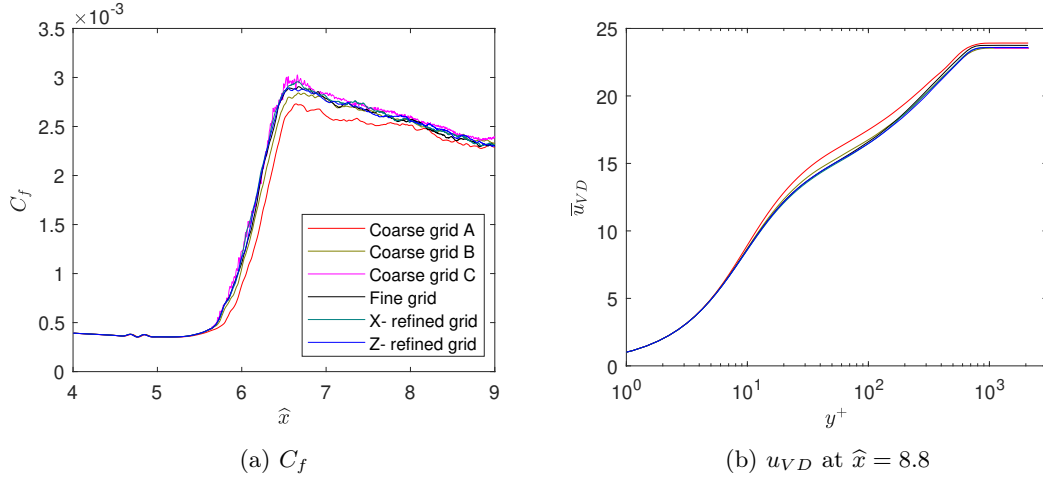


Figure 6.3: Grid independence of air case.

6.2.2 Dense-vapour Cases

For two organic gases, three cases with different thermodynamic states are simulated located in the dilute-gas region, near the saturation line, and in the supercritical region of each gas, respectively. They are named by Cases R1 - R3 and Cases M1 - M3, and they are the same as the cases in

Chapter 5. The characteristic thermodynamic states for the flat-plate flows are defined as the states of uniform incoming flows (T_∞, ρ_∞) and correspond to those of the channel flow cases in Chapter 5, which are already shown in T-S diagrams in Figure 5.3 (a) and (b). Detailed information of dense-vapour cases is shown in Table 6.2. The relative temperature and density $(T_\infty/T_{cr}$ and $\rho_\infty/\rho_{cr})$ of the cases increase from Case R1 to R3 and also from Case M1 to M3 (see Table 6.2), and the compressibility factor Z_∞ , the fundamental derivative of gasdynamics Γ_∞ and the normalised heat capacity $c_{v,\infty}/R$ are also listed. In these dense-vapour cases, the Reynolds number Re_∞ and the Mach number Ma_∞ are the same as in Case AIR. It should be noted that the characteristic length L_{char} in dense-vapour cases is no longer one inch to obtain the same Re_∞ , and their values are at one or two orders of magnitude than that in Case AIR (see Table 6.2). The leading edge of the flat plate starts at $\hat{x} = 0$ and inlet boundary of DNS simulation domain starts at $\hat{x} = 4$ in all dense-vapour cases, and the inlet boundary layer thickness are listed in Table 6.2. Three definitions of boundary layer thickness are used here: 99% velocity thickness δ_{99} , displacement thickness δ_1 , and momentum thickness θ . δ_{99} is defined as the wall distance of the position with $\bar{u} = 0.99U_\infty$, and the other thicknesses are defined as follows [294]:

$$\delta_1 \equiv \int_0^\infty \left(1 - \frac{\rho u}{\rho_\infty U_\infty}\right) dy, \quad (6.8)$$

$$\theta \equiv \int_0^\infty \frac{\rho u}{\rho_\infty U_\infty} \left(1 - \frac{u}{U_\infty}\right) dy. \quad (6.9)$$

θ_{in} of Case AIR is approximately equal to those of dense-vapour cases (except Case R3), but $\delta_{99,in}$ and $\delta_{1,in}$ of Case AIR is not the same to those of dense-vapour cases.

The spatial resolutions in three directions $(\Delta x^+, \Delta y_w^+, \Delta z^+)$ are shown in Table 6.2. The spatial resolution for Case AIR is at the same level as in the works of Li [295] and Pirozzoli [292], while the resolution in the X- and Z- directions is larger and corresponds to the 'Grid B' in the work of Pirozzoli [292]. The results of dense-vapour cases calculated on this grid are compared with those on 'X- refined grid' and 'Z- refined grid' whose information is already given in Table 6.1, and the results of Cases R3 and M3 are shown in Figure 6.4. It can be seen that the simulation results of Cases R3 and M3 on the 'Fine grid' are only slightly different from those on the other grids, so the results of dense-vapour cases are independent of the number of grid nodes, and the spatial resolutions in these two directions are considered large enough here.

Line styles for flat-plate DNS cases of the following figures in this chapter (if not specifically claimed) are shown in Table 6.3. The black line refers to Case AIR, the red lines refer to R1233zd(E) cases and the blue lines refer to MDM cases.

Case	AIR	R1	R2	R3	M1	M2	M3
Gas	Air	R1233zd(E)			MDM		
T_∞/T_{cr}	-	0.86	0.98	1.03	0.86	0.98	1.03
ρ_∞/ρ_{cr}	-	0.02	0.27	1.00	0.02	0.27	1.00
Z_∞	1	0.96	0.67	0.32	0.96	0.68	0.33
Γ_∞	1.2	1.01	0.82	1.90	0.97	0.59	1.62
$c_{v,\infty}/R$	2.5	13.4	15.7	17.3	53.1	58.3	61.9
Re_∞	635,000	635,000	635,000	635,000	635,000	635,000	635,000
Ma_∞	2.25	2.25	2.25	2.25	2.25	2.25	2.25
$L_{char}[mm]$	25.4	2.59	0.33	0.26	4.07	0.52	0.38
$\hat{\delta}_{99,in}$	0.0180	0.0136	0.0133	0.0126	0.0128	0.0127	0.0126
$\hat{\delta}_{1,in}$	0.0096	0.0054	0.0053	0.0047	0.0046	0.0046	0.0045
$\hat{\theta}_{in}$	0.0016	0.0017	0.0016	0.0013	0.0017	0.0017	0.0016
Δx^+ at $\hat{x} = 8.8$	16.0	31.6	34.1	41.7	37.5	38.3	40.4
Δy_w^+ at $\hat{x} = 8.8$	0.25	0.49	0.52	0.64	0.58	0.59	0.62
Δz^+ at $\hat{x} = 8.8$	6.4	12.7	13.7	16.8	15.1	15.4	16.3

Table 6.2: Set-up information for flat-plate DNS cases.

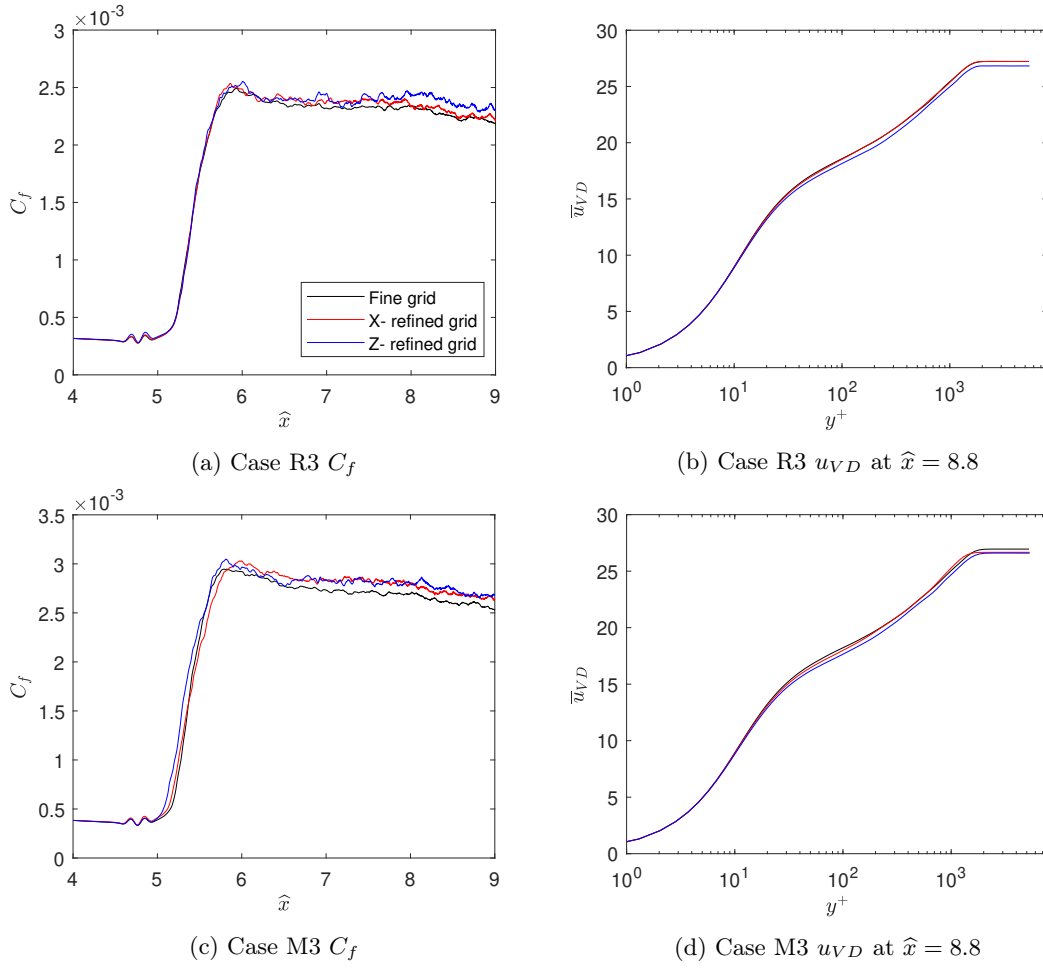


Figure 6.4: Grid independence of dense-vapour cases.

Case	AIR	R1	R2	R3	M1	M2	M3
Line style	—	—	- - -	- . .	—	- - -	- . .
	(black)	(red)	(red)	(red)	(blue)	(blue)	(blue)

Table 6.3: Line styles for DNS cases of flat-plate flows.

6.2.3 Pre-simulation of laminar boundary layers

The growth of the laminar boundary layer from the leading edge of the flat plate to the beginning of the DNS simulation domain is achieved by a pre-simulation for each case. The simulation domain of the pre-simulation is shown in Figure 6.5. In the streamwise direction, this domain is in the region $-5 < \hat{x} < 15$; and in wall-normal direction, it is in the region $0 < \hat{y} < 0.22$.

The boundary thickness under three definitions is given in Figure 6.6. The theoretical thickness

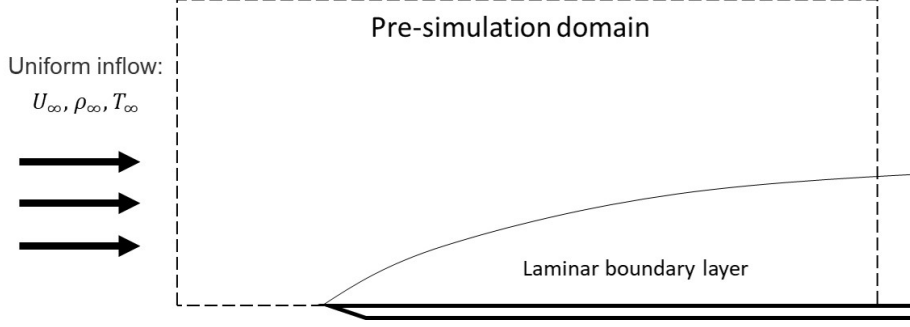


Figure 6.5: Pre-simulation domain of 2D laminar flows at the leading edge of flat plate.

calculated from the Blasius solution conditions [294] is also in Figure 6.6, which is given by:

$$\delta_{99} \approx 5.0 \frac{x}{\sqrt{Re_x}}, \quad (6.10)$$

$$\delta_1 \approx 1.72 \frac{x}{\sqrt{Re_x}}, \quad (6.11)$$

$$\theta \approx 0.664 \frac{x}{\sqrt{Re_x}}. \quad (6.12)$$

For δ_{99} and δ_1 , the Case AIR deviates further from the theoretical values than dense-vapour cases due to the larger variation in density and viscosity; while for θ , the cases with stronger non-ideal effects deviate further from the theoretical values, and the largest deviation is seen in Case R3.

The flow properties at the DNS inlet boundary ($\hat{x} = 4$) are compared in Figure 6.7. The comparison of the dense-vapour cases with Case AIR shows that the wall temperature is lower in cases with stronger molecular-complexity effects (MDM cases) and stronger non-ideal effects (Cases R3 and M3), while the wall density is lower in cases with stronger molecular-complexity effects but weaker non-ideal effects. These differences can be explained in a similar way as introduced in Chapter 5.3.1, so they are not repeated again here. The trends of dynamic viscosity profile in cases with strong non-ideal effects (Cases R3 and M3) are opposite to those in the other cases, which is a ‘liquid like’ behaviour. This behaviour is also found in the turbulent channel flows (also see Chapter 5.3.1).

In summary, even Case AIR has the same $Re_{x,in}$ as dense-vapour cases, whose boundary layer thicknesses are not the same due to the different profiles of thermal properties. Case AIR has a similar inlet θ to dense-vapour cases, but δ_{99} and δ_1 are not. This difference is due to different thermal property profiles, which are influenced by both molecular-complexity effects and non-ideal effects.

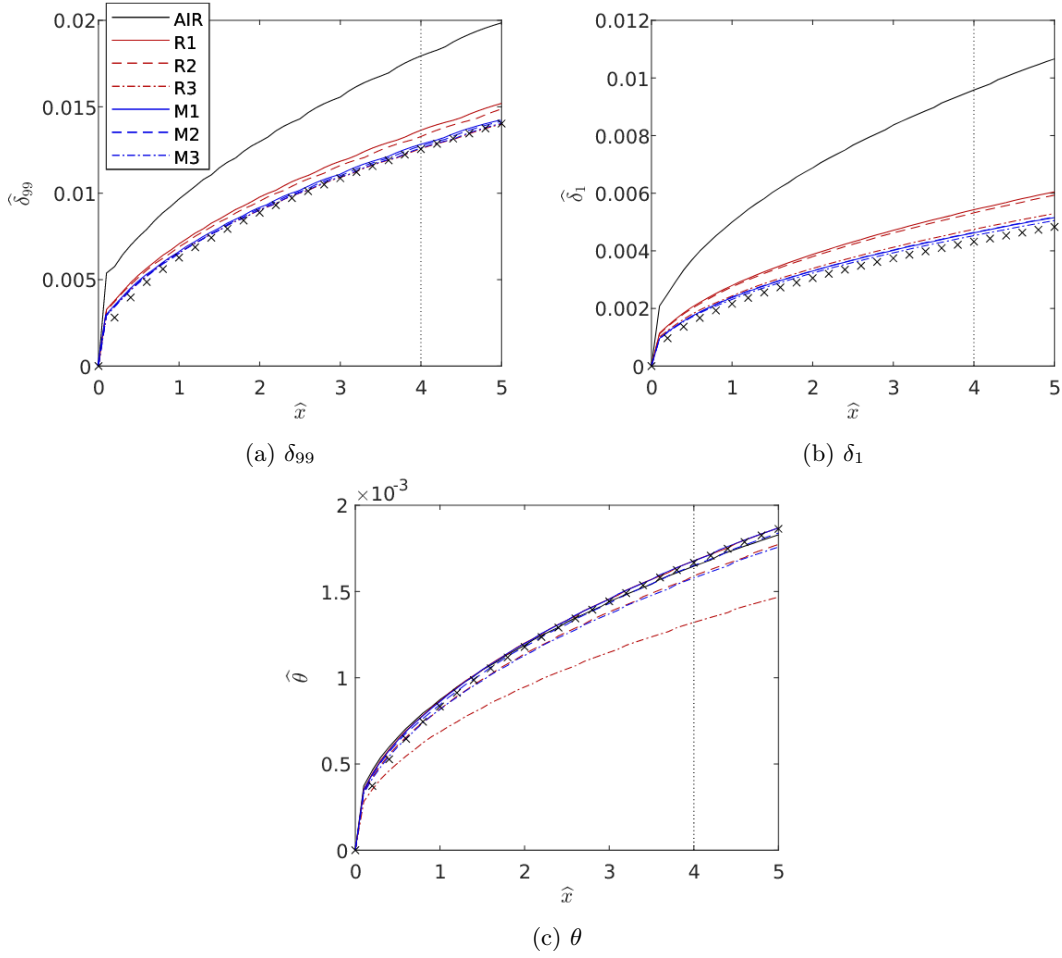


Figure 6.6: Laminar boundary layer thickness. Lines refer to the pre-simulation results of each case, and dots 'x' refer to theoretical thickness.

6.2.4 Validation of Flat-Plate Flow DNS method

The DNS method used in this chapter is compared with the work of Pirozzoli [292] and Li [293]. It should be noted that there are only published experimental and numerical results of flat-plate flows using air, so the DNS method is validated by comparing the results of the air case results with the reference. C_f distribution and $\bar{u}_{VD}$ profile at $\hat{x} = 8.8$ are compared with those of the reference. C_f is the skin friction coefficient which is defined as follows:

$$C_f \equiv \frac{2\tau_w}{\rho_\infty U_\infty^2}, \quad (6.13)$$

and $\bar{u}_{VD}$ is the mean streamwise velocity after VD transformation (see Equation 5.11 in Chapter 5.3.3). Figure 6.8 (a) shows that the distribution of C_f in this work is similar to that in the work of Li [295], while C_f in the work of Pirozzoli [292] increases earlier due to different treatments of the inlet boundary and blowing-and-suction boundary. The slopes of C_f profiles in the transition

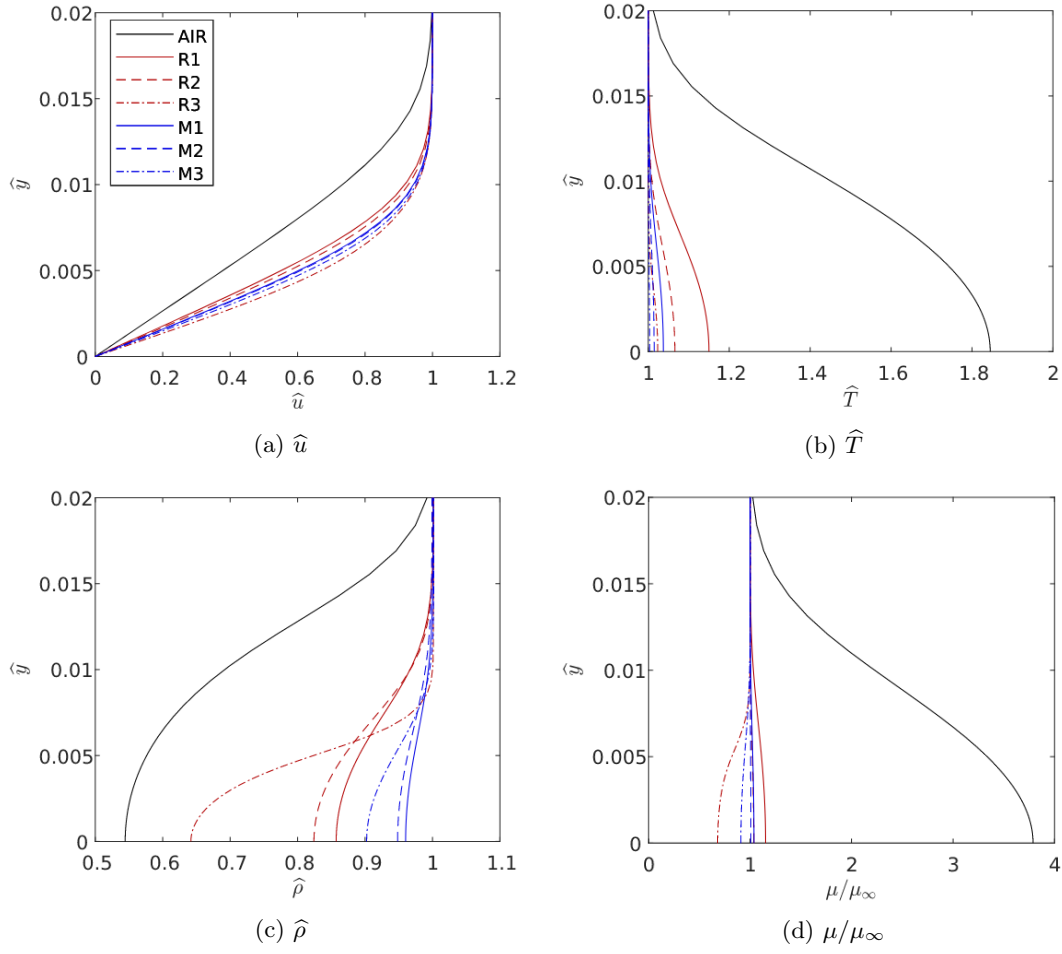


Figure 6.7: The distribution of flow properties at the inlet boundary of the DNS domain.

region and in the fully-developed turbulent region are almost identical. Figure 6.8 (b) shows that the velocity profiles are almost congruent, and $\bar{u}_{VD}$ in this work in the region far from the wall ($y^+ > 100$) is slightly larger than that in two reference works. In summary, the DNS method used in this chapter is valid. Further experimental tests with dense-vapour flat-plate flows are expected to validate this DNS method in dense-vapour flows.

6.3 Statistics of Laminar-Turbulent Transition

6.3.1 Boundary Layer Thickness

The boundary layer thickness profiles of the laminar-turbulent transition in all cases are shown in Figure 6.9. Figure 6.9 (a) shows that $\hat{\delta}_{99}$ increases rapidly at the end of the laminar boundary layer, and the starting point of the rapid increase of $\hat{\delta}_{99}$ is listed in Table 6.4 (represented by $\hat{x}_{br,s}$). $\hat{x}_{br,s}$ can be a signal that the breakdown process has started. $\hat{x}_{br,s}$ of all dense-vapour cases are

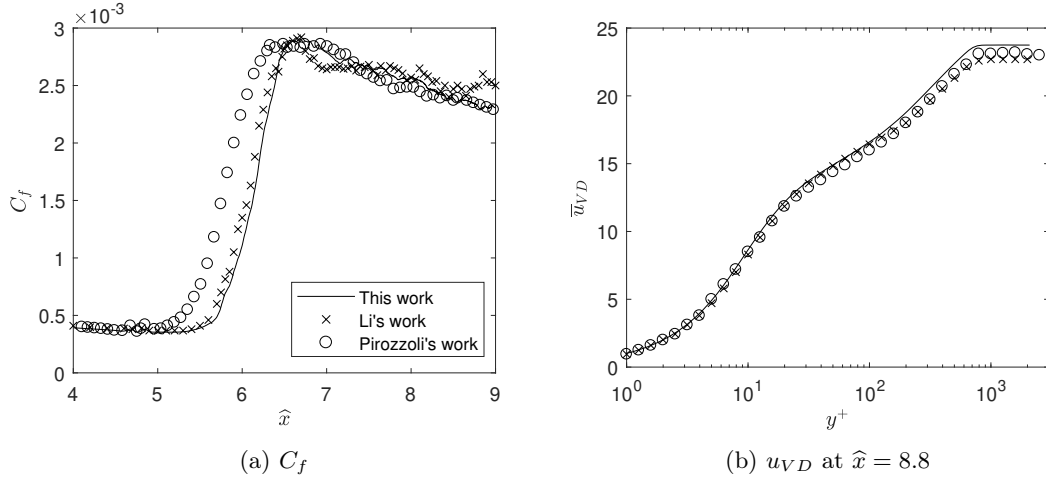


Figure 6.8: Validation of flat-plate DNS method.

significantly earlier than Case AIR, which means the breakdown process in all dense-vapour cases is earlier than in Case AIR.

Case	AIR	R1	R2	R3	M1	M2	M3
$\hat{x}_{br,s}$	5.94	5.39	5.31	5.26	5.26	5.24	5.24

Table 6.4: Start position of the rapid increase of δ_{99} .

Figure 6.9 (b) shows that in all cases the displacement thickness $\hat{\delta}_1$ first decreases and then increases after the breakdown starts. $\hat{\delta}_1$ is larger in Case AIR than in dense-vapour cases as the breakdown starts, and it also increases much faster. Figure 6.9 (c) shows that the momentum thickness $\hat{\theta}$ increases monotonically after the breakdown starts. $\hat{\theta}$ is smaller in Case AIR than in dense-vapour cases (except Case R3), and the slope of this increase is slightly larger in Case AIR. In summary, the difference between air case and dense-vapour cases is significant but the difference between each dense-vapour cases is insignificant (except Case R3).

6.3.2 Skin Friction Coefficient

The distributions of C_f in the streamwise direction are shown in Figure 6.10. In all cases, a significant rise in C_f is seen, which indicates the transition. It shows that C_f starts to increase earliest in MDM cases (blue lines), where the molecular-complexity effects are the strongest. This increasing slope of the profile is also larger in dense-vapour cases than in Case AIR. The position of the end of the breakdown, $\hat{x}_{br,e}$, is defined at the peak point of the C_f profile, and the values for all cases are also listed in Table 6.5. The understanding of the transition process will be discussed in the next section (Chapter 6.4) with the analysis of vortex structures, while the distribution of

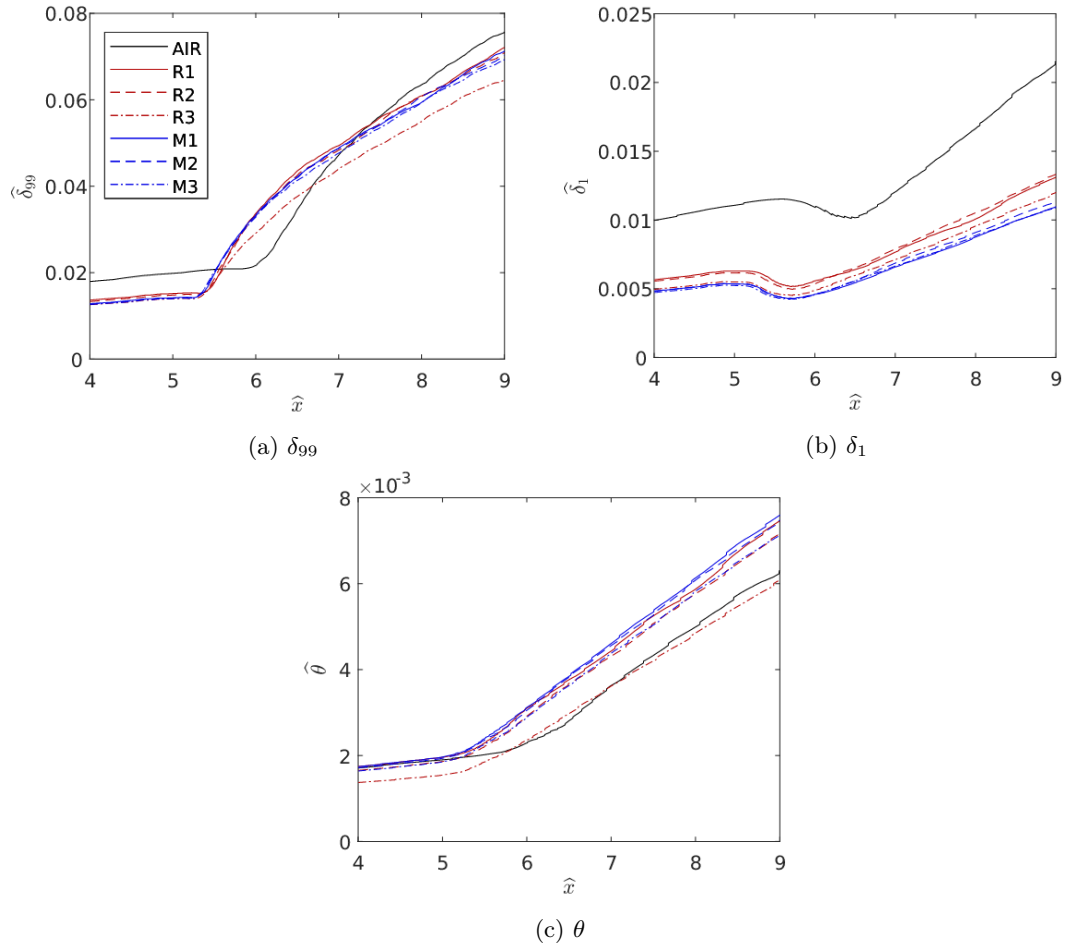


Figure 6.9: Boundary layer thickness. (a) 99% velocity thickness, (b) displacement thickness, and (c) momentum thickness.

C_f before and after the transition is discussed and compared with current theory here.

Case	AIR	R1	R2	R3	M1	M2	M3
$\hat{x}_{br,e}$	6.62	5.92	5.95	5.94	5.80	5.80	5.79

Table 6.5: The position of the end of breakdown process.

From the inlet boundary of the DNS simulation domain ($\hat{x} = 4$) to the end of blowing-and-suction wall boundary ($\hat{x} = 5$), the boundary is still nearly laminar (see Figure 6.10). The profiles of C_f are compared with their theoretical values in Figure 6.11(a) and (b), where the laminar theoretical C_f is given by the following equation [296]:

$$C_{f,lam} = \frac{0.644 C_w^{0.5}}{Re_x^{0.5}}, \quad (6.14)$$

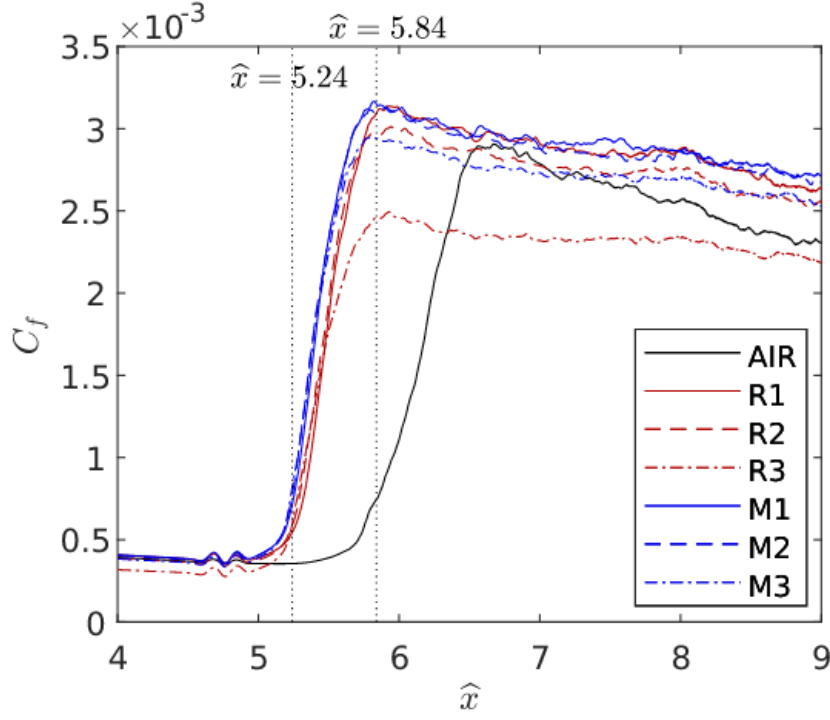


Figure 6.10: Skin friction coefficient.

where

$$C_w = \frac{\bar{\rho}_w \bar{\mu}_w}{\bar{\rho}_e \bar{\mu}_e}. \quad (6.15)$$

The subscript 'e' refers to the edge of the boundary layer. In Equation 6.14, a coefficient C_w is used to consider the impact of the different thermal property between the near-wall region and outside of the boundary. It shows that the Case R3 has the minimum laminar C_f in Figure 6.11 (a) and also the minimum theoretical value in Figure 6.11 (b). It means that the difference in laminar C_f can be explained by the difference of the thermal property ratio between outside the boundary and at the wall $C_w = \frac{\bar{\rho}_w \bar{\mu}_w}{\bar{\rho}_e \bar{\mu}_e}$.

For the fully-developed turbulent boundary layer, C_f from the DNS results is compared with the theoretical results and shown in Figure 6.11(c) and (d). The theoretical results of C_f over adiabatic walls are calculated by the following equation [296]:

$$C_{f,t} = \frac{0.455}{S^2 \ln^2 \left[\frac{0.06}{S} Re_x \frac{\bar{\mu}_e}{\bar{\mu}_w} \sqrt{\frac{\bar{T}_e}{\bar{T}_w}} \right]}, \quad (6.16)$$

where

$$S = \frac{(\bar{T}_w/\bar{T}_e - 1)^{1/2}}{\arcsin A}, \quad A = \left(\frac{\gamma - 1}{2} Ma_e^2 \frac{\bar{T}_e}{\bar{T}_w} \right)^{1/2}. \quad (6.17)$$

For dense-vapour cases where ideal-gas law is not applied, Equation 6.16 is replaced by the following

equation, since it is already found in Chapter 5 that the enthalpy should replace the temperature in non-ideal gases:

$$C_{f,t} = \frac{0.455}{S^2 \ln^2 \left(\frac{0.06}{S} Re_x \frac{\bar{\mu}_e}{\bar{\mu}_w} \sqrt{\frac{\bar{h}_e}{\bar{h}_w}} \right)}, \quad (6.18)$$

where

$$S = \frac{(\bar{h}_w/\bar{h}_e - 1)^{1/2}}{\arcsin A}, \quad A = \left(\frac{\bar{u}_e^2 \bar{T}_e}{2\bar{h}_e \bar{T}_w} \right)^{1/2}. \quad (6.19)$$

Figure 6.11(c) shows that C_f decreases more slowly in dense-vapour cases than in the air case, and C_f is larger in dense-vapour cases than in the air case in the region $\hat{x} > 7.5$ (except Case R3). This trend is also found in the theoretical results (see Figure 6.11(d)), even the theoretical C_f decreases slightly slower than the DNS results. By the theoretical calculation of $C_{f,t}$, the $C_{f,t}$ can be predicted the lowest in Case R3, and it can be predicted higher in all other dense-vapour cases than in Case AIR. It means that the difference in turbulent C_f can also be explained by the difference of thermal property ratio between outside the boundary and at the wall ($\frac{\bar{\mu}_w}{\bar{\mu}_e}$ and $\frac{\bar{h}_w}{\bar{h}_e}$).

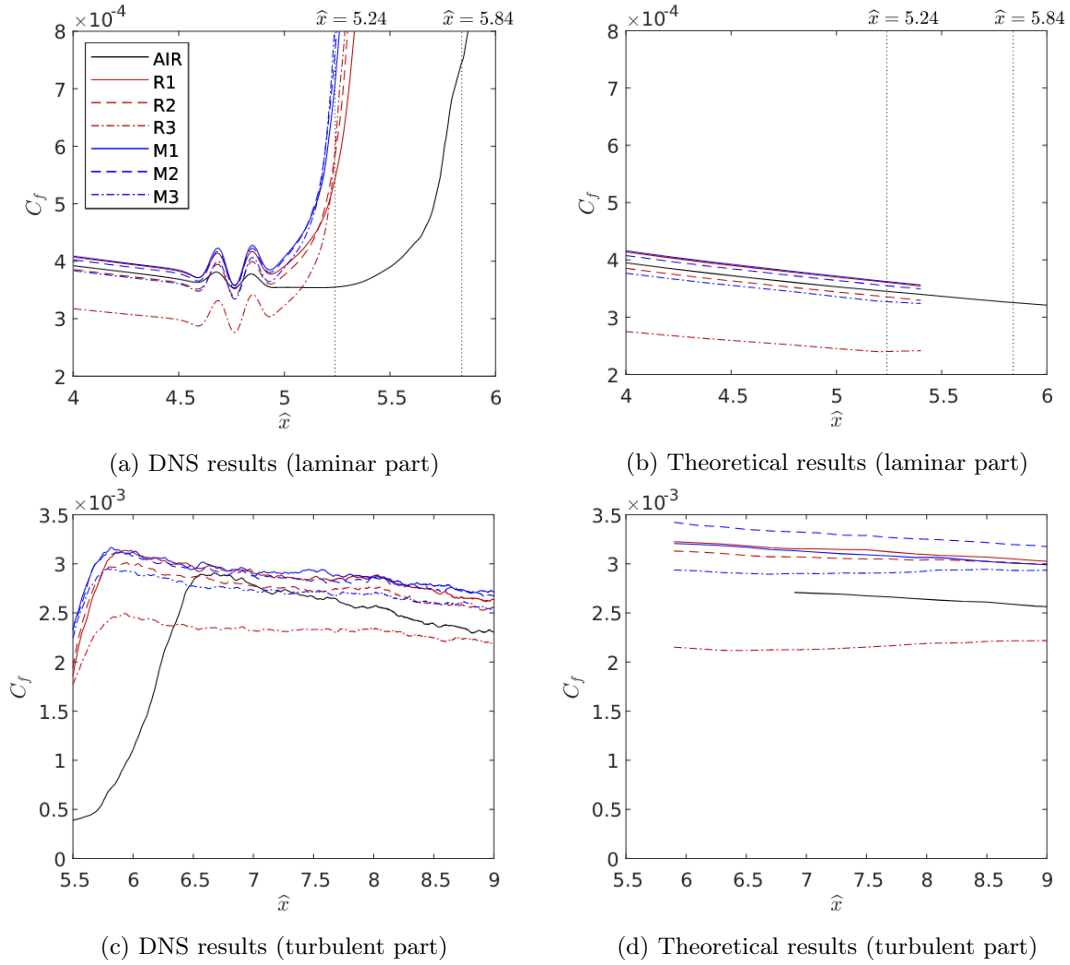


Figure 6.11: Comparison of skin friction coefficients from DNS results and theoretical results.

In summary, C_f starts to increase rapidly after $\hat{x}_{br,s}$ and the increasing speed is greater in dense vapours than in air. The current theoretical calculation of C_f , which considers the thermal property ratio between outside the boundary and at the wall, is able to predict the trend of the C_f distribution for dense vapours in the laminar flows or fully turbulent flows. It means the impact of non-ideal effects and molecular-complexity effects on the distribution of C_f is due to their influence on the thermal property ratios between outside the boundary and at the wall.

6.4 Coherent Structures of Laminar-Turbulent Transition

6.4.1 Vortex structures

The Q criterion [264] is used to identify vortices, and the instantaneous vortex structures in 3D views at a reference time point ($\hat{t}_0$) of five cases are shown in Figure 6.12. Here, the reference time point is considered the beginning of a period of the turbulence evolution, the iso-surfaces are at $Q = 100$, and the color counter shows the wall distance $\hat{y}$.

Figure 6.12(a) shows the vortex structures in Case AIR. The first hairpin vortex can be seen before $\hat{x}_{br,s}$, which is usually considered to be the exact position of the start of breakdown, where the background randomness starts to be amplified [162]. After $\hat{x}_{br,s}$, more symmetric and asymmetric Ω -vortices are observed, whose head rolls upward from the wall, significantly increasing the boundary layer thickness δ_{99} . As the flow moves downstream, the vortex region increases until it eventually occupies the entire flow domain in the spanwise direction. At $\hat{x}_{br,e}$, the flow is completely turbulent and homogeneous in spanwise direction. In dense-vapour cases (see Figure 6.12(b)-(e)), the similar vortex structure is found: the first hairpin vortex is seen before $\hat{x}_{br,s}$; more symmetric and asymmetric Ω -vortices are observed after $\hat{x}_{br,s}$; the vortex region occupies the entire flow at $\hat{x}_{br,e}$.

In all cases, two turbulent spots are seen in the leading region of the breakdown (labeled by ‘A’ and ‘B’ in Figure 6.12(a)-(e)), although the positions of these two spots are different in these cases. In Cases AIR, the leading edge of turbulent spot A is obviously at the upstream of the spot B. Within a period, two turbulent spots form alternately and move downstream, so they are never located at the same $\hat{x}$. These two turbulent spots are separated from the turbulent boundary layer when they first form, and they alternately merge into the downstream turbulent boundary layer. While in dense-vapour cases, the leading edge of the two turbulent spots is on a similar $\hat{x}$ (see Figure 6.12(b)-(e)), then they are connected to the downstream turbulent boundary layer. The differences between dense-vapour cases are insignificant. For the position in spanwise direction, both turbulent spots are at $\hat{z} \approx 0$ in Case AIR, but spot A forms at $\hat{z} \approx 0.02$ and spot B forms at

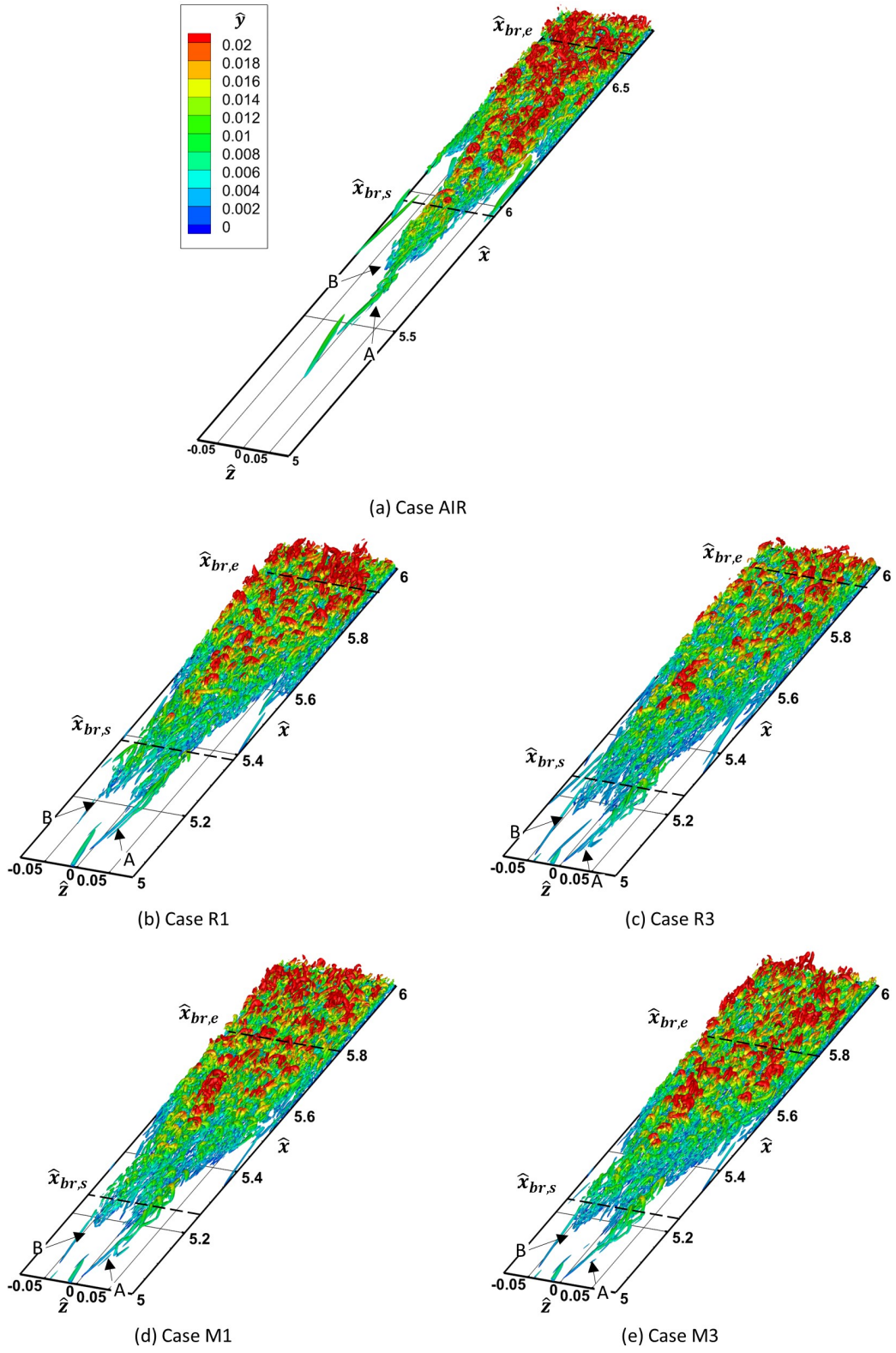


Figure 6.12: Vortex structure in 3D view.

$\hat{z} \approx -0.04$ in dense-vapour cases.

The generation and evolution of turbulent spots within a period (the period of blowing and suction wall boundary $\hat{t}_{p,bs}$) in Case AIR and M3 are compared and shown in Figure 6.13 and Figure 6.14. These figures also show the iso-surface of $Q = 100$, which is the same as the previous figures.

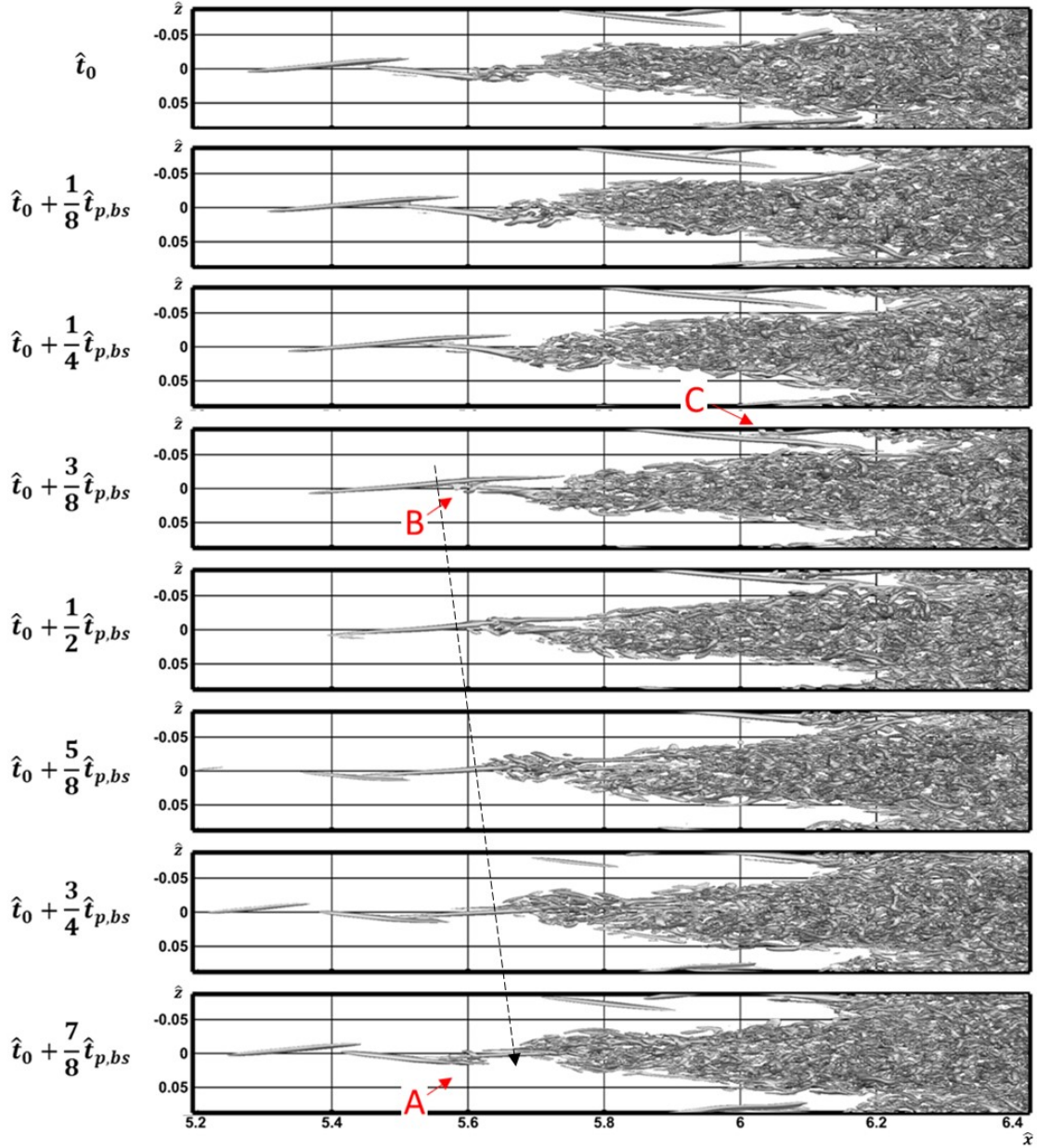


Figure 6.13: Generation and evolution of turbulent spots in Case AIR.

In Case AIR (Figure 6.13), two streamwise vortices develop, one slightly tilted in the direction $+\hat{z}$ (named ‘SV+’) and the other slightly tilted in the direction $-\hat{z}$ (named ‘SV-’), moving downstream and elongating in each period. ‘SV+’ forms at $\hat{x} = 5.4$, $\hat{t} = \hat{t}_0 + \frac{1}{2}\hat{t}_{p,bs}$, and ‘SV-’ forms

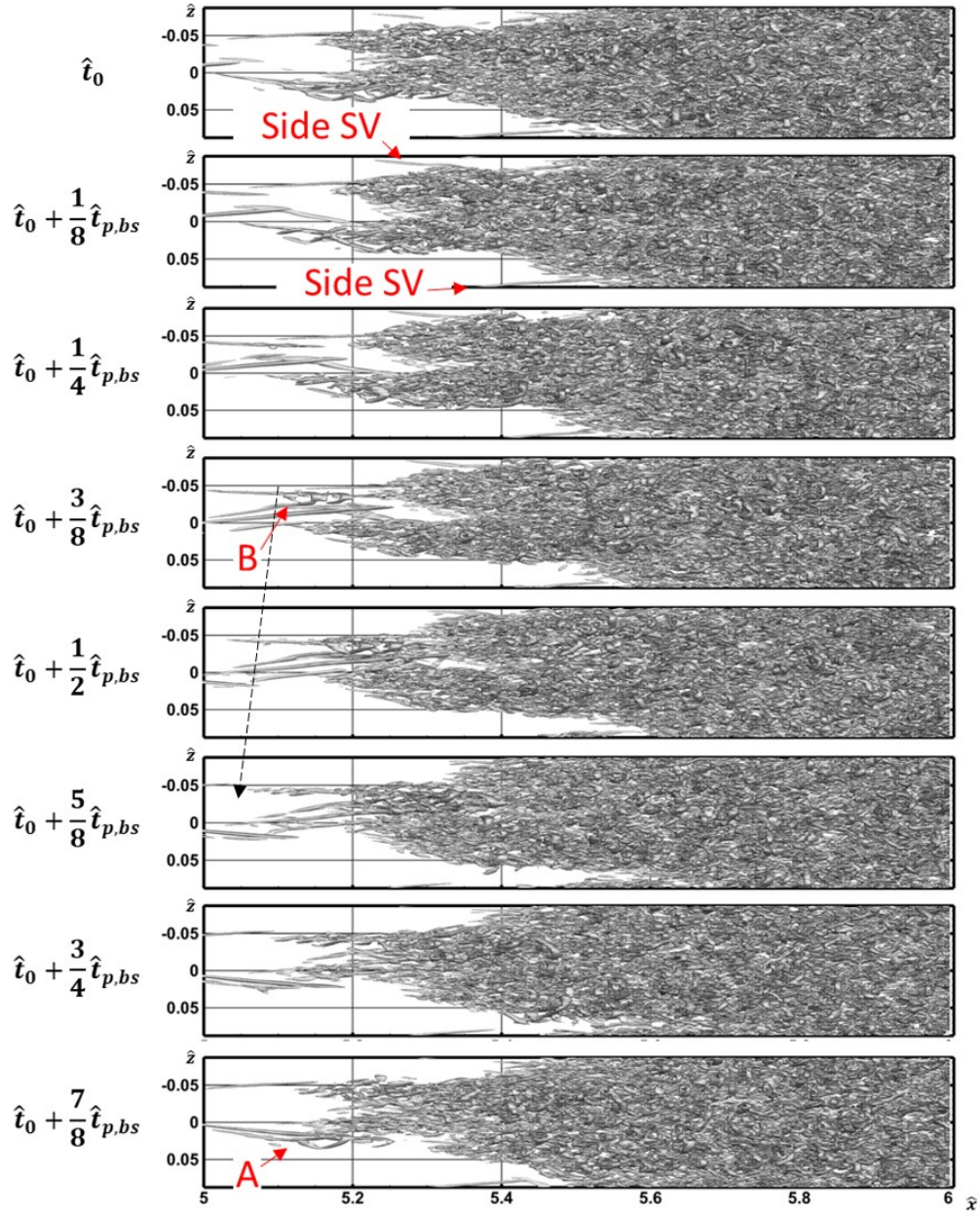


Figure 6.14: Generation and evolution of turbulent spots in Case M3.

at $\hat{x} = 5.2$, $\hat{t} = \hat{t}_0 + \frac{5}{8}\hat{t}_{p,bs}$. Both streamwise vortices are generated (or observed by Q criterion at $Q = 100$) downstream of the blowing-and-suction region ($4.5 < \hat{x} < 5$). The turbulent spot A and B mostly generate at the same $\hat{x}$ but with a gap of half a period (shown in Figure 6.13). The breakdown occurs at the closet point between two streamwise vortices, where a high shear layer leads to Kelvin-Helmholtz (KH) instability. After the breakdown, the turbulent spot increases in size due to the propagation of the instability. This instability propagates along the streamwise vortex in both directions, but the speed of the propagation towards upstream is less than the speed of streamwise vortex movement, so the entire turbulent spot moved downstream (see the dash arrow

in Figure 6.13). Then the turbulent spot merges into the downstream turbulent boundary layer. In fact, there is another turbulent spot (named ‘turbulent spot C’, show in Figure 6.13) downstream of turbulent spot A and B covering the remaining laminar region.

In Case M3 (Figure 6.14), more than two streamwise vortices located upstream of the turbulent spots are observed to have already formed within the blowing-and-suction region, which is different from Case AIR. This means that the effects of blowing and suction are more significant in Case M3 than in Case AIR. The turbulent spots A and B also form at half-period intervals (the same as Case AIR), but they form in different ways. The turbulent spot A forms at the connecting part of the head of a downstream ‘SV-’ and the tail of an upstream ‘SV+’ (see the note in Figure 6.14 at $\hat{t} = \hat{t}_0 + \frac{7}{8}\hat{t}_{p,bs}$), and the turbulent spot B forms at the joining part of the two tails of a ‘SV-’ and a ‘SV+’ (see the note in Figure 6.14 at $\hat{t} = \hat{t}_0 + \frac{3}{8}\hat{t}_{p,bs}$). Note that the turbulent spot B does not follow the dynamics of K-breakdown, where the first Λ -vortex induces aligned downstream Λ -vortices downstream. Both turbulent spot A and B are the result of KH instability which propagates both upstream and downstream along the streamwise vortices. Unlike Case AIR, the propagation speed of KH instability is faster than the moving speed of turbulent spots, so the leading edge of the turbulent spot can be earlier than the position where it originates (see the evolution of turbulent spot B from $\hat{t} = \hat{t}_0 + \frac{3}{8}\hat{t}_{p,bs}$ to $\frac{5}{8}\hat{t}_{p,bs}$ in Figure 6.14). There is no obvious turbulent spot downstream, instead lateral SVs are observed. These lateral SVs generate and touch the turbulent region, then the instability propagates upstream along these SVs and the turbulent structures dominate the entire region in the spanwise direction.

To summarise, the interaction of two streamwise vortices in opposite directions leads to periodic turbulent spots in both air and dense-vapour bypass transitions, which is the dominant vortex structure. Although the blowing-and-suction boundary is the same in all cases, it induces more streamwise vortices in all dense-vapour cases than in Cases AIR. These vortices lead to two different generating types of turbulent spot: in Case AIR, the turbulent spot occurs by the interaction between two head-to-tail streamwise vortices; in Case M3, it occurs by the interaction between two tail-to-tail streamwise vortices. Two main turbulent spots are located almost at the same $\hat{x}$ for dense-vapour transitions, but they are successive in air transitions. A third turbulent spot occupies the remaining laminar region in Case AIR, while the propagation of instability along the lateral streamwise vortex fills the remaining laminar region in dense-vapour cases.

6.4.2 Instantaneous Fluctuation Field

Instantaneous velocity fluctuation field on the X-Z plane at $y = \frac{1}{2}\delta_{99,br,s}$ is shown in Figure 6.15 and Figure 6.16, which show the u -component and v -component of velocity. $\delta_{99,br,s}$ is the boundary

thickness at $\hat{x}_{br,s}$, and they show the flow field at the time point $\hat{t} = \hat{t}_0$. The fluctuation fields of Cases AIR and M3 are compared.

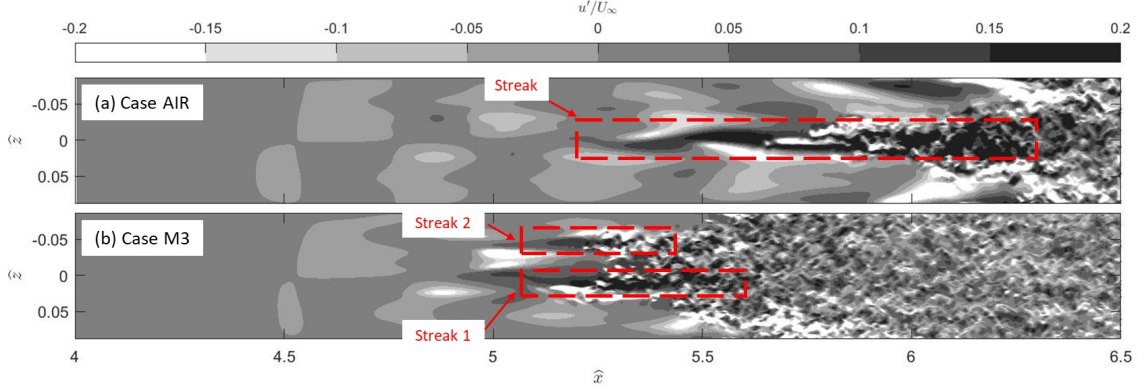


Figure 6.15: u -component velocity fluctuation field on the X-Z plane at $y = \frac{1}{2}\delta_{99,br,s}$.

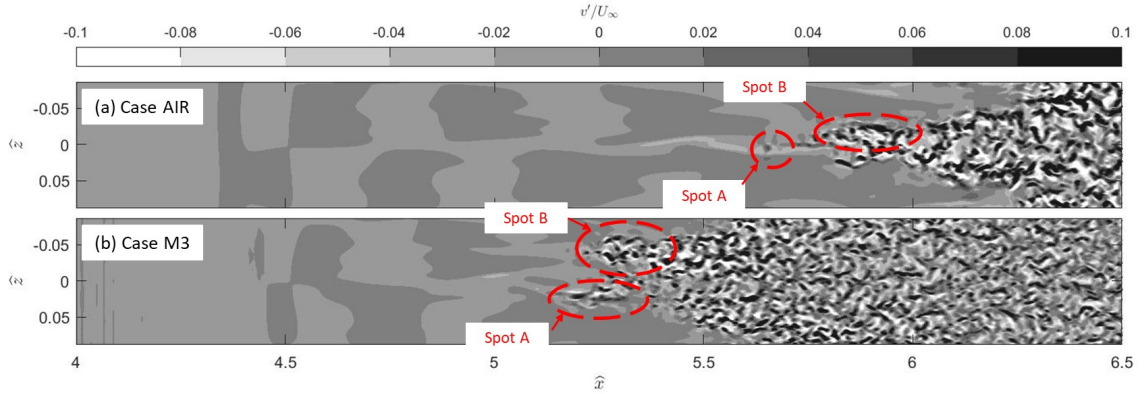


Figure 6.16: v -component velocity fluctuation field on the X-Z plane at $y = \frac{1}{2}\delta_{99,br,s}$.

In Case AIR (Figure 6.15(a)), long streaks of u -component velocity perturbations are observed, corresponding to the phenomena of the bypass transition in the work of Jacob [14]. The long streaks in Case AIR are the result of streamwise vortices, which is a ‘high speed’ streak caused by two tail-to-head vortices with opposite directions of rotation. The instability of the streak leads to turbulence. Similar phenomena are also observed in Case M3, with two ‘high speed’ streaks instead of one. This is consistent with our finding from the analysis of the vortex structure that more streamwise vortices are observed at the leading of transition in Case M3 than in Case AIR. The ‘streaks’ are also shorter in Case M3 than in Case AIR. In Figure 6.16(a) and (b), v -component velocity fluctuation field highlights the location of turbulent spot, which is consistent with the results of Jacob [14].

The instantaneous field of temperature and pressure fluctuations is shown in Figure 6.17 and Figure 6.18. The long streak of low temperature is still observed in Case AIR (Figure 6.17(a)),

which is similar to the high-speed streak, but this streak is not found in Case M3 (Figure 6.17(b)). The disappearance of ‘streak’ structure is due to the larger impact of pressure fluctuation in dense-vapour flows on the temperature fluctuation, the mechanism of which was discussed in Chapter 5. The pressure fluctuation shows the ‘spot’ structure in both Case AIR and M3 (see Figure 6.18), and this ‘spot’ structure disturbs the ‘streak’ structure in the temperature fluctuation field in Case M3.

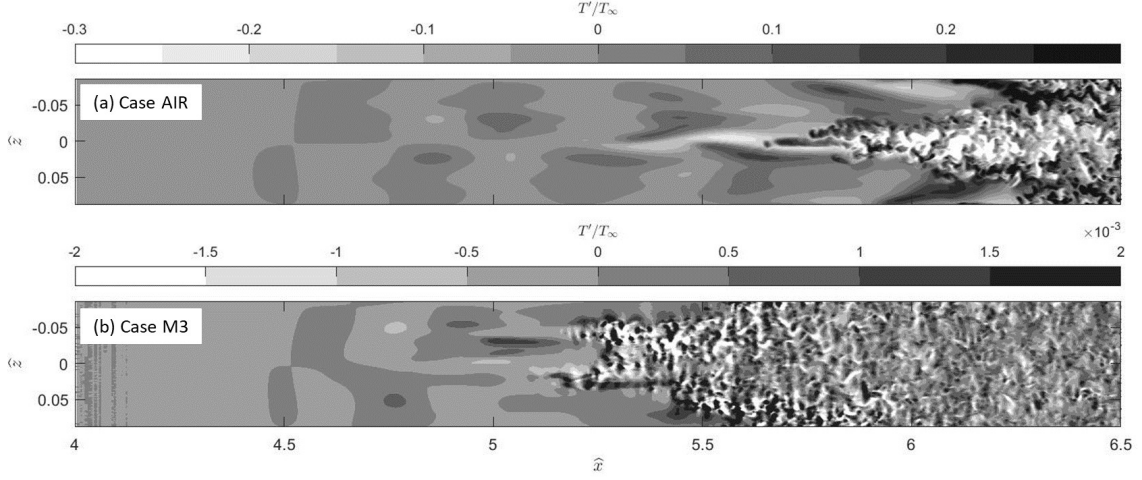


Figure 6.17: T fluctuation field on the X-Z plane at $y = \frac{1}{2}\delta_{99,br,s}$.

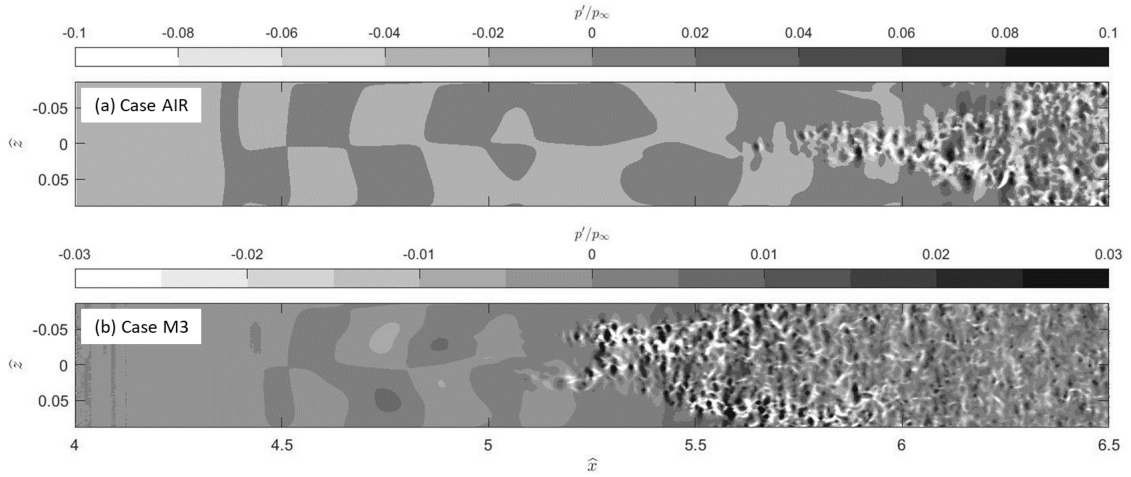


Figure 6.18: p fluctuation field on X-Z plane at $y = \frac{1}{2}\delta_{99,br,s}$.

In summary, a high-speed ‘streak’ structure is observed in u -component of velocity fluctuation field in both air and dense-vapour cases, but the number of streak is larger in Case M3, confirming our findings in the analysis of the vortex structure. The ‘spot’ structure highlights the location of the turbulent spots in both cases, which is consistent with the conclusion of Jacobs’ work [14]. The ‘streak’ structure remains in the field of temperature fluctuation in Case AIR, but disappears

in Case M3 due to the larger impact of pressure fluctuations in dense-vapour flows.

6.5 Proper Orthogonal Decomposition (POD) analysis

Flow fields in Cases AIR and M3 are analysed by POD. Here, the flow fields in the early stage of the transition process are studied. They are first interpolated into a uniform grid, then this interpolated flow field is decomposed using POD. This grid starts at $\hat{x}_{pod,s} = 5$ and ends at $\hat{x}_{pod,e}$, which is the position where C_f increases to half of $C_{f,max}$. $\hat{x}_{pod,e}$ is equal to 6.158 in Case AIR and equal to 5.381 in Case M3. The element number of the uniform grid is $N_x \times N_y \times N_z = 70 \times 50 \times 100$ (350,000 elements in total).

The POD method presented in Chapter 3.2.3 is used. The number of snapshots for both cases is $M = 193$, which come from three periods with an interval of $\frac{1}{64}\hat{t}_{p,bs}$. Then, the data matrix ($\mathbf{P}_{N \times M}$) is created with $N \times M = 350,000 \times 193$.

The results of POD give 193 modes, and the eigenvalues of the first 100 modes (except the first mode) are shown in Figure 6.19. λ_i are shown in pairs in both Case AIR and Case M3. This feature is typical of KH instability, and Charkrit [297] believes that this is a proof that KH instability plays an important role in the transition. The value of eigenvalue in POD refers to the 'energy' contained in the corresponding POD mode. The first four pairs of eigenvalues in Case M3 are larger than in Case AIR, implying that vortices absorb more kinetic energy from the mean flow field and transfer more energy to smaller vortices. The energy transfer from large vortices smaller vortices refers to the breakdown process, in which the large vortices break into smaller ones. This can help explain our earlier finding that the transition is faster in dense-vapour cases than in the air case.

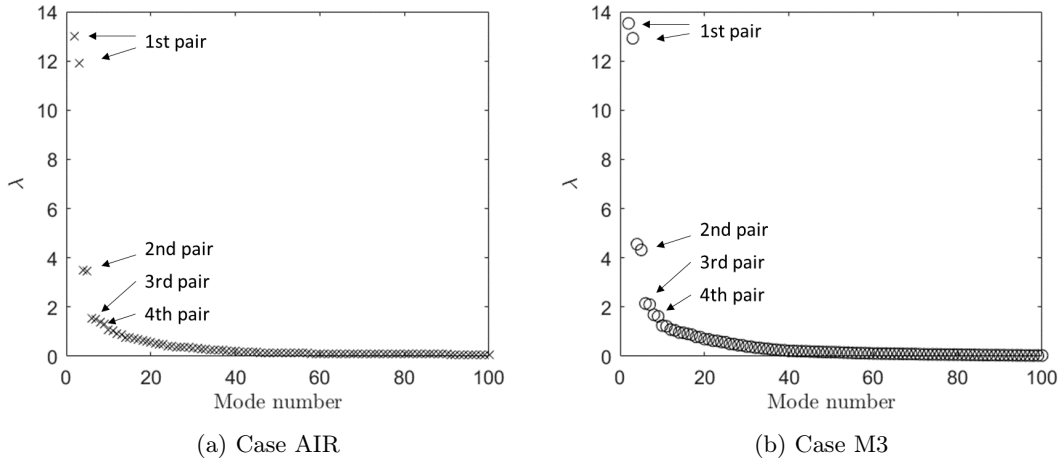


Figure 6.19: The distribution of eigenvalues of POD modes.

The summed energy within the first r modes is shown in Figure 6.20, which is defined as follows:

$$\epsilon(r) = \frac{\sum_{i=1}^r \lambda_i}{\sum_{i=1}^{193} \lambda_i}. \quad (6.20)$$

Most of the energy is contained in the first POD mode, which refers to the mean flow. The fluctuation is only located in the boundary layer, so the remained modes share a small proportion of the overall energy. As the number of modes increases, the $\epsilon(r)$ increases, which means the total energy contained in the first r modes takes larger proportion of the overall 'energy'. It is found that $\epsilon(r)$ is more than 0.99995 in both cases if r is larger than 51. If the first mode is not considered (which is very large), the next 50 mode contains more than 85% fluctuation 'energy' in both cases. Here, the reconstructed flow field, which takes the first 51 POD modes, is compared with the original flow field, aiming to validate the POD analysis method. The reconstructed and original flow fields for both cases are compared in Figure 6.21. It shows that the vortex structures are similar in the reconstructed and the original fields, see the comparison between Figure 6.21 (a) and (b), (c) and (d). The good agreement between the reconstructed and the original flow fields indicates that this POD method is valid.

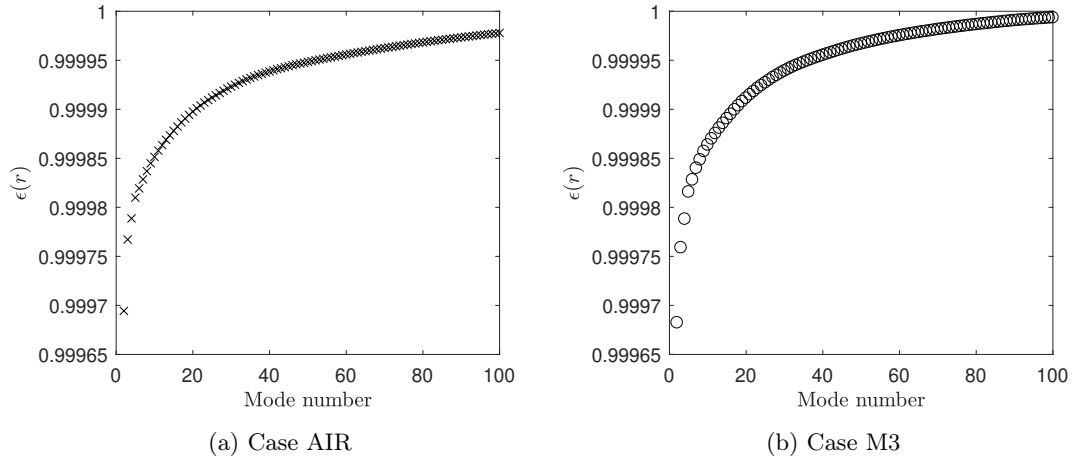


Figure 6.20: The distribution of $\epsilon(r)$.

The vortices in the first four pairs of POD modes for Case AIR and Case M3 are shown in Figure 6.23 and Figure 6.24, respectively, identified by iso-surface of the Q criterion. In Case AIR (Figure 6.23), streamwise vortices are observed in POD modes, and they are organised in a conical region where is also the vortex region shown in Figure 6.13. The shapes of the vortices in each pair of POD modes are similar. As the POD mode number increases, these streamwise vortices are shorter and occur more frequently the in X-direction, and these streamwise vortices are tilted at a greater angle to two sides. This means that the turbulent kinetic energy is mainly contained

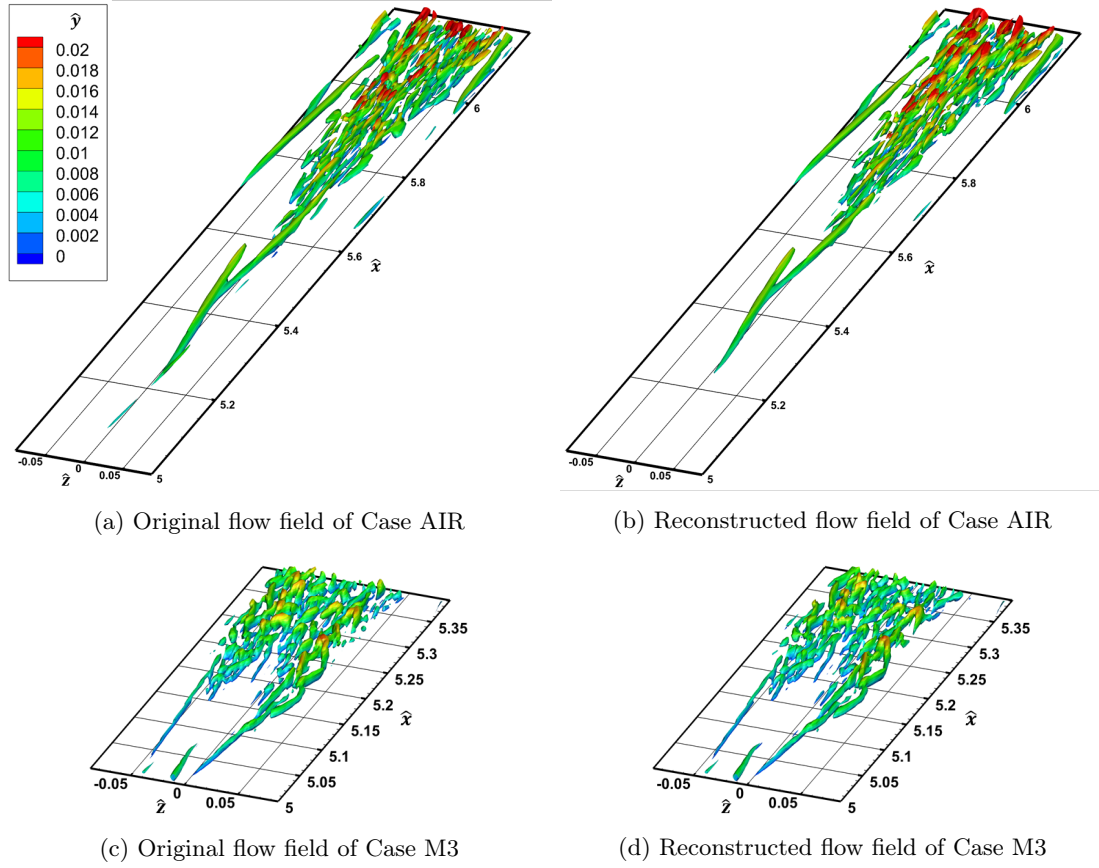


Figure 6.21: Reconstructed flow fields (shown by iso-surface of Q criterion).

in streamwise vortices at different scales and that longer vortices break into smaller ones during the breakdown. These features of streamwise vortices are also observed in Case M3 (Figure 6.24), although these streamwise vortices are not strictly organised in a conical region. A weak group of streamwise vortices is observed away from the main conical region, where the position of turbulent spot B is located (see Figure 6.14). This result is consistent with the finding in the vortex structure analysis, that two nearly parallel turbulent spots dominate the early stage breakdown in Case M3.

To summarise, the eigenvalues of POD modes are shown in pairs and the shapes of a pair of modes are similar for both air and dense vapour. This is taken as a proof that the KH instability plays an important role in the basic mechanism of breakdown by Charkrit [297]. The first four pairs of the eigenvalues in Case M3 is larger than in Case AIR, which shows that the large vortices absorb more energy from the mean flow and transfer to smaller vortices. It can help explain that the breakdown is earlier in dense-vapour cases. Streamwise vortices are observed in all POD modes, and they occur more frequently with increasing mode number. This also supports our finding that the streamwise vortices breakup is the dominant mechanism of early stage breakdown in both

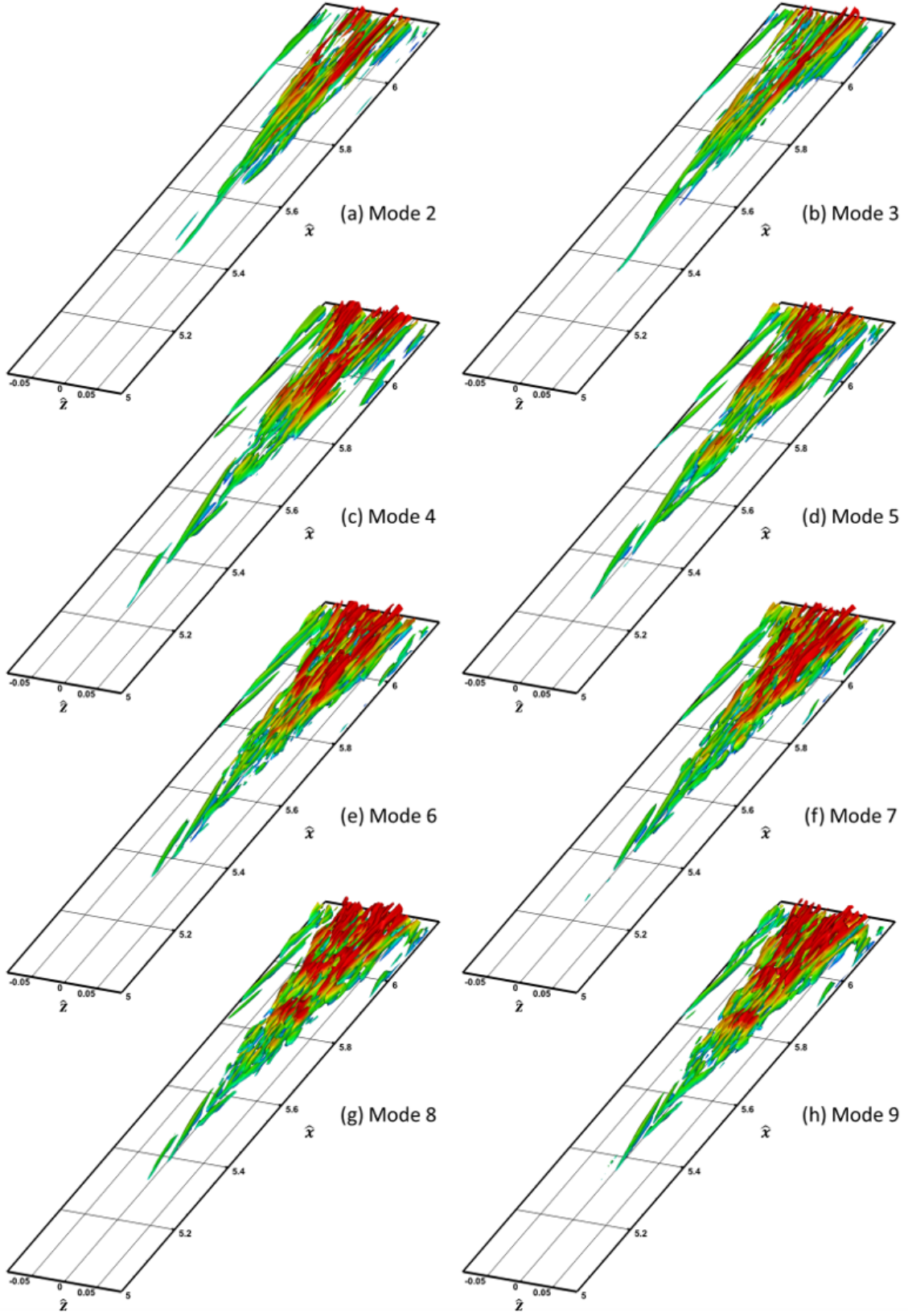
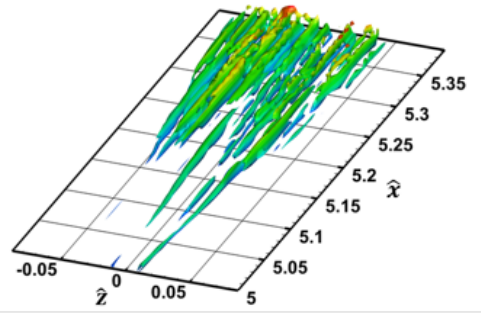
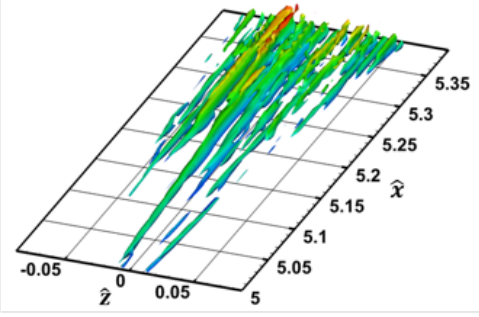


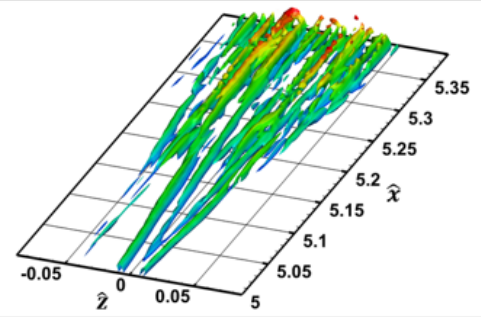
Figure 6.23: POD modes of Case AIR (shown by iso-surface of Q criterion).



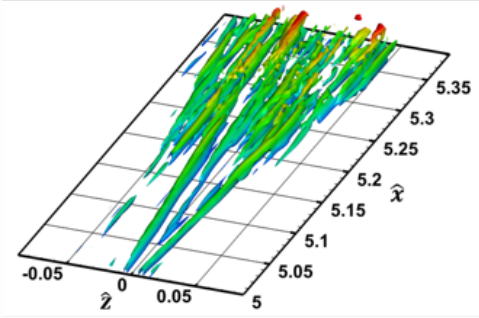
(a) Mode 2



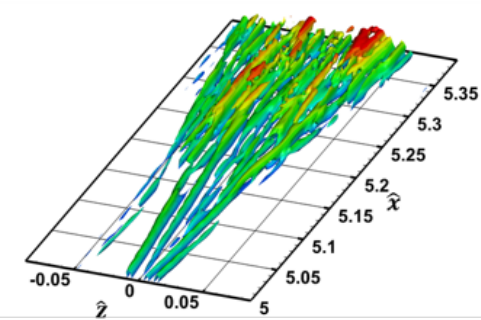
(b) Mode 3



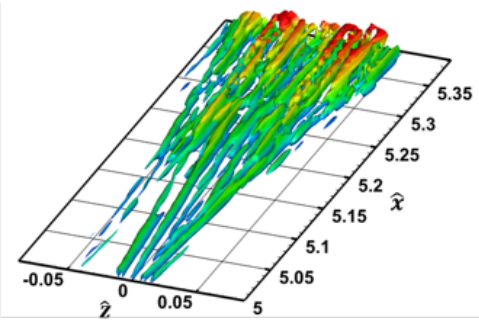
(c) Mode 4



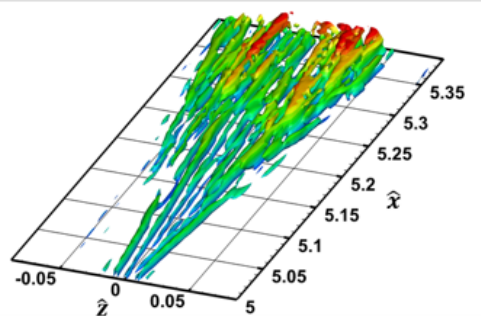
(d) Mode 5



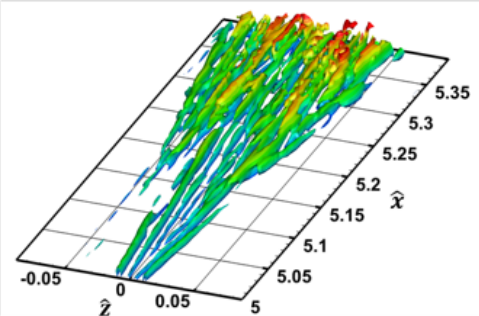
(e) Mode 6



(f) Mode 7



(g) Mode 8



(h) Mode 9

Figure 6.24: POD modes of Case M3 (shown by iso-surface of Q criterion).

cases.

6.6 Chapter Summary

The bypass-type laminar-turbulent transition of dense-vapour boundary layers over a flat plate is simulated by DNS. Two organic gases, R1233zd(E) and MDM, are studied and compared with air, and three different thermodynamic states of each organic gas are considered. $Re_\infty = 635,000$ and $Ma_\infty = 2.25$ are the same in all DNS cases for comparability. A blowing-and-suction wall boundary is used to induce a bypass-type transition.

The breakdown of laminar flow starts earlier in the gas with more complex molecules in the cases of this study. All investigated dense-vapour boundary layers breakdown significantly earlier than air boundary layers, but only a small difference between dense-vapour cases is shown. After breakdown, C_f increases faster in two organic gases than in air, and it decreases more slowly after reaching the peak value in dense vapours. The impact of non-ideal effects and molecular-complexity effects on the distribution of C_f before and after transition is found due to their influence on the thermal property ratios between outside the boundary and at the wall.

The mechanism of breakdown in both air and dense-vapour flows is that the interaction of two streamwise vortices in opposite directions of rotation leads to periodic turbulent spots. The KH instability is found at the closet point between the two streamwise vortices, and the instability subsequently propagates along the vortex. In dense-vapour cases, more streamwise vortices are observed, and the propagation speed of KH instability is also faster, so the leading edge of the turbulent spots is located earlier in dense-vapour cases and therefore the breakdown occurs earlier. The vortex structure looks the same between dense-vapour cases.

The POD analysis is applied to an air case (Case AIR) and a dense-vapour case (Case M3). By comparing the reconstructed flow fields with the original fields, this POD method is validated. In both cases, the eigenvalues of POD modes are shown in pairs and the shapes of a pair of modes are similar, which is considered by Charkrit [297] as a proof that KH instability plays an important role in the basic mechanism of breakdown. The larger eigenvalues in the first four pairs of POD modes supports that the energy transfer from the mean flow to the large vortices and then to the smaller vortices is more significant in dense-vapour cases. The shape of POD modes also supports that the breakup of streamwise vortices is the main mechanism of the early stage breakdown in both air and dense vapours.

Chapter 7

Conclusion and Future Work

7.1 Synopsis

This thesis presents the study of the fundamental flow phenomena in dense vapours used in ORC turbines, including the gasdynamic behaviour in a blade-shaped supersonic nozzle and the turbulent behaviours in benchmark wall-bounded flows. An experimental method for testing a supersonic nozzle is designed, and a preliminary test is introduced can compared with CFD results. A Direct Numerical Simulation (DNS) method for dense vapours is developed and applied on fully-developed turbulent channel flows and the transition flows over a flat plane. The impact of molecular-complexity effects and non-ideal effects on the turbulent behaviours are studied.

7.2 Conclusions

Main conclusions of this thesis are summarised here in line with the objectives set out in the thesis.

1. The establishment of an experimental test facility for a supersonic nozzle using dense vapours (measuring the pressure distribution and Schlieren images), and the preliminary test of a supersonic nozzle.

A experimental method for testing supersonic flows of dense vapour is established, in which the pressure distribution can be measured and Schlieren images can be taken. A 'Sandwich' structure is designed to make these two functions work together. The pressure is measured on two nozzle surfaces, and the Schlieren images is taken with the help of a back mirror and a front quartz window. This experimental method is applied in the preliminary test of a blade-shaped nozzle.

A supersonic cascade is designed by MOC-based method, and the performance of the designed geometry is analysed by RANS simulation method. The simulation results shows that the design

is able to achieve a nearly uniform outflow with $Ma \approx 2$. A nozzle using the cascade blade shape is designed. It is tested in two working fluids: nitrogen and R1233zd(E). The preliminary test results of nitrogen test shows that an adverse pressure gradient is found on both two surfaces of the nozzle, and a shock train is observed in the corresponding position by the Schlieren images. The R1233zd(E) test also shows an adverse pressure gradient, but the the flow features in Schlieren images are distrubed by two-phase flows. This problem has to be solved in the future work.

2. The study of fully-developed turbulent boundary layers in a channel, allowing to understand the molecular-complexity effects and non-ideal effects on wall-bounded turbulent behaviours and turbulent modelling issues.

A DNS method for non-ideal gases is developed and applied on channel flows. The impacts of molecular-complexity effects and non-ideal effects on wall-bounded supersonic turbulent dense-vapour flows are studied in two organic gases: R1233zd(E) and MDM. The statistical mean flow properties, including temperature, density and velocity, are found quantitatively influenced by the molecular-complexity effects and non-ideal effects. Non-dimensional numbers $Pr_G Ec_G$ will influence the mean temperature profile, and non-ideal thermodynamic derivative $\left(\frac{\partial \rho}{\partial T}\right)_p$ will influence the mean density profile. The influence of the two effects on the mean velocity profile is due to their impact on mean density profile and mean viscosity profile; therefore, by applying Trettel & Larsson [11] (TL) transformation and the semi-local normalised wall distance y^* , the mean velocity profile in dense vapours can nearly coincide with that in ideal air. Walz's equation in terms of enthalpy instead of temperature is checked in dense vapours, and the error of Walz's equation in dense-vapour cases is with in $\pm 3\%$ (smaller than in air) when compared with DNS results.

For turbulent fluctuation fields, the results show that molecular-complexity effects and non-ideal effects can lead to qualitative difference between dense vapours and ideal air. The intensities of temperature, pressure and density fluctuations (T'_{rms} , p'_{rms} and ρ'_{rms}) are no longer of the same order of magnitude in dense vapours, because T'_{rms} is significantly reduced by both molecular-complexity effects and non-ideal effects. A new relationship between T'_{rms} , p'_{rms} and ρ'_{rms} is proposed with a maximum deviation of 2% in dense vapours when compared with DNS results. It is found that the sound-wave mode rather than the vorticity mode is the dominant mode for generation of thermodynamic property fluctuations in the inner layer of dense-vapour cases with strong molecular-complexity effects or non-ideal effects. This is because that molecular-complexity effects significantly increase the density fluctuation induced by sound-wave mode and non-ideal effects significantly increase the temperature fluctuation induced by sound-wave mode. Therefore the correlations between T' , p' and ρ' within the inner layer are qualitatively affected. Near-wall turbulence structure is analysed and also supports this finding.

Some important modelling issues are discussed in the boundary layer of dense vapours based on DNS results. The strong Reynolds analogy (SRA) is invalid when non-ideal effects are strong, because the deviation between velocity mixing length scale and enthalpy mixing length scale becomes very large. BY comparing different turbulent eddy viscosity model for boundary layers, it is found that the Shih [287] model has a better estimate in the log-law region than the other two models in all dense-vapour cases. The models of viscous transport term and turbulent transport term in the $k - \varepsilon$ RANS method still follow the trend of their exact profile (achieved by DNS results), and the error of these models is not significantly increased by molecular-complexity effects or non-ideal effects. The viscosity fluctuation can lead to an error of up to 25% in the decomposition of ε in dense vapours. The assumption of a constant turbulent Prandtl number at $Pr_t = 0.9$ is still acceptable with an error of about $\pm 30\%$, which is not worse than other complex models in dense gases.

3. The understanding of the laminar-turbulent transition over a flat plate in the present of fluids with molecular complexity and non-ideal effects.

The developed DNS method is applied on bypass transition flows over a flat plane for two organic gases: R1233zd(E) and MDM. A blowing-and-suction wall boundary is used to induce the bypass-type transition. The breakdown of laminar flow starts earlier in dense-vapour cases studied than in the air case, but the difference between dense-vapour cases is much smaller than the difference between air and dense vapours. The impact of molecular-complexity effects and non-ideal effects on the C_f distribution is due to their influence on the thermal property ratio between outside the boundary and at the wall.

The mechanism of breakdown in both air and dense-vapour flows is the interaction of two streamwise vortices in opposite rotation directions, and this lead to periodic turbulent spots due to the Kelvin-Helmholtz (KH) instability. Streamwise vortices breaks up and the instability subsequently propagates along the vortices. More streamwise vortices are induced by blowing-and-suction boundary conditions for dense vapours than for air, and the propagation speed of KH instability is higher than the speed of turbulent spots in dense-vapour cases, so turbulent spots occur earlier in dense vapour which means the breakdown starts earlier. A Proper Orthogonal Decomposition (POD) procedure is applied to analyse the flow field of the early stage of transition. Streamwise vortices caused by blowing-and-suction boundary conditions are confirmed as the dominant feature in the POD analysis.

7.3 Future Work

In this thesis, a blade-shaped supersonic nozzle was tested in a preliminary experiment. The wall-bounded turbulent behaviour is studied in fully-developed turbulent channel flows and in the laminar-turbulent transition on a flat plate. As shown below, there is scope for future work based on this thesis:

7.3.1 Experimental Works

The Schlieren images of the test with R1233zd(E) are disturbed by two-phase flows in the current tests. Firstly, the heating system of this test rig is going to be improved. In the current test rig, only one heater is applied to make the liquid working fluid evaporate, but it is not able to heat the vapour to a required overheating temperature. Meanwhile, there is some cold vapour in the pressure vessel which will mix with the charged hot vapour, and it is also influence the heating performance of the rig. To improve the heating performance and make the controlling of the thermodynamic state within the pressure vessel more convenient, a vapour heating system inside the pressure vessel will be installed. It can help to warm up the pressure vessel before the charging process, and also help to achieve a required overheating temperature in the charging process.

Secondly, the pipework upstream of the test section should also be improved. It is found that there are some liquid fluids on the pipe wall and in corners of the pipework. These liquid will mix with the blowdown vapour and lead to a two-phase flow. A pipe-wall heating system should be installed to warm up the pipes upstream of the test section. Meanwhile, a drain-pipe should also be design, because there may be amount of liquid fluids stored in the pipes. The test section and the pipework upstream of the test section located in the lowest position of the test rig, so the liquid fluids can store in the test section and the pipework when the rig is cold down. These liquid fluids should be drained before the first test of a day, and a drain-pipe at the bottom will help.

Currently, the nozzle was tested under the working conditions where the inlet total pressure is lower than the design conditions. A test with higher inlet total pressure will be considered in the future. The limitation of the inlet pressure is due to the limitation in the volume of the current pressure vessel. The pressure regulator requires a period of time to achieve a stable inlet condition, and the pressure in the pressure vessel should stay above the target inlet pressure within this period of time. This requires either a higher initial vessel pressure or a larger volume of the vessel. If the safety pressure cannot be improved, the increase of the vessel volume is a solution. Another one or two pressure vessel will be installed paralleling with the current pressure vessel, so as to increase the vessel volume.

The back pressure controlling system cannot work well due to leaking problems, so the expansion ratio in current tests are smaller than the design condition. The influence of the leaking problem will be reduced in the future work. The sealing between nozzle plates and the quartz window is difficult, because the quartz window is easily broken when it is pressed on its back. These leaking flow will block the nozzle downstream of the nozzle throat, which lead to a high back pressure. To reduce this back pressure, the long straight channel downstream the blade shape will be shorten in the future work, it helps to discharge the leaking flows and reduce the back pressure.

A test of cascade flows is also planned, in which at least five channels are included. The flow capacity of the current pressure regulator and controlling valves is not enough for the cascade flow test, so they should be re-designed according to the requirement of cascade flows.

7.3.2 Numerical Works

The DNS numerical method proposed in this thesis will be validated by comparing with published non-ideal flow data. Even though there is no experimental data for dense-vapour flows, but there is supercritical CO₂ experimental data available, and it can be used to validate the current numerical method. Meanwhile, there is also other numerical data of dense-vapour flows, which can also be used. The inhomogeneous part $\frac{\partial \mathbf{F}_{j,inh}}{\partial x_j}$ is discretized by the upwind scheme, but it is meaningful to discuss whether it is the best scheme for this term.

The turbulent behaviour of dense vapours with a zero pressure gradient has already been studied, and more benchmark flows should be studied in the future. Two ongoing studies as a consequence of this thesis are underway: the interaction between turbulent boundary layer and oblique shock wave, and the flows over airfoils. The mixing flows in dense vapours are also research interests, since the mixing loss play an important role in the ORC turbines. It can help to understand the trailing-edge wake features and predict the mixing loss more accurate. These studies will help to further improve the understanding of fundamental issues in the internal flows of ORC turbines. Turbulent models also need to be studied in more benchmark flows than just flat-wall-bounded turbulent flows to improve the generality of turbulent models in dense vapours.

Turbulent modelling issues of $k-\varepsilon$ RANS method are discussed in this thesis, with several issues still open. First, the fluctuation of the viscosity has a significantly impact on the decomposition of ε , but the impact on the ε model equation is not fully understood due to the unclear physical meaning of the model equation and the complex expression of the exact transport equation of ε . This is a task for future work. Turbulent modelling issues for other RANS methods and Large Eddy Simulation (LES) should also be discussed by comparing with the current DNS results.

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