Large eddy simulations (LES) of inclined dense jets in coastal waters

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**NANYANG
TECHNOLOGICAL
UNIVERSITY**

**LARGE EDDY SIMULATIONS (LES)
OF INCLINED DENSE JETS IN COASTAL
WATERS**

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SCHOOL OF CIVIL AND ENVIRONMENTAL ENGINEERING
2016**

LARGE EDDY SIMULATIONS (LES) OF INCLINED DENSE JETS IN COASTAL WATERS

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Summary

Desalination plants are increasingly common to augment the freshwater supply to ease the pressure on the demand of freshwater due to the rapid global urbanization. In view of potential environmental impacts, the brine outfall of desalination plants must be properly designed to ensure good mixing with the surrounding ambient seawater. Many previous studies had been performed experimentally on the mixing behavior of inclined dense jets, and analytical models had also been developed based on these experimental results to aid the outfall design. However, the accuracy of predictions by these models still needs further improvement.

The Computational Fluid Dynamics (CFD) approach offers another alternative to predict the mixing behavior of inclined dense jets in coastal waters. So far, only a few CFD studies using the Reynolds Averaged Navier-Stokes (RANS) approach have been reported in the literature. In the present study, the mixing behavior of the inclined dense jet is investigated with the Large Eddy Simulation (LES) approach, which is theoretically more advanced in terms of resolving the large coherent eddies involved.

To build capability and experience, LES was first carried out to investigate two related topics: (a) flow separation around a circular cylinder (for wall interactions), and (b) a circular turbulent wall jet without buoyancy (for concentration spreading along the wall boundary). In (a), the velocities within a square pipe with an

embedded cylindrical tube were simulated by both RANS and LES. Experimental measurements were also carried out. In comparison, RANS with the $k-\epsilon$ closure and wall function yielded the least accurate results particularly in the wake region; while the $k-\omega$ closure was in satisfactory agreement with the experimental data near to the cylinder but grossly over-predicted in the far field. LES with near wall modelling provided the best predictions of the experimental data. Thus, the results illustrated that LES with near wall modelling can better predict the flow field around boundaries including possible flow separation. In (b), LES with near wall modelling was able to predict the strong anisotropy of the concentration spreading of walls jet near the boundary, while RANS with different turbulence closures and the wall function failed to do so. The LES results also agreed well with the available experimental data in the prediction of turbulence intensity near the wall.

Given the experience, LES with near wall modelling was then employed to predict the mixing behavior of inclined dense jets in coastal waters. The results showed that LES predicted the geometrical characteristics of the inclined dense jet reasonably well in general, and the accuracy was much better than the existing integral models. The LES predictions on dilution were also much better than the existing integral models, but still with an under-prediction of $\sim 20\%$ compared with the experimental data. The turbulence intensity was predicted satisfactorily by LES in the outer half of the inclined dense jet but not in the inner half, suggesting that the current mesh scheme was not able to fully capture the convective turbulence by the unstable stratification in the inner half. With the bottom impact, LES with near wall modelling was able to reproduce the localized concentration build-up at the impact point reported by Abessi and Roberts (2015), while RANS with the $k-\epsilon$ closure and wall function was unable to do so. The profiles of normalized mean concentration

and concentration fluctuation along the spreading layer predicted by LES were close to previous experimental data, showing self-similarity. However, the dilution and thickness were under-predicted.

Overall, the results in the present study demonstrated that, with the current mesh scheme, LES with near wall modelling was a better alternative to predict the mixing behavior of inclined dense jets in coastal waters than the existing integral models and RANS with the $k-\epsilon$ closure and wall function compared herein.

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List of Symbols

a	Sound speed
a^*	Low Reynolds number correction
$a_0^* a_\infty^*$	Constants in standard k - ω closure
A_0, A_s	Coefficients in realizable k - ε closure
b_c	Concentration spread width
C_0	Initial discharge concentration
C_1, C_2	Constant coefficients dependent on the discharge inclination angle
$C_{1\varepsilon}, C_{2\varepsilon}, C_\mu$	Constants in standard k - ε closure
$C_{2\varepsilon}, C_{2\varepsilon}^*$	Coefficients in RNG k - ε closure
C_c	Centerline concentration
C_{m0}	Maximum streamwise concentration
C_ε	Constant in DKE SGS model
C_k	Constant in DKE SGS model
C_S	Smagorinsky constant
C_v	Constant in RNG k - ε closure
C_w	Constant in WALE SGS model
C^+	Empirical constant in log-law of the wall
C_ϕ	Correction term in dynamic Smagorinsky SGS model
d	Nozzle diameter of circular wall jet
d_{wall}	Distance to the wall
D	Diameter of discharge port of inclined dense jet

D_ω	Cross-diffusion term
f_i	External force in the i direction
F_1, F_2	Blended functions
Fr	Densimetric Froude number
g	Gravitational acceleration
g_i	Gravitational acceleration in the i direction
G_b	Generation of the turbulence kinetic energy due to buoyancy
$G_k, \hat{G}_k$	Generation of the turbulence kinetic energy due to the mean velocity gradients
G_ω	Generation of the specific dissipation rate
h	port height to the bottom
h	Distances from the nozzle center to the bottom
H_d	Distances from the nozzle center to the surface
H_s	Spreading layer width
k	Turbulent kinetic energy
k_{sgs}	SGS turbulence kinetic energy
L_b	Distances from the nozzle center to the back
L_f	Distances from the nozzle center to the front
L_M	Jet characteristic length scale
L_{sp}	Displacement of the “seeding” particles
L_S	Mixing length
p	Pressure
Pr_t	Turbulent Prandtl number
Q_0	Flow rate
Q_j	Turbulent (SGS) scalar flux
r	Radial distance

Re	Reynolds number
R_ε	Additional term in RNG k - ε closure
Re_t	Coefficient in standard k - ω closure
R_j	Coefficient in dynamic Smagorinsky SGS model
R_k	Constant in standard k - ω closure
s	Distance from the nozzle center along the jet centerline
S	Strain rate
Sc_t	Turbulent (SGS) Schmidt number
S_i	Dilution of the impact point
S_L	Dilution at a certain location
S_m	Dilution of the centerline peak
S_r	Dilution of the return point
S_s	Dilution of the end of the mixing zone
S_{ij}	Strain rate tensor
S_{ij}^d	Coefficient in WALE SGS model
$S_k, S_\varepsilon, S_\omega, S_\phi$	Source terms
t	Time
t_s	Simulation time
T'	Temperature fluctuation
T_0	Initial discharge temperature
T_a	Ambient temperature
T_m	Maximum spanwise temperature
T_{m0}	Maximum streamwise temperature
T_{ms}	Maximum temperature in respective offset sections
T_{sp}	Specific time interval of seeding particle

$\mathbf{u}$	Velocity vector
u, v, w	Velocities in x, y and z directions
u', v', w'	u -, v -, and w -components of velocity fluctuations
$\bar{u}_i$	mean velocity components
u_i	Velocity component in the i direction
u'_i	Fluctuating velocity component in the i direction
u_τ	Friction velocity
u^+	Dimensionless velocity
U_0	Jet exit velocity or cross-section averaged velocity
U_m	Maximum spanwise velocity
U_{m0}	Maximum streamwise velocity
U_{ms}	maximum velocity at the offset section
U_{sp}	Velocity of seeding particles
V	Cell volume
W	Distances from the nozzle center to the left and right sides
x, y or z	Cartesian coordinates
x_i	Impact point location
x_m	Horizontal location of centerline peak
x_r	Return point location
x_s	End of the mixing zone
$y_{cm/2}$	Concentration half-height
$y_{m/2}$	Velocity half width
Y_M	Contribution of fluctuating dilatation in the compressible turbulence
Y_k	Dissipation of the turbulent kinematic energy
Y_ω	Dissipation of specific dissipation rate

$z_{cm}/2$	Concentration half-height
z_m	Vertical location of centerline peak
$z_{m/2}$	Velocity half height
z_t	Terminal rise height
$z_{tm}/2$	Temperature half-height
z^+	Dimensionless distance to the wall
z_I^+	Dimensionless distance of the first wall node to the wall
α_k	Inverse effective Prandtl numbers for k
α_ε	Inverse effective Prandtl numbers for ε
α^*	Low Reynolds number correction
β	Constant in RNG k - ε model
β^*	Coefficient in standard k - ω model
δ_{ij}	Kronecker delta
ε	Dissipation rate
ε_j	Coefficient in dynamic Smagorinsky SGS model
η	Constant in RNG k - ε closure
η_0	Constant in RNG k - ε closure
θ	Discharge inclination angle
κ	Von Karman constant
λ	Second viscosity
μ	First (dynamic) viscosity
μ_t	Turbulent (SGS) viscosity
μ_{eff}	Effective viscosity
ρ	Fluid density
ρ_a	Density of the ambient water

ρ_b	Density of the brine
σ_k	Turbulent Prandtl numbers for k
σ_ε	Turbulent Prandtl numbers for ε
$\sigma_{\omega,2}$	Constant in SST k - ω closure
τ_{ij}	Viscous, Reynolds or SGS stress
τ_{kk}	Isotropic part of the SGS stress
τ_w	Wall shear stress
ϕ	Scalar variable
ϕ'	Scalar fluctuation
ω	Specific dissipation rate
Γ	Viscous diffusivity
Γ_k	Effective diffusivities for turbulence kinetic energy
Γ_t	Turbulent diffusivity
Γ_ω	Effective diffusivities for specific dissipation rate
Δ	Grid scale
Δ_f	Filter-size
$\varnothing_o$	Outer diameter
$\varnothing_i$	Inner diameter
Ω_{ij}	Rate of rotation tensor

List of Abbreviations

BVM	Bousinesq-Viscosity Model
CCD	Charge-Coupled Device
CFD	Computational Fluid Dynamics
DNS	Direct Numerical Simulation
DKE	Dynamic Kinetic Energy
ED	Electro-Dialysis
EIA	Environmental Impact Assessment
EMA	Escaping Mass Approach
EASM	Explicit Algebraic Stress Model
FEM	Finite Element Method
FVM	Finite Volume Method
GUI	Graphical User Interface
GCI	Grid Convergence Index
LES	Large Eddy Simulation
LIF	Laser Image Fluorescence
LA	Light Attenuation
MSF	Multi-Stage Flash
MED	Multi-state Effect Distillation
NF	Nano-Filtration
PIV	Particle Image Velocimetry
PLIF	Planar Laser Induced Fluorescence
PDF	Probability Density Function

RBF	Reduced Buoyancy Flux
RNG	Re-Normalization Group
RO	Reverse Osmosis
RANS	Reynolds Averaged Navier-Stokes
SWRO	Seawater Reverse Osmosis
SST	Shear Stress Transport
S-L	Smagorinsky-Lilly
SGS	Sub-Grid Scale
3DLIF	Three-Dimensional Laser-Induced Fluorescence
UV	Ultra-Violet
WALE	Wall-Adapting Local Eddy-Viscosity

1 Introduction

1.1 Background

The rapid global urbanization in the past decades has exerted significant pressures on natural resources, among which the demands of freshwater are particularly in constraint. As a result, there is increasing interest to explore alternative methods to augment the situation. In cities near the coast, seawater desalination, especially seawater reverse osmosis (SWRO), is gaining popularity as an alternative of freshwater supply (Lattemann et al., 2010). At present, a large number of desalination plants are either built or being planned in the Middle East as well as other regions including the United States, Europe and Asia (Tularam and Ilahee, 2007; Lattemann et al., 2010).

The desalination processes essentially remove the suspended matters and dissolved minerals from seawater to produce potable water; while the waste stream of concentrated fluid, or so called brine, is typically directly discharged back to the coastal waters for economical purposes. However, the disposal of desalination brine containing elevated concentrations of dissolved substances, waste heat as well as suspended particles, is drawing increasing attention to their potential environmental impact on the coastal waterborne species (Morton et al., 1997; Tularam and Ilahee, 2007; Lattemann and Höpner, 2008; Roberts et al., 2010; Dрами et al., 2011).

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In the literature, mortality rate analysis had been carried out to assess different salinity tolerances of different waterborne species (Pillard et al., 1999), and a salinity of 40 g/L was suggested as the general threshold for acute toxicity (Yoon and Park, 2011). The typical salinity of SWRO desalination brine, however, is around 60 - 90 g/L, and it is therefore essential to dilute the desalination brine to a prescribed level. In addition, the heavier desalination brine has a tendency to sink towards the seabed, and the salinity does not decay spontaneously in the seawater due to its chemical stability. As a result, the salinity may accumulate near the discharge area over a period if the outfall is not properly designed. Overall, to mitigate the potential environmental impacts, a brine outfall must be properly configured and placed so as to efficiently mix with the surrounding ambient seawater to reduce the salinity within prescribed levels at the end of a small regulated mixing zone (Del Bene et al., 1994; California Coastal Commission, 2004).

A submerged inclined outfall configuration is typically adopted for desalination brine discharges with a single-port outfall or a multi-port diffuser in coastal waters. With the inclined configuration, the inclined dense jet exhibits a longer curvilinear trajectory before impacting the sea bed, leading to more efficient mixing with the entrained ambient water (Shao and Law, 2010). Figure 1.1 illustrates the schematic side view of the inclined dense jet in stagnant ambient, where h is port height to the bottom and θ is the discharge inclination angle; x_m , z_m , z_t , x_r , x_i , x_s and H_s are the horizontal location of centerline peak, vertical location of centerline peak, terminal rise height, return point location, impact point location, end of the mixing zone and spreading layer width, respectively; S_m , S_r , S_i and S_s are the dilution of the centerline peak, return point, impact point and end of the mixing zone, respectively. It shows that the inclined dense jet first rises up due to the discharge momentum until a

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maximum height is reached. Subsequently, the dense jet turns downward due to the negative buoyancy and impacts onto the seabed (Roberts et al., 1997). Entrainment takes place continuously along the jet trajectory. After the bottom impact, the diluted dense effluent then spreads along the seabed as a gravity current, exhibiting behavior similar to a spreading layer. A transition from the near field region to the far field region can be determined in the spreading layer at the end of the near field region.

Figure 1.1 Schematic side view of a typical inclined dense jet in stagnant ambient

Many analytical and experimental studies have been performed on the subject of submerged inclined dense jets to optimize the design of the brine outfall (Roberts and Toms, 1987; Roberts et al., 1997; Kikkert et al., 2007; Shao and Law, 2010; Lai and Lee, 2012; Oliver et al., 2013b). These experimental results indicated that the kinematic and mixing behavior of the inclined dense jet in stagnant ambient are dependent on the diameter (D) of the discharge port as well as the discharge densimetric Froude number (Fr) as:

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$$\frac{X}{FrD} = C_1(\theta) \quad (1.1)$$

$$\frac{S_L}{FrD} = C_2(\theta) \quad (1.2)$$

$$Fr = \frac{U_0}{\sqrt{\frac{\rho_b - \rho_a}{\rho_a} gD}} \quad (1.3)$$

where X represents the geometrical parameters in the horizontal, vertical or lateral direction; S_L is the dilution at a certain location; U_0 is the jet exit velocity; g is the gravitational acceleration; ρ_a and ρ_b are the density of the ambient water and brine, respectively; C_1 and C_2 are constant coefficients dependent on the discharge inclination angle.

Previous findings had helped assess the potential environmental impact of brine discharges and thus enable the design of the outfall in an optimal configuration. At the same time, the cost of brine outfall construction is still a major concern to cope with the rapidly growing capacity of desalination plants. More work is still needed to investigate inclined dense jets under various scenarios to further reduce the cost of the brine outfall.

1.2 Objectives and Scope

The design of brine outfalls desires further investigations of inclined dense jets in various flow conditions for the subsequent assessment of potential environmental

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impact. Previous studies have been mostly performed experimentally on inclined dense jets, including both kinematic and mixing behavior and thus the dilution characteristics. Based on these experimental results, analytical or integral models have also been developed as an efficient means to predict the geometrical parameters as well as the dilution of inclined dense jets (Cipollina et al., 2004; Kikkert et al., 2007) to aid the outfall design. However, improvement on the accuracy of predictions is still very much desired from these models (Palomar et al., 2012).

Numerical simulations based on Computational Fluid Dynamics (CFD) approaches offer another alternative to predict the mixing behavior of inclined dense jets in coastal waters. With the rapid advancement of computing hardware in recent years, the adaptation of CFD is also becoming more and more feasible. In the literature, only a few CFD studies using the Reynolds Averaged Navier-Stokes (RANS) approach have been reported so far, and they also focused on only limited characteristics of the inclined dense jet. The key objective of the present study is therefore to investigate comprehensively the mixing behavior of the inclined dense jet in coastal waters with CFD approaches. In particular, the numerical methodology adopted in the present study is the Large Eddy Simulation (LES) approach, which is theoretically anticipated to provide a better prediction of the mixing behavior due to its improved accuracy in resolving the large coherent eddies than the conventional RANS approach.

For brine discharges from a submerged outfall into coastal waters, the bottom impact of the inclined dense jet is inevitable, and the dilution at the impact point is

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an important consideration for the assessment of potential environmental impact. Therefore, another objective of the present study is to investigate numerically the impact of the inclined dense jet onto the bottom boundary. With the LES approach, detailed coherent structures and mixing mechanisms near the bottom can be explored, which are usually very difficult to be quantified experimentally due to the limitation of experimental techniques. After the bottom impact, the diluted dense effluent then spreads along the seabed as a gravity current, exhibiting behavior similar to a spreading layer. It is also essential to examine the mixing behavior in the spreading layer for the assessment of regulatory compliance at the end of mixing zone. The present study also addresses this issue.

Since wall interactions with bottom impact are of critical importance in this study, to build the capability and experience, LES studies are first carried out to investigate two related topics: (a) flow separation around a circular cylinder (for wall interactions), and (b) a circular turbulent wall jet without buoyancy (for concentration spreading along the wall boundary). These two configurations enable a detailed investigation of the numerical modelling approaches coupling LES for the larger flow domains with the boundary layer simulations, particularly with the considerations of the associated mixing behavior. This is to pave the way for the follow-up investigation with the simulations of the bottom impact of the inclined dense jet. In reality, wall jets are also sometimes used for effluent discharge in the industry when the effluent port is located near the bottom (Findikakis and Law, 1998).

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1.3 Outline

The present thesis consists of 8 chapters. Chapter 1 introduces the background of inclined dense jets, research motivation and objectives of the present study. Chapter 2 reviews the literature regarding the development of seawater desalination, potential environmental impact of brine discharges, inclined dense jets, turbulent circular wall jets and simulations of UV reactor flow for ballast water treatment. Chapter 3 presents the numerical methodology adopted in the present study including the turbulence closures of the CFD approach and near-wall simulations of wall-bounded flows. Chapter 4 illustrates an experimental validation of the LES approach in simulating the complex flow with wall interactions. Chapter 5 introduces the LES simulation results of turbulent circular wall jets. In Chapter 6, the LES simulation results of inclined dense jets into stagnant ambient are presented, together with the experimental validation of the numerical predictions. Chapter 7 investigates the bottom impact of the inclined dense jet as well as the characteristics of the spreading layer by means of LES. Finally, Chapter 8 summarizes the major findings and conclusions in the present study, and recommends possible future works.

2 Literature Review

2.1 Development of Seawater Desalination

Seawater and brackish water desalinations were firstly adopted in arid regions such as the Middle East (Saudi Arabia, United Arab Emirates, etc.), and nowadays have been among the most important sources of potable water. It is now more and more common to adopt desalination technologies to supplement freshwater supply in a large number of industrialized or developing countries including United States, Europe, Australia, China and etc. (Tularam and Ilahee, 2007; Lattemann and Höpner, 2008; Lattemann et al., 2010).

Desalination consists of a series of treatment processes that remove suspended matters (plankton, particles and etc.) and dissolved salt and other minerals from seawater or brackish water to produce potable water. A pioneering major seawater desalination facility was built in Saudi Arabia in 1938, and major development was made during World War II to supply water for military purpose (NRC, 2008). These early projects mainly operated desalination using distillation technology, and subsequently the Multi-state Effect Distillation (MED) process had been adopted in industry for a long time. MED was later replaced by the Multi-Stage Flash (MSF) developed in the 1950s due to its simpler operation and more reliable process (NRC, 2008; Lattemann et al., 2010). In the early 1970s, the commercialization of Reverse Osmosis (RO) in seawater desalination began (Buros, 2000). RO is a separation process via membranes that the water is separated from the dissolved matters by a

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semipermeable membrane barrier. Compared to MSF or MED, RO requires no heating or phase change which usually consumes a huge amount of energy. The major energy for SWRO is instead to pressure the feed seawater to flow through the membrane barrier, which is typically lower in energy consumption than distillation.

To conclude, desalination technology has been significantly developed in the past century from MED to MSF, and RO has gained dominated popularity in the past decades. With the development of technology, the capability of seawater desalination, especially SWRO, is growing rapidly to cope with the huge demand of freshwater arising from the growing population, urbanization and industrialization. For example, the world's largest operating RO system in 1969 was a capability of 380 m³ per day in Dallas, Texas, while nowadays the largest RO system can produce over 330,000 m³ per day (Lattemann et al., 2010). According to the statistics from the 20th International Desalination Association (IDA) Worldwide Desalting Plant Inventory, the capacity of worldwide installed desalination plants was 44.1 million m³ per day in 2006 (IDA and GWI, 2008). Figure 2.1 shows the yearly growth of the installed daily capacity before 2007 as well as the estimated growth from 2007 to 2015. From the figure, the installed capacity in 2007 was over 40 million m³ per day, and it is projected that the capacity will reach almost 100 million m³ per day by 2015. Among these installed desalination plants by 2007, RO processes take the majority of total capacity at 51% according to the statistics, and MSF and MED account for 32% and 8%, respectively. The remaining 9% is shared by other minor desalination processes including membrane-based Nano-Filtration (NF) and Electro-Dialysis (ED) processes.

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Figure 2.1 Yearly growth of the desalination market before 2007 and projected growth from 2007 – 2015 (IDA and GWI, 2008)

In other words, although the distillation processes still play the dominant role to produce freshwater (IDA and GWI, 2008) in countries from the Middle East, RO is fast becoming the dominant process outside the Middle East region, including the United States, Australia, and China. Singapore is also in great need for SWRO to diversify the water supply and is currently operating two large RO plants, meeting 25% of water demand in total. A recent plan is that Singapore is going to install the third desalination plant in 2017 with a capacity of 136,000 m³ per day (PUB Singapore's National Water Agency, 2015).

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2.2 Environmental Impacts of Brine Discharge

With the growth of desalination plants in many coastal regions, the desalination activities nowadays also draw increasing concerns on the potential environmental impact to the local ecology. An immediate concern is from the intake of desalination plants. Seawater desalination plants usually receive feed water from open seawater intakes. The existence of the intake can affect water exchange and sediment transport, and may result in losses of waterborne species which adhere to the intake screens or are pumped into the plants together with the feed water. This issue can be avoided or minimized by constructing infiltration galleries and placing the intake in a proper location. Another concern during the operation of desalination plants is their brine discharges into coastal waters. In the following sections, a review of the potential environmental impact of brine discharges is presented.

The desalination brine contains the concentrate of dissolved matters such as salt, suspended solid as well as possible thermal energy received from thermal desalination plants (Lattemann et al., 2010). Morton et al. (1997) compared the brine components of MSF and RO plants. The concentrate of distillation plants mainly contains increased temperature, salinity, pretreatment chemicals such as residual chlorine and chlorination by-products and heavy metals such as copper and nickel. Comparatively, the concentrate of SWRO plants typically contains elevated salinity and chlorination by-products, but residual chlorine is usually removed to protect the RO membranes.

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The distribution of marine species in coastal area is highly dependent on favorable environmental conditions including salinity, temperature, chemicals and metals, and therefore the desalination brine discharges may have adverse impact on these marine species. Drami et al. (2011) studied the environmental impact of a dual plant consisting of a SWRO plant and power plant. They observed that the salinity and temperature caused a decrease in the cell number of chlorophyll-a and picophytoplankton. Another study by Yoon and Park (2011) also revealed the ecotoxicological effects of desalination brine on marine species. It was found that different phytoplankton species have different sensitivities to the desalination brine, among which *Isochrysis galbana* has the lowest tolerance with over 50% mortality at 65 ppt of salinity. The high sensitivity to the salinity not only happens to phytoplankton, but also the macroalgae and fish. In general, a salinity of 40 g/L has been suggested as the threshold for acute toxicity. The average salinity of the world's oceans is 35 g/L, while the SWRO plants typically produce brine with a salinity of around 60 ~ 90 g/L. To conclude, the desalination brine may adversely affect the waterborne species near the outfall area. Therefore, an Environmental Impact Assessment (EIA) is usually required to be carried out for a proposed desalination project to identify and evaluate all potential impacts (Mabrook, 1994; Höpner and Windelberg, 1997; Hoepner, 1999; Lattemann and Höpner, 2008).

2.3 Inclined Dense Jets in Stagnant Ambient

As noted previously, it is essential to design the brine outfall in an optimal manner to achieve a rapid mixing of the brine effluent with ambient waters. Hence, a good prediction of the outfall performance is important for the design of desalination systems.

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A submerged inclined outfall is typically adopted in coastal waters for desalination brine discharges due to its longer curvilinear trajectory as shown in Figure 1.1. In the past decades, many analytical and experimental studies have been conducted on inclined dense jets to optimize the design of the brine outfall. The following section reviews previous studies on inclined dense jets in stagnant ambient, including experimental observations, integral modelling as well as numerical simulations.

2.3.1 Experimental observations

Zeitoun et al. (1970) performed a pioneering experiment on inclined brine outfalls with various inclinations (relative to horizontal) including 30° , 45° , 60° and 90° into stagnant ambient. They observed the longest trajectory at the angle of 60° and hence the maximum dilution at the terminal rise height. The 60° inclination was then investigated in many subsequent experimental investigations (Pincince and List, 1973; Roberts et al., 1997; Shao and Law, 2010).

Pincince and List (1973) performed a study on brine discharges in an estuary. Based on laboratory assessment, they suggested a dilution of 100:1 before the jet impacted the sea bed. They also compared their experimental results with integral modelling predictions, and concluded that the integral model was able to predict the flow geometrical trajectories with reasonable accuracy but significantly underestimated the dilution. Through dimensional analysis, the terminal rise height and its dilution

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were observed to be related to the inclination angles of the discharge port as well as densimetric Froude numbers (Fr).

Roberts and Toms (1987) investigated the dilution as well as terminal rise height of inclined dense jets in flowing currents. With a steady flowing current, the dilution of the inclined dense jet was observed to increase when the orientation of the outfall to the current direction changed from the same direction (co-flow) to adverse direction (counter-flow). When the current speed became zero, i.e., in stagnant ambient, it was also found that the inclined dense jet was preferable than the vertical dense jet with much higher dilution and lower terminal rise height as well.

With the development of laser imaging techniques, Planar Laser Induced Fluorescence (PLIF) began to be applied for the observation of two-dimensional concentration distribution fields. Roberts et al. (1997) adopted PLIF to quantify the instantaneous concentration distribution of a 60° inclined dense jet at the center plane. Their investigation covered the jet geometrical and mixing characteristics including the terminal rise height, impact point location and dilution, which were summarized into coefficients by dimensional analysis. In their study, the jet spread along the bottom boundary beyond the impact point was also reported whereby the dilution continued to increase. They determined the end of the mixing zone by the location where the scalar turbulence intensity dropped to 5%.

Another experimental study of vertical dense jets was performed by Zhang and Baddour (1998). They found that, for $Fr > 7$, the source mass flux had a negligible effect on the maximum jet penetration, resulting in a proportionality relationship

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between the densimetric Froude number and maximum height. However, for $Fr < 7$, it was found the derived proportional coefficients were not consistent with previous results, which they attributed to the effect due to the source mass flux at small densimetric Froude numbers.

In recent decades, comprehensive experimental studies on inclined dense jets have been performed covering both geometrical characteristics including the centerline peak, terminal rise height and return point and mixing characteristics including the dilution along the jet trajectory (Cipollina et al., 2005; Shao and Law, 2010; Papakonstantis et al., 2011a; Papakonstantis et al., 2011b; Lai and Lee, 2012). Cipollina et al. (2005) performed an experimental study on inclined dense jets in stagnant ambient with various configurations including different diameters of the discharge port, inclination angles and flow conditions including various brine densities and jet flow rates. The geometrical parameters, including the centerline peak, terminal rise height and return point, were found to be proportional to the densimetric Froude numbers instead of the Reynolds numbers. They also determined the geometrical coefficients for different discharge inclinations including 30° , 45° and 60° .

Shao and Law (2010) conducted an experimental study on 30° and 45° inclined dense jets in stagnant ambient using combined PIV and PLIF techniques to simultaneously measure the velocity and concentration distributions, respectively. If PIV and PLIF were to be conducted separately, potential errors may be involved when repeating the experiments for the measurements. A comprehensive investigation was conducted in their study, including the centerline trajectory and

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other geometrical coefficients. The mixing characteristics were also covered, including the centerline peak dilution, return point dilution and cross-sectional concentration distributions. They also examined the bottom effects on the inclined dense jet. It was found that the influence of the bottom boundary on the mixing behavior was significant if the nozzle height to the bottom was insufficient.

Papakonstantis et al. (2011a) performed an experimental study on inclined dense jets with six inclinations from 45° to 90° in stagnant ambient to measure the geometrical characteristics correlations with the densimetric Froude numbers as well as inclinations. From their observation, the maximum final terminal rise occurred at 80° . In their other study (Papakonstantis et al., 2011b), the mixing characteristics was reported for 45° , 60° and 75° in stagnant ambient. The dilution at the maximum height and return point were compared with previous experimental results. Furthermore, they also studied the second-order mixing characteristics, e.g., the concentration turbulence intensity. It was found that, at the same horizontal location, the vertical location of the maximum concentration turbulence intensity was systematically higher than the jet trajectory.

Lai and Lee (2012) reported a comprehensive study of inclined dense jets in stagnant ambient using PIV and PLIF for the observation of velocity and concentration distributions, respectively, with inclinations from 15° to 60° . The jet trajectories and mixing characteristics were investigated and compared with the integral model VISJET's predictions. They found that the maximum terminal rise and associated dilutions were generally under-predicted by VISJET. In their study, the concentration turbulence intensity was also investigated, and the vertical location

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of the concentration turbulence intensity at the terminal rise was observed to be beyond the centerline peak which was consistent with Papakonstantis et al. (2011b).

2.3.2 Integral modeling

In addition to experimental studies, many analytical studies had also been performed. With integral analysis, the governing equations, including the continuity, momentum and scalar transport equations, are integrated typically with an assumption of the Boussinesq approximation that the density differences between the brine and seawater is sufficiently small. Another main assumption of integral analysis is that the cross-sectional distribution of the jet trajectory can be expressed using a shape function of either Gaussian or Top-hat for the integration.

Integral modelling of positively buoyant jets had been extensively performed in the past (e.g. Morton (1959), Abraham (1963), Wang and Law (2002) and Fischer et al. (2013)). Comparatively, fewer studies had been carried out for negatively buoyant jets. To facilitate the design of the brine disposal diffusers, Cipollina et al. (2004) developed a model of inclined dense jets in stagnant ambient, which had four input parameters: the inclination, discharge port diameter, flow rate and fluid density. Their model was able to predict the jet centerline, impact point and horizontal location of the centerline peak in reasonable agreement with the experimental data, while the jet boundary and terminal rise height were under-predicted. They also revealed that the jet at a smaller inclination than 60° produced a larger dilution when a sloping seabed was involved.

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Kikkert et al. (2007) derived a new analytical model for the mixing behavior of inclined dense jets. They found that the analytical solution predicted the trajectory of the inclined dense jet with reasonable accuracy for different inclinations from 0 to 75°, but the integrated dilution was underestimated. In particular, the inner spreading of the inclined dense jet was also under-predicted.

Palomar et al. (2012) recently compared systematically the predictions of inclined dense jets by integral models including CORMIX, JetLag and UM3 with previous experimental data. The comparison was carried out in stagnant ambient with inclinations ranging from 30° to 60°, as well as in dynamic ambient including co-flowing, counter-flowing and transverse-flowing currents. In stagnant ambient, the three integral models generally under-estimated the geometrical coefficients including terminal rise height, centerline peak and return point location. In particular, the dilution characteristics were significantly under-predicted by at least 50% from these integral models. In dynamic ambient, the integral models were also found to under-predict the terminal rise height with increasing current speeds, and the deviation was the worst in transverse-flowing currents. Regarding the dilution, the integral models were found to under-predict at the return point with small current speeds, while over-predict with high current speeds except for UM3, which showed under-predictions for different current speeds in general.

2.3.3 Numerical modeling

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The approach of CFD has been introduced in the last two decades to numerically study the inclined dense jet. Previous studies mostly focused on vertical fountains (Kuang and Lee, 1999; Zeng and Huai, 2005; Mier-Torrecilla et al., 2012). The fountain is inherently different from the inclined dense jet because it re-entrains the negatively buoyant fluid which falls back around the vertical discharge.

The first CFD study on inclined dense jets was reported by Vafeiadou et al. (2005) in the literature. They employed the RANS approach and Shear Stress Transport (SST) $k-\varepsilon$ turbulence closure for the simulations in stagnant ambient at various discharge inclinations. The results on the terminal rise height were 15% to 40% lower compared to Roberts et al. (1997). They also found that the impact point distance was significantly under-predicted by CFD compared to Roberts et al. (1997)'s experimental results. At a given inclination, the terminal rise height from the CFD predictions was found to be proportional to the increasing densimetric Froude number.

Oliver et al. (2008) performed a numerical investigation on the initial mixing of inclined dense jets using the RANS approach with standard and calibrated $k-\varepsilon$ turbulence closures. They investigated the center plane concentration profiles, centerline integrated dilution at the maximum centerline peak, horizontal and vertical locations of the centerline peak, maximum elevation of the flow edge, and spreading widths. The results show that the centerline integral dilution at the maximum height was relatively under-predicted by the $k-\varepsilon$ closure compared to the experimental data, but was closer to the analytical solution. The $k-\varepsilon$ predicted integral dilution was also found to be dependent on the initial discharge inclination

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which was not evident in the experimental measurements. The $k-\varepsilon$ predicted spreading layer was significantly thinner than the reported experimental data, and the authors suggested that the $k-\varepsilon$ closure overestimated the stability of density gradient in the lower region of the inclined dense jet. Overall, they concluded that the RANS predictions provided more accurate representation of the inclined dense jets than integral models.

Recently, Gildeh et al. (2015) conducted a comprehensive numerical study using various turbulence closures, including RNG $k-\varepsilon$, realizable $k-\varepsilon$, nonlinear $k-\varepsilon$ and two Reynolds Stress Models (LRR and Launder-Gibson), to investigate the geometrical, velocity and concentration characteristics of 30° and 45° inclined dense jets. The cross-sectional velocity and concentration profiles were presented and compared with the experimental data. However, based on their results, the dilution at the return point showed very little differences between the 30° and 45° discharge inclinations, while previous experimental studies suggested that 45° should be more optimal in terms of dilution.

2.4 Bottom Impact of Inclined Dense Jets

In shallow coastal waters, the inclined dense jet would eventually impact onto the seabed. As noted previously, it is essential to predict the dilution at the impact point for the consideration of potential environmental impact. In addition, after the bottom impact, the diluted dense effluent then spreads along the seabed which forms a spreading layer. The spreading layer can further dilute the dense effluent (Roberts et

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al., 1997), and it is therefore essential to examine the mixing behavior of the spreading layer.

When the discharge port of a jet is placed close to a seabed bottom, the Coanda effect may occur which can affect the trajectory and mixing behavior, resulting in reduced dilution. The Coanda effect on positively buoyant jets was experimentally investigated previously by Sobey et al. (1988), and on negative dense jets by Shao and Law (2010). In most other cases, the Coanda effect was intentionally avoided (Jiang et al., 2014).

Roberts et al. (1997) investigated the 60° inclined dense jet with bottom impact using the laser-induced fluorescence (LIF) technique. They found that the terminal rise height was in good agreement with Roberts and Toms (1987), but the impact dilution was relatively higher. Besides the terminal rise height and impact point dilution, the flow characteristics beyond the impact point were also measured. The dilution at the end of the spreading layer, which was defined as the location where the concentration turbulence intensity falls to 5%, was found to be 60% higher than the impact point. They also determined the thickness and vertical concentration distribution in the spreading layer at different horizontal locations.

Nemlioglu and Roberts (2006) conducted a similar study on inclined dense jets using three-dimensional laser-induced fluorescence (3DLIF), which they extended the range of discharge angles to 15° - 90° . The dilution at the impact point was found to be essentially independent of discharge angles from 30° to 75° . The three-

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dimensional instantaneous concentration contours were also compared among different inclination angles in their study.

Papakonstantis and Christodoulou (2010) performed an experimental study on inclined dense jets from 45° to 85° as well as positively buoyant jets to investigate the transient evolution of the spreading along a horizontal bottom. They found that, for the inclined dense jet, the outer boundary of the density current was almost radial, and the transient variation of the radial distance to the impact point was computed to be proportional to the square root of time. Using non-dimensional analysis, they showed that the radial distance normalized by the local jet parameters was independent of the inclination angles and densimetric Froude numbers.

Crowe (2013) compared the results of inclined dense jets with and without bottom boundary to examine its possible influence on the mixing characteristics of the inclined dense jet. Based on his results, the presence of the bottom boundary had no influence on the characteristics at the maximum height, but had substantial influence at the return point. The jet spreading width was also affected by the bottom boundary when approaching the return point. From their data, the minimum nozzle height (H_d) necessary to avoid the boundary effect can be further determined for different inclination angles.

More recently, Palomar (2014) investigated inclined dense jets with inclinations from 15° to 75° using Particle Image Velocimetry (PIV) and PLIF, focusing on the behavior within the spreading layer. They measured the mean and turbulence fluctuation characteristics of velocity and concentration fields, which the normalized

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cross-sectional distributions were found to be self-similar. They also presented the velocity centerline from the discharge port up to the end of the mixing zone. In addition, they also investigated the dilution and spreading layer thickness at the end of mixing zone and compared with Roberts et al. (1997). They found that the decay of the concentration along the spreading layer was significant, and the ratio of the dilution at the impact point and at the end of the mixing zone ranged from 45% (30°) to 63% (75°).

The experimental studies mentioned above investigated the dilution variation at the impact location, but detailed information was typically missing in terms of the localized concentration distribution around the impact location. Recently, Abessi and Roberts (2015) added more information to this issue. They studied the effect of the discharge inclinations on the inclined dense jet in stagnant ambient, with measurements from the discharge port to the end of the mixing zone. All jet parameters were found to be dependent on the discharge angle, while the impact dilution was relatively insensitive to angles from 45° to 65°. An important observation in their study was that there existed a localized concentration build-up at the impact location in a time-averaged manner. In other words, the time-averaged concentration which was reducing along the trajectory due to entrainment, increased locally at the impact point before continuing the decay along the spreading layer. This localized build-up has important implications towards the determination of the impact dilution at the boundary.

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2.5 Turbulent Circular Wall Jets

For a free circular jet, the jet flow expands in an axisymmetrical manner. However, when a jet is placed next to an impermeable wall, i.e., a turbulent wall jet, the flow becomes asymmetrical due to the no flux condition at the wall. There are extensive applications of turbulent circular wall jets in the industry, such as film-cooling of the wall of a turbine (Launder and Rodi, 1983) and effluent discharges into shallow waters where the effluent port is located near the bottom (Findikakis and Law, 1998). Substantial experimental and numerical studies on turbulent wall jets had been conducted to investigate their hydrodynamics and thermodynamics (Sforza and Herbst, 1970; Rajaratnam and Pani, 1974; Launder and Rodi, 1983; Padmanabham et al., 1991; Craft and Launder, 2001; Law and Herlina, 2002; Bouda et al., 2008).

2.5.1 Experimental observations

Sforza and Herbst (1970) performed experimental measurements on the mean characteristics of three-dimensional turbulent wall jets, with air jets from various orifices discharging parallel to a flat wall into stagnant air ambient. Based on the observed axial maximum velocity decay, they characterized the wall jet into three distinct regions: the potential core, characteristic decay and radial type decay region. Their results showed that the decay rate of the maximum velocity in the near field was dependent on the orifice geometry, while this dependency became negligible in the far downstream. In terms of the mixing layer normal to the wall, the spanwise

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growth was independent of the nozzle shape, except for the region near the discharge nozzle.

Rajaratnam and Pani (1974), and Padmanabham et al. (1991) later investigated the velocity distribution of turbulent wall jets. The vertical cross-sectional velocity distribution was divided into two distinct regions. The region below the maximum velocity was named the boundary layer region and that above was named the free mixing region. A similarity of velocity profiles was observed in both the streamwise and spanwise directions in the zone of established flow. The characteristic scales for the similarity scaling are defined in Figure 2.2.

Figure 2.2 Schematic diagram of velocity distribution within a three-dimensional wall jet

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The maximum streamwise and spanwise time-averaged velocities, U_{m0} and U_m , were chosen as the characteristic velocity scales in the respective directions; the vertical distance from the bottom to the position where the time-averaged velocity is half of the maximum time-averaged velocity U_{m0} (i.e., velocity half height), $z_{m/2}$, was chosen as the vertical characteristic length scale; and the lateral characteristic length scale, $y_{m/2}$, was defined in a similar manner. Rajaratnam and Pani (1974) showed that, in the region of fully developed flow, the velocity scale, U_{m0} , decreased with the streamwise distance whereas both $z_{m/2}$ and $y_{m/2}$ increased linearly, with $y_{m/2}$ increasing at 4 to 5 times faster than $z_{m/2}$.

Law and Herlina (2002) performed a comprehensive experimental study on a circular three-dimensional wall jet using a non-intrusive laser imaging technique, developed by Law and Wang (2000). The analysis focused on the characteristics within the zone of established flow from 20 to 50 nozzle diameters (d). Both the velocity and concentration profiles were found to be self-similar in either streamwise or spanwise direction. They also analyzed the variations in the velocity, concentration, and length scales. The decays of maximum velocity and concentration were expressed by the following equations:

$$\frac{U_{m0}}{U_0} = 9.23 \left(\frac{x}{d} \right)^{-1.066} \quad (2.12)$$

$$\frac{C_{m0}}{C_0} = 6.97 \left(\frac{x}{d} \right)^{-1} \quad (2.13)$$

where x is the streamwise distance from the nozzle, C_{m0} is the streamwise maximum concentration and C_0 is the initial source concentration at source. The velocity-half-

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height and velocity-half-width were found to be increasing linearly from 20 to 50 nozzle diameters and can be expressed by the following linear fitting functions:

$$\frac{z_{m/2}}{d} = 0.042 \frac{x}{d} + 0.60 \quad (2.14)$$

$$\frac{y_{m/2}}{d} = 0.21 \frac{x}{d} - 1.91 \quad (2.15)$$

Similarly, the variations in concentration half-heights and half-widths were described as

$$\frac{z_{cm/2}}{d} = 0.061 \frac{x}{d} + 0.31 \quad (2.16)$$

$$\frac{y_{cm/2}}{d} = 0.31 \frac{x}{d} - 3 \quad (2.17)$$

where $z_{cm/2}$ and $y_{cm/2}$ are the concentration half-height and half-width, respectively. As compared to the gradients of linear fitting curves in Eqs. (2.14) to (2.17), the lateral profiles spread about 5 times faster than the vertical profiles for both velocity and concentration. The velocity ratio was consistent with the observation of Rajaratnam and Pani (1974), while the concentration ratio was identified for the first time in their study.

In addition to the mean flow behavior, Herlina and Law (2002) also extended the experimental observation to the turbulence characteristics of the circular wall jet, using the combined PIV and PLIF techniques. The turbulence characteristics included the distribution of velocity fluctuation, concentration fluctuation and turbulent mass transport both spanwise and streamwise, covering the streamwise displacement up to 50 nozzle diameters. It was found that the induced turbulence was still evolving within the region investigated. The turbulence intensity of

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velocity and concentration increased downstream in general, while the turbulent mass transport generally decreased with increasing distance from the nozzle. More experimental investigations on turbulent wall jets had also been performed by Abrahamsson et al. (1997), Gerodimos and So (1997), and Eriksson et al. (1998).

2.5.2 Numerical modelling

Craft and Launder (2001) conducted a numerical investigation on three-dimensional turbulent wall jets using the RANS approach with various turbulence closures. The mechanism for the larger lateral spreading rate, as observed by Rajaratnam and Pani (1974), was investigated. The differences among the turbulence closures were due mainly to the variants of the second moment closure used to resolve the Reynolds stresses. The results showed that the higher rate of lateral spread arose from induced stream-wise turbulent vortices, rather than asymmetric diffusion. The spreading ratio was observed to be sensitive to the choice of pressure-strain model.

Lubcke et al. (2003) performed a numerical study on the spreading mechanism of three-dimensional turbulent wall jets with a modified Explicit Algebraic Stress Model (EASM) to resolve the turbulent secondary motion near the wall. They compared the quartic EASM results with linear Bousinesq-viscosity model (BVM), quadratic EASM, as well as previous experimental results. They found that the quartic EASM was able to capture the turbulence secondary motion. However, the predicted lateral to vertical spreading ratio was 2.97 which was still much less than the experimental ratio of about 5.

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Dejoan and Leschziner (2005) explored the mean flow and turbulence characteristics of a plane turbulent wall jet, or two-dimensional wall jet, by means of the LES approach. They captured all scales larger than 10 Kolmogorov lengths with fine grid spacing (with 8.4 million grids in total). The numerical results were generally in agreement with the experimental data from Eriksson et al. (1998). They also analyzed the budgets for the turbulence energy and Reynolds stresses to study the interactions between the near-wall and outer shear layer, and demonstrated that turbulent transport, among a number of mechanisms, played a decisive role.

Recently, Li et al. (2012) examined numerically the circular wall jet using LES, and compared the predictions with previous experimental data. They simulated the mean velocity and turbulence characteristics in both spanwise and streamwise directions. The Probability Density Function (PDF) of the streamwise velocity fluctuation, cross-sectional profiles of turbulent Reynolds stresses at various downstream locations and the vortex structure near the wall were also presented. However, their results did not agree well with the experimental data from Law and Herlina (2002) and Herlina and Law (2002).

2.6 Simulations of UV Reactor Flow for Ballast Water Treatment

Ballast waters have been widely used in vessels for centuries to compensate the imbalance caused by the asymmetric distribution of cargos or passengers in ships, and to maintain the stability in the presence of lateral forces and moments generated

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by winds or waves during the sea journey. Ballast water is taken in by ships from the port of departure, and transported via oceans or rivers to the destination, where the water might be discharged or exchanged during the loading and unloading processes. The large amount of ballast water discharge had raised great threats to the worldwide aquatic ecosystems as well as the health of human beings, as ballast water carries large amount of organisms which may invade the endemic water (Carlton, 1985; Ruiz et al., 2000). To control the species invasion from ballast water, International Maritime Organization (IMO) (2004) issued a regulation that the ballast water was required to be treated to fulfil certain criteria before being discharged.

Ultra-Violet (UV) disinfection, as an efficient method to treat ballast waters with no by-products, is reported to be a good alternative for the treatment of ballast water (Werschkun et al., 2012). On the other hand, it is essential to control the energy consumption in UV disinfection processes, as it can be extremely high when treating the huge volume of ballast water within a ship. Due to the limited time and resources, the optimization of UV reactors can be better achieved through numerical simulations rather than experiments. In addition, experiments can be used for the validation of numerical studies. Typically, an integrated numerical simulation for UV disinfection consists of the CFD modelling for the flow field, modelling for the UV fluence rate (intensity distribution) and modelling for the microbial response to UV.

Liu et al. (2007) performed an integrated numerical simulation for the assessment of UV disinfection of ballast waters. He evaluated six commonly used RANS

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turbulence closures for the flow field prediction. The flow field and microbial inactivation were found to vary with the choice of the turbulence closure. However, none of them yielded consistent results compared to the experimental data. Therefore, a better approach than RANS was suggested to cope with the predictions of the complex flow field of the UV reactor.

Wols et al. (2010) compared the results of hydrodynamic predictions in a long square flume by RANS with $k-\epsilon$ closure and LES. The flow rate adopted was 5 L/s, and the mean velocity could be calculated as 0.031 m/s based on their configuration. Note that this relatively low velocity usually occurs in conventional water treatment while ballast water treatment requires a much higher velocity. The prediction of flow around the UV lamp was shown to be more accurate using LES.

3 Numerical Methodology

3.1 Introduction

CFD has been developed for decades. As a branch of fluid mechanics, it uses numerical methods to solve problems involving fluid flows, heat transfer, and related phenomena such as chemical reactions. If done properly and accurately, it can augment the investigation of fluid phenomena beyond experimental and analytical studies. As the CFD theory develops, more accurate results can be obtained. As a result, CFD is becoming more and more popular in academic research as well as industrial applications. This chapter discusses all the CFD approaches involved in the present study.

3.1.1 Computational fluid dynamics

An integrated CFD modelling consists of three main elements: a pre-processor, a main solver and a post-processor (Versteeg and Malalasekera, 2007). The pre-processing usually consists of the definition of the computational domain for a physical model, subsequent mesh generation, setting of boundary conditions and definition of physical properties. Regarding the solver, it involves the integration of the governing equations over all the control volumes within the computational domains, and the selection of discretization methods (to convert integrated equations into a serial of algebraic equations) and solution methods (to solve the algebraic

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equations). Besides, other related functions involving the computing speed and stability are also included in the solver. The post-processing displays or exports the velocity vector maps, velocity or concentration field contours, particle tracking, turbulence characteristics and other aspects.

Among the elements, the solver is the most important. Based on the numerical methods in the solver, the CFD approach can be classified into the finite volume, finite element, finite difference and other numerical methods. The Finite Difference Method (FDM) is one of the oldest among them, first developed by Richardson (1910) and adopted for numerical solution by Thom (1933). FDM is easy to implement, but is restricted to simple grids and the equations do not conserve on coarse grids. Compared to FDM, the Finite Element Method (FEM) is more often used nowadays in CFD programs for its higher accuracy with coarse grids. FEM was initially developed for structural mechanics (Courant, 1943) and thereafter began to be adopted for fluid flows in 1970s. The disadvantages of FEM are the slower speed to compute large domains.

Later, the Finite Volume Method (FVM) was developed for flow problems (Evans et al., 1957; Gentry et al., 1966). It solves the conservation problems with FDM and greatly reduces the computation time for very large domains which FEM cannot handle. Therefore, it has become the predominant numerical method for CFD nowadays. Many commercial CFD codes, for example, Ansys Fluent, Ansys CFX, Phoenix and Comsol, as well as open source codes such as OpenFOAM are established based on FVM.

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3.1.2 Summary of well-known CFD codes

3.1.2.1 ANSYS Fluent

In the present study, Ansys Fluent is chosen as the solver in Chapters 4 and 5. Ansys Fluent is a well-established CFD package that has been widely used in fluid flow, heat transfer, and chemical reactions with complex geometries. It is written in the C computer programming language, thus flexible solver control is possible. ANSYS Fluent provides complete flexibility for mesh schemes, and therefore it is very convenient to compute using unstructured meshes for very complex geometries that structured meshes cannot deal with. Supported mesh types include triangular, quadrilateral, tetrahedral, hexahedral, wedges and hybrid meshes. Gambit can be used for the geometrical creation as well as the mesh generation before importing the model to ANSYS Fluent.

The capabilities of Ansys Fluent range from two-dimensional to three-dimensional flows, steady to transient flows, laminar to turbulent flows, Newtonian to non-Newtonian flows, and single-phase to multi-phase flows. It provides a friendly user-interface for the setting of boundary conditions, physical properties, numerical schemes and the post-processing. In addition, the parallel processing capability in ANSYS Fluent speeds up simulation for large domains.

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3.1.2.2 OpenFOAM

OpenFOAM (Open source Field Operation And Manipulation) is a C++ library that allows users to create their own applications for the solutions of CFD. OpenFOAM was originally created by Weller et al. (1998) to develop a more flexible simulation platform for general use, and therefore it was written in C++ rather than FORTRAN computer language which was more commonly used for CFD in the past. It is currently released and maintained by the OpenFOAM Foundation (OpenFOAM, 2015) as an open source code under the protection of the GNU General Public License.

The capabilities of OpenFOAM solvers include the steady and unsteady flows, incompressible flow and compressible flow, multiphase flow and etc. Various turbulence closures can be implemented in OpenFOAM with the RANS approach, and both LES and Direct Numerical Simulation (DNS) are also available. In terms of mesh generation, OpenFOAM provides a utility namely blockMesh for the structured mesh generation, and a utility namely snappyHexMesh for complex geometry meshes. Besides, OpenFOAM accepts grids generated by third-party tools and converts them to the OpenFOAM format. Many pre- and post-processing utilities are also provided in OpenFOAM.

One of the strengths of OpenFOAM is that, in addition to the embedded utilities, customized solvers and pre-/post-processing tools can be created in C++ language. In contrast to ANSYS Fluent, all the parameters of the solver within OpenFOAM

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are open, and users are free to change the solver parameters to adjust to the flow problems. A disadvantage of OpenFOAM is the absence of an integrated graphical user interface (GUI) other than the simple post-processing GUI, namely paraFOAM.

3.2 Governing Equations

The flow of a viscous fluid is governed by the continuity and momentum equations as follow (Pope, 2002):

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0 \quad (3.1)$$

x-momentum equation:

$$\begin{aligned} \frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} \\ = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho f_x \end{aligned} \quad (3.2)$$

y-momentum equation:

$$\begin{aligned} \frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho vw)}{\partial z} \\ = -\frac{\partial p}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} + \rho f_y \end{aligned} \quad (3.3)$$

z-momentum equation:

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$$\begin{aligned} \frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho u w)}{\partial x} + \frac{\partial(\rho v w)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z} \\ = -\frac{\partial p}{\partial z} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} + \rho f_z \end{aligned} \quad (3.4)$$

where u , v and w are the velocities in the x , y and z direction, respectively; ρ is the fluid density, t is the time, p is the pressure, f_i (i represents x , y or z) is the external force in the respective direction, and τ_{ij} are the viscous stresses.

For a Newtonian fluid, the viscous stresses, τ_{ij} , are proportional to the rates of deformation (Versteeg and Malalasekera, 2007), given by

$$\tau_{xx} = 2\mu \frac{\partial u}{\partial x} + \lambda \text{div}(\mathbf{u}) \quad (3.5)$$

$$\tau_{yy} = 2\mu \frac{\partial v}{\partial y} + \lambda \text{div}(\mathbf{u}) \quad (3.6)$$

$$\tau_{zz} = 2\mu \frac{\partial w}{\partial z} + \lambda \text{div}(\mathbf{u}) \quad (3.7)$$

$$\tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \quad (3.8)$$

$$\tau_{xz} = \tau_{zx} = \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \quad (3.9)$$

$$\tau_{yz} = \tau_{zy} = \mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \quad (3.10)$$

where $\mathbf{u}$ is the velocity vector, μ is the first (dynamic) viscosity and λ is the second viscosity. The effect of second viscosity typically is small, and an empirical value for gas flows (Schlichting, 1979) is given by

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$$\lambda = -\frac{2}{3}\mu \quad (3.11)$$

For an incompressible liquid, the mass conservation equation (see Eq. (3.1)) can be simplified to $\text{div}(\mathbf{u}) = 0$ and the second viscosity term can be neglected.

Substituting Eqs. (3.5) - (3.10) into Eqs. (3.1) - (3.4), the following simplified governing equations, namely the well-known Navier-Stokes equations, can be obtained:

$$\frac{\partial \rho}{\partial t} + \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (3.12)$$

$$\begin{aligned} \frac{\partial(\rho u)}{\partial t} + \rho \left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) \\ = -\frac{\partial p}{\partial x} + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + \rho f_x \end{aligned} \quad (3.13)$$

$$\begin{aligned} \frac{\partial(\rho v)}{\partial t} + \rho \left(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right) \\ = -\frac{\partial p}{\partial y} + \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) + \rho f_y \end{aligned} \quad (3.14)$$

$$\begin{aligned} \frac{\partial(\rho w)}{\partial t} + \rho \left(u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) \\ = -\frac{\partial p}{\partial z} + \mu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + \rho f_z \end{aligned} \quad (3.15)$$

In addition, the scalar equation can be written as

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$$\begin{aligned} \frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho u\phi)}{\partial x} + \frac{\partial(\rho v\phi)}{\partial y} + \frac{\partial(\rho w\phi)}{\partial z} \\ = \frac{\partial}{\partial x} \left(\Gamma \frac{\partial\phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\Gamma \frac{\partial\phi}{\partial y} \right) + \frac{\partial}{\partial z} \left(\Gamma \frac{\partial\phi}{\partial z} \right) + S_\phi \end{aligned} \quad (3.16)$$

where ϕ is the scalar variable, Γ is the viscous diffusivity and S_ϕ is the source term.

3.3 Turbulence Closures

3.3.1 Introduction

In theory, the governing equations (Eqs. (3.12) - (3.16)) for continuity, momentum and scalar transport can be directly applied to all the viscous flows. At the same time, it is very difficult to resolve turbulent flows directly using the continuity equation and momentum equations because the flow fluctuation requires much smaller grids and time step than laminar flows.

To reduce computational cost, the Reynolds averaging method was widely adopted for solving the turbulent flow (Launder and Spalding, 1972; Launder and Spalding, 1974; Yakhot and Orszag, 1986; Yakhot et al., 1992; Menter, 1994; Shih et al., 1995; Wilcox, 1998). In this approach, the instantaneous velocity is decomposed into two components:

$$u_i = \bar{u}_i + u'_i \quad (3.17)$$

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where $\bar{u}_i$ and u'_i are the mean and fluctuating velocity components ($i = 1, 2, 3$), respectively. Other scalar variables (ϕ), for instance the pressure, can also be expressed in a similar way:

$$\phi = \bar{\phi} + \phi' \quad (3.18)$$

Substituting the above expressions into the continuity and momentum equations yields (Launder and Spalding, 1974)

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}}{\partial x} + \frac{\partial \bar{\rho} \bar{v}}{\partial y} + \frac{\partial \bar{\rho} \bar{w}}{\partial z} = 0 \quad (3.19)$$

$$\begin{aligned} \frac{\partial \bar{\rho} \bar{u}}{\partial t} + \bar{\rho} \left(\bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} + \bar{w} \frac{\partial \bar{u}}{\partial z} \right) \\ = - \frac{\partial p}{\partial x} + \mu \left(\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + \frac{\partial^2 \bar{u}}{\partial z^2} \right) \\ + \left(- \frac{\partial \overline{\bar{\rho} u' u'}}{\partial x} - \frac{\partial \overline{\bar{\rho} u' v'}}{\partial y} - \frac{\partial \overline{\bar{\rho} u' w'}}{\partial z} \right) + \bar{\rho} f_x \end{aligned} \quad (3.20)$$

$$\begin{aligned} \frac{\partial \bar{\rho} \bar{v}}{\partial t} + \bar{\rho} \left(\bar{u} \frac{\partial \bar{v}}{\partial x} + \bar{v} \frac{\partial \bar{v}}{\partial y} + \bar{w} \frac{\partial \bar{v}}{\partial z} \right) \\ = - \frac{\partial p}{\partial y} + \mu \left(\frac{\partial^2 \bar{v}}{\partial x^2} + \frac{\partial^2 \bar{v}}{\partial y^2} + \frac{\partial^2 \bar{v}}{\partial z^2} \right) \\ + \left(- \frac{\partial \overline{\bar{\rho} u' v'}}{\partial x} - \frac{\partial \overline{\bar{\rho} v' v'}}{\partial y} - \frac{\partial \overline{\bar{\rho} v' w'}}{\partial z} \right) + \bar{\rho} f_y \end{aligned} \quad (3.21)$$

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$$\begin{aligned}
\frac{\partial \bar{\rho} \bar{w}}{\partial t} + \bar{\rho} \left(\bar{u} \frac{\partial \bar{w}}{\partial x} + \bar{v} \frac{\partial \bar{w}}{\partial y} + \bar{w} \frac{\partial \bar{w}}{\partial z} \right) \\
= -\frac{\partial p}{\partial z} + \mu \left(\frac{\partial^2 \bar{w}}{\partial x^2} + \frac{\partial^2 \bar{w}}{\partial y^2} + \frac{\partial^2 \bar{w}}{\partial z^2} \right) \\
+ \left(-\frac{\partial \bar{\rho} \bar{u}' \bar{w}'}{\partial x} - \frac{\partial \bar{\rho} \bar{v}' \bar{w}'}{\partial y} - \frac{\partial \bar{\rho} \bar{w}' \bar{w}'}{\partial z} \right) + \bar{\rho} f_z
\end{aligned} \tag{3.22}$$

Taking the time average, dropping the overbar on the mean velocity components and replacing the body force term with the gravity, the Reynolds-Averaged Navier-Stokes (RANS) equations can be written in Cartesian tensor form as

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0 \tag{3.23}$$

Momentum equation:

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \rho g_i + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} \right) \right] + \frac{\partial \tau_{ij}}{\partial x_j} \tag{3.24}$$

In addition, scalar transport equation:

$$\frac{\partial}{\partial t} (\rho \phi) + \frac{\partial}{\partial x_j} (\rho \phi u_j) = \frac{\partial}{\partial x_j} \left[\Gamma \left(\frac{\partial \phi}{\partial x_j} \right) \right] + \frac{\partial Q_j}{\partial x_j} \tag{3.25}$$

where g_i is gravitational acceleration in the i direction. Compared to the Navier-Stokes equations, the RANS equations involve additional terms, $\tau_{ij} = -\rho \overline{u'_i u'_j}$ and $Q_j = -\rho \overline{\phi' u'_j}$, which are the Reynolds stresses and turbulent scalar flux, respectively. These terms must be solved by additional equations to ensure the closure of equations.

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3.3.2 Reynolds averaged Navier-Stokes closures

Within the scope of RANS, many turbulence closures were developed based on various assumptions as the derivation of Reynolds stresses is difficult by theoretical calculations. An alternative is to introduce an approximation, the Boussinesq hypothesis, which assumes that the stresses can be incorporated through turbulent viscosity or eddy viscosity in the following manner (Launder and Spalding, 1974):

$$\tau_{ij} = -\rho \overline{u'_i u'_j} = \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \left(\rho k + \mu_t \frac{\partial u_k}{\partial x_k} \right) \delta_{ij} \quad (3.26)$$

where μ_t is the turbulent viscosity, u_i is the mean velocity component, δ_{ij} is the kronecker delta, and k is the turbulent kinetic energy which is calculated by

$$k = \frac{\overline{u'_i u'_i}}{2} = \frac{1}{2} (\overline{u'^2} + \overline{v'^2} + \overline{w'^2}) \quad (3.27)$$

Similarly, by analogy that the turbulent transport of scalar is proportional to the gradient of the mean quantity, we have the expression for the turbulent scalar flux:

$$Q_j = -\rho \overline{\phi' u'_j} = \Gamma_t \frac{\partial \phi}{\partial x_j} \quad (3.28)$$

where Γ_t is the turbulent diffusivity.

Together with the expressions in Eqs. (3.26) - (3.28), the RANS equations can be closed only if the turbulent viscosity and turbulent diffusivity can be properly expressed. Since the turbulent transport of momentum and scalar is assumed to be due to the same mechanism, it is naturally expected that there exists a correlation

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between the turbulent diffusivity and turbulent viscosity, which is known as the Reynolds analogy as follow (Versteeg and Malalasekera, 2007):

$$Sc_t = Pr_t = \frac{\mu_t}{\Gamma_t} \quad (3.29)$$

where Sc_t and Pr_t are the turbulent Schmidt number and turbulent Prandtl number for scalar and heat, respectively.

The Boussinesq hypothesis has been adopted in many closures among which the $k - \varepsilon$ type and $k - \omega$ type closures are two popular closures. The differences among them are the way to solve the turbulent viscosity, μ_t . The disadvantage of Boussinesq hypothesis is that the turbulent viscosity is assumed to be isotropic which may not be always true, and would lead to false results. However, the assumption requires very low computational cost to calculate the turbulent viscosity. Therefore, closures based on the Boussinesq hypothesis have been widely used in industrial applications.

The following sections illustrate the RANS type approaches which were adopted in the present study to compare with the LES predictions, including a group of $k - \varepsilon$ closure as well as $k - \omega$ closure. The $k - \varepsilon$ closure involves a group of two-equation turbulence closure, including the standard $k - \varepsilon$ closure, Re-normalization Group (RNG) closure, and realizable $k - \varepsilon$ closure, in which the two transport equations involving the turbulence kinetic energy (k) and its dissipation rate (ε) are introduced to solve for the turbulent viscosity.

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3.3.2.1 Standard $k - \varepsilon$ closure

In the standard $k - \varepsilon$ closure, the flow is assumed to be fully turbulent and the molecular viscosity is neglected. The turbulence kinetic energy and its dissipation rate can be computed from the following equations (Launder and Spalding, 1972)

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \quad (3.31)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) \\ = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \\ + S_\varepsilon \end{aligned} \quad (3.32)$$

where $G_k = -\rho \overline{u'_i u'_j} \frac{\partial u_j}{\partial x_i}$ is the generation of the turbulence kinetic energy due to the mean velocity gradients; $G_b = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right) g_i \frac{\mu_t \partial T}{Pr_t \partial x_i}$ is the generation of the turbulence kinetic energy due to buoyancy; $Y_M = 2\rho \varepsilon \left(\sqrt{\frac{k}{a^2}} \right)^2$ is the contribution of fluctuating dilatation in the compressible turbulence to the dissipation rate, with a is the sound speed, S_k and S_ε are user-defined source terms; and σ_k and σ_ε are the turbulent Prandtl numbers for k and ε , respectively.

After the turbulent kinematic energy and its dissipation rate are obtained, the turbulent viscosity can be calculated by

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$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (3.33)$$

The constants involved in Eqs (3.31) - (3.33) include $C_{1\varepsilon}, C_{2\varepsilon}, C_\mu, \sigma_k, \sigma_\varepsilon, Pr_t$. The values of these constants are listed in Appendix A.

3.3.2.2 RNG $k - \varepsilon$ closure

Based on the standard $k - \varepsilon$ closure, two other closures (RNG and realizable $k - \varepsilon$ closures) have been developed to improve the performance. The RNG $k - \varepsilon$ closure is developed from the standard $k - \varepsilon$ closure with refinements based on the renormalization group theory (Yakhot and Orszag, 1986).

The transport equations of RNG $k - \varepsilon$ closure are similar to those of the standard closure (Yakhot et al., 1992):

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left(\alpha_k \mu_{eff} \frac{\partial k}{\partial x_j} \right) + G_k + G_b - \rho \varepsilon - Y_M + S_k \quad (3.34)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) \\ = \frac{\partial}{\partial x_j} \left(\alpha_\varepsilon \mu_{eff} \frac{\partial \varepsilon}{\partial x_j} \right) + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \\ - R_\varepsilon + S_\varepsilon \end{aligned} \quad (3.35)$$

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where α_k and α_ε are the inverse effective Prandtl numbers, and μ_{eff} is the effective viscosity calculated by RNG theory, which calculates the turbulent viscosity as

$$d\left(\frac{\rho^2 k}{\sqrt{\varepsilon\mu}}\right) = 1.72 \frac{\frac{\mu_{eff}}{\mu}}{\sqrt{\left(\frac{\mu_{eff}}{\mu}\right)^3 - 1 + C_v}} d\left(\frac{\mu_{eff}}{\mu}\right) \quad (3.36)$$

The R_ε term is calculated by

$$R_\varepsilon = \frac{C_\mu \rho \left(\frac{Sk}{\varepsilon}\right)^3 \left(1 - \frac{Sk}{\varepsilon \eta_0}\right) \varepsilon^3}{1 + \beta \left(\frac{Sk}{\varepsilon}\right)^3} \frac{1}{k} \quad (3.37)$$

where η_0 , and β are constants. Using Eq. (3.37), the ε equation (3.35) can be rewritten as

$$\begin{aligned} \frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_i}(\rho\varepsilon u_i) \\ = \frac{\partial}{\partial x_j} \left(\alpha_\varepsilon \mu_{eff} \frac{\partial \varepsilon}{\partial x_j} \right) + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon}^* \rho \frac{\varepsilon^2}{k} \end{aligned} \quad (3.38)$$

where $C_{2\varepsilon}^*$ is computed by

$$C_{2\varepsilon}^* = C_{2\varepsilon} + \frac{C_\mu \rho \left(\frac{Sk}{\varepsilon}\right)^3 \left(1 - \frac{Sk}{\varepsilon \eta_0}\right)}{1 + \beta \left(\frac{Sk}{\varepsilon}\right)^3} \quad (3.39)$$

The value of $C_{2\varepsilon}^*$ varies with S , which represents the strain rate. When $S = 0$, $C_{2\varepsilon}^* = C_{2\varepsilon}$, which is consistent with the standard closure. Therefore, the RNG closure is more sensitive to the effects of strain rate.

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In summary, compared to the standard $k - \varepsilon$ closure, the RNG closure improves the accuracy for rapidly strained flows by inserting an additional term in ε equation, and considering the low-Reynolds-number effects (in near-wall region) by developing an analytical differential formula for effective viscosity. The default values of the constants are summarized in Appendix A.

3.3.2.3 Realizable $k - \varepsilon$ closure

The realizable $k - \varepsilon$ closure differs from the standard $k - \varepsilon$ closure by two additional modifications: an alternative formulation for the turbulent viscosity, and a modified transport equation for ε . The term “realizable” means that certain mathematical constraints need to be satisfied on the Reynolds stresses, which is consistent with the physics of the turbulent flows. The limitation of the realizable $k - \varepsilon$ closure is that, for the computational domain containing both stationary fluid zones and rotating zones, it can produce non-physical turbulent viscosities.

The transport equations with the realizable $k - \varepsilon$ closure can be written as (Shih et al., 1995):

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \quad (3.40)$$

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$$\begin{aligned}
\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_i}(\rho\varepsilon u_i) \\
= \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + \rho C_1 S \varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}} \\
+ C_{1\varepsilon} \frac{\varepsilon}{k} C_{3\varepsilon} G_b + S_\varepsilon
\end{aligned} \tag{3.41}$$

Similar to other $k - \varepsilon$ closures, the turbulent viscosity is calculated by Eq. (3.33).

Here, C_μ is no longer a constant. Instead, it is calculated by

$$C_\mu = \frac{1}{A_0 + A_s \frac{kU^*}{\varepsilon}} \tag{3.42}$$

where

$$U^* \equiv \sqrt{S_{ij}S_{ij} + \tilde{\Omega}_{ij}\tilde{\Omega}_{ij}} \tag{3.43}$$

The default values of the constants A_0 and A_s as well as expression of $\tilde{\Omega}_{ij}$ are summarized in Appendix A.

3.3.2.4 Standard $k - \omega$ closure

The standard $k - \omega$ closure is an empirical closure based on transport equations for the turbulence kinetic energy and specific dissipation rate, ω , instead of the dissipation rate. The turbulence kinetic energy and the specific dissipation rate can be calculated by (Wilcox, 1998)

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$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\Gamma_k \frac{\partial k}{\partial x_j} \right] + G_k - Y_k + S_k \quad (3.44)$$

$$\frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_i}(\rho \omega u_i) = \frac{\partial}{\partial x_j} \left[\Gamma_\omega \frac{\partial \omega}{\partial x_j} \right] + G_\omega - Y_\omega + S_\omega \quad (3.45)$$

where $G_k = -\rho \overline{u'_i u'_j} \frac{\partial u_j}{\partial x_i}$ is the generation of the turbulent kinetic energy by the averaged velocity gradients; $G_\omega = \alpha \frac{\omega}{k} G_k$ is the generation of the specific dissipation rate; $Y_k = \rho \beta^* f_\beta^* k \omega$ and $Y_\omega = \rho \beta f_\beta \omega^2$ are the dissipation of the turbulent kinematic energy and specific dissipation rate, respectively; $\Gamma_k = \mu + \frac{\mu_t}{\sigma_k}$ and $\Gamma_\omega = \mu + \frac{\mu_t}{\sigma_\omega}$ are effective diffusivities for the turbulence kinetic energy and specific dissipation rate, respectively; and S_k and S_ω are source terms.

After solving the transport equations, the turbulent viscosity can be expressed as

$$\mu_t = \alpha^* \frac{\rho k}{\omega} \quad (3.46)$$

where α^* is the low Reynolds number correction, given by

$$\alpha^* = a_\infty^* \left(\frac{a_0^* + Re_t/R_k}{1 + Re_t/R_k} \right) \quad (3.47)$$

where $Re_t = \frac{\rho k}{\mu \omega}$, $R_k = 6$, and $a_0^* = 0.024$. When the Reynolds number increases, Re_t increases accordingly and finally $\alpha^* = a_\infty^* = 1$. The values of the constants involved herein are summarized in Appendix A.

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3.3.2.5 SST $k - \omega$ closure

The Shear-stress transport (SST) $k - \omega$ closure is developed by combining the formulation of the $k - \omega$ closure in the near-wall region with the $k - \varepsilon$ closure in the far field, which hereby is converted into the $k - \omega$ formulation. Compared to the standard $k - \omega$ closure, the SST $k - \omega$ closure includes some refinements and is more accurate and reliable for flows including transonic shock waves and adverse pressure gradient flows.

The transport equations for the SST $k - \omega$ closure are similar to the standard $k - \omega$ closure (Menter, 1994):

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\Gamma_k \frac{\partial k}{\partial x_j} \right] + \hat{G}_k - Y_k + S_k \quad (3.48)$$

$$\frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_i}(\rho \omega u_i) = \frac{\partial}{\partial x_j} \left[\Gamma_\omega \frac{\partial \omega}{\partial x_j} \right] + G_\omega - Y_\omega + D_\omega + S_\omega \quad (3.49)$$

where $\hat{G}_k = \min(G_k, 10\rho\beta^*k\omega)$ is the generation of turbulence kinetic energy due to the mean velocity gradients; $G_\omega = \frac{\omega}{k}\hat{G}_k$ is the generation of specific dissipation rate; $Y_k = \rho\beta^*k\omega$ and $Y_\omega = \rho\beta f_\beta\omega^2$ are the dissipation of turbulent kinematic energy and specific dissipation rate, respectively, due to the turbulence; $D_\omega = 2(1 - F_1)\rho \frac{1}{\omega\sigma_{\omega,2}} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}$ is the cross-diffusion term; and S_k and S_ω are source terms.

The turbulent viscosity is obtained by

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$$\mu_t = \frac{\rho k}{\omega} \frac{1}{\max\left[\frac{1}{\alpha^*}, \frac{SF_2}{a_1\omega}\right]} \quad (3.50)$$

where S is the strain rate magnitude, and F_2 is the blended function. The values of the constants are summarized in Appendix A.

3.3.3 Large eddy simulation

The RANS closures require very low computational cost but predict the flow with a low accuracy in many complex cases. An alternative method is to solve the Navier-Stokes equations without any hypothesis or any turbulence closure, which is termed the DNS approach. The solution of DNS is the most accurate among all simulation methods while requires the highest computational cost as the meshes have to be fine enough to capture the smallest eddies and the time step must be small enough to ensure numerical stability. However, observation reveals that the scale of eddies ranges from macro-scale to micron-scale and most of the energy is contained in the large eddies (Kolmogorov, 1941). Therefore, one alternative is to compute the relatively large eddies using DNS and simulate the small eddies by a suitable turbulence sub-grid model, which forms the basis of the LES approach.

3.3.3.1 Introduction

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In turbulent flows, the transports of mass, momentum, energy, and other quantities are mainly affected by the large eddies which are strongly determined by the boundary conditions, and thus anisotropic (Pope, 2002). On the contrary, the small eddies are isotropic or tend to be isotropic and rarely affected by boundaries, thus the turbulence closures are more suitable in this case. In LES, eddies are filtered into large and small parts based on the local grid sizes, and large eddies are computed directly by the instantaneous Navier-Stokes equations while small ones are modelled based on the Boussinesq hypothesis. The RANS closures are also based on the Boussinesq hypothesis, however, eddies of all scales are assumed to be isotropic, and thus they cannot resolve the large eddies accurately. Therefore, by direct simulations of large eddies, LES is expected to yield better predictions of the flow than the RANS closures. For small eddies, the Boussinesq hypothesis can give reasonable results even with relatively coarse grids. Therefore, the computational cost involved with LES is lower than that with DNS, although generally still higher than the RANS closures.

With the LES approach, the filtered continuity, momentum and concentration transport equations based on the instantaneous Navier-Stokes equations in Cartesian coordinates for LES are as follows (Smagorinsky, 1963):

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho \tilde{u}_j) = 0 \quad (3.51)$$

Momentum equation:

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$$\frac{\partial}{\partial t}(\rho \tilde{u}_i) + \frac{\partial}{\partial x_j}(\rho \tilde{u}_i \tilde{u}_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial \tilde{u}_i}{\partial x_j} \right) \right] + \frac{\partial \tau_{ij}}{\partial x_j} \quad (3.52)$$

Scalar transport equation:

$$\frac{\partial}{\partial t}(\rho \tilde{\phi}) + \frac{\partial}{\partial x_j}(\rho \tilde{\phi} \tilde{u}_j) = \frac{\partial}{\partial x_j} \left[\Gamma \left(\frac{\partial \tilde{\phi}}{\partial x_j} \right) \right] + \frac{\partial Q_j}{\partial x_j} \quad (3.53)$$

where the tilde indicates spatially filtered variables; $\tau_{ij} = -\rho \tilde{u}_i \tilde{u}_j - \rho \tilde{u}_i \tilde{u}_j$ and $Q_j = -\rho \tilde{\phi} \tilde{u}_j - \rho \tilde{\phi} \tilde{u}_j$ are the sub-grid scale (SGS) stresses and SGS scalar flux, respectively.

In Eqs. (3.51) – (3.53), eddies are classified into different scales through the filtering operation. Large eddies can be resolved directly, while small eddies are represented by subgrid-scale stresses which require further modelling. The subgrid-scale turbulence closures are typically based on the Boussinesq hypothesis, which calculates the subgrid-scale turbulent stresses as (Smagorinsky, 1963; Lilly, 1967)

$$\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2\mu_t \tilde{S}_{ij} \quad (3.54)$$

$$Q_j = -\frac{\mu_t}{Sc_t} \frac{\partial \tilde{\phi}}{\partial x_j} \quad (3.55)$$

where μ_t is the SGS viscosity, τ_{kk} is the isotropic part of the SGS stresses which can be added to the filtered static pressure term or neglected, $Sc_t = 0.7$ (Yimer et al., 2002; Law, 2006) is the SGS turbulent Schmidt number, and $\tilde{S}_{ij}$ is the strain rate tensor given by:

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$$\tilde{S}_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \quad (3.56)$$

Similar to the RANS closure, it can be observed from Eqs. (3.51) – (3.55) that the only unresolved variable for LES is the SGS viscosity, μ_t , which can be calculated by the SGS models as to be introduced in the following.

3.3.3.2 Smagorinsky SGS model

The Smagorinsky SGS model was originally developed by Smagorinsky (1963) for the closure of SGS viscosity. Later, Lilly (1967) further developed the model, and thus the model is also called Smagorinsky-Lilly SGS model. The subgrid-scale turbulent viscosity is modelled in the Smagorinsky SGS model as:

$$\mu_t = \rho L_S^2 |\tilde{S}| \quad (3.57)$$

where $|\tilde{S}| \equiv \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$ and L_S is the mixing length given by:

$$L_S = \min(\kappa d_{\text{wall}}, C_S \Delta) \quad (3.58)$$

with κ is the Von Karman constant, d_{wall} is the distance to the wall, Δ is the grid scale and C_S is the Smagorinsky constant which usually ranges from 0.1 – 0.2. However, C_S may not be a universal constant, thus limiting the prediction capability.

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3.3.3.3 Dynamic Smagorinsky SGS model

In the dynamic Smagorinsky SGS model, C_s is no longer regarded as a constant. In fact, it can be better determined by a localized dynamic procedure proposed by Germano et al. (1991) and further modified by Lilly (1992) as follow:

$$C_s^2 = \frac{\langle L_{ij} M_{ij} \rangle}{2 \langle M_{ij} M_{ij} \rangle} \quad (3.59)$$

$$L_{ij} = \tilde{u}_i \tilde{u}_j - \hat{\tilde{u}}_i \hat{\tilde{u}}_j \quad (3.60)$$

$$M_{ij} = \Delta^2 |\widehat{\tilde{S}}| \tilde{S}_{ij} - \hat{\Delta}^2 |\hat{\tilde{S}}| \hat{\tilde{S}}_{ij} \quad (3.61)$$

where the angular brackets indicate a spatial averaging procedure over directions of statistical homogeneity, and the caret indicates a spatial filtered quantity on the test-filter.

This procedure was further developed to include the scalar transport as (Lilly, 1992)

$$Sc_t = \frac{C_s^2}{C_\phi^2} \quad (3.62)$$

$$C_\phi^2 = \frac{\langle \varepsilon_j R_j \rangle}{\langle R_j R_j \rangle} \quad (3.63)$$

$$\varepsilon_j = \widehat{\tilde{u}_j \tilde{\phi}} - \hat{\tilde{u}}_j \hat{\tilde{\phi}} \quad (3.64)$$

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$$R_j = \Delta^2 |\tilde{S}| \frac{\partial \tilde{\phi}}{\partial x_j} - \Delta^2 |\hat{S}| \frac{\partial \hat{\phi}}{\partial x_j} \quad (3.65)$$

3.3.3.4 Dynamic kinetic energy SGS model

In the Dynamic Kinetic Energy (DKE) model, the transport of the SGS turbulence kinetic energy is defined by (Kim and Menon, 1997)

$$k_{sgs} = \frac{1}{2} (\overline{u_k^2} - \bar{u}_k^2) \quad (3.66)$$

which is obtained by solving the transport equation

$$\rho \frac{\partial \bar{k}_{sgs}}{\partial t} + \rho \frac{\partial \bar{u}_j \bar{k}_{sgs}}{\partial x_j} = -\tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j} - C_\varepsilon \rho \frac{k_{sgs}^{3/2}}{\Delta_f} + \frac{\partial}{\partial x_j} \left(\frac{\mu_t \partial \bar{k}_{sgs}}{\sigma_k \partial x_j} \right) \quad (3.67)$$

where the constant σ_k is equal to 1 and the constant C_ε is determined dynamically.

The subgrid-scale turbulent viscosity is thus computed by

$$\mu_t = C_k \rho k_{sgs}^{1/2} \Delta_f \quad (3.68)$$

where C_k is a constant which is determined dynamically, and Δ_f is the filter-size that can be computed by

$$\Delta_f \equiv V^{1/3} \quad (3.69)$$

where V is the volume of the computational cell. The SGS stress is thus different and can be written as

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$$\tau_{ij} - \frac{2}{3}\rho k_{sgs}\delta_{ij} = -2\mu_t C_k \rho k_{sgs}^{1/2} \Delta_f \bar{S}_{ij} \quad (3.70)$$

3.3.3.5 Wall-adapting local eddy-viscosity SGS model

In the Wall-Adapting Local Eddy-viscosity (WALE) model, the subgrid-scale turbulent viscosity is modelled as (Nicoud and Ducros, 1999)

$$\mu_t = \rho L_s^2 \frac{(S_{ij}^d S_{ij}^d)^{3/2}}{(\bar{S}_{ij}^d \bar{S}_{ij}^d)^{5/2} + (S_{ij}^d S_{ij}^d)^{5/4}} \quad (3.71)$$

where L_s and S_{ij}^d are computed by:

$$L_s = \min(\kappa d, C_w V^{1/3}) \quad (3.72)$$

$$S_{ij}^d = \frac{1}{2}(\bar{g}_{ij}^2 + \bar{g}_{ji}^2) - \frac{1}{3}\delta_{ij}\bar{g}_{kk}^2, \bar{g}_{ij} = \frac{\partial \bar{u}_i}{\partial x_j} \quad (3.73)$$

where $C_w = 0.325$.

3.4 Near-Wall Treatments

The presence of walls can significantly affect the turbulent flows due to the no-slip condition of the wall. In particular, the flow velocity and turbulence are rapidly reduced toward the wall due to the viscous damping and kinematic blocking in the

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very near-wall region (Kim, 1989; So et al., 1996). Hence a special treatment for the low-*Re*-number near-wall flow is required.

3.4.1 Law of the wall

In turbulent flows, the velocity is increasingly reduced when approaching a wall boundary. Previous studies revealed that the time-averaged velocity at a certain position close to the wall is proportional to the logarithm of the distance from the location to the wall, namely the law of the wall (Vandriest, 1956; Tennekes and Lumley, 1972). Later on, the wall region is further investigated, and the logarithmic of the wall is found to be only valid when the location is within the inner boundary layer but far enough from the wall where the viscous effects can be negligible (Tennekes and Lumley, 1972). In other words, the near-wall region consists of three layers, including a viscous sub-layer, a buffer layer and a fully turbulent layer, as shown in Figure 3.1. The distance to the wall is usually represented by z^+ which is normalized by the friction velocity and dynamic viscosity expressed as follow (Schlichting et al., 2000):

$$z^+ \equiv \frac{\rho u_\tau z}{\mu} \quad (3.74)$$

$$u_\tau = \sqrt{\frac{\tau_w}{\rho}} \quad (3.75)$$

where z is the distance to the wall, u_τ is called friction velocity, τ_w is the wall shear stress.

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Figure 3.1 Subdivisions of the near wall region (Schlichting et al., 2000)

The viscous sub-layer resides below around $z^+ = 5$, where the flow is almost laminar and the viscosity dominates the momentum and heat transfer. The relationship between the velocity and the wall distance in this layer follows the following equation (Schlichting et al., 2000):

$$u^+ = z^+ \quad (3.76)$$

where u^+ is the dimensionless velocity expressed as

$$u^+ = \frac{u}{u_\tau} \quad (3.77)$$

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Further away from the wall, i.e. z^+ is large enough to be within the fully turbulent layer, or the log-law layer, where the turbulence plays a major role while the laminar effect becomes negligible. Within the fully turbulent layer, the mean velocity is proportional to the logarithm of the distance from the wall as follow (Schlichting et al., 2000)

$$u^+ = \frac{1}{\kappa} \ln z^+ + C^+ \quad (3.78)$$

where κ is the Von Karman constant and C^+ is the empirical constant, and they can be determined to 0.41 and 5, respectively (Schlichting et al., 2000). In the buffer layer between the viscous sub-layer and the log-law layer, the velocity neither follows Eq. (3.76) or the log-law in Eq. (3.78). Laminarity and turbulence both play equally important roles in the buffer layer.

3.4.2 Wall functions

Resolving the viscous sub-layer requires very fine grid on the wall, and the flow in the buffer layer is complex to model. Therefore, one alternative is to establish a “bridge” between the wall and far field instead of directly resolving the boundary layer, forming the wall function. With the wall function, semi-empirical formulas are used to bridge the region between the wall and the outer fully-turbulent layer instead, and it has been vastly used in RANS simulations due to its relative simplicity (Craft and Launder, 2001; Huai et al., 2010).

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The shortcoming of the wall function is that it may give wrong results due to improper near-wall meshes that the first node falls into viscous sub-layer or buffer layer instead of the fully turbulent layer. The general application of this approach is thus limited due to the empiricism involved.

3.4.3 Near-wall modelling

Compared to wall functions, the near-wall modelling approach, instead, resolves the near-wall region directly, which necessitates a sufficient resolution of the boundary layer. Without semi-empirical formulas, the near-wall modelling approach is expected to simulate the near-wall region in higher accuracy. Since the viscous sub-layer is of the order of $z^+ \sim 5$, the first mesh node in LES should reside around $z^+ = 1.0$ for near-wall modelling (Piomelli and Balaras, 2002; Dejoan and Leschziner, 2005). In the present study, proper direct near-wall modelling is adopted for the LES simulations.

4 Evaluation of RANS with various Turbulence Closures and LES with various SGS Models in Simulating Flows with Wall Interactions

In this chapter, an experimental validation of the LES approach is performed in terms of its performance to simulate complex flows with wall interactions. The validation was performed within a customized closed conduit in which the flow passed a cylinder, with the configuration which is originated from a cross-flow UV reactor for the ballast water treatment (Wols et al., 2011). Various RANS closures were also included for comparisons with the LES predictions.

4.1 Introduction

In the present study, the LES approach is introduced to simulate the complex flow in UV reactors. The LES predictions were compared with various commonly used RANS turbulence closures, and validated by the experimental measurement within a customized closed conduit in which the flow passed a horizontally orientated cylinder. The configuration originated from a cross-flow UV reactor for ballast

*This chapter is written based on “Evaluation of RANS with various turbulence closures and LES with various SGS models in simulating flows with wall interactions”, In preparation.

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water treatment (Wols et al., 2011). The general principle of the cross-flow reactor is for the lamp sleeves to be usually placed perpendicular to the flow with a staggered pattern, so as to force the water to move close to the lamp surfaces thus increasing the UV intensity. With the simplified model, the superior performance of LES than RANS in dealing with flow predictions within such complex configuration is demonstrated.

4.2 Experimental Methodology

4.2.1 Experimental setup

In the present study, a lab-scale model was fabricated using transparent acrylic sheets with a thickness of 10 mm to quantify the hydrodynamics behind the single lamp sleeve of cross-flow UV reactors. As illustrated in Figure 4.1, the cylinder (sleeve) had an outer diameter ($\varnothing_o$) of 30 mm and was placed at the mid-depth of the model. The reactor was designed with a rectangular cross-section of 71 mm (height) $\times$ 50 mm (width), as it was more convenient for PIV measurements to be conducted with a flat surface rather than a curved surface (as with a circular cross-section). The reactor began with a circular inlet tube having an inner diameter ($\varnothing_i$) of 24 mm, and followed by an abrupt change in the cross-sectional area of the conduit which would lead to flow separation. To achieve a uniform flow, a plastic porous block was placed near the inlet tube and an acrylic sheet with 56 holes was attached to the bounded wall to hold the porous block. The upstream region occupied approximately 1.3 meters within which the flow became fully turbulent.

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Figure 4.1 Lab-scale UV reactor (unit in mm): (a) three-dimensional view; and (b) top view

4.2.2 Particle image velocimetry

PIV is a non-intrusive optical based technique to measure the two-dimensional instantaneous velocity field and corresponding post-processed mean velocity field (Law and Wang, 2000; Law and Herlina, 2002; Weitbrecht et al., 2002). In this chapter, PIV was adopted to quantify the velocity fields in the customized model for the validation of the LES predictions.

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PIV technique is based on the determination of the displacement (L_{sp}) of a group of “seeding” particles with cross-correlation within an Imaging Area (IA) during a specific time interval (T_{sp}), and the particle velocity (U_{sp}) is then calculated by the following equation:

$$U_{sp} = \frac{L_{sp}}{T_{sp}} \quad (4.1)$$

By assuming that the group of particles is passively advected by the fluid flow, the particle velocity thus represents the flow field. To satisfy the assumption, the density of the seeding particles must be approximately neutrally buoyant so that they can be suspended in the fluid; and the particle sizes must be efficiently small to track the flow, yet large enough to scatter sufficient light for the camera to capture. In the present study, the particle size was chosen to be 50 μm for all the experiments.

To capture the motion of seeding particles in the model, a dual-cavity frequency-doubled pulsed Nd:YAG laser and a charge-coupled device (CCD) camera were combined as an integral system. The pulsed laser system emitted a light sheet with a wavelength of 532 nm for illumination. The CCD camera captured the images with a resolution of 1600×1186 at a frame rate of 15 Hz. The specifications of the system were summarized in Table 4.1.

4.2.3 Experiment procedures

During the experiments, the flow circulation was maintained by connecting the model with a reservoir tank. Water was pumped continuously from the reservoir,

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and the flow rate was controlled by a digital flow meter. The laser light sheet was adjusted to coincide with the center plane parallel to the vertical direction, and the camera was focused on the laser sheet to capture the scattered light. The seeding particles were added to the tank to obtain a fully mixing solution with a concentration of 0.1 g/L. The time interval (T_{sp}) between two frames were adjusted according to various flow rates, and determined through calibration runs. The measurements were conducted at three flow conditions, as shown in Table 4.2.

Table 4.1 Specifications of the laser system

Items	Specifications
Laser model	Dantec Dynamics DualPower 50-100
Camera	Dantec Dynamics FlowSense 2M
Lasing medium	Nd:YAG
Minimum pulse duration	4 ns
Wavelength	532nm
Maximum output	400mJ

To investigate the hydrodynamics around the cylinder, especially the variations of velocity profiles behind the cylinder where a recirculation zone (wake region) is usually present in turbulent flows (Williamson, 1996), a total of 279 image pairs were recorded at 2 Hz during each measurement which lasted for 138 seconds. These image pairs were post-processed using the Dantec Dynamic Studio software for the time-average velocity field. The velocity field was first derived through “Adaptive Correlation” based on recorded images, and then filtered by “Moving Average Validation”. A time-averaged velocity vector map was finally generated by

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averaging the vector fields at individual time instances. To examine the velocity field, velocity profiles were extracted along vertical lines at seven locations, which included 75 mm upstream, and then 50, 75, 100 and 125 mm downstream. The streamwise velocity profiles along streamwise centreline ($y = z = 0$) were also extracted to investigate velocity variation along the centerline.

Table 4.2 Flow conditions of experiments

Cases	1	2	3
Flow Rate Q_0 (L/s)	0.63	1.18	1.55
Cross-Sectional Avearged Velocity U_0 (m/s)	0.176	0.332	0.437
Re	6,600	12,400	16,400

4.3 Numerical Methodology

4.3.1 Numerical setup

Figure 4.2 shows the three-dimensional computational domain created in Gambit which was a mesh generator for ANSYS Fluent, where the origin of coordinate was set to the center of the cylinder (tube sleeve). The computational domain was based on the physical setup in the experiments as shown in Figure 4.1, with the same dimensions but a simplification of the upstream configuration. Within the physical setup shown in Figure 4.1, there was a substantial distance (over 1.5 m) upstream for the flow to develop into fully turbulent state before reaching the cylinder.

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However, the region of interest was mainly the area behind the sleeve where flow separation happened. In order to save computational effort, only a 0.3 m length in the upstream domain was simulated, and it was numerically examined to be sufficient to cover the upstream region (about 0.05 m based on the experiments as presented in the following sections) affected by the presence of the cylinder.

4.3.2 Meshing and boundary conditions

The domain was meshed into structural meshes with 2 million cells. The grid size ranged from 0.5 mm to 2 mm, and the near wall regions were further refined by adaption. To check the grid independence, the results from three grid schemes were compared with each other. Figure 4.3 shows the velocity profiles of $Re = 12400$ at $x = 100$ mm downstream simulated based on the standard $k-\varepsilon$ closures and the LES approach with WALE SGS model with three different grid schemes. The grid scheme with 2 million cells was found to be sufficient for both $k-\varepsilon$ and LES simulations. The inlet boundary condition was set to uniform velocity, with three corresponding inlet velocities of 0.176, 0.332, and 0.437 m/s. The turbulence intensity was estimated to be 2% for the inlet. The outlet was set to pressure outlet and the other boundaries were set to no-slip wall boundary.

Figure 4.2 Model geometry: (a) overview, and (b) top view

4.3.3 Solver settings

ANSYS Fluent was adopted as the solver for the simulations, and the pressure-based transient solver was used. In the present study, the LES approach with SGS models including the Smagorinsky-Lilly (S-L), WALE and DKE, as well as the RANS approach with the standard, RNG and realizable $k-\varepsilon$, and standard and SST $k-\omega$ closures were performed for comparisons. The near-wall modelling approach was chosen for LES, and the log-law wall function was chosen for the $k-\varepsilon$ closures and $k-\omega$ closures. The time step was adjusted by Courant-Friedrichs-Lewy condition (Courant et al., 1967) so that the Courant number was less than 1. The convergence criteria for the continuity, velocities, and k were all set to 10^{-6} .

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Figure 4.3 Velocity profiles of $Re=12400$ at $x = 100$ mm

To determine the necessary duration for time averaging of the LES simulation results, the velocity profiles at $x = 100$ mm obtained from various time durations are compared in Figure 4.4, where the results were obtained from the LES (results were time-averaged from $t = 0$ to the specific time) and standard $k-\epsilon$ closure predictions (results were extract at the specific time). Even though the RANS model solved the flow in a Reynolds averaged manner, the sufficient simulation time still needed to be determined to avoid the effect of the initial condition. From the comparison of different time durations, the simulation time of 15 s was found to be fully sufficient for RANS predictions, and the duration of 25 s was sufficient for LES.

Figure 4.4 Velocity profile of $Re = 6600$ at $x = 100 \text{ mm}$

4.4 Results and Discussion

The mean velocity characteristics at the center plane were obtained from various turbulence closures and were compared with the present experimental data. The velocity profiles along the vertical direction (z axis) were first extracted from the center plane ($y = 0$) at various streamwise locations (x axis) including $x = -75 \text{ mm}$, 50 mm , 75 mm , 100 mm , and 125 mm . The effect of Reynolds numbers could be assessed by comparing the velocity profiles at the same streamwise location under various Reynolds numbers. The longitudinal velocity profiles along the centerline ($y = z = 0$) from $x = -75 \text{ mm}$ to $x = 300 \text{ mm}$ were also extracted to investigate the velocity variation along the centerline in this section.

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4.4.1 Velocity profiles in upstream region

It is critical to examine the steady flow profile in the upstream section before the cylinder. Figure 4.5 shows the vertical velocity profiles in the upstream at $x = -75$ mm with the three Reynolds numbers. From the experimental data, it can be observed that the velocity profile was slightly more uniform for higher Reynolds numbers. This suggests that the flow field might not be fully developed at the lowest Re , and it was probably due to the insufficient upstream length.

Despite the experimental imperfection, all the numerical results obtained from the different approaches collapsed into a single curve and were somewhat close to the experimental data, revealing the similar performance of these approaches in the predictions of upstream steady flow. A slight difference of the velocities at the centerline between the experimental data and predicted results can be observed at the highest Re , with the variation around 2%, which was within the experimental uncertainty.

4.4.2 Velocity profiles in wake region

It was concluded from Figure 4.5 that the different approaches all provided reasonably good predictions of the steady flow profile in the upstream section. However, behind the cylinder, there existed a wake region in which velocity fields

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were significantly affected by the cylinder (Williamson, 1996), and the performance of conventional RANS closures was reported to yield poor accuracy (Liu et al., 2007) in this region. Therefore, the characteristics of the flow in the wake region behind the cylinder required further investigation. In this section, the mean velocity profiles were extracted from various turbulence closures as well as experimental results at different streamwise locations for comparison.

Figure 4.6 shows the comparison of velocity profiles at $x = 50$ mm obtained from the various CFD approaches and experimental observations. From the figure, the velocity profile was featured by two peaks and one trough, with a local minimum along the centerline. The two peaks were due to flow acceleration with the presence of the walls both at top and bottom where the velocity decreased to zero. The presence of a trough located at the centerline in the wake region was consistent with previous studies (Cantwell and Coles, 1983; Breuer, 2000) when the flow passed a cylinder. From the figure, both LES and RANS with the $k-\omega$ closure were found to yield better agreement with the experiments, while RANS with the $k-\varepsilon$ closure yielded much higher peaks and lower local minimum value. In terms of the trough, LES produced better predictions with a higher Re .

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Figure 4.5 Velocity profiles at $x = -75$ mm: $Re =$ (a) 6600, (b) 12400, and (c) 16400

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Figure 4.6 Velocity profiles at $x = 50$ mm: $Re =$ (a) 6600, (b) 12400, and (c) 16400

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Further downstream, the velocity profiles at $x = 75$ mm were extracted and plotted in Figure 4.7, which the curves also generally had two peaks and one trough. Comparing with Figure 4.6, the differences between the extreme values (peaks and trough) became smaller, indicating the effect of the cylinder was weakened. From the figure, RANS with the three different $k-\varepsilon$ closures still far over-predicted the peak values and under-predicted the minimum values. RANS with the three different $k-\omega$ closures gave much better predictions of the minimum values but over-predicted on the peak values. In comparison, LES, especially the DKE and WALE SGS models, showed its capability of simulating both extreme values reasonably well.

Figure 4.8 shows the velocity profiles at $x = 100$ mm. Compared with Figure 4.6 and Figure 4.7, the flow profile tended to be much more uniform. In general, RANS with the $k-\varepsilon$ closures were unable to reproduce this trend. Among the $k-\omega$ closures, the standard $k-\omega$ closure better predicted the minimum values at the centerline, but both the standard and SST $k-\omega$ closures over-predicted the peaks. In comparison, the LES predictions were consistent with the experimental results. Within LES, the WALE and DKE SGS models were found to be better than the S-L model, which tended to yield more uniform results at large and medium Re .

In summary, RANS with the $k-\varepsilon$ closures were not able to reproduce the velocity variations in the wake region, and the $k-\omega$ closures provided better predictions but over-predicted the peaks when the flow went downstream from the cylinder. In general, LES, especially the WALE and DKE SGS models, provided the closest results to the experimental data in the wake region.

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Figure 4.7 Velocity profiles at $x = 75$ mm: $Re =$ (a) 6600, (b) 12400, and (c) 16400

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Figure 4.8 Velocity profiles at $x = 100$ mm: $Re =$ (a) 6600, (b) 12400, and (c) 16400

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4.4.3 Velocity profiles beyond wake region

With increasing distance from the cylinder in the downstream, the effect of the cylinder eventually disappears and the velocity profiles become uniform in general. Figure 4.9 shows the velocity profiles at $x = 125$ mm, and from the figure the velocity became almost uniform, proving that the influence of the wake region can be negligible at this point.

From the figure, it can be observed that RANS with the $k-\varepsilon$ closures were not able to simulate this transition and they tended to predict a much larger wake region. The $k-\omega$ closures generally captured this transition better, even though the standard $k-\omega$ closure tended to reproduce large wake region at high Re . However, both the standard and SST $k-\omega$ closures predicted much higher velocity compared with the experimental data. In comparison, LES was able to capture this transition well and the predicted velocities were closer to the experimental data, and among all the LES models the LES S-L model was the best performer.

4.4.4 Longitudinal velocity profiles at centerline

Figures 4.6 - 4.9 illustrated how the mean velocity profiles changed along the flow direction behind the cylinder. To better understand the flow characteristics, the magnitude of streamwise velocity along the centerline of the reactor was plotted from $x = -75$ to 300 mm, as shown in Figure 4.10. It was found that the centerline

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velocity started to drop from $x = -50$ mm until reaching zero at the surface of the cylinder. Once the flow passed the cylinder, the velocity increased from zero to a local peak and then decreased again to a local minimum located at around $x = 42$ mm and seemed invariant with Re . The minimum location was the location where the direction of streamwise velocity changed from negative to positive (Cantwell and Coles, 1983). Beyond that, the velocity began to positively increase until reaching a steady state.

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Figure 4.9 Velocity profiles at $x = 125$ mm: $Re =$ (a) 6600, (b) 12400, and (c) 16400

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Figure 4.10 Longitudinal variation of velocity at the centreline: $Re =$ (a) 6600, (b) 12400, and (c) 16400

4.5 Conclusions

The hydrodynamics of the flow passing a cylinder within a closed conduit was investigated by both RANS and LES approaches with various turbulence closures and LES SGS models, respectively. Overall, RANS with the $k-\varepsilon$ closures yielded the least accurate results with far under-estimations of the longitudinal velocity in the wake region; while the $k-\omega$ closures were in satisfactory agreement with the experimental data near to the cylinder but continuously over-predicted in the far field; and LES provided the best fit to the experimental data. Overall, the results illustrated that LES is a better approach than RANS in predicting the flow field around complex boundaries including possible flow separation, and is thus more suitable for the flow field predictions within a UV reactor.

5 Large Eddy Simulations of Turbulent Circular Wall Jets

5.1 Introduction

As discussed above, the occurrence of turbulent circular wall jets is common in many industrial applications, such as film-cooling of the wall of a turbine (Launder and Rodi, 1983) and effluent discharges into shallow water where the effluent port is located near the bottom (Findikakis and Law, 1998). In the literature, many studies were performed on turbulent wall jets by means of experiments (Law and Herlina, 2002) as well as numerical modelling (Craft and Launder, 2001).

The previous numerical studies on three-dimensional turbulent wall jets focused only on the kinematic characteristics, while the mixing behavior or scalar transport had not been addressed so far. The understanding of the scalar transport of the circular wall jet is important for engineering assessment, and it also contributes towards the fundamental understanding of wall bounded shear flows. In this study, we employ LES with proper near-wall modelling to evaluate both the kinematic and scalar mixing characteristics of the turbulent circular wall jet. Based on the results,

*This chapter is written based on “Large eddy simulations of turbulent circular wall jets”, *International Journal of Heat and Mass Transfer* (2015).

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we shall demonstrate that the performance of LES in simulating the three-dimensional turbulent wall jet with proper near-wall modelling is satisfactory. The LES results are found to be superior to the results from RANS models with wall functions.

5.2 Computational Methodology

In the present study, two RANS closures (standard k - ϵ and standard k - ω) and LES approach with the Smagorinsky SGS model were adopted to simulate three-dimensional circular wall jets. The governing equations for the closures were discussed in Chapter 3.

5.2.1 Flow configuration

The computational domain was configured based on the experimental setup in Law and Herlina (2002) in Cartesian coordinates. As shown in Figure 5.1, U_0 and U_{m0} are the inlet velocity and maximum streamwise mean velocity, respectively, and $y_{m/2}$ and $z_{m/2}$ are velocity-half-width and velocity-half-height, respectively. The computational domain had dimensions of 1.5 m length, 0.6 m width and 0.2 m height. A circular inlet with a diameter (d) of 5.5 mm was centered at a height (h) of 3.75 mm from the wall. The mesh was a hybrid type with a total of 1.6 million cells. The grid size ranged from 0.3 mm to 13 mm, with a higher resolution near the inlet and the bottom wall boundary as shown in Figure 5.2, in which the grid size

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gradually increased from the origin of the coordinates towards the outer region in three dimensions. Particularly, the size of the grid decreases towards the bottom wall in the z -direction. The minimum grid spacing in the x and y directions were 0.8 mm and 0.3 mm, respectively.

Figure 5.1 Schematic diagram of the computational domain

The grid convergence had been tested using the Grid Convergence Index (GCI), which is a widely used method for the estimation of uncertainty due to the discretization in CFD simulations (Roache, 1997; Celik et al., 2008), with both coarser (0.9 million cells) and finer (3.1 million cells) schemes. Figure 5.3 presents the uncertainty of the results along the centerline at the nozzle height, where the GCI value is plotted in the form of error bars. From the figure, the maximum uncertainty was about 10%, and the uncertainty at most places was small. To simulate the near-wall region, a log-law wall function was applied to both the $k - \varepsilon$ and $k - \omega$ closures.

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The proper near-wall modelling was adopted for LES that the near-wall meshes were further refined such that the first mesh node (z_l^+) is less than 1.0 due to the anticipation of wall significance in this case.

Figure 5.2 Mesh in the near-inlet region and on the bottom wall for near-wall modelling

5.2.2 Computational setup

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In terms of boundary conditions, the inlet was set to have a uniform inflow velocity (U_0) of 2.23 m/s and a temperature (T_0) of 305 K. With an ambient temperature (T_a) of 300 K and an insulated wall, the temperature difference could then be utilized as tracer of the scalar concentration distribution within the jet mixing. It should be noted that the scalar mass transport revealed through the temperature distribution was the key objective in the present study. The hydraulic diameter and turbulent intensity at the inlet were estimated to be 5.5 mm and 5%, respectively. For the LES simulations, artificial turbulence of the inflow was set using the spectral synthesizer method (Kraichnan., 1970; Smirnov et al., 2001). In this method, the random flow is generated by synthesizing divergence-free vector fields from a sample of Fourier harmonics, accounting for the effects of inhomogeneity and anisotropy of turbulent shear stresses. Therefore, the method is particularly suited for the wall jet study using LES with which the effects of inhomogeneity and anisotropy are of primary importance. Based on the inlet diameter and the kinematic viscosity of water (1×10^{-6} m²/s), the Reynolds number was calculated to be $Re = 12200$, which was fully turbulent. The bottom was specified as a wall boundary with no-slip condition, and the top surface was set as slip condition. The other four boundaries were set as zero gradient boundary conditions.

The numerical software used in the present study was ANSYS Fluent version 13 based on the FVM. The governing equations were discretized based on the FVM with the SIMPLE algorithm for the pressure-velocity coupling. Least Squares Cell Based method was chosen to compute the gradient. In RANS models, the second-order upwind scheme was used for the momentum and turbulent kinetic energy discretization, and the first-order upwind scheme was used for the dissipation rate. In LES, bounded central differencing was used for the momentum discretization.

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Time was discretized using the second-order implicit scheme, and the standard scheme was introduced for the pressure interpolation. The convergence criterion of 10^{-5} was set for the continuity, velocities, and k , and 10^{-6} for energy. Moreover, the time step for LES was determined so that the Courant number was less than 1.

Figure 5.3 (a) Velocity variation and corresponding uncertainty along the centreline; (b) Scalar concentration variation and corresponding uncertainty along the centreline

5.3 Results and Discussion

The results of numerical simulations were compared at two planes: the horizontal plane (at $z = 3.75$ mm) and the vertical symmetry plane (at $y = 0$). They illustrated the lateral and wall-normal spread of the wall jet, respectively. In this study, the time-averaged LES results were sampled from 30 to 160 s of the simulation time, as such period was judged to be quasi-steady and the profiles fully developed.

5.3.1 Velocity characteristics

The instantaneous ($t = 160$ s) velocity vector maps obtained from LES at the two planes are shown in Figure 5.4. The direction of the vectors shows how the flow spreads streamwise and spanwise within the domain, and the length of the vectors indicates the magnitude of the velocity. In Figure 5.4a, the vectors show the small spreading in the streamwise direction, and the vectors of large magnitude exist in a narrow region near to the bottom wall. Comparatively, the vectors shown in Figure 5.4b show the larger spreading in the spanwise direction, and the vector magnitudes are generally higher than those in Figure 5.4a. The velocity contours are shown in Figure 5.5, where both the instantaneous and mean velocities at the two planes are plotted. From the figure, it can be observed that the velocity field starts to show significant fluctuations at around $x/d = 10$ in the two planes, and the wider mean velocity contours as shown in Figure 5.5d correspond to the larger spanwise vectors in Figure 5.4b. The spreading angles of the mean velocity profiles are also indicated

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in Figure 5.5. From the figure, it is obvious that the spanwise spreading angle is much larger than the streamwise spreading angle.

Figure 5.4 Vector maps of instantaneous velocity at: (a) symmetry plane, and (b) $z = 3.75$ mm

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Figure 5.5 Velocity contours (m/s): (a) instantaneous velocity in the symmetry plane, (b) instantaneous velocity at $z = 3.75$ mm, (c) mean velocity in the symmetry plane, and (d) mean velocity at $z = 3.75$ mm

5.3.1.1 Streamwise velocity profiles

In Figure 5.6, the results of LES, standard $k-\omega$ and standard $k-\varepsilon$ closures are compared with the experimental measurements by Law and Herlina (2002) in terms of the streamwise (x - z) velocity profiles along the centreline from $x/d = 20$ to 50. U_m is the velocity in the center plane. It should be noted that only the average similarity profiles at different cross sections obtained by RANS models are presented for

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brevity. All the streamwise velocity profiles from numerical simulations tended to collapse into a single curve, which coincided with the experimental data. However, clearly the LES results were in better agreement with the experimental data than the standard $k-\epsilon$ and $k-\omega$ models, both of which showed larger deviations, especially the standard $k-\omega$ model. Verhoff (1963)'s empirical curve for the two-dimensional wall jet, shown in Figure 5.6, was also in very good agreement with the numerical simulations. This agreement indicated that there was no significant difference in the streamwise velocity profiles between two-dimensional and three-dimensional wall jets, which was also noted by Law and Herlina (2002).

Figure 5.6 Streamwise velocity profiles along centreline

The LES results of streamwise velocity profiles at offset sections were also extracted and compared with experimental data shown in Law and Herlina (2002) in Figure 5.7. $z_{m/2}$ and U_{ms} represent the local velocity-half-height and maximum

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velocity at the offset section, respectively. The numerical data along the centerline and various offset sections were observed to be also self-similar and in good agreement with the experimental measurements. It can thus be concluded that the self-similarity is also applicable to the velocity distribution in the offset sections, and that the velocity distributions between the centerline and various offset sections are similar within the range of the investigation.

Figure 5.7 Nondimensional profile of streamwise velocity at offset sections

5.3.1.2 Spanwise velocity

The spanwise (x - y) velocity profiles were extracted from the horizontal plane as shown in Figure 5.8 at the height where the centerline of the inlet was located. All the LES results were nearly self-similar and in agreement with the experimental data,

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while the standard k - ϵ model showed larger deviations in the region near the centerline. It should be noted that this similarity was also reported by Rajaratnam and Pani (1974) and Padmanabham and Gowda (1991). However, their measurements only focused on the near-centreline region up to $y/y_{m/2} = 1.6$, while the simulations here extended to $y/y_{m/2} = 3$. The Goertler solution for free jets from Schlichting (1979) and the previous numerical results by Huai et al. (2010) are also plotted in Figure 5.8 for comparison. Note that Huai et al. (2010) used the realizable k - ϵ closure instead of the standard k - ϵ closure. It can be observed that, compared with the experimental data, the results from LES and all RANS models all under-predicted the velocity magnitudes after about $y/y_{m/2} = 1$.

Figure 5.8 Spanwise velocity profiles

5.3.1.3 Decay of maximum mean velocity

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Sforza and Herbst (1970) divided the longitudinal spreading of turbulent wall jet into the following regions based on the maximum mean velocity decay rate: a potential core region, a characteristic decay region, and a radial-type decay region. In the radial-type decay region, the maximum mean velocity would decrease almost linearly with the downstream distance. In Figure 5.9, the decay of maximum velocity in the third region from LES, standard $k-\varepsilon$ and standard $k-\omega$ closures are compared with the experimental measurements as well as the numerical simulation of Li et al. (2012). From the figure, it is obvious that the LES results provide the best agreement. Comparatively, both the standard $k-\varepsilon$ and $k-\omega$ closures over-predict the decay measurements significantly.

Figure 5.9 Decay of maximum mean velocity

5.3.1.4 Variations of velocity length scales

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The variations of velocity-half-height and velocity-half-width are presented in Figure 5.10 and Figure 5.11, respectively. In addition, Rajaratnam and Pani (1974)'s experimental results are also plotted in Figure 5.10, and Li et al. (2012)'s numerical results are shown in both figures.

Figure 5.10 Variation of velocity-half-height

A linear relationship between the velocity-half-height (width) and longitudinal distance was reported by Law and Herlina (2002) and Rajaratnam and Pani (1974). As shown in Figure 5.10, the standard $k-\epsilon$ and $k-\omega$ closures over-predict the velocity-half-height measurements while the LES results are in good agreement with the experimental measurements. The linear fitting curve based on LES results could be described by

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$$\frac{z_{m/2}}{d} = 0.056 \frac{x}{d} + 0.53 \quad (5.1)$$

Li et al. (2012) simulated the circular wall jet using LES with the SGS model of DKE. DKE is a relatively new SGS model proposed by Kim and Menon (1997) which accounts for the transport of the SGS turbulence kinetic energy, while the Smagorinsky SGS model is based on an assumption of the local equilibrium between the transferred energy through the grid-filter scale and the dissipation of the kinetic energy at small SGS. DKE is thus more advanced than Smagorinsky for wall-bounded flows in theory. However, from the two figures, Li et al. (2012)'s results far exceed the experimental data for the velocity-half-height, and are similar to the results of $k-\varepsilon$ and $k-\omega$ models. Note that the present study used a hybrid mesh while Li et al. (2012) adopted a structured mesh. Therefore, it is possible that the grid arrangement near the wall boundary was coarser in their simulations.

In Figure 5.11, the results of the $k-\varepsilon$ and $k-\omega$ closures both under-predict the experimental data. In comparison, the LES results have the best agreement with the previous experimental and numerical measurements, and could be described by a linear fitting function as

$$\frac{y_{m/2}}{d} = 0.31 \frac{x}{d} + 4.40 \quad (5.2)$$

Overall, LES results provide the best predictions of the kinematic characteristics collectively for all the three decay rates, and the accuracies are well within the

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experimental variations. The LES growth rate of velocity-half-width is 5.5 times as large as that of velocity-half-height, which is close to the experimental data.

5.3.2 Scalar characteristics

The relative scalar characteristics (based on the temperature differences) obtained from LES are shown in Figure 5.12, where both the instantaneous and mean scalar concentration at the two planes are plotted. The behaviors of the concentration fields are basically similar to those of the velocity fields (as shown in Figure 5.5). The concentration fields also start to fluctuate after around $x/d = 10$, and the spreading rate is higher in the spanwise direction. It can also be observed that the scalar spreading is generally larger than the velocity spreading both in the streamwise and spanwise directions, by comparing Figure 5.12 with Figure 5.5.

5.3.2.1 Streamwise scalar profiles

In Figure 5.13, the results of LES, standard $k-\varepsilon$ and standard $k-\omega$ predictions are compared with the experimental measurements in terms of the streamwise scalar concentration profiles along the centerline from $20d$ to $50d$. T_m and T_{m0} are the centerline concentration and centerline maximum concentration, respectively, and $z_{tm/2}$ is the scalar-half-height. All the streamwise scalar profiles from the numerical simulations tend to form similar curves with $(T_m - T_a)/(T_{m0} - T_a)$ decreased exponentially from a maximum value at the wall. However, the standard $k-\varepsilon$ and

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standard $k-\omega$ results show over-predictions when $z/z_{tm/2} > 1$, while the LES results are in better agreement with the experimental data.

The LES results of the streamwise scalar distribution at offset sections are reported for the first time, as shown in Figure 5.14, where $z_{tm/2}$ and T_{ms} are the local scalar-half-height and maximum scalar concentration in respective offset sections, respectively. Similar to the velocity profiles in Figure 5.7, it can be concluded that self-similarity is also applicable to the scalar distribution in the offset sections.

Figure 5.11 Variation of velocity-half-width

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Figure 5.12 Temperature difference contours (K): instantaneous temperature (a) in the symmetry plane and (b) at $z = 3.75$ mm; mean temperature (c) in the symmetry plane and (d) at $z = 3.75$ mm

Figure 5.13 Streamwise scalar concentration profiles

Figure 5.14 Nondimensional profile of streamwise scalar concentration at offset sections

5.3.2.2 Spanwise scalar profiles

The spanwise scalar profiles extracted from the horizontal plane are plotted in Figure 5.15, where $y_{tm/2}$ is the scalar-half-width. All models reproduce reasonable agreement with the experimental data within $y/y_{tm/2} = 1$. However, similar to the spanwise velocity profiles, the results from LES and two RANS models all under-predict the spanwise scalar distribution beyond $y/y_{tm/2} = 1$.

Figure 5.15 Spanwise scalar concentration profiles

5.3.2.3 Decay of maximum mean scalar concentration

The decay of maximum mean scalar concentration in the plane of symmetry from $20d$ to $50d$ is presented in Figure 5.16. Similar to the observations of the decay of maximum mean velocity, LES results have better agreement with the experimental measurements, while the two RANS closures over-predict the maximum scalar concentration decay.

5.3.2.4 Variation of scalar length scales

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Figures 5.17 and 5.18 show the variations of scalar-half-height and scalar-half-width, respectively. In Figure 5.17, all the numerical results are in reasonable agreement with the experimental data. The linear fitting curve of LES can be quantified as

$$\frac{z_{tm/2}}{d} = 0.092 \frac{x}{d} - 0.6 \quad (5.3)$$

Figure 5.16 Decay of maximum mean concentration

In Figure 5.18, similar to the under-prediction of the velocity-half-height, the standard $k-\epsilon$ and standard $k-\omega$ models also under-predict the development of scalar-half-width. Comparatively, the LES results are in good agreement with the experimental data. The simulation results based on LES can be described by the following equation derived by linear curve fitting:

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$$\frac{y_{tm/2}}{d} = 0.44 \frac{x}{d} - 7.3 \quad (5.4)$$

The ratio between the decay rate of the scalar-half-width and the scalar-half-height is found to be best reproduced by LES, which gives a predicted ratio of 4.9 near to the value of 5.0 obtained by Law and Herlina (2002).

Figure 5.17 Variation of scalar-half-height

Comparing the spreading rates between the scalar and velocity, the scalar field spreads faster than the velocity field in both the lateral and vertical directions. The LES results have scalar-to-velocity ratios of 1.64 in the lateral direction and 1.42 in the vertical direction, which are in reasonable agreement but somewhat higher than the experimental measurements by Law and Herlina (2002) which recorded the ratios to be 1.45 and 1.47, respectively.

Figure 5.18 Variation of scalar-half-width

5.3.3 Turbulence characteristics

LES with proper near-wall modelling has been demonstrated in the above sections to be superior to other RANS closures for the wall jet simulations in terms of the velocity and scalar characteristics. Therefore, the LES results are further explored herein. In this section, the LES turbulence intensity distributions are compared with previous experimental measurements and numerical data.

5.3.3.1 Streamwise turbulence characteristics

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The turbulence intensity contours in the symmetry plane are shown in Figure 5.19 and Figure 5.20, where u' and w' are the u - and w -components of velocity fluctuations, respectively. In Figure 5.19, the u -component of turbulence intensity remains at a low value near the inlet, increases sharply to a maximum value within the region from $x/d = 10$ to 15, and then decreases in the downstream region. In Figure 5.20, the w -component of turbulence intensity shows similar characteristics and the maximum turbulence intensity occurs in the same place as in u -component. Comparing Figure 5.19 and Figure 5.20, it can be observed that the magnitude of turbulence intensity in the u -direction is much larger than in the w -direction.

Figure 5.19 Contour (m/s) of u -component turbulence intensity ($\sqrt{u'^2}$) in the symmetry plane

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Figure 5.20 Contour (m/s) of w -component turbulence intensity ($\sqrt{w'^2}$) in the symmetry plane

The profiles of u -component turbulent intensity at the symmetry plane obtained from $x/d = 20$ to 40 are shown in Figure 5.21. All the LES results show self-similar curves within the range in x direction with the maximum turbulence intensity occurring at around $0.6z_{m/2}$, which is consistent with the experimental measurements by Herlina and Law (2002) and Abrahamsson et al. (1997). The peak of the turbulence intensity remains relatively constant at a value of 29% and is also in reasonably agreement with the experimental data. In comparison, Li et al. (2012)'s results show large turbulence intensity when $z_{m/2} > 1$, which may be due to the coarser grid arrangement near the wall as discussed earlier.

Figure 5.21 Streamwise variation of u -component turbulence intensity

The profiles of w -component turbulence intensity at the symmetry plane are shown in Figure 5.22. The LES results are in general agreement with experimental data. The peak of the turbulence intensity is about 20% and slightly larger than the experimental data. The location of the peak value is found to be around $0.7z_{m/2}$, which lies between Herlina and Law (2002)'s and Abrahamsson et al. (1997)'s results. Compared with the u -component turbulent intensity in Figure 5.21, the peak of w -component turbulent intensity is lower and the location is slightly further downstream.

The profiles of scalar concentration turbulence intensity are also examined in Figure 5.23, where T' is the scalar concentration fluctuation. As seen in the figure, the turbulence intensity increases with the distance from the wall up to a maximum of around 30% which is consistent with experimental data, and then decreases. The

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position of the maximum intensity is at $\sim 0.4z_{m/2}$ while the experimental results show higher position. In general, all the LES results are in very reasonable agreement with the experimental results from Herlina and Law (2002).

Figure 5.22 Streamwise variation of w -component turbulence intensity

5.3.3.2 Spanwise turbulence characteristics

The turbulence intensity contours at the horizontal plane are shown in Figure 5.24 and Figure 5.25, where v' is the v -component velocity fluctuation. In Figure 5.24, the u -component of turbulence intensity shows symmetry with respect to the centerline and the variation of turbulence intensity along x direction is similar to that in Figure 5.19. In Figure 5.25, the v -component of turbulence intensity has similar distribution to the u -component while smaller magnitude. Same as the streamwise

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turbulence intensities, the maximum u - and v -component of turbulence intensities in the horizontal plane also occurs at approximately $x/d = 10$ to $x/d = 15$.

Figure 5.23 Streamwise variation of temperature fluctuation

Figure 5.24 Contour of u -component turbulence intensity ($\sqrt{u'^2}$) at $z = 3.75$ mm

Figure 5.25 Contour (m/s) of v -component turbulence intensity ($\sqrt{v'^2}$) at $z = 3.75$ mm

The profiles of u -component turbulence intensity in the spanwise direction are shown in Figure 5.26. The results of LES coincide with the experimental data within $y/y_{m/2} = 1$, and the peak of the u -component turbulence intensity is around 25% which agrees with experimental data. Beyond $y/y_{m/2} = 1$, the LES results show a faster decay, which is consistent with the observations in the spanwise velocity and scalar profiles. This may be attributable to the weakness of the Smagorinsky SGS models in dealing with the low-level turbulence in the downstream region.

The profiles of v -component turbulence intensity in the spanwise direction are shown in Figure 5.27. The LES results are close to the experimental measurements from Herlina and Law (2002), and the peak of the v -component turbulence intensity is around 18%.

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Figure 5.26 Spanwise variation of u -component turbulence intensity

Figure 5.27 Spanwise variation of v -component turbulence intensity

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Herlina and Law (2002) explored the spanwise variation of the concentration turbulence intensity at $z = 3.75$ mm up to $y/y_{tm/2} = 1.6$. They found that the intensity increased from the centerline up to $y/y_{tm/2} = 0.3$ and then started to decrease. In Figure 5.28, the LES results are compared with the experimental data in terms of the spanwise scalar turbulence intensity. In general, the LES results are in reasonable agreement with the experimental data. However, the maximum intensity occurs at the centerline for the LES, which is somewhat different from the experimental measurements. The maximum intensity is approximately 28% at the center which is also higher.

Figure 5.28 Spanwise variation of temperature fluctuation

5.3.4 Vorticity characteristics

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The coherent structure of the wall jet is essential for understanding the flow development. The eddy structures of LES from $x/d = 15$ to 55 are compared with the experimental images in a time sequence at 1 second interval as shown in Figure 5.29. The experimental images were obtained by the PLIF approach. Due to the limited extent of the laser sheet illumination, the left and right ends of the experimental images are darker than the central region, and thus they can only provide qualitative illustration of the eddy structures. Comparatively, the eddy structures of the LES are visualized by plotting the concentration contours in a gray scale. From the figure, the large coherent eddy structures of LES show similar length scales to those in the experimental images. However, the small eddy structures widely observed in the experimental images are filtered out in LES.

Figure 5.30 to Figure 5.32 further show the x -, y -, and z -components of vorticity in the symmetry plane, respectively. Compared with the vorticities in the x and z directions, the vorticity in the y direction plays a dominant role in the jet interactions with the wall. The large vorticity near the wall is caused by the no-slip condition at the wall. The vorticity near the upper layer of the jet shows an opposite direction due to the shearing of the jet with the ambient fluid.

The contours of vorticities at the horizontal plane are plotted in Figure 5.33 to Figure 5.35. The vorticity in the z direction are symmetrical with respect to the central axis, and has larger magnitude in general. Discrete peak regions can also be observed which are signature of the three-dimensional near-wall eddies. This is also attributed to the interactions of the jet with the ambient fluid. Comparing these

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figures, it is easy to find that these vortices are three-dimensional and their sizes increase linearly in the downstream direction.

Figure 5.29 Vertical eddy structures at the central plane: (Left) experimental images; (Right) LES results

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Figure 5.30 Contour (s^{-1}) of x -direction vorticity at symmetry plane

Figure 5.31 Contour (s^{-1}) of y -direction vorticity at symmetry plane

Figure 5.32 Contour (s^{-1}) of z -direction vorticity at symmetry plane

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Figure 5.33 Contour (s^{-1}) of x -direction vorticity at $z = 3.75$ mm

Figure 5.34 Contour (s^{-1}) of y -direction vorticity at $z = 3.75$ mm

Figure 5.35 Contour (s^{-1}) of z -direction vorticity at $z = 3.75$ mm

5.4 Conclusions

In the present study, the turbulent circular wall jet was simulated numerically using LES with proper near-wall modelling and two RANS models with enhanced wall functions. The simulations covered the velocity and scalar concentration characteristics in both the streamwise and spanwise directions. The numerical results were then compared with previous experimental measurements in the literature.

The results demonstrated that LES is superior to the two RANS models in reproducing both the kinematic and scalar mixing characteristics. The LES results provide better agreements with the experimental data in general, though with some under-prediction for the spanwise velocity profiles away from the jet centreline. Comparatively, the two RANS models fail to predict the strong anisotropic ($dy_{m/2}/dz_{m/2}$ and $dy_{tm/2}/dz_{tm/2} \approx 5:1$) spreading of the wall jet near the boundary. In terms of the turbulence intensities and vorticity distribution, the LES results agree well with experimental data in both the streamwise and spanwise directions. It is however noted that the spanwise turbulence intensity in the region far from the centreline also decreases faster, which can be attributed to the weakness of the Smagorinsky SGS model in dealing with low turbulence intensity in those regions. In the symmetry plane, the vorticity distribution is dominated by the y -direction vorticity driven by the presence of the wall, while in the horizontal plane, the z -direction vorticity caused by the shearing of the jet flow with the ambient fluid plays the primary role.

6 Large Eddy Simulations of 45° Inclined Dense Jets

As noted previously, the brine effluent must be sufficiently diluted within a regulated mixing zone for EIA, and thus it is essential to design the outfall in an optimal manner to achieve a rapid mixing of the brine effluent with ambient waters. This chapter shall investigate numerically the mixing behavior of inclined dense jets in stagnant ambient.

6.1 Introduction

As discussed in previous chapters, many analytical and experimental studies were conducted on inclined dense jets (Zeitoun et al., 1970; Roberts et al., 1997; Shao and Law, 2010). A few CFD studies were also reported in literature by means of the RANS approach (Vafeiadou et al., 2005; Oliver et al., 2008; Gildeh et al., 2015). In the present study, we employ the LES approach to simulate the submerged 45° inclined dense jet discharged into stagnant ambient removing bottom impact. The objective is to evaluate the performance of LES on the predictions of both the kinematic and mixing behavior of the inclined dense jet in the near field. Experimental measurements are also performed for the validation of the LES predictions. The numerical and experimental results are presented and compared to

*This chapter is written based on “Large eddy simulations of 45° inclined dense jets”, *Environmental Fluid Mechanics* (2016).

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the available data in the literature. The LES approach shall be demonstrated to predict the inclined dense jet in satisfactory agreement with the experimental data.

6.2 Computational Methodology

In this chapter, the LES approach with Smagorinsky and dynamic Smagorinsky SGS models were adopted for the predictions of inclined dense jets. The governing equations for the two SGS models were discussed in Chapter 3, and the OpenFOAM platform was adopted to implement the LES governing equations. OpenFOAM has been used and validated for mixture flow of two incompressible fluids in many studies including jets (Gruber et al., 2011; Lai et al., 2014).

6.2.1 Flow configuration

The simulation domain was configured based on a fully submerged inclined jet with an inclination of 45° . As shown in Figure 6.1, the origin of Cartesian coordinates was set at the center of the discharge nozzle, the diameter of which was D . The distances from the nozzle center to the back (L_b), front (L_f), left and right sides (W), surface (H_d) and bottom (h) boundaries were equal to or larger than $0.7D_{Fr}$, $6D_{Fr}$, $1.8D_{Fr}$, $2D_{Fr}$, and $1D_{Fr}$, respectively. Particular attention was paid to the nozzle's cover water depth (h) to avoid the surface contact of the inclined dense jet (Jiang et al., 2014). In the present study, all the cases satisfied the criteria for fully submerged 45° inclined dense jet ($h > 1.6D_{Fr}$).

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Figure 6.1 Schematic diagram of the computational domain

The computational domain was discretized with a stretched and structured mesh with increasing grid spacing from the center of the nozzle to the boundaries, as shown in Figure 6.2a. A double refinement was performed within a region that covered the core of the jet. The grids attached to the nozzle tube were generated by a tool of OpenFOAM, namely snappyHexMesh, which can divide a base cell into several sub-cells and then snap the sub-cell boundaries onto the surface of the nozzle tube, as shown in Figure 6.2b. The fluid viscosity and diffusivity were $10^{-6} \text{ kg}\cdot\text{m}^{-1}\text{s}^{-1}$ and $10^{-9} \text{ m}^2/\text{s}$, respectively. The other parameters for each case and their corresponding meshes are summarized in Table 6.1.

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Figure 6.2 (a) A structured mesh of the domain; (b) Detailed grids near the nozzle at the center plane

Table 6.1 Physical parameters and grid sizes

Cases	D (mm)	U_0 (m/s)	ρ_b (kg/m ³)	ρ_a (kg/m ³)	Fr	Number of grid cells (Million)	SGS model
S1	6.0	0.513	1032	997	11.3	2.5	Smagorinsky
S2	6.0	0.679	1032	997	15.0	3.3	Smagorinsky
S3	6.0	0.909	1032	997	20.0	5.6	Smagorinsky
S4	6.0	0.909	1013	997	30.0	10.1	Smagorinsky
S5	8.0	0.547	1027	997	11.3	3.1	Smagorinsky
D1	6.0	0.513	1032	997	11.3	2.5	Dynamic Smagorinsky
D2	6.0	0.679	1032	997	15.0	3.3	Dynamic Smagorinsky
Present experiment	5.8	0.515	1034	997	11.3	--	--

To examine the grid convergence, the method of GCI (Celik et al., 2008) was used for the estimation of uncertainty in the CFD simulations. With GCI, the uncertainty

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is determined by a formula incorporating the results of two additional simulations of which a coarser mesh and a finer mesh are used individually. Figure 6.3 shows the dilution (represented in a line) and its uncertainty (represented in vertical bars) near the return point (at $\sim 3.6FrD$) in Case S1. C and C_0 are the local and initial concentrations, respectively. From the figure, the uncertainty near the return point can be observed to be relatively small.

Figure 6.3 Dilution at the nozzle height level near the return point

6.2.2 Computational setup

The boundary condition at the top surface was set to free slip, while a zero gradient open boundary was used for the other five outer boundaries. The nozzle surface was

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set as a velocity inlet with a uniform discharge velocity at a turbulence intensity of 10%. The corresponding dense fluid density was specified in Table 6.1. The other surfaces of the discharge tube were taken to be wall boundaries. A second order implicit backward scheme was used for the discretization of the temporal term. An upwind and a linear scheme were chosen to compute the divergence term and the Laplacian term, respectively. The convergence criterion of 10^{-6} was set for the continuity, velocities as well as scalar concentrations. The time step interval was adjusted to ensure that the Courant number was less than 1.0. The computations were performed using parallel processors in the High Performance Computing centre of the Nanyang Technological University. As an example, for Case S2, the flow was computed up to 50 seconds, with a real-time computing duration exceeding 7 days with 4 nodes (each node having 16 cores).

6.2.3 Experimental validation

In addition to the numerical simulations, the velocity and concentration distributions of the 45° inclined dense jet at the center plane were also experimentally determined in the present study using the laser imaging techniques of PIV and PLIF, respectively. The experiments were performed in a glass test tank at the Nanyang Technological University, Singapore.. The following shall discuss the experimental setup and methodology.

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6.2.3.1 Experimental setup

The experimental observation of mixing behavior of inclined dense jets was conducted within a glass tank with dimensions of 2.8 m long, 0.8 m wide and 1.0 m tall. In terms of the tank, the walls and bottom are made of transparent glass, and the bottom was elevated at 0.85 m above the floor so as to spare enough space for the installation of the laser. A Perspex platform with dimensions of 1.5 m long, 0.75 m wide and 10 mm thick was placed horizontally above the tank bottom as a false seabed. In the present experiments, the nozzle had an inner diameter of 5.8 mm, and the center of the nozzle was set at 50 mm above the perspex bottom to avoid the influence of the bottom boundary.

Together with the glass tank, two peristaltic pumps (Cole-Parmer Instrument Co., Masterflex 77200-52) were adopted to continuously provide the source solution for the constant head tank. During the experiments, the brine solution was pumped from the source container to the constant head tank at a flowrate, which is 20 - 30% higher than the discharge flowrate, to maintain the solution in the constant head tank at a constant water level. Two electromagnetic flowmeters (KROHNE, Altometer SC80AS; YOKOGAWA, AXF015G) were adopted to monitor the real time discharge flowrate of the discharge nozzle. In the present study, the fluctuation of flowrate was found to be less than 2%, which can be considered constant.

6.2.3.2 Planar laser induced fluorescence

The laser system as described in Table 4.1 was adopted to quantify velocity and concentration fields by means of PIV and PLIF, respectively. The PIV approach has been introduced in Chapter 4. PLIF is an optical measurement technique to determine the instantaneous and mean scalar (including temperature and concentration) distribution fields (Law and Wang, 2000; Law and Herlina, 2002; Shao and Law, 2010). The setup of PLIF is similar to PIV but the working principle is even simpler. With PLIF, the intensity of the fluorescent light by the dye tracer excited by the laser illumination is captured which is proportional to the dye concentration. In the present study, Rhodamine B was used as the dye tracer.

In order to convert the captured fluorescence light to the actual dye concentration, a calibration was performed before the experiments (Law and Wang, 2000). During an experiment, the laser was adjusted to coincide with the center plane of the inclined dense jet. The camera began to capture images after the inclined dense jet was initiated for a while. The concentration distribution based on the images was post-processed using the Dantec Dynamic Studio software. The flow conditions of the experiments are listed in Table 6.1.

6.3 Results and Discussion

In the following discussion, the LES predictions were compared with the experimental results obtained in the present study as well as previous experimental and numerical studies (Cipollina et al., 2005; Kikkert et al., 2007; Oliver et al., 2008; Shao and Law, 2010; Papakonstantis et al., 2011a; Papakonstantis et al., 2011b; Lai and Lee, 2012; Palomar et al., 2012; Oliver et al., 2013c), including the jet trajectories, geometrical and dilution parameters, and turbulence characteristics. Except for the eddy structures shown in Figure 7.16, all the results were time-averaged over the period starting from 15 or 120 s (for simulation and experimental measurements, respectively), and lasting for approximately 60 to 80 s.

As noted previously, Crowe (2013) investigated the possible influence of bottom impact on the mixing characteristics of the inclined dense jet. Based on his results, for the 45° inclined dense jet, the minimum nozzle height (h) necessary to avoid the boundary effect is $\sim 0.6DFr$. The previous studies with and without a bottom boundary were included for a comprehensive comparison herein, and the potential boundary effect has been clearly indicated for those with a bottom boundary.

6.3.1 Jet trajectory and overall flow characteristics

Figure 6.4 shows the mean velocity magnitude and normalized concentration contours (C/C_0) of Case S1 at the centerline plane. From the velocity contours, the

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inclined dense jet first rises due to the initial discharge momentum until it reaches the peak height as shown in Figure 6.4. The concentration contours also show a similar pattern. Subsequently, the negative buoyancy becomes dominant, and the inclined dense jet sinks downwards. The following jet characteristics, including the jet trajectory, geometrical and dilution characteristics, cross-sectional profiles and jet spread widths, can be obtained from the velocity magnitude and concentration contours at the center plane.

The jet centerline, also known as the trajectory, is a main geometrical feature of the inclined dense jet. The jet centerline can be defined as the locus of the maximum velocity or concentration at various cross sections from the respective velocity or concentration contour maps shown in Figure 6.4. Figure 6.5 presents the normalized jet concentration and velocity centerlines, with different Fr obtained from the LES predictions (with both Smagorinsky and Dynamic Smagorinsky models) and experimental measurements, where $L_M = (\pi/4)^{1/4} DFr$ is the jet characteristic length scale. The experimental results from Kikkert et al. (2007) and Oliver et al. (2013c) as well as three different integral modelling predictions (Corjet, UM3 & Visjet) from Palomar et al. (2012) are also included for comparison. From the figure, the normalized LES predictions with different Fr were similar to each other with slight divergences towards the downstream direction. The predictions with the Dynamic Smagorinsky model (D1) were almost identical to the Smagorinsky model (S1) for the jet trajectory. Compared with the present experimental results and those from previous studies, the LES predictions coincided with them near the nozzle and then diverged after the peak height, which was somewhat over-predicted. However, the divergence between the LES and experimental results was relatively smaller

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compared with the integral modeling predictions from Palomar et al. (2012). It is noted that both the velocity (solid line) and concentration centerlines (dotted line) almost coincided with each other, which had also been noted in previous experimental studies (Shao and Law, 2010). In the following discussion, the centerline refers to the concentration centerline if not indicated otherwise.

6.3.2 Geometrical and mixing features

To assess the environmental impact of the brine discharge, the analysis must include the determination of the geometrical features of the inclined dense jet, including the terminal rise height, return point location as well as dilution at different locations. As discussed earlier, previous studies had verified that the various normalized geometrical and mixing quantities of the inclined dense jet for a specific nozzle inclination are proportional to Fr . The various geometrical and mixing quantities predicted by LES are summarized in Table 6.2 together with the experimental results from the present and previous studies, with S_m and S_r being the dilution at the centerline peak height and return point, respectively.

In Table 6.2, the coefficients of the LES results are average values from the simulation runs shown in Table 6.1. The maximum variations of the coefficients from the Smagorinsky LES results are also indicated in the table. Based on the simulations, the variations were within around 10%, and most of them were approximately within 5%. The trend lines of the Smagorinsky LES results are also plotted for comparison based on these average coefficients in Figure 6.6 - 6.9.

Figure 6.4 Non-dimensional mean (a) velocity (m/s) and (b) concentration contours at the center plane for Case S1

Figure 6.5 Comparison of normalized centerline trajectories

6.3.2.1 Terminal rise & centerline peak

The terminal rise height, z_t , is crucial to the assessment of the environmental impact of the brine discharge. The criteria to determine the terminal rise height were different among the previous studies. Herein, the terminal rise height is defined as the peak height at the location where the concentration drops to 5% of the centerline peak concentration. Figure 6.6 presents the terminal rise height derived from the mean concentration fields at the centerline plane. The previous experimental and numerical results are included for comparison. It should be noted that the results of Oliver et al. (2013) are represented by a trend line based on the averaged coefficient. From the figure, the LES predictions with the Smagorinsky and dynamic Smagorinsky SGS models coincided with each other, and they were close to the

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experimental results from Oliver et al. (2013), Cipollina et al. (2005), Kikkert et al. (2007), et al.. The trend line based on the LES predictions (with the Smagorinsky SGS model) is plotted in the figure as well. The LES trend line was obviously closer to the experimental trend line from Oliver et al. (2013) than the prediction of integral models presented by Palomar et al. (2012).

Once the centerline was determined, the horizontal and vertical locations of the centerline peak, x_m and z_m , can be derived which are plotted against Fr in Figure 6.7. From the figure, it can be observed that the LES predictions agree well with the present experimental results as well as the results from previous studies. The normalized horizontal location x_m/D and vertical location z_m/D increased linearly with increasing Fr . The trend lines based on the averaged coefficients of the LES are also plotted in the respective figures. The scattering of the LES data points from the trend lines was relatively small, which demonstrated the consistency and accuracy of the predictions.

6.3.2.2 Return point location

Upon reaching the peak height, the inclined dense jet falls back onto the bottom due to its negative buoyancy. The location of the impact point, where the downward flow impinges onto the bottom, and the associated dilution are important parameters for the environmental impact analysis. The impact location can be dependent on the site conditions, including the source height and bed slope (Jirka, 2008; Oliver et al., 2013a). Here, the bottom effect was not considered, and the return point position

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(where the downward flow returns to the source height), is examined instead. The LES predictions were compared with corresponding experimental measurements from the literature.

Table 6.2 Comparison of coefficients

Quantities		$\frac{x_m}{DFr}$	$\frac{z_m}{DFr}$	$\frac{z_t}{DFr}$	$\frac{x_r}{DFr}$	$\frac{S_m}{Fr}$	$\frac{S_r}{Fr}$	Bottom boundary
LES (Smagorinsky)		2.06 ± 0.12	1.26 ± 0.13	1.46 ± 0.09	3.71 ± 0.19	0.26 ± 0.03	1.06 ± 0.09	No
LES (Dynamic)		2.03	1.22	1.43	3.57	0.27	1.02	No
Present experiment		1.82	1.13	1.68	3.24	0.41	1.49	No
Kikkert et al. (2007)		1.84	1.06	1.60	3.26	-	-	No
Oliver et al. (2013)		1.75	1.09	1.65	3.13	0.39	1.22	No
Palomar et al. (2012)	CORJET	1.52	0.99	1.41	2.65	-	0.65	No
	UM3	1.32	0.85	1.24	2.32	-	0.63	No
	JETLAG	1.52	0.95	1.27	2.68	-	0.76	No
Cipollina et al. (2005)		1.80	1.17	1.61	2.82	-	-	Yes
Shao and Law (2010)		1.69	1.14	1.47	2.83	0.46	1.26	Yes
Papakonstantis et al. (2011a & b)		2.03	1.17	1.58	3.78	0.52	1.55	Yes
Lai and Lee (2012)		2.09	1.19	1.58	3.34	0.45	1.09	Yes

Figure 6.8 shows the normalized horizontal location of the return point against Fr . The trend line based on the averaged LES coefficient is plotted in the figure as well. The differences between the two SGS models were small. It can be observed that the LES predictions were close to the experimental data especially from Kikkert et al. (2007) but with slight over-predictions.

Figure 6.6 Comparison of normalized terminal rise height

6.3.2.3 Dilution

The dilution at a specific location is defined as the initial concentration at the source over the local concentration, C_0/C . In the present study, the dilution at the return point is plotted against Fr in Figure 6.9. It can be observed that the results of previous studies deviated from each other, which may be due to their various bottom conditions as suggested by Oliver et al. (2013). Seen from the figure, the LES predictions were close to the results from Oliver et al. (2013) but slightly lower. The LES averaged trend line based on the Smagorinsky results is also plotted in the figure. In comparison, the LES trend line still somewhat under-predicted the experimental results, but the agreement was much better compared to the integral modeling predictions from Palomar et al. (2012).

Figure 6.7 Comparison of normalized centerline peak: (a) horizontal and (b) vertical locations

Figure 6.8 Comparison of normalized return point location

Figure 6.9 Comparison of normalized dilution at the return point

6.3.3 Cross- sectional profiles

Figure 6.10 shows the normalized velocity and concentration profiles at different cross sections along the respective jet trajectories based on the Smagorinsky model. The cross sections began at $s = 0.1FrD$, where s is the distance from the nozzle center along the jet centerline, and the interval between the sections was $0.3FrD$. As can be observed from the profiles, the flow pattern can be divided into the inner (or lower) and outer (or upper) halves in the regions below and above the trajectories of velocity or concentration maxima, respectively. Both the velocity and concentration profiles showed symmetry with respect to the centerline trajectory in the initial stage ($s < 1.0FrD$). After $s \approx 1.0FrD$, asymmetry developed and the velocity or concentration profiles in the inner half were now wider than the outer half. Further downstream, the distributions became even more flattened.

In Figure 6.11, the non-dimensional cross-sectional profiles of the concentration C/C_c from Case S1 are plotted against r/b_c , where r is the radial distance (negative represents upper half), b_c is the concentration spread width and C_c is the centerline concentration. A Gaussian profile is also plotted here for comparison. The results from previous studies are included by re-normalizing s/D into s/FrD . In the near-nozzle region, the cross-sectional profiles obtained by LES showed self-similarity and distributed in the Gaussian manner. In the downstream region, the inner half began to deviate from the Gaussian profile, and the distortion increased with the distance from the nozzle within the range of the investigation in the present study. This phenomenon was also noted in previous experimental studies (Kikkert et al.,

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2007; Shao and Law, 2010) and numerical study (Oliver et al., 2008), which can be attributed to the additional spreading by the buoyancy induced instability.

Figure 6.10 Cross-sectional profiles of (a) velocity and (b) concentration fields
(Case S1)

6.3.4 Jet spread

In the present study, the jet spread widths are characterized based on the distance from the centerline to the 5% value of the centerline maximum. Figure 6.12 presents the velocity and concentration spread widths along the centerline trajectory. The LES predictions were nearly identical between the Smagorinsky and dynamic Smagorinsky models, and the spread widths of the LES predictions in the upper region were closer to the experimental data. However, the LES spread width was smaller in the inner region. Clearly, the enhanced inner spreading due to the buoyancy-induced instability was again not sufficiently captured by LES.

The variation of the jet spread width along the trajectory is further examined in Figure 6.13. In the figure, the upper and lower spread widths of the LES predictions with both the Smagorinsky and dynamic Smagorinsky SGS models are extracted from Figure 6.12, and re-plotted against normalized s . Consistent with Figure 6.12, the differences between the Smagorinsky and dynamic Smagorinsky models were small as shown in Figure 6.13a. Starting from the nozzle, the upper and lower spread widths of the LES predictions increased almost linearly in the beginning matching closely the experiment results, and then the rate of increase began to decline after $s \approx 2.0FrD$ where the centerline peak was located. Around the peak region, the vertical momentum of the inclined dense jet became weak physically, while the buoyancy-induced instability at the bottom became prominent and drove the centerlines significantly lower, resulting wider spread widths in the experimental results. From the figure, the LES predictions were not able to fully capture this phenomenon due to the inadequacy of the SGS models with the adopted grid

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spacing. Subsequently, the spread widths resumed its increase at $s \approx 2.7FrD$ in the downward plume region.

Figure 6.11 Non-dimensional cross-sectional distributions of normalized concentration at (a) $s/D Fr = 0.5 \sim 1.2$ and (b) $s/D Fr = 1.2 \sim 2.5$

Figure 6.12 Comparison of the jet velocity and concentration spread widths

6.3.5 Turbulence characteristics and eddy structures

In Figure 6.14, the concentration turbulence intensity of the LES predictions at the centerline peak is computed and compared with the experimental data from Oliver et al. (2013) and Papakonstantis et al. (2011). From the figure, the LES and experimental results showed similar distributions, having a peak value at $r/b_c \approx -0.7$ in the outer region. Compared to Oliver et al. (2013), LES under-predicted the turbulence intensity in the inner region where the buoyancy-induced momentum and instability were present.

Figure 6.13 Variation of (a) upper and (b) lower jet spread widths along the trajectory

Figure 6.14 Concentration turbulence intensity at the centerline peak in the (a) vertical and (b) lateral directions

The concentration turbulence intensity in the lateral direction was also extracted at the concentration peak and compared with the experimental data from Papakostas et al. (2011) and Lai and Lee (2012). It is noted, however, that both Papakostas et al. (2011) and Lai and Lee (2011) performed their experiments with the bottom boundary, while the present simulations were conducted without the boundary. The predictions of the Smagorinsky and Dynamic Smagorinsky models were comparably similar to the experimental data from Lai and Lee (2012), but generally lower than Papakostas et al. (2012), with twin peaks at $r/b_c \approx \pm 0.5$.

Figure 6.15 shows the concentration turbulence intensity at the return point. In Figure 6.15a, the azimuthal (normal to the jet centerline) distribution of the LES turbulence intensity is compared to Oliver et al. (2013). Similar to the centerline peak, the turbulence intensity at the return point also had a peak value at $r/b_c \approx -0.7$.

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However, the turbulence intensity at the return point preserved the linear decline in the inner region. Compared to the experimental data, the LES predictions somewhat over-predicted the turbulence intensity. The lateral turbulence intensity at the return point is also plotted in Figure 6.15b. Unlike in Figure 6.14b, the turbulence intensity at the return point did not show the twin peaks in Figure 6.15b, and the Smagorinsky model predicted higher turbulence intensity in general.

The coherent structure of the inclined dense jet is important to the understanding of the flow development, and can aid in the analysis of the mixing characteristics as well as the turbulence intensity. The LES eddy structures from Case S1, visualized by plotting the concentration contours in a diverging color map at the center plane, are compared with the present experimental PLIF images in a time sequence of 0.5s interval as shown in Figure 6.16. From the figure, the LES predictions had similar length scales to the experimental images in terms of the size of the coherent large eddies. Particularly, a series of similar-size vortex rings can be observed in the lower region below the centerline in the LES images. In contrast, the experimental images showed a fuller spectrum of large eddy sizes in the lower region. This discrepancy of the eddy sizes explained the lower turbulence intensity of the LES predictions in Figure 6.14, and also revealed the weakness of the SGS models with the adopted grid spacing in resolving the convective mixing by buoyancy-induced instability in the lower region.

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Figure 6.15 Concentration turbulence intensity at the return point in the (a) azimuthal and (b) lateral directions

Figure 6.16 Eddy structures at the central plane: (Left) experimental images; (Right) LES predictions (Case S1)

6.4 Conclusions

In the present study, the 45° inclined dense jet was simulated numerically using LES with both the Smagorinsky and Dynamic Smagorinsky SGS models, and the simulation results were compared with the experimental measurements performed in the present study as well as from previous studies in the literature. The comparison covered the geometrical and dilution characteristics, the spread width characteristics and the eddy structures at the center plane.

In summary, both the Smagorinsky and the dynamic Smagorinsky SGS models predicted the geometrical characteristics reasonably well, including the return point location, horizontal and vertical location of the centerline peak, with a slight over-prediction of $\sim 10\%$ compared with the experimental data. Hence, the LES approach performed much better than the existing integral models in terms of the geometrical characteristics. LES is also much superior to the integral models in predicting the dilution at the return point. For dilution, the LES results had an under-prediction of $\sim 20\%$ compared with the experimental data, while the comparison with integral modeling results in Palomer et al. (2012) yielded $\sim 50\%$ under-predictions. Note, however, that the recent improvements in integral modelling approach such as Reduced Buoyancy Flux (RBF) model from Oliver et al. (2013b) and Escaping Mass Approach (EMA) from Yannopoulos and Bloutsos (2012) had achieved better results. In terms of the jet spread widths, the LES predictions were in reasonable agreement with the experimental measurements near the nozzle region, but beyond the centerline peak the under-prediction became prominent. The predicted turbulence intensity was satisfactory in the upper half but not the inner half.

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Together with the comparison of the eddy structures, it is obvious that, with the currently used mesh sizes, both the Smagorinsky and dynamic Smagorinsky SGS models are not fully able to capture the convective turbulence under the influence of buoyancy. Improvement of the SGS model is therefore necessary in this direction, and it is being pursued in a further study.

7 Large Eddy Simulations of 45° and 60° Inclined Dense Jets with Bottom Impact

As discussed before, inclined dense jets eventually impact onto the seabed, and it is important to investigate the mixing process near the bottom impact. The mixing behavior of inclined dense jets without bottom impact has been studied numerically in Chapter 6. In this chapter, we shall focus on the bottom impact of inclined dense jets using the LES approach.

7.1 Introduction

As noted previously, many experimental and numerical studies on inclined dense jets were performed in the literature. A few studies were also performed experimentally to investigate the bottom impact of inclined dense jets. However, numerical investigations of the bottom impact have not been reported as far as we are aware. In the present study, we performed a numerical study using the LES approach to simulate inclined dense jets with 45° and 60° inclinations in stagnant ambient, including the impact and spreading processes on the bottom boundary. The objective was to evaluate the performance of LES on the predictions of both the

*This chapter is written based on “Large eddy simulations of 45° and 60° inclined dense jets with bottom impact”, *Journal of Hydro-environment Research* (2015), Submitted.

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kinematic and mixing behavior of the inclined dense jet with bottom boundary in the near field region. RANS simulations with the k - ε turbulence closure were also carried out for a direct comparison.

7.2 Computational Methodology

In this chapter, the LES approach with dynamic Smagorinsky SGS model was used and discretized in the open source code OpenFOAM. The standard k - ε closure was adopted herein for comparison and was also performed within OpenFOAM. The governing equations for the LES approach as well as the standard k - ε closure were discussed in Chapter 3.

7.2.1 Physical properties

A series of computational domains was configured for the simulations of inclined dense jets with two inclinations of 45° and 60° at various flow conditions, as listed in Table 7.1. The fluid viscosity and diffusivity were $10^{-6} \text{ kg}\cdot\text{m}^{-1}\text{s}^{-1}$ and $10^{-9} \text{ m}^2/\text{s}$, respectively. The density of the ambient water was 997 kg/m^3 , and the port diameter was 6 mm. Fr was varied from 10 to 30 by adjusting ρ_b and U_0 , and the values are shown in Table 7.1 together with corresponding Re for each case.

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Table 7.1 Flow conditions of each case

Cases	θ	D (mm)	U_0 (m/s)	ρ_b (kg/m ³)	ρ_a (kg/m ³)	Fr	Re	Turbulence models	Grid amounts (million)	t_s (s)
F1	45	6	0.68	1032	997	14.9	4080	LES	6.9	60
F2	45	6	0.45	1032	997	10.0	2700	LES	6.5	60
F3	45	6	0.76	1015	997	23.3	4560	LES	10.0	80
F4	45	6	0.45	1032	997	10.0	2700	$k - \varepsilon$ (wall function)	1.8	20
F5	45	6	0.45	1032	997	10.0	2700	$k - \varepsilon$ (near-wall modelling)	1.9	20
S1	60	6	0.91	1015	997	27.9	5460	LES	10.2	80
S2	60	6	0.62	1015	997	19.0	3720	LES	8.2	80
S3	60	6	0.45	1015	997	13.8	2400	LES	6.7	60
S4	60	6	0.37	1015	997	11.4	2220	LES	10.0	180

7.2.2 Computational domain

The computational domain is shown in Figure 6.1, but with different dimensions. The distances from the port to the back (L_b), front (L_f), left and right sides (W), front distance (L_f) and surface (H_d) boundaries for each case were always larger than 1 DFr , 6 DFr , 8 DFr and 4 DFr , respectively, to ensure sufficient space to resolve the dense jet under full submergence (Jiang et al., 2014). The clearance distance to the bottom boundary (h) was fixed at 27 mm, which was sufficient to avoid the Coanda effect (Shao and Law, 2010), while not exceedingly far for the bottom impact. L_f for Case S4 was further extended to 15 DFr for the observation of the spreading layer up to the end of the near field region.

7.2.3 Grid scheme

The computational domain was discretized with a stretched and structured mesh with increasing grid spacing from the center of the port to the boundaries, as shown in Figure 7.1. In particular, a double refinement was performed within a region that covered the core of the jet. The grids attached to the discharge tube were generated by snappyHexMesh, as shown in Figure 7.1b. In total, the number of grid points varied from 6 to 10 million, as indicated in Table 7.1. For the k - ϵ simulations, the number of grid was much lower at 1.8 million, and the execution was much faster than LES. The maximum number of grid points for the LES simulations was constrained by the available computing resources for this study. In theory, if the LES grid spacing is sufficiently small into the inertial range, the sub-grid model would then be able to represent the flow within the cell in a near exact manner. However, this requirement was too demanding with respect to the computing resources available. As an alternative, the method of GCI (Celik et al., 2008) was used instead to examine the gross grid convergence which was similar to Chapter 6.

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Figure 7.1 (a) A structured mesh of the domain, and (b) detailed grids of the discharge tube

Wall modeling was critical to the present configuration in order to resolve the bottom impact and spreading processes. We adopted the near-wall modeling approach instead for LES whereby a refined grid resolution near the wall was required. To assess the grid sufficiency near the wall, z^+ analysis was conducted with the present mesh. Figure 7.2 shows the non-dimensional distance (divided by z^+) of the first grid point (indicated as z_1^+) above the bottom boundary calculated from the instantaneous flow characteristics at $t = 60$ s. It can be seen that the first grid resided roughly around $z_1^+ = 1$ and most of them were below $z_1^+ = 2$ in most cases. Thus, the near wall modeling objective was generally achieved. With the $k-\epsilon$ simulations, we performed two cases using the log-law wall function and near-wall modelling respectively for comparison.

7.2.4 Boundary conditions

The boundary condition at the top surface of the computational domain was set to free slip, while a zero gradient open boundary was used for the left, right, back and front boundaries. A no-slip condition was applied to the bottom boundary. The port opening was set as a velocity inlet with a uniform discharge velocity at a turbulence intensity of 10%. The corresponding dense fluid density was specified in Table 7.1. The other surfaces of the discharge tube were taken to be wall boundaries. A second order implicit backward scheme was used for the discretization of the temporal term. An upwind and a linear scheme were chosen to compute the divergence term and the Laplacian term, respectively. The convergence criterion of 10^{-6} was set for the continuity, velocities as well as scalar concentrations. The time step interval was adjusted to ensure that the Courant number was less than 1.0.

The simulations were performed with parallel computing at the High Performance Computing Centre at Nanyang Technological University. The meshes of each case were decomposed and simulated on parallel runs using 64 or 128 cores. The simulation time of each case, t_s , from the beginning of the discharge is indicated in Table 7.1. In particular, t_s for Case S4 was extended up to 180 s to provide sufficient time-averaged results within the spreading layer. For most of the LES simulations, the real-time computing duration ranged from 7 - 20 days, while it was less than 3 days for the k - ϵ simulations.

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Figure 7.2 z_1^+ of the bottom grid along the center plane near the impact point: (a) 45° and (b) 60°

7.3 Results and Discussion

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The instantaneous and time-averaged contours of the normalized concentration (C/C_0) from the LES Case S3 are shown in Figure 7.3 as a typical illustration of the simulation results. From the instantaneous contours at $t = 60$ s in Figure 7.3a, the trajectory of the inclined dense jet was consistent with the physical expectation as noted previously. Vortices are also observed around the inclined dense jet in the figure. In particular, circulating vortices can be seen beneath the dense jet itself which might be due to the peeling detrainment at the bottom boundary of the jet with the unstable stratification. Figure 7.3b shows the time-averaged contour of the concentration during $t = 15\sim 60$ s. From the figure, the decay in jet concentration along the trajectory due to entrainment can be clearly identified. It can also be observed that the mean concentration in the inner region below the trajectory was higher than the outer region, which can be attributed to the buoyancy induced instability with the unstable stratification noted above in Figure 7.3a.

In the following discussion, the LES predictions were time-averaged from $t = 15$ s until the end of the run time, t_s , for all cases. This was except Case S4 whereby the time-averaging started from $t = 60$ s instead to minimize the effect of initial conditions to the spreading layer characteristics. The time-averaged LES predictions were then compared with relevant results from previous studies in the following.

7.3.1 Jet trajectory and overall flow characteristics

The jet centerline trajectory is a main geometrical feature of the inclined dense jet. It is defined as the locus of the maximum concentration or velocity at various cross-sections from the respective contour maps of mean concentration or velocity

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respectively. The concentration trajectory and velocity trajectory were shown to almost coincide with each other in previous studies (Shao and Law, 2010). In the present study, we thus only present the concentration trajectory for brevity.

Figure 7.3 (a) Instantaneous and (b) time-averaged concentration contours of Case S3

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Figure 7.4 shows the normalized jet concentration centerlines with different Fr obtained from both the LES and $k-\varepsilon$ predictions at 45° and 60° , where $L_M = (\pi/4)^{1/4} DFr$ is the jet characteristic length scale. The available experimental data from previous studies (Shao and Law, 2010; Lai and Lee, 2012; Palomar, 2014) are included for comparison. In Figure 7.4a, the normalized LES predictions at 45° with different Fr coincided with each other, and were thus nearly self-similar. Compared with the experimental results, the LES predictions agreed very well with the data from Shao and Law (2010) and Lai and Lee (2012). In comparison, the trajectory from Palomar (2014) was somewhat over-predicted in the region beyond the centerline peak. With respect to the $k-\varepsilon$ predictions, they were not sensitive to the wall modeling approach as the two cases of log-law wall function and near-wall modeling (listed in Table 7.1) did not differ significantly. The predicted trajectory for both was however far below the experimental data as well as LES predictions.

In Figure 7.4b, the LES predictions of concentration trajectories at 60° are plotted and compared with the experimental measurements from Palomar (2014). The LES predictions at low Fr were close to the experimental data but generally with lower centerline peak, which was consistent with the situation in Figure 7.4b. Compared to 45° , the LES predictions presented larger divergences at 60° among different Fr beyond the centerline peak.

7.3.2 Geometrical features and return point dilution

7.3.2.1 Overview of geometrical coefficients

Once the concentration trajectory was identified, the geometrical features of the inclined dense jet, including the locations of maximum centerline peak, return point, and impact point, can be determined. The coefficients for these geometrical features with both 45° and 60° inclinations are summarized in Tables 7.2 and Table 7.3, respectively. In addition to the previous studies with bottom boundary (indicated in ‘Y’) mentioned before, the experimental results from earlier studies on inclined dense jets without a bottom boundary (indicated in ‘N’) are also included in the table for comparison.

In Table 7.2, the LES coefficients represent the average values for all the 45° LES cases. Compared to the LES results in Chapter 6 without the bottom boundary, the geometrical coefficients were slightly smaller here. Correspondingly, the dilution coefficients were also reduced with the shorter trajectory, which was expected physically.

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Figure 7.4 Comparison of normalized concentration centerline trajectories: (a) 45° and (b) 60°

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Table 7.2 Comparison of coefficients with 45° inclination

Quantities		$\frac{x_m}{D Fr}$	$\frac{z_m}{D Fr}$	$\frac{z_t}{D Fr}$	$\frac{x_r}{D Fr}$	$\frac{x_i}{D Fr}$	$\frac{S_m}{Fr}$	$\frac{S_r}{Fr}$	$\frac{S_i}{Fr}$	wall
LES		1.97	1.13	1.35	3.32	3.78	0.32	1.00	0.82	Y
$k - \varepsilon$ (wall function)		1.38	0.72	1.04	2.45	2.97	0.45	0.74	0.87	Y
$k - \varepsilon$ (near-wall modelling)		1.30	0.74	1.06	2.38	2.89	0.44	0.71	0.86	Y
Nemlioglu and Roberts (2006)		-	-	2.0	-	3.2	-	-	1.7	Y
Lai & Lee (2012)		2.09	1.19	1.58	3.34	-	0.45	1.09	-	Y
Shao and Law (2010)		1.69	1.14	1.47	2.83	-	0.46	1.26	-	Y
Cipollina et al. (2005)		1.80	1.17	1.61	2.82	-	-	-	-	Y
Papakonstantis et al. (2011 a & b)		2.03	1.17	1.58	3.16	-	0.52	1.55	-	Y
Palomar (2014)		-	-	-	-	-	-	1.40	1.03	Y
Gidde et al. (2015)	RNG	1.59	1.08	1.47	2.67		0.39	0.89		Y
	Real	1.80	1.23	1.59	3.31		0.46	1.21		
	Nonlinear	2.20	1.47	1.81	3.85		0.36	0.81		
	L-G	1.78	1.10	1.50	2.89		0.42	1.07		
	LRR	1.76	1.16	1.58	3.10		0.44	1.15		
Chapter 6		2.06	1.26	1.46	3.71	-	0.26	1.06	-	N
Kikkert et al. (2007)		1.84	1.06	1.60	3.26	-	-	1.71		N
Oliver et al. (2013)		1.75	1.09	1.65	3.13		0.39	1.22		N
Palomar et al. (2012)	CORJET	1.52	0.99	1.41	2.65		-	0.65		N
	UM3	1.32	0.85	1.24	2.32		-	0.63		
	JETLAG	1.52	0.95	1.27	2.68		-	0.76		

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Table 7.3 Comparison of coefficients with 60° inclination

Quantities	$\frac{x_m}{D Fr}$	$\frac{z_m}{D Fr}$	$\frac{z_i}{D Fr}$	$\frac{x_r}{D Fr}$	$\frac{x_i}{D Fr}$	$\frac{S_m}{Fr}$	$\frac{S_r}{Fr}$	$\frac{S_i}{Fr}$	wall
LES	1.75	1.70	2.00	2.86	2.67	0.35	1.29	1.10	Y
Roberts et al. (1997)	-	-	2.2	-	2.4	-	-	1.6	Y
Cipollina et al. (2005)	1.42	1.77	2.32	2.25	-	-	-	-	Y
Nemlioglu and Roberts (2006)	-	-	2.2	-	2.4	-	-	1.6	Y
Palomar (2014)	-	-	-	-	-	-	1.61	1.41	Y
Lai & Lee (2012)	1.78	1.64	2.08	2.84	-	0.44	1.07	-	Y
Papakonstantis et al. (2011 a & b)	1.83	1.68	2.14	2.75	-	0.56	1.68	-	Y
Kikkert et al. (2007)	1.6	1.6	2.27	2.72	-	-	1.81	-	N
Palomar et al. (2012)	CORJET	1.20	1.39	1.85	2.22	-	-	0.70	N
	UM3	1.09	1.16	1.60	1.97	-	-	0.62	
	JETLAG	1.32	1.36	1.69	2.33	-	-	0.79	

7.3.2.2 Horizontal and vertical locations of maximum centerline peak

The horizontal and vertical locations of the centerline peak, x_m and z_m , are plotted against Fr in Figure 7.5 and Figure 7.6, respectively. Previous experimental results from Cipollina et al. (2005), Shao & Law (2010), Papakonstantis et al. (2011) and Lai & Lee (2012) are included for comparison. It can be observed in Figure 7.5 that the 45° LES predictions agreed well with the experimental data. A trend line of the LES predictions was also plotted in the figure, which was close to the experimental

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trend line of Lai and Lee (2012). Similar observation can also be seen in Figure 7.5b, where the 60° LES predictions were very close to the experimental results especially from Papakonstantis et al. (2011), and the LES trend line was nearly identical to that of Lai & Lee (2012).

The maximum centerline peak height is particularly important to assess the submergence of the inclined dense jet in a water body. In Figure 7.6, the centerline peak heights of 45° and 60° are plotted separately to compare with the previous experimental results. The LES predictions for 45° were in reasonably agreement with the experimental data. Similar conclusion can be drawn for 60° particularly with Papakonstantis et al. (2011), although slight under-prediction was noted.

7.3.2.3 Return point location

The horizontal location of the return point from the LES predictions is plotted against Fr in Figure 7.7. From the figure, the 45° LES predictions were close to the experimental data in general, while the 60° LES predictions were in good agreement with Papakonstantis et al. (2011) and Lai and Lee (2012), but somewhat larger than those of Cipollina et al. (2005). Overall, it can be concluded that the LES simulations were able to reproduce well the geometrical characteristics of the inclined dense jet.

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Figure 7.5 Horizontal location of centerline peak: (a) 45° and (b) 60°

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Figure 7.6 Centerline peak height: (a) 45° and (b) 60°

Figure 7.7 Return point location: (a) 45° and (b) 60°

7.3.2.4 Return point dilution

The return point dilution of both 45° and 60° is normalized by and plotted against Fr in Figure 7.8a and b, respectively. Previous experimental results from Shao & Law (2010) and Lai & Lee (2012) were included, as well as the trend lines based on the

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average coefficients from Palomar (2014) and Papakonstantis et al. (2011). A trend line of the LES predictions based on the average coefficient was plotted as well. From Figure 7.8a, the LES predictions generally under-predicted the normalized dilution at 45° compared to previous experimental results. It should be noted that the experimental data for dilution was generally more scattered compared to the geometrical parameters. This under-prediction also occurred at 60° in Figure 7.8b. We noted only one exception that the experimental results of Lai & Lee (2012) showed even lower dilution than the present LES predictions at 60° . The under-predictions of the return point dilution by the LES approach can be attributed to the inaccuracy of the LES SGS model in simulating the turbulence subjected to the stable and unstable stratifications around the inclined dense jet with the adopted mesh scheme.

7.3.3 Impact point dilution analysis

Figure 7.9 presents the contour of mean concentration around the impact region. It can be clearly observed that, along the jet trajectory and when approaching the bottom, the dilution increased continuously due to entrainment until a localized maximum was reached. Subsequently, the trend reversed and the dilution decreased instead near the impact point. To illustrate clearly the concentration variation near the impact location, the LES predicted dilution along the concentration centerline from the port to the bottom impact location are plotted against s/Dfr shown in Figure 7.10, where s is the streamwise distance along the centerline. Clearly, beyond the return point, the dilution continued to increase up to the maximum and then decreased until reaching the bottom. This phenomenon was earlier noted by Abessi

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and Roberts (2015) in their experimental measurements. The physical reasons behind the concentration build-up at the boundary are unclear at this point, but it is likely to be linked to the characteristics of turbulence fluctuations around the impact point. Nonetheless, the present study shows that the LES approach with near-wall modeling was able to reproduce this important feature of the inclined dense jet.

Comparatively, the predicted dilution variation from the k - ϵ predictions along the centerline near the impact point is also plotted for comparison in Figure 7.11. In the figure, s was re-defined as the distance along the centerline from the impact point for better illustration. Clearly, the predictions with the k - ϵ closure were lower compared to LES, and the localized minimum at the bottom impact point was not reproduced. The local contour of the mean concentration from the k - ϵ predictions is presented in Figure 7.12 for better illustration. The concentration in the figure changed smoothly and again no localized build-up at the bottom were observed. We note that the RANS approach with k - ϵ closure adopts more empirical simplifications, and it is thus not surprising that the turbulence characteristics around the impact location was not reproduced as accurately compared to the LES approach. The current results demonstrated the necessity of adopting LES for the simulation of inclined dense jets if the bottom impact is of key interest to the outfall design, despite the higher demand of computing resources required.

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Figure 7.8 Return point dilution: (a) 45° and (b) 60°

Figure 7.9 Concentration distribution from LES results of Case F2 near the impact point

7.3.4 Spreading layer characteristics

This section presents the concentration variation from the LES predictions in the spreading layer for the 60° inclination. The results were obtained from Run S4 which extended the computational domain beyond the end of the mixing zone.

7.3.4.1 Overview of the spreading layer

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Figure 7.13 shows the mean concentration contour of the spreading layer beyond the impact point. From the figure, the mean concentration continued to decrease along the spreading layer which was relatively thin. It was also observed that the thickness of the spreading layer continued to decrease until a minimum is reached, and then it started continuously growing. The concentration fluctuation is presented in Figure 7.14. From the figure, the distribution of concentration fluctuation was similar to that of mean concentration in Figure 7.14 except the centerline of maximum concentration fluctuation, which was significantly elevated beyond the boundary.

Figure 7.10 Dilution along centerline from the discharge port to bottom impact point (dash line indicates the approximate location of the return point independent of Fr ; short solid lines indicate the bottom impact locations)

7.3.4.2 Bottom dilution

The normalized bottom dilution with different Fr on the center plane is plotted in Figure 7.15. The experimental results from Nemlioglu & Roberts (2006) are included for comparison. The LES predictions with different Fr were close to each other before the impact point (generally at around $x/Dfr = 3$), after which the curve began to diverge. Thus, the results showed that Fr is a significant factor influencing the spreading layer, with a higher Fr leading to a higher fluctuation and additional mixing within the layer. Compared to the experimental results, the LES predictions were generally under-predicting the dilution which were similar to the situation before the impact, and can be attributed to the inaccuracy with the adopted SGS model and mesh scheme. It should be noted that the decrease of the bottom dilution by Nemlioglu and Roberts (2006) beyond $x/Dfr = 7$ might be attributed to the presence of the vertical wall in streamwise in their experimental measurements.

Figure 7.11 Comparison of dilution between the LES and $k-\epsilon$ results along centerline near the impact point

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Figure 7.12 Concentration distribution from $k-\varepsilon$ simulation of Case F5 near the impact point

Figure 7.13 Contour of mean concentration of Case S4 in the spreading layer

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Figure 7.14 Contour of mean concentration fluctuation of Case S4 in the spreading layer

Figure 7.15 Comparison of bottom dilution along centerline up to the end of the near field region for 60°

7.3.4.3 Streamwise profiles of concentration and concentration fluctuation

To further examine the concentration variation along the spreading layer, the streamwise concentration profiles are normalized and plotted at various locations in Figure 7.16, where z is re-defined as the vertical distance from the wall and C_c is the centerline concentration. From the figure, all the profiles collapsed into similar curves, showing self-similarity. The LES predictions were also close to the experimental results from Palomar (2014), but again with over-predictions in the elevated distances from the bottom. Due to the no-flux condition at the bottom boundary, it can be expected that the maximum concentration in the spreading layer occurs close to the boundary itself. However, we note that for a three-dimensional gravity current, the maximum point might be slightly elevated from the boundary, due to the small elevated head nose of the gravity current (Ooi et al., 2009).

Figure 7.17 shows the concentration fluctuation profiles along the spreading layer. With x/D_{Fr} less than 6, the profiles from the LES predictions were in reasonable agreement with previous experimental results. Beyond $x/D_{Fr} > 7$, however, the concentration fluctuation remained high even at the elevated region far from the bottom. This observation is consistent with the wider concentration fluctuation near the bottom beyond $x/D_{Fr} > 6.5$ in Figure 7.14.

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Figure 7.16 Normalized concentration profiles along the spreading layer from Case S4

Figure 7.17 Comparison of concentration fluctuation along the spreading layer from Case S4

7.3.4.4 End of the near field region

Roberts et al. (1997) defined the end of the near field region as the location where the intensity of concentration fluctuation drops to 5%, and they concluded a value of $x/Dfr = 9$ based on their measurements. In the present study, the end of the near field region was also determined to be $x/Dfr = 9$ for comparison. The spreading layer thickness and centerline dilution at the end of the near field region were compared with previous experimental data in Figure 7.18 and 7.19, respectively.

Figure 7.18 Spreading layer thickness at the end of the near field region

From the figures, LES predicted a relatively thinner spreading layer compared to the experiments, with lower dilution as well. The coefficients of the spreading layer thickness and the centerline dilution were summarized in Table 7.4. The ratios of the

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return point and impact point dilution to the dilution at the end of the near field were also summarized in the table to be 58% and 46%, respectively, which were very close to Palomar (2014)'s observations.

Figure 7.19 Centerline dilution at the end of the near field region

Table 7.4 Comparison of coefficients of spreading layer with 60° inclination at the end of near field

Quantities	$\frac{x_s}{DFr}$	$\frac{H_s}{DFr}$	$\frac{S_s}{DFr}$	$\frac{S_r}{S_s}$	$\frac{S_i}{S_s}$
LES	9	0.54	1.57	0.58	0.46
Roberts et al. (1997)	9	0.7	2.6	-	-
Palomar (2014)	9	0.8	2.7	0.60	0.52

7.3.5 Eddy structures

A key advantage of the LES approach is the availability of the transient information on the coherent eddy structure of the inclined dense jet which is helpful in understanding the flow development and can aid in the analysis of the mixing characteristics. As an illustration, LES eddy structures from Case S4 were extracted and displayed by plotting the concentration contours at the center plane. Figure 7.20 shows the images of the eddy structures from $t = 40 - 43$ s at 0.5 s interval.

From the figure, a series of vortex rings can be observed along the trajectory as well as in the lower region below the trajectory. These vortices evolved with distance and grew larger in size approaching the impact point. Upon impact, they were then broken down into smaller vortices and spread along the bottom. These small vortices remained within a thin layer on the bottom which formed the spreading layer. Note that due to the adaptation of SGS modelling for the grid scale turbulence, small eddies were inevitably missing in the visualization of the LES results.

Figure 7.20 Sequence of the eddy structure of Case S4 during $t = 40 - 43$ s

7.4 Conclusions

In the present study, the inclined dense jets of 45° and 60° inclinations with bottom boundary were simulated, using LES approach with the dynamic Smagorinsky SGS model combined with near-wall modeling for the bottom boundary. RANS simulations with $k-\varepsilon$ turbulence closure were also performed with both wall function and near wall modelling for direct comparison. Experimental measurements from previous studies were included for verification.

The overall results showed that with the present mesh scheme, LES can predict well the geometric characteristics of the inclined dense jet, including the horizontal and vertical locations of the centerline peak and the return point location. The magnitude of the return point dilution was however underestimated by $\sim 20\%$ corresponding to the grid resolution adopted compared to previous experimental data. This underestimation showed that there are still challenges to simulate accurately the mixing behavior of the inclined dense jet as well as the wall interaction processes. At the same time, LES was able to reproduce the localized concentration build-up at the impact point reported recently by Abessi and Roberts (2015), while $k-\varepsilon$ predictions were unable to do so and were generally far below the LES predictions as well as previous experimental data in terms of the geometrical and dilution characteristics.

The spreading layer was simulated up to the end of the near field region at $x/D_{Fr} = 9$ as defined by Roberts et al. (1997). The characteristics of the spreading layer was analysed including the normalized concentration profiles, normalized concentration

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fluctuation profiles, spreading layer thickness and the dilution at the end of the near field region. The profiles of the normalized mean concentration and concentration fluctuation along the spreading layer were close to previous experimental data, showing self-similarity. The dilution and thickness of the spreading layer were however under-predicted.

The present study demonstrates the adaptation and accuracy of using the LES approach for the simulation of inclined dense jets. We believe that further improvement can be foreseen in the near future with improved SGS models that incorporate the density stratification, as well as acceleration in the computing hardware architecture.

8 Conclusions and Recommendations

8.1 Conclusions

8.1.1 Evaluation of RANS with various Turbulence Closures and LES with various SGS Models in Simulating Flows with Wall Interactions

In chapter 4, the performance of both RANS and LES approaches on the flow simulations with wall interactions was evaluated in terms of the kinematic behavior of the steady flow within a UV reactor with an embedded cylindrical tube. Experimental measurements were performed within the UV reactor model for validation of the CFD predictions.

The CFD results were generally in very good agreement with the experimental data in the upstream region (i.e., before reaching the cylinder), while deviations started to amplify in the downstream region, especially where the flow separation occurred. However, RANS with the $k-\varepsilon$ closures yielded the least accurate results with far under-estimations of the longitudinal velocity in the wake region; while the $k-\omega$ closures were in satisfactory agreement with the experimental data near to the cylinder but continuously over-predicted in the far field; and LES provided the best fit to the experimental data. Overall, the results illustrated that LES is a better approach than RANS in predicting the flow field around complex boundaries

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including possible flow separation, and is thus more suitable for the flow field predictions within a UV reactor.

8.1.2 Large Eddy Simulations of Turbulent Circular Wall Jets

In Chapter 5, the LES simulations of turbulent circular wall jets were performed and compared with the k - ϵ and k - ω closures as well as previous experimental data. Both the velocity and scalar characteristics were investigated in the streamwise and spanwise directions. The lateral spreading ratios of the wall jet on the boundary were investigated for both velocity and scalar. The LES predictions were demonstrated to well predict the strong anisotropic of the wall jet near the boundary, while the RANS closures were not able to predict it. The LES results also agreed well with experimental data in the prediction of the turbulence intensity. The vorticity distribution was also discussed in the present study. The vorticity distribution was found to be dominated by the y -direction vorticity in the symmetry plane driven by the presence of the wall. In the horizontal plane, the vorticity distribution was dominated by the z -direction vorticity caused by the shearing of the jet flow with the ambient fluid plays the primary role.

8.1.3 Large Eddy Simulations of 45° Inclined Dense Jets

Chapter 6 investigated the mixing behavior of 45° inclined dense jets with bottom impact using the LES approach with both the standard Smagorinsky and the

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dynamic Smagorinsky SGS models, including the geometrical coefficients, dilution behavior and turbulence characteristics. Experiments were also performed to validate the LES predictions. The results demonstrated that the LES approach predicted the geometrical characteristics reasonably well with a slight over-prediction in general, and much better than the existing integral models which were compared in the present study. In terms of dilution, the LES results had an under-prediction of $\sim 20\%$ compared with the experimental data, but were much better than the integral model predictions from Palomar (2012) as well. The turbulence intensity was predicted satisfactorily by LES in the upper half but not the inner half. The LES approach with both the Smagorinsky and dynamic Smagorinsky SGS models were not fully able to capture the convective turbulence under the influence of buoyancy.

8.1.4 Large Eddy Simulations of 45° and 60° Inclined Dense Jets with Bottom Impact

In Chapter 7, the bottom impact of inclined dense jets was investigated by means of the LES approach with dynamic Smagorinsky SGS model. RANS simulations with k - ϵ turbulence closure were also performed with both wall function and near wall modelling for comparison.

With the present mesh scheme, LES can predict well the geometric characteristics of the inclined dense jet with bottom impact. The dilution at the return point was again underestimated by $\sim 20\%$ compared to previous experimental data, which was

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consistent with the finding in Chapter 6. LES was able to reproduce the localized concentration build-up at the impact point reported by Abessi and Roberts (2015), while k - ϵ predictions were unable to do so which were generally far below the LES predictions. The spreading layer up to the end of the near field region was also analyzed by means of the LES approach. The profiles of the normalized mean concentration and concentration fluctuation along the spreading layer were close to previous experimental data, showing self-similarity, and the dilution and thickness of the spreading layer were also presented by LES, with under-predictions.

8.2 Recommendations

The mixing behavior of inclined dense jets and associated wall interactions were investigated in detail by means of the LES approach in the present study. The LES approach was found to be superior to the RANS approach with various turbulence closures adopted in the present study in the predictions of wall interactions as well as kinematic characteristics. However, LES was still limited in the predictions of the dilution along the trajectory and in the lower region of the inclined dense jet, with somewhat under-predictions.

In the lower region of inclined dense jets, the mixing mechanism is driven by buoyancy-induced instability which behaves as unstably stratified flow, and may produce small eddies in an anisotropic manner. With the current grid scheme, however, the LES approach with adopted SGS models was not fully able to capture such small motions. Either LES simulations with much finer grids or more suitable

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SGS models are suggested for the dilution of the inclined dense jet in the future work. There were a few LES studies that simulate stratified turbulence in atmosphere and oceans by incorporating positive buoyancy effect into the SGS models (Canuto and Minotti, 1993; Cheng and Canuto, 1994). These SGS models with stratification modified the expressions of the reduced vertical length scale so as to better represent the anisotropy in the stably stratified flow. The development and validation of these SGS models for unstable stratification such as the mixing mechanism of the inclined dense jet are therefore recommended.

In addition, the numerical simulations of the mixing behavior of inclined dense jets in a dynamic ambient are also recommended for future work. The LES performance on predicting the inclined dense jet in stagnant ambient has been investigated comprehensively in the present study. However the performance of LES in the dynamic ambient is still unclear. The evolution of inclined dense jets in the dynamic ambient with time and space can be further revealed using the LES approach.

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Appendix A

Values of Constants and Coefficients in RANS closures

A.1 Standard $k - \varepsilon$ Closure

$$C_{1\varepsilon} = 1.44 \tag{A.1}$$

$$C_{2\varepsilon} = 1.92 \tag{A.2}$$

$$C_\mu = 0.09 \tag{A.3}$$

$$\sigma_k = 1.0 \tag{A.4}$$

$$\sigma_\varepsilon = 1.3 \tag{A.5}$$

$$Pr_t = 0.85 \tag{A.6}$$

A.2 RNG $k - \varepsilon$ Closure

$$C_{1\varepsilon} = 1.42 \tag{A.7}$$

$$C_{2\varepsilon} = 1.68 \tag{A.8}$$

$$\eta_0 = 4.38 \tag{A.9}$$

$$\beta = 0.012 \tag{A.10}$$

A.3 Realizable $k - \varepsilon$ Closure

$$C_1 = \max \left[0.43, \frac{S \frac{k}{\varepsilon}}{S \frac{k}{\varepsilon} + 5} \right] \quad (\text{A.11})$$

$$C_{1\varepsilon} = 1.44 \quad (\text{A.12})$$

$$C_2 = 1.9 \quad (\text{A.13})$$

$$\sigma_k = 1.0 \quad (\text{A.14})$$

$$\sigma_\varepsilon = 1.2 \quad (\text{A.15})$$

$$A_0 = 4.04 \quad (\text{A.16})$$

APPENDIX A

A.4 Standard $k - \omega$ Closure

$$f_{\beta^*} = f(\chi) = \begin{cases} 1, & \chi_k < 0 \\ \frac{1 + 680\chi_k^2}{1 + 400\chi_k^2}, & \chi_k \geq 0 \end{cases} \quad (\text{A.17})$$

$$\chi_k \equiv \frac{1}{\omega^3} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} \quad (\text{A.18})$$

$$\beta^* = \beta^* = \beta_{\infty}^* \left(\frac{\frac{4}{15} + (Re_t/R_{\beta})^4}{1 + (Re_t/R_{\beta})^4} \right) \quad (\text{A.19})$$

$$\beta_{\infty}^* = 0.09 \quad (\text{A.20})$$

$$R_{\beta} = 8 \quad (\text{A.21})$$

$$\zeta^* = 1.5 \quad (\text{A.22})$$

$$\alpha_{\infty}^* = 1 \quad (\text{A.23})$$

$$\beta_i = 0.072 \quad (\text{A.24})$$

$$R_{\omega} = 2.95 \quad (\text{A.25})$$

$$\sigma_k = 2.0 \quad (\text{A.26})$$

$$\sigma_{\omega} = 2.0 \quad (\text{A.27})$$

A.5 SST $k - \omega$ Closure

$$\sigma_k = \frac{1}{F_1/\sigma_{k,1} + (1 - F_1)/\sigma_{k,2}} \quad (\text{A.28})$$

$$\sigma_\omega = \frac{1}{F_1/\sigma_{\omega,1} + (1 - F_1)/\sigma_{\omega,2}} \quad (\text{A.29})$$

$$F_1 = \tanh(\phi_1^4) \quad (\text{A.30})$$

$$\phi_1 = \min \left[\max \left(\frac{\sqrt{k}}{0.09\omega y}, \frac{500\mu}{\rho y^2 \omega} \right), \frac{4\rho k}{\sigma_{\omega,2} D_\omega^+ y^2} \right] \quad (\text{A.31})$$

$$D_\omega^+ = \max \left[2\rho \frac{1}{\sigma_{\omega,2}} \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}, 10^{-10} \right] \quad (\text{A.32})$$

$$F_2 = \tanh(\phi_2^2) \quad (\text{A.33})$$

$$\phi_2 = \max \left[2 \frac{\sqrt{k}}{0.09\omega y}, \frac{500\mu}{\rho y^2 \omega} \right] \quad (\text{A.34})$$

$$\beta_i = F_1 \beta_{i,1} + (1 - F_1) \beta_{i,2} \quad (\text{A.35})$$

$$\sigma_\omega = 2.0 \quad (\text{A.36})$$

$$\sigma_{k,1} = 1.176 \quad (\text{A.37})$$

$$\sigma_{\omega,1} = 2.0 \quad (\text{A.38})$$

$$\sigma_{k,2} = 1.0 \quad (\text{A.39})$$

$$\sigma_{\omega,2} = 1.168 \quad (\text{A.40})$$

$$a_1 = 0.31 \quad (\text{A.41})$$

APPENDIX A

$$\beta_{i,1} = 0.075 \tag{A.42}$$

$$\beta_{i,2} = 0.082 \tag{A.43}$$