Modelling and simulation of single- and multi-phase impinging jets

A thesis submitted to The University of Manchester for the degree of Nuclear Engineering Doctorate in the faculty of Engineering and Physical Sciences

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Abstract

Title: “Modelling and simulation of single- and multi-phase impinging jets”

Impinging jets are a flow geometry that is of interest in many chemical and processing engineering applications for a wide range of industries. Of particular interest in the current research is their application to particle re-suspension in nuclear reprocessing activities such as the HAS (highly active storage) tanks at Sellafield, UK. The challenging nature of these operations and their environment means that in-situ experimental work is impossible. Therefore, when designing and optimising equipment such as HAS tanks, engineers often turn to computational modelling to help gain an understanding about what effects certain modifications may have on the performance of the jet. The challenge then becomes obtaining physically realistic predictions using the methods available to industry.

Impinging jets are complex and complicated flow geometries that have caused a number of problems for computational modellers over the years. Indeed, several turbulence models and approaches have been developed specifically with impinging jets in mind to help overcome some of the more difficult aspects of the flow. The work presented herein compares Reynolds-averaged Navier-Stokes (RANS) commercial codes readily available to industrial users for single- and multi-phase flows with RANS and large eddy simulation (LES) codes developed in an academic research environment. The intention is to contrast and compare and highlight where industrial-based computational models fall short and how these might be improved through implementing schemes with fewer simplified terms.

The work conducted for this Engineering Doctorate has modelled a series of impinging jets with varying jet heights and Reynolds numbers using a range of RANS turbulence models within commercial and academic-based codes. This allows not only the discussion of the performance of the applied turbulence models, but also the effects of varying jet height. The predictions are validated against available experimental data for assessment of the performance of the scheme used. The degree of alignment with real, physical data is an indication of the performance of a model and is used to conclude where a particular model has failed or whether it is more suited than another. Different particle sizes have also been considered to determine the ability of different particle tracking schemes to predict particle behaviour based on their response to the continuous phase. Multi-phase data is also validated against limited available experimental data. Finally, LES has been used to demonstrate the next step in complexity in terms of simulation and prediction of continuous phase flows in difficult engineering applications and how these can greatly improve upon predictions from RANS methods.

Submitted by Matthew Garlick for the degree of Nuclear Engineering Doctorate at the University of Manchester on December 2014.
Declaration

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## Nomenclature

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<tbody>
<tr>
<td>$Ac$</td>
<td>Acceleration number</td>
</tr>
<tr>
<td>$A_0$</td>
<td>Empirical constant</td>
</tr>
<tr>
<td>$a_1, a_2, a_3...$</td>
<td>Drag coefficient constants</td>
</tr>
<tr>
<td>$b_{ij}$</td>
<td>Reynolds stress anisotropy tensor (Fluent)</td>
</tr>
<tr>
<td>$C$</td>
<td>Model constant/coefficient</td>
</tr>
<tr>
<td>$C^2$</td>
<td>Smagorinsky parameter (LES)</td>
</tr>
<tr>
<td>$Cd$</td>
<td>Drag coefficient</td>
</tr>
<tr>
<td>$C_R$</td>
<td>Coefficient of restitution</td>
</tr>
<tr>
<td>$C_{ij}$</td>
<td>Convection term</td>
</tr>
<tr>
<td>$D$</td>
<td>Diameter of jet nozzle</td>
</tr>
<tr>
<td>$D_T$</td>
<td>Turbulent diffusion term</td>
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<td>$D_L$</td>
<td>Molecular diffusion term</td>
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<td>$d$</td>
<td>Diameter</td>
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<td>Energy</td>
</tr>
<tr>
<td>$E'$</td>
<td>Empirical constant</td>
</tr>
<tr>
<td>$F$</td>
<td>Force/additional force</td>
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<tr>
<td>$F_{ij}$</td>
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<td>$g$</td>
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<td>$K$</td>
<td>Saffman coefficient = 2.594</td>
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<tr>
<td>$k$</td>
<td>Turbulent kinetic energy</td>
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<td>$L$</td>
<td>Leonard stress tensor, length scale of energy containing motions</td>
</tr>
<tr>
<td>$l$</td>
<td>Length scale of turbulence ($A \equiv l$)</td>
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<td>Mach number</td>
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<td>$m$</td>
<td>Mass</td>
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<td>$P_k$</td>
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<td>Time</td>
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<tr>
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<tr>
<td>$U_{mag}$</td>
<td>Mean velocity magnitude = $\sqrt{u^2 + v^2 + w^2}$</td>
</tr>
<tr>
<td>$u, v, w$</td>
<td>x, y, z- components of instantaneous velocity</td>
</tr>
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<td>$u_e$</td>
<td>Friction velocity</td>
</tr>
<tr>
<td>$V$</td>
<td>Volume</td>
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Relative velocity = $u_f - u_p$

Cartesian co-ordinate

Height of first grid cell

Thickness of viscous sublayer

**Greek symbols**

- $\alpha$: Empirical material specific constant for $C_R$
- $\beta$: Density ratio = $\rho_f / \rho_p$
- $\Delta$: Filtering length scale
- $\delta_{ij}$: Kronecker delta
- $\epsilon$: Turbulent energy dissipation rate
- $\eta$: Kolmogorov length scale
- $\kappa$: von Karman constant
- $\lambda$: = $1/(1 + 0.5\beta)$
- $\mu$: Dynamic viscosity
- $\mu_t$: Turbulent eddy-viscosity
- $\nu$: Kinematic viscosity
- $\Omega_{ij}$: Rate of rotation tensor
- $\phi_{ij}$: Pressure-strain term
- $\phi_{ij, 1}$: Slow pressure-strain term
- $\phi_{ij, 2}$: Rapid pressure-strain term
- $\phi_{ij, w}$: Wall correction to the pressure-strain term
- $\omega$: Angular velocity
- $\rho$, $\rho_f$: Density of fluid
- $\rho_p$: Density of particle
- $\sigma_k$, $\sigma_\epsilon$: Model constant = 1.0, = 1.2 respectively
- $\tau$: Dummy variable for time (Particle equation of motion)
- $\tau_{ij}$: Stress tensor
- $\tau_p$: Particle response time
- $\tau_r$: Transit time
- $\tau_e$: Eddy lifetime
- $\tau_{e, w}$: Wall shear stress
- $\zeta$: Normally distributed random number

**Subscript**

- $0$: Initial value
- $A$: for added mass
- $f$: of fluid
- $H$: for the Bassett history
- $p$: of particle
- $i, j, k$: Indices of unit vector
- $n$: First cell in domain from boundary
- $\mu$: Viscous/ of viscosity

**Superscript**

- $a$: Anisotropic part of tensor
- $\bar{\phi}$: Mean quantity
- $\phi'$: Fluctuating quantity
- $\tilde{\phi}$: Filtered quantity
- $n$: $n^{th}$ timestep
## Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>ASM</td>
<td>Algebraic stress model</td>
</tr>
<tr>
<td>BNFL</td>
<td>British Nuclear Fuels Ltd</td>
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<tr>
<td>CFD</td>
<td>Computational fluid dynamics</td>
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<tr>
<td>DNS</td>
<td>Direct numerical simulation</td>
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<tr>
<td>GUI</td>
<td>Graphical user interface</td>
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<tr>
<td>HALES</td>
<td>Highly active liquid evaporation and storage</td>
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<tr>
<td>HAS</td>
<td>Highly active storage</td>
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<tr>
<td>HLW</td>
<td>High level waste</td>
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<tr>
<td>ILW</td>
<td>Intermediate level waste</td>
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<tr>
<td>$k$-$\varepsilon$</td>
<td>$k$-epsilon model</td>
</tr>
<tr>
<td>$k$-$\omega$</td>
<td>$k$-omega model</td>
</tr>
<tr>
<td>LES</td>
<td>Large eddy simulation</td>
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<tr>
<td>LDA</td>
<td>Laser Doppler anemometry</td>
</tr>
<tr>
<td>LLW</td>
<td>Low level waste</td>
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<tr>
<td>LPT</td>
<td>Lagrangian particle tracker</td>
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<tr>
<td>NDA</td>
<td>Nuclear decommissioning authority</td>
</tr>
<tr>
<td>NNL</td>
<td>National Nuclear Laboratory</td>
</tr>
<tr>
<td>PIV</td>
<td>Particle image velocimetry</td>
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<tr>
<td>RANS</td>
<td>Reynolds-averaged Navier-Stokes</td>
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<tr>
<td>r.m.s</td>
<td>Root mean square</td>
</tr>
<tr>
<td>RNG</td>
<td>Re-normalisation group</td>
</tr>
<tr>
<td>RSTM</td>
<td>Reynolds stress turbulence model</td>
</tr>
<tr>
<td>SGS</td>
<td>Subgrid scale</td>
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<tr>
<td>SSG</td>
<td>Speziale-Sarkar-Gatski</td>
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<tr>
<td>SST</td>
<td>Shear stress transport</td>
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Chapter 1  Introduction

The Sellafield site in Cumbria, England is one of the world’s largest spent fuel reprocessing plants. For over 30 years it has stored and reprocessed fuel from the UK’s nuclear fleet as well as imported spent nuclear fuel from overseas for reprocessing. Whilst the site has changed hands over the decades and has gradually been decommissioned, the treatment and temporary storage of spent fuel in the UK is still centralised at Sellafield. In 2005 the site passed from the hands of British Nuclear Fuels Ltd (BNFL) to the Nuclear Decommissioning Authority (NDA) and is now operated by Sellafield Ltd. The site still contains the legacy of Britain’s civil and military nuclear programme and is currently undergoing a huge decommissioning effort to dismantle the remaining Calder Hall and Windscale facilities, as well as management of the nuclear waste on the site. Central to the operations at Sellafield is the safe handling and storage of spent nuclear fuel and reprocessing waste streams. These materials require considerable care and bespoke storage units. This introduction outlines where these wastes arise in the nuclear fuel cycle and the problems they pose to safe storage. The research reported in this thesis then contributes to answer the question of how can numerical methods be used to help design and optimisation of equipment used in the process and improve storage of these hazardous materials?
1.1 Motivation behind the research

The nuclear fuel cycle is a complex and difficult area of expertise which handles the mining, enrichment, manufacture, usage, reprocessing, storage and disposal of nuclear fuel. There is considerable debate as to whether to adopt an open or closed cycle. In an open fuel cycle, nuclear fuel is passed once through a reactor before being sent for treatment, encapsulation and eventual disposal at a deep geological facility. Given the nature of the encapsulation and disposal of the open fuel cycle, it is unlikely that the spent fuel will be recoverable again. In a closed fuel cycle, the spent nuclear fuel is reprocessed, recovering the reusable uranium and plutonium, which can be manufactured back into new fuel elements. This produces a very problematic waste stream which must ultimately be disposed of in a similar manner to spent nuclear fuel in an open cycle. As it may be difficult to choose between the two at the present time, many countries have opted for an interim third option in which spent nuclear fuel is stored until a decision can be made on the best way of treating it.

Spent nuclear fuel contains the remainder of the fissile isotope uranium-235 as well as uranium-236, plutonium, minor actinides (neptunium, americium and curium) and fission products. Reprocessing separates the fuel into re-useable material for fuel fabrication and waste which ultimately must be disposed of. Within the nuclear industry it is important to understand the classification of the waste streams and how each must be handled. The classification of waste is generally handled on a safety case basis as well as radioactivity and concentration of short- and long-lived nuclides, fitting into one of three bands shown in Table 1.1

At the Sellafield site, spent nuclear fuel arrives from UK nuclear power stations and its overseas customers. The fuel is received in shielded flasks and contained in storage racks which are placed in a preliminary storage pond to allow the short-lived radionuclides time to further decay. After around 100 days the contents have significantly decayed and can be removed from the storage ponds and sent to stripping operations. During this stage the uranium pellets are exposed by stripping the fuel cladding away allowing the spent fuel rods to be sent for mechanical cropping. The cropped fuel is then dissolved in nitric acid followed by the primary separation phase which constitutes 18 counter-current mixer-settlers in series and a solvent extraction system using tributyl phosphate and odourless kerosene. During the process the uranium (~96%) and plutonium (~1%) are separated as nitrates into the solvent phase, leaving the fission products and minor actinides (~3%) in the nitric acid or aqueous phase. This aqueous phase (also known as the PS1 aqueous raffinate) is then steam stripped to remove entrained solvent before being transported to the Highly Active Liquid Evaporation and Storage (HALES) facility on the Sellafield site for further processing.
### Classification Overview

#### Disposal Options

<table>
<thead>
<tr>
<th>Classification</th>
<th>Overview</th>
<th>Disposal Options</th>
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<tbody>
<tr>
<td>Low level waste (LLW)</td>
<td>Activity levels are above clearance levels for exempt waste (&gt;4MBq/Te) but do not qualify for ILW. A precise activity limit is difficult to establish due to the range of criteria that different wastes might fulfil to be classified. Wide classification of wastes and LLW tends to be further categorised into short-lived waste and very low level waste.</td>
<td>Suitable for near-surface disposal for up to a few hundred years. Depth is dependent on the activity of the waste itself. Requires little shielding and only robust provisions for duration of storage.</td>
</tr>
<tr>
<td>Intermediate level waste (ILW)</td>
<td>Waste containing higher concentrations of long-lived radionuclide requiring a greater degree of containment and isolation are classified as ILW. The boundary between LLW and ILW is somewhat indistinguishable as the safety case for different waste types vary significantly.</td>
<td>Disposal underground at a depth of 10-100m is indicated for ILW. This has the potential to provide safer storage and reduce chances of exposure to the environment beyond reliable institutional control.</td>
</tr>
<tr>
<td>High level waste (HLW)</td>
<td>Surprisingly, HLW need not have significantly higher radioactivity than ILW, however, should the concentration of short- and long-lived radionuclide be sufficient to generate heat then the waste must be classified as HLW. A much greater degree of shielding and provisions for containment must be considered as well as heat dissipation methods.</td>
<td>HLW requires deep geological disposal with heat dissipation taken into account. At present, HLW is stored in ponds or in convection cooled facilities on the surface.</td>
</tr>
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</table>

Table 1.1 – LLW, ILW & HLW classification and disposal options

The main purpose of the HALES facility is to reduce the volume of HLW in order to make long term storage feasibly possible. Approximate Sellafield throughput is 5 tonnes of spent fuel per day, which results in 25m³ of highly active dilute liquid waste, the majority of which is nitric acid. To reduce the volume of waste within the HALES facility there are a number of kettle-type evaporators through which the raffinate is sent to. During the evaporation phase the acid is distilled, increasing the concentration of waste products and solids content up to 50%. The nature of this waste makes it extremely difficult to measure or characterise. With the acid removed, water is added to the waste to dilute it and avoid corrosion and particle build-up-related issues downstream before the liquors are cooled and discharged to storage tanks. These evaporators are operated by control over the pressure within the vessel and generally operate at around 50°C. At elevated temperatures the risk of corrosion becomes significant and it is desirable to keep this risk as low as possible.

The liquors are held in large vessels called Highly Active Storage (HAS) tanks based in the HALES facility. It is these tanks (Figure 1.1) which are the main motivation behind the current research and are discussed in some detail here. As these tanks have been developed, many issues have arisen and each generation of tank has seen design improvements. The latest model
of HAS tanks are approximately 150m$^3$ and contain seven cooling coils, a base and side cooling jacket, instrumentation, ventilation, jet ballasts and air lifts. The liquors are held in the tanks at an optimal temperature of around 55°C which ensures enhanced corrosion does not occur and reduces the rate of precipitation. The solids which do precipitate out of the liquor are considered highly active and therefore heat-generating. As these particles settle under gravity at the bottom of the tank they form a layer and can cake unless re-suspended. A bed of these particles can result in the formation of localised hot spots which can accelerate corrosion and damage the base of the tank or the cooling coils. Therefore the HAS tanks have methods of keeping particles suspended, or re-suspending those which do settle on the base in the form of air lifts and jet ballasts.

Figure 1.1 – HAS tank at Sellafield highlighting (A) central jet ballast, (B) cooling coil arrangement, (C) radial impinging jets, (D) air lifts

The jet ballasts are impinging jets located around the edges of the tank with a large one in the centre. The peripheral jets are angled at the wall and base of the tank which deflects the flow inwards to form a wall jet, re-suspending solid particles around the edges of the tank. The central jet ballast is normal to the base of the tank and forms an axisymmetric turbulent jet. The peripheral and central jets create a clearance zone sufficient to keep the majority of particles on the base mobile. The cycle starts by pressurising the central jet ballast with air to rapidly drive the liquor out of the nozzle at reasonably high velocities (typically around ~15m/s) which re-suspends solids from the bottom. The jet ballast ullage is vented and the liquor reverse flows through the nozzle of the jet to refill the jet ballast for the next cycle. Alternatively, at low liquor levels, to maintain the performance of the jet, the liquor is vacuum lifted during the venting phase of the cycle. At the completion of the firing phase of the first jet, the second jet
fires and repeats the same process as the first. The complete sequence of firing, venting and re-filling all jets can take around 10-30 minutes.

The performance of these jets has been evaluated by experimental methods and some basic computational studies. The former consisted of a 1/10th rig located at the Workington laboratory owned by National Nuclear Laboratory (NNL). These experiments utilise test solids to simulate the contents of the HAS tanks. At present, studies are being conducted to determine more in-depth characteristics of these simulants so that more representative experiments can be performed in the test rig. Both experiments and simulations have shown the resultant clearance of particles on the base of HAS tanks as a ‘star’ shape. When the area of clearance is not sufficient (i.e. the clearance areas do not overlap) regions of settled particles in-between clearance areas remain unsuspended and the risk of localised hotspots is increased. In practice it has been found that the jets perform to an acceptable level but not to their design specifications; therefore there was a desire to improve the computational capabilities of modelling impinging jets. If this could be achieved, multiple variables could be changed to examine how the important parameters influence the behaviour of the impinging jet and therefore strongly influence future experiments to validate the performance of the jets. Furthermore, an improved computational model should be capable of looking at multi-phase systems and the distribution of particles in an impinging jet. This data is highly valuable during the design and optimisation of these tanks and could ascertain whether full floor clearance was being achieved by the impinging jet configuration. Whilst computational fluid dynamics in industry is not limited to commercial codes, they are certainly more widely used than bespoke codes which may have been developed for a specific purpose. A comparison between such commercial codes and codes used in academia would be beneficial to determine which provides more accurate and reliable data and potentially where certain codes fail.

1.2 Impinging Jets

Turbulent jets are used in a wide range of industrial applications and can be found in many different configurations. They are a class of turbulent shear flow that has been of considerable interest within both academia and industry. The impinging jet is one such configuration of turbulent jet in which a fluid is discharged from a nozzle on to a flat, solid surface. This approach is commonly used in heating, cooling and drying operations. Furthermore, the turbulent behaviour of the impinging jet makes them ideal for multi-phase mixing and particle re-suspension when mechanical mixing is not appropriate. The heat transfer characteristics of the system are known to be directly affected by the scale of turbulence; turbulence which is, in-
turn, affected by a number of other factors. Plenty of studies are available which detail how different configurations and varying certain parameters can affect the performance of the heat and mass transfer properties of a jet. It is the purpose of this thesis to investigate some of these factors though turbulence modelling and simulation techniques. By obtaining suitable flow field and turbulence statistics one might then determine how these affect mixing and mass transfer.

Impinging jets used to facilitate mixing fluids or multi-phase systems are often used when mechanical mixing is not an option. It is a difficult task to design and optimise impinging jet configurations to ensure an acceptable level of mixing or particle suspension and often requires experiments to determine which configuration will achieve the desired results. This can be an expensive process. The experimental approach must include, and try to justify, a host of variables, including the nozzle diameter, shape, height, exit velocity and angle of incidence. Data then must be analysed and compared to see the impact of these variables on operating conditions, including particle distributions and velocities, attrition or coagulation estimations. These conditions can have subsequent effects on other factors such as heat transfer which is particularly important in combustion chambers. Through use of computational fluid dynamics (CFD) these factors can be investigated and narrowed down to well-informed estimates which can strongly direct any experimental testing.

Multi-phase modelling requires a good understanding of fluid-solid and solid-solid interactions. These interactions dominate the behaviour of the flow and so must be well understood to help the design, optimisation and development of process equipment. Both the underlying physics and case specifics are equally important. Contact between solids is likely to cause attrition or coagulation. Wear and erosion must be considered to vessel walls, internal heating/cooling coils and agitator blades and particle density distributions are essential to ensure that adequate mixing can be achieved. Most commercial CFD codes have very simple multi-phase models which industry must rely upon. Therefore, more extensive experimental testing is needed to ensure the operations work correctly, which can be extremely expensive. The low confidence in multi-phase CFD is an issue which must be addressed. Other methods are available with a greater degree of accuracy for multi-phase flows, typically in academia. If the methods typically employed in academic codes can be used to improve commercial CFD codes then this would be immensely beneficial to industries which rely on CFD.
1.3 Scope and objectives of the research

Considering the motivation and background discussed, it is important to outline the scope of the present research and the objectives it is hoped to be achieved. The thesis focuses on the modelling of single- and multi-phase impinging jets using a variety of different approaches. It is essentially split into two themes: the first concerns single-phase simulations and the second considers multi-phase simulations. Within each theme are three sub-sections which concern the different computational methods that have been used.

The industrial relevance of the impinging jet, and the challenging flow features it presents, makes it an ideal system to use for comparison and evaluation of mathematical models. Literature surrounding impinging jets is reviewed in Chapter 2 and from this three impinging jets have been considered in this research. The primary variable is the jet height or the separation distance between the jet nozzle and the impingement plate. The jet heights considered represent three different categories of impingement in order to provide a different angle of discussion between turbulence models and modelling methods.

Commercial CFD codes are now very common in industrial practice. Their general robustness, intuitive GUI and fast computational times make them ideal. However, the turbulence models which come with CFD packages are typically designed to give a solution for any system at the expense of accuracy. Further to this, some generalisations and assumptions are made for basic models which contradict practices used in more advanced codes making their use questionable at even the simplest of levels. However, commercial CFD codes have brought to light the benefit that computational modelling can provide in design and development engineering across a wide range of industries. This allows for more efficient designs, reducing development costs and bringing products to market more rapidly and economically than has been possible before its introduction. As a result of this it is equally as important to evaluate the performance of such commercial CFD codes as it is the more advanced academic methods such as LES or DNS.

ANSYS Fluent is a well-known and commonly used commercial CFD code package found in industry. In order to obtain an understanding of what is offered in ANSYS Fluent, it is important to use a variety of turbulence models including 2-equation and 5-equation variants. Using three turbulence models from ANSYS Fluent 13.0, the components of these models can be compared and the shortcomings of each identified. These models are discussed in full in Chapter 3. The first model to be investigated is the realisable $k$-$\varepsilon$ model, a simple and robust 2-equation model. The performance of this is then compared with that of a linear and non-linear variant of the RSTM. The latter might be expected to perform better than the other two due to the non-linear nature of the pressure-strain correlation in an impinging jet. However, it is
unlikely that all three models will accurately predict a flow system which falls in line with experimental data. As these are RANS models, the system can be simplified to a 2D axisymmetric problem to save computational resources and time.

Moving on from industrial to academic methods, the RANS STREAM code has been developed with a number of turbulence models to choose from. These range from standard $k$-$\varepsilon$ models to advanced non-linear RSTM. Of interest in this code is the non-linear RSTM with wall reflection developed by Craft (1991). This model was designed with impinging jets in mind and therefore, it is expected to perform well. A good impinging jet solution will show that RANS methods are still a viable method of simulation when used without assumptions that compromise the integrity of the underlying physics. As with the ANSYS Fluent simulations, the RANS STREAM code is capable of 2D axisymmetric simulations and these will be used to save time and computational resources.

The next stage of the present work involves LES. LES require significantly more computational resources and are often more difficult to operate than RANS methods. In LES the large scale turbulence structures are directly solved whilst the smaller scales are modelled. This approach is based upon the more realistic assumption that turbulent mixing is only really affected by the larger scale turbulence, whilst the smaller scales can be considered as isotropic. Spatial filtering is applied to the Navier-Stokes equations, effectively providing a decomposition to define large- and small-scale turbulence. Often this filtering process is linked to the mesh and numerical approximation. This places additional sensitivity upon the mesh used with LES and often proves to be the most challenging aspect. The subgrid-scale stresses are modelled using an eddy-viscosity approach based on the Smagorinsky model. This should serve to illustrate the problems that RANS can have with non-trivial flow systems. Placing particles into the solution is also a unique aspect of this work and should provide realistic insight into the behaviour and deposition of particles in an impinging jet.

The addition of particles to the above-discussed RANS and LES approaches completes the range of areas this study aims to investigate and brings it much closer to the industrial application of the research. That is, the HAS tanks and the impinging jets used to suspend particles on the base of the tanks. Particles have not been visualised in an impinging jet using reliable computational methods to date, and the present work should thus provide an excellent opportunity to determine where the distribution and behaviour of particles in an impinging jet. The potential for recirculation of particles back to the jet axis is one of great interest as this would readily replace the particles that had recently been cleared from the base of the tank. Although the geometry of the present simulations is not specifically based on the HAS tanks, a general approach allows the work to be applied to many other applications of impinging jets.
Chapter 2  Literature Review

This chapter is aimed at exploring and discussing the current and on-going research into turbulent impinging jets. A large amount of literature has been published for both experimental and computational impinging jet studies but mostly for single-phase systems. Dividing the literature review into experimental and computational studies will allow for easier discussion and comparison of studies which are to be used as the benchmark for the current research.

It is necessary to consider both single- and multi-phase studies of impinging jets for validation purposes and to seek areas which authors have so far neglected. Very few studies consider multi-phase impinging jets which gives room for advancement in this area. An overview of turbulent impinging jets is also provided to outline the fundamentals of the jet structure which will be referred to throughout the thesis.

2.1  Overview of Impinging Turbulent Round Jets

The structure of an impinging jet is dependent upon a number of variables the impact of which we have come to understand through experimental and computational analysis. Experimental studies for instance lead us to develop empirical correlations for the variables and their impact on jet behaviour. These correlations can then be used in computational studies to improve predictions and investigate finer details of the jet structure. Furthermore, there are certain features of impinging jets which are difficult to model. If these difficulties can be overcome then this will improve the ability of CFD models to model impinging jets and flow configurations which have similar features.

Figure 2.1 shows the structure of two basic impinging jet configurations. A significant feature of impinging jets is labelled the jet potential core in Figure 2.1 which is where the fluid has not begun to mix at the interface between the developing jet and the surrounding ambient fluid. The notable difference is the jet height, defined as the distance between the jet nozzle and the impingement plate.
Figure 2.1 – Illustration of an impinging jet on a flat surface (a) transitional flow impingement and (b) impingement within the potential core

Narayanan et al (2004) identify the different regimes shown in Figure 2.1 as:

a) The case where the jet impinges once the potential core has started to decay as a result of the growth of the developing jet boundary layer (also known as the jet mixing layer)

b) Impingement occurs before the potential core has begun to decay. The jet boundary layer may still be relatively small at the time of impingement for small jet heights.

The current work investigates both of these cases to analyse the impact each configuration has on the resultant jet structure. An additional case is also investigated in which the impingement plate is placed at the point where the potential core is just about to decay to the centreline also known as the transitional case.

Concerning the structure and behaviour of the impinging jet, three distinct regions can be identified and are highlighted in Figure 2.1.

(1) The free jet region, as noted by Abramovich (1963) is located prior to any strong interaction forces as a result of impingement. The free jet region then comprises the initial discharge of the jet where the thickness of the jet edge mixing layer is at a minimum. As the jet proceeds into the region of stagnant fluid the jet boundary begins to grow as surrounding fluid or particles are entrained. As the jet boundary layer grows, momentum is exchanged with the adjacent shear layers, thus the potential core is
eventually “eaten up” through shear forces acting on the jet by the surrounding fluid (Schlichting, 1979). Provided the jet height is sufficiently large, this region is almost completely identical to that of a fully free jet which may never impinge on a surface. Should the jet height be large enough then the potential core will eventually decay completely resulting in the gradual decay of the axial velocity along the centreline. The length of the potential core is typically dependent on the inlet conditions of the jet and the properties of the fluid. Studies by Albertson et al (1950), Gardon & Akrifat (1965), Martin (1977) and Narayanan et al (2004) have estimated the length of the potential core to be 5-6 times the diameter of the jet.

(2) The impingement region or stagnation region in which the strong interaction forces born from impingement produce a change in the direction of the flow. These forces were demonstrated to appear within the final 16% of the approach to the stagnation region by Tani & Komatsu (1964) whilst Beltaos & Rajaratnam (1974) found it to be 14%. The impact of these forces causes the axial velocity to rapidly decay and sees a fast build up of the static pressure at the impingement region. At the point of impingement, the fluid motion comprises a nearly irrotational normal straining, as opposed to simple shear, whilst developing to a combination of strong rotationality and streamline curvature towards the edge of the impingement region. The static pressure causes the radial acceleration of the fluid outwards, away from the stagnation region. The boundary layer in this region was investigated by Schrader (1961) who concluded that the boundary layer begins to thicken beyond a radial distance of 1.1D, the so-called jet deflection region or flow acceleration region.

(3) Beyond the impingement region, the wall jet region forms and begins to develop. This region constitutes the remainder of the development of the radial wall jet. The flow is now dominantly radial and concerns the wall forces/interaction (boundary layer) and free shear as the wall jet moves against stagnant fluid on the other side (free mixing layer). The development of the wall jet is quite complex and was investigated by Launder & Rodi (1983). In the wall jet region, the rate of growth of the jet soon becomes linear. This implies that the profile of the jet does not change once normalised and is so called “self-similar” and was demonstrated by Poreh et al (1967). It was found that the rate of spreading is different for axisymmetric (round) jets rather than plane jets (square or slot). Plane jets have been shown to have a higher spreading rate and thus produce a deflected wall jet with a thicker mixing layer. In round jets the axisymmetric expansion of the radial wall jet, which increases the rate of momentum
transfer, ultimately slowing the radial wall jet. This is not the case with the plane jet

The hydrodynamics of impinging flows are also discussed in significant detail by Rajaratnam
(1976) and Martin (1977) who review early literature and theories developed by other authors.
Martin presents a number of equations which can approximate the velocity profiles for the
different regions of the impinging jet flow, with constants that must either be found empirically
or vary depending upon the nozzle type, jet geometry and Reynolds number.

2.2 Experimental studies of turbulent impinging jets

Experimental studies of impinging jets face a number of problems concerning the measuring
techniques used to obtain the flow data. There are a number of measuring techniques available,
where no particular method is free from doubt or questionable reliability. Many studies spend a
good deal of time and effort justifying why they used a particular approach and how they
overcame the disadvantages associated with it. There are considerably more studies which look
at the heat transfer properties of impinging jets and focus less on the turbulence statistics and
flow field data. However, since the present study is not concerned with heat transfer, these are
not reviewed here.

Measuring techniques used in experimental studies on impinging jets are quite varied with pros
and cons to each of them. *Hot-wire anemometry* is an invasive probe method, which correlates
the change in current through a very fine, hot, wire to velocity fluctuations. As flow passes the
wire it has a cooling effect which alters the resistance of the wire. *Laser-Doppler anemometry*
(LDA) is a technique in which neutrally buoyant tracer particles are added to the fluid phase.
The flow then passes through a laser sheet where the particles diffract the light. The diffracted
light is collected by a receiver which allows the calculation of the velocity and other turbulent
statistics. *Particle imaging velocimetry* (PIV) is a more recent, non-intrusive, method that has
been adopted to look at flows. Once again, tracer particles are added to the fluid and an area of
interest is illuminated with a light source. A camera rapidly captures images of the locations of
the tracer particles in-sync with a pulsed laser light. The particles are translated as pixels into a
PIV software package and flow statistics can be obtained by monitoring the progress of the
particles. Furthermore, a significant advantage of PIV is that it can potentially be used to obtain
multi-phase data by ensuring the discrete phase particles are larger/identifiable from the tracer
particles. In theory this allows velocity and turbulent data to be obtained from both phases
simultaneously.
Studies detailing flow field and turbulence statistics are important to this research for validating computational simulations with physically real data. Furthermore, the configuration of jets varies quite considerably making certain studies more desirable for validation than others.

### 2.2.1 Single-phase studies

Single-phase impinging jet studies have been of interest both academically and industrially for many decades in an attempt to develop relationships between the variables which make up impinging jets and the effect they have on their behaviour. These empirical relationships are then used in developing and designing impinging jets within industry. One of the earliest studies of turbulent round impinging jets was by Poreh et al (1967), which set the benchmark for impinging jet studies in subsequent years. The authors presented measurements of mean velocities, turbulence intensities, Reynolds stresses and the wall friction within the radial wall jet in addition to some theoretical considerations of the wall jet region. The study noted that the height of the jet discharge made an impact upon the resultant wall jet but focused on the variation of the Reynolds number. It was found that after non-dimensionalising the data, Reynolds number did not have a significant effect on the turbulent statistics. In their study, the authors contradicted some earlier observations by Glauert (1956) by stating that in an axisymmetric jet, the rate of jet spreading is found to be smaller and the rate of decay of the radial velocities is greater than in a radial free jet.

Following Poreh et al (1967), studies by Rajaratnam (1974), Era & Saima (1975) and Ennojji & Asanuma (1982) took similar measurements of impinging jets using hot-wire anemometry. These studies were mostly aimed at developing relationships for velocity profiles and variables such as Reynolds number and jet height.

A slightly more recent study is that of Cooper et al (1993), who also used hot-wire anemometry to provide an extensive set of measurements for an axisymmetric turbulent impinging jet. The study built upon some important features used by Baughn & Shimizu (1989), such as a well-defined inlet condition and jet heights as low as 2D. The Cooper et al study provided a comprehensive set of impinging jet data specifically for comparison and validation purposes in its sister paper by Craft et al (1993). Using two Reynolds numbers of 23,000 and 70,000, Cooper et al conducted a series of experiments to obtain velocity and turbulence statistics whilst Baughn & Shimizu measured heat transfer data for several jet heights. The jet heights reported in the literature are h/D = 2, 3, 4, 6 and 10, although greater emphasis is shown to h/D = 2, 6 and 10 as these correspond to impingement in different regions of the jet. Ensuring a fully-developed pipe flow with a sufficient length of straight pipe preceding the jet nozzle is useful.
This gives a clear description of the inlet conditions at the jet nozzle which can be replicated. Surprisingly few other studies specify this condition which narrows down the literature that could be reliably used to validate computational solutions. Since Cooper et al, more studies have used fully-developed profiles and described their inlet conditions more clearly.

Measurements were made using hot-wire anemometry which is often found to be unreliable in areas of high turbulence or flow reversal such as the stagnation point. Cooper et al comment that close to the wall (y/D < 0.1), the hot-wire anemometer is highly sensitive to velocity fluctuations parallel to the wall which leads to inaccuracies. This problem has been shared by other authors such as Chevray & Tutu (1978) and Knowles & Myszko (1998). Furthermore, the stagnation region is highly turbulent with unsteady flow reversals and separations making multiple velocity measurements very difficult for hot-wire anemometers. However, the authors go on to explain that the study was primarily for validation purposes and data very close to the wall, although desired, was not critical to the study. Validation of the overall turbulence model can be achieved without data very close to the wall, however if evaluation of wall treatment methods was the focus it would require a different technique capable of near-to-wall measurements. Craft et al (1993) published a sister paper which used data from Cooper et al (1993) to assess several turbulence models using a RANS approach with various improvements.

Knowles & Myszko (1998) used the study of Cooper et al (1993) to verify their experimental findings. The authors found a linear rate of jet spreading which is a well-established and accepted feature of impinging jets which is also in line with the findings of Cooper et al (1993). Their study also found that the jet height has a significant effect on peak turbulence levels up to r/D = 4; lower jet heights caused an increase in the peak level measured in the stagnation region and as the jet height was increased, the turbulence production in the radial wall jet was reduced. This is due to smaller radial velocities and smaller radial velocity gradients normal to the wall which results in a thicker wall-jet.

Yokobori et al (1979) confirmed the existence of counter-rotating, large-scale vortices at positions along the jet. It was this early discovery which suggested that these vortices were enhanced when the jet impinged at a transitional jet height. The structures were instrumental in the increased rate of heat and mass transfer in the stagnation region. Difficulties arise when measuring the velocity field in the near field of the stagnation zone. An early study by Landreth & Adrian (1990) noted that PIV should resolve measurements of complex turbulent systems with suitable accuracy. Their study was limited in terms of jet height, Reynolds number and did not use a fully-developed pipe flow at the jet exit but served to demonstrate that PIV could be used effectively in this setup. With PIV, the instantaneous velocity fields that were measured could detect the presence and impact of secondary vortices on the turbulence statistics. Using ensemble averaging, the authors were able to determine the mean velocities and plot reasonable
flow characteristics although only eleven realisations were used, which gives an approximate mean value for the velocity vectors. Landreth & Adrian comment that the primary vortex weakens as it propagates downstream prior to producing secondary vortices. The authors also comment on the satisfactory accuracy of the PIV and its agreement with LDV measurements. Slightly more recently, Nishino et al (1996) comment that PIV is more suitable for velocity measurements in high turbulence regions such as the stagnation region as it is able to resolve flow reversals and capture two or three velocity components simultaneously. Their study captured highly turbulent statistics including the velocity fluctuations and turbulent stresses in the flow near the stagnation. Analysis in three dimensions showed the turbulence was axisymmetric about the centreline. The study itself used a submerged nozzle jet directed at a flat impingement plate, however the setup did not use a fully-developed profile at the nozzle exit which limits its use for comparison to computational studies. Unfortunately, PIV also fails to adequately obtain data close to the wall due to the size of the camera and interference from reflections on the surface.

Fairweather & Hargrave (2002) and Hargrave et al (2006) performed measurements on an air jet using PIV at a jet height of 2D and found their results were in reasonable alignment with other authors such as Cooper et al (1993) and Dianat & Jones (1995) who used probe techniques. Although some differences do occur between the two techniques, there are advantages and disadvantages of using both. PIV is limited by the maximum spatial resolution, unlike hot-wire anemometry, however it can distinguish the directionality of the flow more reliably than probe techniques and avoids the problem associated with intrusive measurement techniques.

Barata et al (1993) used LDA to visualise a high-Reynolds-number round impinging jet at a height of 5D from the impingement plate into a cross-flow. The authors also used computational methods to simulate the regions where there is no experimental data. The LDA technique was able to clearly detect the vortex structures which showed a strong recirculation zone, largely due to the cross flow, and the study provided two mean and turbulent velocity profiles at different radial distances parallel to the jet axis. The study showed the strengths of combining experimental and computational techniques although as the jet involves a cross flow its applicability is limited in the present research. Birch et al (2005) also used LDA to measure flow statistics of a methane impinging jet at a height of 12.82D above the impinging plate. Their findings indicated anticipated trends based on the previous work of Poreh et al (1967) and Cooper et al (1993). They demonstrate the influence of the plate at the familiar distance of 16% of the jet height, and the steadily increasing fluctuating velocity up until this region. The use of LDA did not permit them to make measurements close enough to the wall to see the sudden drop in wall-normal fluctuations which is seen in Cooper et al (1993) due to the wall dampening effect on the turbulence. Proof of the radial wall jet collapsing into self-similar profiles is
illustrated, indicating no systematic deviation and the lack of buoyancy forces acting on the tracer particles. A slight negative mean velocity above the radial wall jet suggests a recirculation zone has formed. Similar observations were made by Fairweather & Hargrave (2002) as well as an early study by Bradshaw & Love (1961).

The recirculation zone occurs due to the entrainment of the quiescent fluid into the developing jet. Fairweather & Hargrave (2002) followed up on experimental work by Dianat et al (1995) who found a strong recirculation zone in an impinging jet with air. When the domain is confined (i.e. a solid surface located just above the jet nozzle) the fluid is forced to follow the radial entrainment of the fluid towards the jet axis. In the case of an unconfined jet, the recirculation will be significantly weaker as fluid is drawn from above the jet nozzle axially as well as radially. It should also be mentioned that Birch et al (2005) only found a recirculation zone in the air jet due to its significantly higher velocities than in the water jet. The presence of a recirculation zone has an impact on the transport of particles from the outer reaches of the radial wall jet back to the stagnation region and is discussed a little further in the following section.

Geers et al (2004) directed a study comparing PIV and LDA techniques for jet arrays and a single jet. Their results showed that whilst there are some differences between the two measurement methods, they were within reasonable, often excellent, agreement. The critical issue with the PIV measuring technique, is that it is unable to obtain flow statistics close to the wall. The closest Geers et al were able to get to the wall was 0.9mm with PIV whereas the first measuring station for LDA was at 0.1mm. Since most of the interesting flow statistics occur close to the wall, this limits the use of studies which use PIV for the time being.

2.2.2 Multi-phase studies

The literature investigating multi-phase impinging jets is somewhat limited in terms of its usefulness for validating computational models. The majority of these studies focus primarily on heat transfer aspects such as the impact particles have on the heat transfer properties of the jet which is not useful for validating multi-phase models which do not account for heat transfer. Actual flow field data of continuous and particulate phases have scarcely been published as of 2014. It is notoriously difficult to obtain continuous and multi-phase data from complex systems so experimental setups are often based on simplified geometries.

The free jet region in Figure 2.1(a) can be compared with a fully free, turbulent jet that does not impinge on a surface at any height as the influence of the wall only appears to have an effect at
a small distance from the impingement plate. Studies by Hishida et al (1992), Modarress et al (1984), Mostafa & Mongia (1987) and Longmire & Eaton (1992) investigated free jets rather than impinging jets. Their conclusions aligned to state that the rate of entrainment of the surrounding fluid was lowered by the presence of the particles. This implies that the rate of jet spreading is less than that of a jet without particles, which has considerable implications for multi-phase impinging jets. Yoshida et al (1990) also reached this same result with a plane impinging jet and found that the results from the free jet region aligned well with studies of fully free jets. Yoshida et al agreed with earlier authors that this smaller rate of jet spreading was primarily due to the momentum exchange between the particles and the fluid, which ultimately reduced the exchange of momentum with the surrounding, stagnant fluid. The particles were also noted to have a modulating effect on the turbulence by damping the velocity fluctuations in the shear layer between the jet and the stagnant fluid.

The study by Yoshida et al investigated the effects of the particles on the turbulence and vice versa as well as the impact on heat transfer. Using an LDA technique for both phases, Yoshida found that as the fluid slowed as it approached the wall the particles had sufficient inertia to overcome this and rebounded heavily off the wall. In the stagnation region, the presence of the particles has a significant damping effect on the axial velocity. The rebounded particles reach a height of 2.5D off the impingement plate. Such a large rebound caused the particles to pass through the shear layer of the jet and the radial wall jet. Despite the modulating effect particles have in the free jet, near the stagnation region the particles actually augment the turbulence. The reason behind this is due to the velocity difference between fluid and particle being such that turbulence is generated in the wake of the particle. The scale of this interaction is governed by the number of particles, the slip velocity and the velocity vectors of both phases and was investigated by Yuan & Michaelides (1992) and Crowe et al. (1985 & 1995). The streamline curvature in the region of the stagnation point also intensifies the axial velocity fluctuations more so than the radial fluctuations, which leads to an augmentation of the overall turbulent intensity in this region and in the radial wall jet region. This conclusion was found to be in line with the work of Hijikata et al (1982). The presence of particles in the radial wall jet was seen to initially decrease the velocity of the gas phase whilst increasing the turbulent intensities. This is arguably the result of the particles having little or no momentum in the radial direction and therefore being a burden on the flow. At greater radial distances, the profiles indicate a decrease in the turbulent intensities of the gas phase which brings it closer to that of the single-phase data and can be attributed to the attenuation of the gas-solid interactions.

Anderson & Longmire (1995) published a study which built upon the work of Yoshida et al and Longmire & Eaton (1992). However, Anderson & Longmire investigated the effects of forced and unforced jets and particle sizes. They used the Stokes number to characterise the flow
based on particle response time and another based on Kelvin-Helmholtz instabilities. The Stokes number is a dimensionless term to characterise the effect of inertial motion of particles in a fluid flow. Particle dispersion and particle concentration have been shown to be highly dependent on the Stokes number. Using instantaneous images of single- and multi-phase paired with particle distribution plots, the behaviour of the particles was investigated. The formation of vortex rings along the interface between the jet and the surrounding fluid has a profound impact on the distribution of particles in the free jet and the behaviour in the stagnation region. It is worth noting that the authors also mention a number of features that were already covered by Yoshida et al (1990). The intermittent vortex rings forming along the interface 'pinched' the particles towards the centreline. In the space between the rings, the particles expanded to the full width of the developing jet. This effect was more evident for particles of larger sizes, which retain negative radial velocities due to their higher inertia. Since smaller particles have less momentum, they are more likely to follow the streamlines of the flow and thus expand radially with the jet. The residence time of particles as they rebound off the plate in the stagnation zone was shown to vary with Stokes number and be effective up to a height of $h/D = 0.1$. Larger particles have a higher residence time in the stagnation zone as they take longer to accelerate into the radial wall jet, whilst smaller particles are more easily swept away with the continuous phase, thus have a lower residence time. For two particle sizes of the same number density this implies that particles with higher Stokes numbers are more likely to remain in the stagnation zone than those with lower Stokes numbers. Such effects of Stokes number would be interesting to see on a computational basis and would lend itself to assess the sophistication of the model.

A big question concerning particle-laden jets is the behaviour of particles along the impingement wall. In practice, jets are often used to clear sediment beds of particles, hence the interaction between beds of particles and the jet is of interest here, particularly with the industrial relevance discussed in Section 1.1. Particle re-suspension in such flows has recently been reviewed by Ziskind (2006) in an attempt to bring together the models and theories developed over years of studies on the subject. It was found that Reeks & Hall (2001) who proposed the rock ’n roll model of particle detachment was the most widely accepted and sophisticated approach to date. Whilst their experiments used a fully-developed turbulent channel flow, the fundamentals which governed when a particle was re-suspended are applicable to the majority of flow geometries. This model brings together many phenomena including aerodynamic forces (mainly shear stress) acting on the particle (mainly drag) and the adhesive forces of the particle and the surface. Furthermore, the authors also recognised the importance of resonant energy transfer as a result of velocity fluctuations near the particle, although these effects were found to be minimal. Young et al (2006) used a round jet impinging normally on a wall to re-suspend particles. The shear stress imposed by the jet close to the
impingement plate is assumed to be directly related to particle removal at the surface. In a comparison with experimental data from Smedley et al (1999) the shear stress results showed reasonable although not perfect alignment. The study by Smedley et al used particle removal to directly infer shear stress, whilst Young et al measured the shear stress directly. This finding supports the widely accepted model of particle removal due primarily to aerodynamic drag whilst the slight deviation from the earlier set of data indicates that smaller forces are playing a part as well.

Further work regarding sediment erosion is reaching the limits of the scope of the present work, however there is much literature regarding jet optimisation for clearing sediment beds which directly relates to the HAS tanks at Sellafield. Studies by Aderibigbe & Rajaratnam (1996), Qi et al (2000), McArthur et al (2012) and Hunter et al (2013) relate the above fundamental theories to sediment bed erosion using impinging jets by varying properties such as jet heights, Reynolds number, particle properties and fluid. Hunter et al found that the scale at which experiments were conducted had an impact upon the rate of re-suspension due to increased recirculation rates in smaller vessels. This led to a higher rate of sediment erosion and reaching a steady state sooner than in larger vessels. Furthermore, the authors determined an optimum jet height for re-suspension of around \( h/D = 10 \).

### 2.3 Computational studies of turbulent impinging jets

There is currently considerable desire in the research community both academically and industrially to develop numerical codes capable of reliably calculating the transport of mass, momentum and often heat in flow geometries of engineering applications. The equations which are used to calculate these are known as the Navier-Stokes equations and can be solved directly using direct numerical simulation (DNS), filtered and solved using large eddy simulation (LES) or time-averaged and modelling with the Reynolds-averaged Navier-Stokes (RANS) method. There are advantages and disadvantages to each approach and selecting the appropriate technique can almost be as difficult as applying it to the actual flow configuration. There must be consideration for the geometry of the system, the turbulence, the Reynolds number, computational resources and reasonable timescales when using computational fluid dynamics. A brief overview of each of these approaches is given here:

1. RANS approaches are based on time averaging the Navier-Stokes equations which describe the motion of the fluid. This is achieved by splitting the instantaneous velocity statistics into mean and fluctuating components. The process of time averaging results in a loss of information which gives unknown terms in the RANS equations which have
been extensively reviewed by Speziale (1994) and are discussed further in Chapter 3. These unknown terms must be modelled using known quantities in order to close the equation set by using turbulence closure models. There are a number of turbulence models which gives RANS methods quite a large range of options, some better than others, making it equally challenging and important to select the correct turbulence model to solve the flow system under examination. Simple turbulence models are based on the eddy-viscosity hypothesis (Boussinesq, 1877) which relates the Reynolds stresses to mean velocity gradients and a turbulent diffusion coefficient. These two-equation schemes falling into this category remain popular in commercial CFD codes and use in industry due to their robust nature. They are able to give a solution for almost any geometry through simplification of certain terms within the models. As geometries get more complex and the physics within them becomes more distant from the assumptions made, the accuracy of the predictions begins to degrade rapidly. Such models are fairly quick to run on a computational basis as well, making them ideal for ballpark solutions or directing future simulations with more advanced techniques.

More advanced turbulence models such as the Reynolds stress transport models or second moment closures solve the transport equations for the individual Reynolds stresses. Reynolds stress models can be expected to give superior results compared with two-equation models in many geometries although at the cost of computation time and general robustness. Now solving for the Reynolds stresses as well requires solving additional equations. The additional equations concern the generation, dissipation and transport of the Reynolds stresses which provides a better framework for the solution. Such models are able to capture the effects of vortices and secondary flows associated with more complex geometries. However, these models can be less robust than the two-equation approach; therefore better initial conditions are needed and control at the boundaries of the computational domain.

(2) DNS simulates the instantaneous turbulent structure with no empirical modelling of the turbulence at all. This requires all scales of the turbulence to be resolved in the computational mesh using the Navier-Stokes equations. The absence of turbulence closure models removes the problems associated with turbulent assumptions and averaging techniques used in RANS methods. As a result of this DNS usually provides highly accurate solutions providing the geometry is compatible with DNS. As all scales are resolved directly, the computational demand is considerably higher than any other approach. Even for simple flows, the range of Reynolds numbers is limited by the computational requirements of the simulation and the computational power at hand. At higher Reynolds numbers the range of instantaneous scales rapidly increases, which
dramatically increases the computational demand. DNS is rarely utilised in industrial applications due to its computational expense and extremely long run times making it impractical for use. Solution stability is also an issue with DNS. However, it is very useful for validation purposes and can enable us to look at variables in geometries which cannot be accessed by experimental methods.

(3) LES is a compromise between RANS and DNS which resolves the larger scales of turbulence directly using spatially filtered Navier-Stokes equations on a suitably refined computational mesh whilst modelling the smaller scale turbulent eddies that fall below the Kolmogorov scale (Piomelli & Baaras, 2002) using a simple turbulence model. The Kolmogorov scale is a measure of the smallest eddies present in high-Reynolds-number flows. The assumption that the smaller scale turbulent eddies have an isotropic effect of turbulence whilst the larger scales are anisotropic is much closer to reality than that used in RANS, thus excellent agreement with physical data is achievable with LES. The cut-off point for resolved turbulence is determined by a filtering function. Scales which fall below this point are modelled using a sub-grid scale model, of which there is a range. A review of SGS models can be found in Vreman et al (1995). In comparison with the previously discussed approaches, LES has the advantages of DNS in being able to compute the instantaneous velocity field without the huge computational cost of DNS. Whilst RANS remains quicker and less computationally demanding than LES, LES resolves large scale turbulence directly – as in DNS. As DNS resolves all scales of turbulence it has significantly longer runtimes than LES for the sake of resolving the smaller scales which can arguably be considered less important. LES then provides an in-between approach capable of resolving key turbulence structures (turbulent eddies) whilst not as computationally demanding as DNS. The BOFFIN code originally started as a RANS based code and was later converted to LES by di Mare & Jones (2003). More details concerning BOFFIN can be found in Chapter 3.

Whilst DNS provides what should be an ideal predictive tool for fluid flow, the computational intensity of the calculation renders it fairly useless on a day-to-day basis for engineering applications. However, computational advancement has certainly put LES predictions within reach of many users of CFD, as such LES now features as an option in Ansys Fluent (Ansys Fluent Theory Guide, 2010). However, for the foreseeable future, the dominant approach is most likely to be RANS methods, due to their being widely implemented in commercial codes, their ease of use and robustness fit well within the requirements of industry.

The majority of the literature is focused around RANS methods on the basis that they are commonly used in industry. Improvements that can be made to RANS techniques therefore
translate directly into improvements for industry (Kendil et al, 2011). This is illustrated when one considers the number of developments for two-equation or second-moment closure models in the literature. Consider the original two-equation model by Jones & Launder (1972) developed at Imperial College, London. This turbulence model was designed for simple shear flows and therefore struggled to accurately predict reasonable flow patterns in more complex systems. The model has seen dramatic development and hundreds of different versions now exist, although some of these still struggle in anything other than shear dominated flows. Some of these have been incorporated into the STREAM code developed at the University of Manchester by Lien & Leschziner (1994). Whilst retaining the two-equation framework, a number of non-linear stress-strain relationships have also been proposed, to deal better with complex strain fields including streamline curvature, and these are discussed in further detail in the upcoming sections.

2.3.1 Single-phase studies

Considerable research is being directed towards the development of reliable methods for simulating and modelling fluid transport. Industrial users of CFD often find themselves limited with simple, robust models contained within commercial CFD packages. Design and optimisation of process equipment requires confidence in both experimental and computational data that is used to justify design changes and features, particularly in the nuclear industry. Academic research of CFD has advanced much further than the commonly used methods in industry, using DNS and LES methods. Historically, these methods have been out of reach for day-to-day use in engineering applications due to their complex setup conditions, computational intensity and extended run-times. Whilst these limitations still largely apply to DNS methods, LES has drawn closer to industrial use and is even available within Ansys Fluent in some capacity. Despite the potential for LES use in engineering applications and its advantages over time-averaged approaches, RANS modelling is still the favoured and most popular approach to industrial users. This highlights the importance to continue development of RANS methods alongside LES and provide as many simulation and modelling options for design and optimisation purposes as possible.

One of the most basic forms of RANS modelling is the $k-e$ two-equation model developed by Jones & Launder (1972). This model linearly relates the Reynolds stress tensors to the mean strain rate tensor by way of the eddy viscosity hypothesis (Boussinesq, 1877). An additional two transport equations are solved to represent the transport of the turbulent properties of the flow alongside the time-averaged versions of the Navier-Stokes equations. The turbulent
kinetic energy, $k$, and its rate of dissipation, $\varepsilon$, are obtained by solving these two equations. The linear stress-strain relation is normally the major problem when predicting moderately complex systems. Also the equations of $k$ and $\varepsilon$ can occasionally result in poor predictions. The two-equation model has been shown by Craft et al (1993), Dianat et al (1996) and Wang et al (2014) to perform poorly in impinging jet geometries when validated against experimental data. Eddy-viscosity models are designed around obtaining the correct shear stresses in a simple shear flow, which does not always give the correct normal stresses. In simple shear flows such as a straight pipe, this result is not unreasonable. In slightly more complex flows more likely encountered in practice when stresses are no longer predominantly in one direction the error in the normal stresses becomes significantly greater and presents major problems. Impinging jets are such a flow type where isotropy cannot be assumed. Bradshaw (1987) stated that the failure of the eddy-viscosity was due to its form rather than its applicability. Pope (1978) claims that the non-linear variation for the eddy viscosity improves the ability of the model to capture normal stress anisotropy, insensitivity to secondary strains and excessive generation of turbulence in regions of streamline curvature. Hence, this move towards more physically realistic stresses reduces the need for realisability.

Craft et al (1993) concluded that the reason behind the over-prediction of the turbulent velocity fluctuations in the stagnation region was due to the linear nature of the eddy viscosity hypothesis, being applied to a region of boundary-induced streamline curvature. The problem had been highlighted much earlier by Lumley (1978) who said that the linear correlation of mean rate of strain through the eddy-viscosity was insufficient and must be made non-linear. Since then, many non-linear (quadratic and cubic) two-equation models have been developed. Apsley & Leschziner (1998), Shih et al (1995), Suga et al (1995) are notable examples who saw improvements over the standard ‘linear’ $k$-$\varepsilon$ turbulence models. The non-linear formulation of the stress-strain correlation has notable advantages when applied to non-homogeneous flows. Using an impinging jet flow Suga et al (1995) show improvement of the model over the Launder & Sharma (1974) model in the stagnation region, however the models eventually coincide with each other in the outer regions of the radial wall jet (where both agree well with experimental data). The dramatic over prediction of the velocity fluctuations in the stagnation region are not seen in the non-linear version of the model. The limited applicability of some of the non-linear $k$-$\varepsilon$ models has been motivation for authors such as Suga et al (1995) to develop a cubic stress-strain relation which was applicable to a wider range of flows.

Another improvement to the $k$-$\varepsilon$ model was made by Shih et al (1995) who developed a realisable Reynolds stress algebraic equation model in which the viscosity coefficient, $C_\mu$, was not constant. This was implemented in their $k$-$\varepsilon$ model (Shih et al, 1995) which has also been shown to provide more physically realistic results than standard $k$-$\varepsilon$ models. The realisable
model uses a variable $C_p$ proposed by Reynolds (1987) rather than a constant value which avoids the possibility of unphysical (negative) values for the normal stresses when certain conditions are met. Verification and validation studies against existing models and experimental data show the realizability of the $k$-$\varepsilon$ model to improve predictive capabilities of the model. The specifics of this model are discussed further in Chapter 3 as it is one of the models used for comparison in the current research.

Jones & Ledin (1990) stated that the first step towards representing the essential features of turbulence is the second-moment closure methods. These consist of the algebraic stress models (ASM) and the Reynolds stress turbulence models (RSTM). The ASM is an intermediate approach which has not been used in the present work. For additional information see Rodi (1976) and Versteeg & Malalasekera (1995). The RSTM approach determines the Reynolds stresses by solving transport equations for the stresses themselves and the turbulent energy dissipation rate, thus shifting the modelling task to unknown higher-order correlations. This is the first step to describing the anisotropy of turbulence through the Reynolds stresses and moving away from the eddy-viscosity assumption. The next step might then be considered how the pressure-strain correlation term is modelled. As this term has a significant impact on almost all turbulent flows it is pivotal to good predictions of turbulent flows when the RSTM approach is used. Early progress was made by Launder et al (1975), with later models and developments appearing from Lumley (1978), Jones & Musonge (1988) and Craft & Launder (1992). The latter model by Craft & Launder was developed with impinging jets specifically in mind. Their addition of a wall reflection term addressed the redistribution of stresses normal to the wall into the radial direction. This modification improved the model’s capability for predicting the normal stresses in the stagnation region showing good comparisons against experimental data. This study is considered in more detail later. The model retained a linear pressure-strain correlation which is known to perform well in plane homogeneous turbulent flows but less so in regions of high anisotropy (Lumley, 1978). Jones & Musonge (1988) adopted a linear model in terms of the Reynolds stress equations to formulate a closure approximation for the fluctuating velocity-pressure gradient correlation. The model is capable of simulating high-Reynolds-number homogeneous flows provided they are far from a wall. Their study shows strong alignment with most experimental data indicating good agreement with such flows, however, the authors also concede that additional closure approximations representing the transport of the Reynolds stresses and scalar fluxes must be added should anisotropic flows be investigated. The model has been developed further by authors such as Durbin (1993a & 1993b), So et al (1994) and Dianat et al (1996a). Dianat et al amongst others acknowledged that wall bounded flows and anisotropic turbulence are very common in engineering applications, which limits the applicability of the model by Jones & Musonge.
Speziale et al (1991) argue that complex nonlinearities involving the anisotropy tensor add very little to the modelling of the pressure-strain correlation, thus the improvement is minimal. They developed a dynamic model termed the SSG model which is linear in the mean velocity gradients with coefficients that are functions of the anisotropy tensor. This has the advantage of retaining a simple, generic model for plane, homogenous, turbulence allowing for the determination of empirical constants based on calibrations with experiments, yet using a non-linear quadratic approach in regions of anisotropic turbulence. This model was shown by the authors to outperform that of Launder et al (1975) for a variety of homogenous turbulent shear flows and the decay of isotropic turbulence.

Dianat et al (1996a) further developed the turbulence closure by Jones & Musonge (1988) to encompass flows influenced by a wall whilst retaining its capability for handling high-Reynolds-number flows. The presence of a wall results in pressure reflections back into the body of the flow which distort the fluctuating pressure field and thus influence the rest of the flow. The introduction of this wall reflection term essentially dampens the stresses normal to the wall but does not affect the predicted shear stresses. The authors validated their predictions against experimental data of an impinging jet flow and verified their modifications against the original turbulence model. The r.m.s fluctuating velocities were dramatically over-predicted in the stagnation region for the original model. The use of the wall reflection model improved the alignment with experimental data, significantly in the stagnation region as the wall-normal stresses were being correctly dampened. Further away from the stagnation region where the principal turbulence generator changes from normal straining to shear, there was little difference between the model predictions as should be expected.

Craft et al (1993) used a standard $k$-$\varepsilon$ model and three RSTM’s of varying complexity to predict an impinging jet based on the experimental setup of Cooper et al (1993). The predicted data was normalised using the bulk velocity and compared to identical data from the experiment to validate each model and determine which models failed to achieve good to strong alignment. The $k$-$\varepsilon$ model was that of Launder & Sharma (1974) and was used to provide a baseline for the RSTM comparisons. The first RSTM was developed by Gibson & Launder (1978) and features a basic linear stress-strain correlation. The remaining two RSTM were developments of the authors through research at UMIST over a prolonged period (Craft & Launder, 1992). The third introduced the wall-reflection term which was discussed previously. The modification dampened wall-normal velocity fluctuations and redistributed these radially. The fourth was developed with a more complex formulation of the pressure-strain correlation. Reynolds numbers considered were 23,000 and 70,000 for jet heights of 2 and 6D respectively. The results indicated that the $k$-$\varepsilon$ model and the more basic Reynolds stress model led to an over-prediction of the turbulence levels near the stagnation point. This being the most complex part
of the flow, this is not surprising. The turbulent statistics at further radial distances from the centreline were also found to show poor agreement with experimental data, mostly assumed to be the result of the very poor predictions upstream. The two RSTM’s which had been developed over a number of years at Manchester University showed that accounting more accurately for the wall effects greatly improved alignment of the turbulence statistics with experimental data, although less so for the fourth RSTM. It was suggested that the modified pressure-strain correlation would improve predictions in the stagnation region but degrade the solution in the radial wall jet where the flow has become a wall-bounded shear flow. However, with better predictions in the stagnation region one can expect better predictions downstream within the radial wall jet which is illustrated in the validation plots.

Wang et al (2014) provided a comparison paper of a huge range of turbulence models using a turbulent jet and a set of experimental studies by Ashforth-Frost & Jambunathan (1994) to provide data for validation. A host of two-equation models, including $k$-$\varepsilon$ and $k$-$\omega$, and second moment closures were used to simulate a confined impinging jet. The shear stress transport (SST) $k$-$\omega$ model (Wilcox, 1998 and Menter, 1994) solves transport equations for $k$ and the specific dissipation rate, $\omega$. The solutions from each of the turbulence models were compared at various radial distances and validated with available experimental data. In some instances it was found that the second-moment closures were actually inferior to the SST $k$-$\omega$ model which is surprising given the advantages concerning anisotropy the RSTM has. Various wall treatments from Ansys Fluent were compared. Standard, scalable, non-equilibrium and enhanced wall treatments were used. Detail on these is given in Chapter 3. The authors found that when an enhanced wall treatment was used with the $k$-$\varepsilon$ model, agreement with experimental data was much better than with other wall treatment methods, although little discussion is given as to why this might be the case. The study by Wang et al highlights what the present work is hoping to achieve: a comparison of available turbulence models (albeit fewer) with more focus on the fundamental physics of each model and why certain models perform better than others. Furthermore, the introduction of particles into an impinging flow stretches the available methods of industry quite thin when compared to academic methods.

Rhea et al (2009) have modelled a plane impinging jet at a practical Reynolds number which coincides with the experimental conditions of Yoshida et al (1990). Both RANS and LES approaches were used and validated against the experimental data. The second moment closure of Dianat et al (1996a & 1996b) was used prior to an LES code using a sub-grid scale model based on the dynamic model of Germano et al (1991). Both approaches yielded good alignment with experimental data, however uncertain inlet conditions and questionable measurement techniques lead to questions over whether the simulation and experiments were ‘like-for-like’. The wall reflection term within the RANS code was shown to produce under-predicted values
for the turbulent velocity fluctuations and shear stresses. The study by Dianat et al (1996a) used the same code, though with a round jet. The fundamental differences between these configurations are sufficient to expect differing behaviour in the stagnation and radial wall jet regions, as has already been discussed at the start of this chapter. Thus, the performance of the RANS model suggests that a modified wall reflection term might be required to account for non-axisymmetric jets. The LES slightly under-predicted the turbulent quantities to a lesser extent although this may be due to the previously mentioned doubts regarding the validation data. Either way, the study serves to illustrate the strength of LES over the RANS approach particularly in geometries where turbulence is highly anisotropic and large eddy structures dominate.

A lesser used model was applied recently by Kubacki, Rockicki & Dick (2011) who investigated the fluid flow and heat transfer of a round impinging jet for several combinations of jet heights and Reynolds numbers using a newly developed $k-\omega$ model by Wilcox et al. (2008) and a number of RANS/LES hybrid models. The simulations were compared with experimental data. For small jet heights and Reynolds numbers, the mean velocity profiles were well predicted by all models, however the fluctuating velocities were only well predicted for the RANS/LES hybrid models. The $k-\omega$ model was reported to over-predict the fluctuating velocity magnitude in the stagnation region and at larger jet heights and Reynolds numbers show inaccurate predictions due to the mixing in the shear layers between the jet and ambient fluid. It was concluded that many of the downfalls of the $k-\omega$ models could be overcome with the hybrid equivalent models if the grid was sufficiently fine to resolve the breakup of the vortices in the shear layers of the jet. The resolution of the grid was also found to be of highest importance in studies by Hadžiabdić & Hanjalić (2008) who used LES to simulate impinging jet flows.

Hadžiabdić & Hanjalić (2008) performed a host of sensitivity studies looking at the impact of grid resolution, boundary conditions, initial conditions and sub-grid-scale models. Of particular interest was their investigation into the impact of the upper boundary conditions surrounding the impinging jet nozzle. The most awkward to define is the entrainment boundary condition. This condition maintains a constant pressure and enables fluid to enter or leave based on the local flow conditions inside the domain. A successful entrainment boundary is one in which it has very little impact on the flow field of interest. The authors looked at a fixed inlet boundary, convective outflow and entrainment boundary and found that as long as the boundary was offset from the entrance of the pipe by approximately half the pipe diameter it had very little effect on the stagnation zone and radial wall jet. The downside of this is the additional nodes that are required above the jet nozzle which are essentially wasted grid nodes. There were noticeable differences in the flow patterns of the quiescent fluid surrounding the jet however with the most intuitive representation of the experimental conditions being represented by the entrainment...
boundary. Boersma (2000) studied different types of entrainment boundary and determined that for free shear flows a pressure boundary was superior to the simple no slip and free slip boundaries when compared with experimental data from Schlichting (1979). Hadziabdic & Hanjlic also considered the instantaneous profiles of the jet. They discussed the presence of Kelvin-Helmholtz type instabilities which lead to vortex rings along the shear layer between the jet and the ambient fluid. Such turbulent structures are discussed in great detail by Yule (1978) for round, free jets. These rings are convected along the jet where they coalesce with other rings and gradually lose their structural coherence. These structures contribute to the growth rate of the shear layer of the developing jet as it entrains more surrounding fluid, leading to the decay of the potential core. In the stagnation region, the now large scale eddy structures resulting from the vortex rings impinge on the surface. The significance of the impact of these structures on the surface is extremely relevant to heat transfer and multi-phase flows and is discussed further in the following section.

2.3.2 Multi-phase studies

Recent advances in computational approaches for multi-phase systems have led to an overall improvement in the capabilities of modelling multi-phase flows commonly found in industrial applications. An impressive number of systems contain multi-phase flows which might benefit from such improved computational models for multi-phase flows. The use of CFD is now at such a stage which makes it indispensable to design and optimisation of process equipment, therefore understanding and improvement of the available models and techniques is very important. To gain an appreciation of what constitutes a multi-phase flow, Crowe et al (1995) amongst others have published the conditions for different types of systems which include dilute gas-particle flows, sludges, bubble flows etc… Furthermore, different modelling techniques are best suited to different types of multi-phase flow. The main two techniques the current review is concerned with are Eulerian-Eulerian and Eulerian-Lagrangian approaches. Essential to these techniques are the different approaches of handling the particles which are mainly selected based on the types of systems mentioned by Crowe et al (1995). A series of studies by Mostafa & Mongia (1987, 1988) compared Eulerian-Eulerian and Eulerian-Lagrangian methods in a spray geometry. The authors found that the Eulerian-Lagrangian model generally performed well throughout, whilst the Eulerian-Eulerian did well under certain flow conditions. This highlights the importance of selecting the correct method for modelling certain multi-phase systems.
The handling of particles can be conducted using one, two or four-way coupling. In one-way coupling the continuous phase exerts force on to the particle as it moves through the flow field and no opposing interaction is considered on the continuous phase. In two-way coupling, the resultant particle motion is used to influence the surrounding continuous phase by adding source terms to the governing equations for the continuous phase. One-way and two-way coupling requires more information about the particle kinetic equilibrium to determine which method is appropriate or necessary in any particular case. The Kolmogorov scale is used to determine whether a particular particle size will have an impact on the fluid. For instance, if the particle characteristics are much smaller than the Kolmogorov scale the influence on the continuous phase is considered negligible. However, even in situations where this condition is not met Gouesbet & Berlemont (1999) have shown the influence of the particle on the fluid can sometimes be neglected and still provide predictions without negative effects, though this is limited to certain materials and geometries. Four-way coupling is essentially the same as two-way coupling but also considers particle-particle interactions; in particularly dilute flows the use of four-way coupling can be avoided, Loth (2000).

There are a number of studies which focus on multi-phase impinging jets, however very few provide turbulence statistics for the continuous phase and multi-phase against which to validate our models. This was highlighted in the experimental section of this chapter due to the difficulty in measuring simultaneous phases. More will be discussed on the fundamentals of the two main approaches to computational multi-phase flows and relevant studies using them with turbulent jets.

The Eulerian-Eulerian technique treats both phases as a continuum and is therefore often known as the “continuum model”. Both phases are solved on a fixed computational domain thus, have the same reference frame. The basis of this approach assumes that phases are in, or close to, kinetic equilibrium with each other and that the relative velocities are somewhat similar. The Eulerian-Eulerian technique allows for systems with a large mass fraction whilst numerical simplicity allows for quick computation times (Sivier et al, 1996). Eulerian models enable both phases to use a consistent discretisation scheme which benefits two-way coupling models. However, this requires the use of a dispersion tensor which may limit the models applicability to certain systems and materials (Faeth, 1987). The most common Eulerian model is the “two-fluid” which was reviewed for a number of complex geometries by Lahey & Drew (2001). The model requires a variable or mechanism in the transport equation for particle number density to account for turbulent dispersion. This model was also used for a free turbulent jet by Lopez de Bertodano (1998) with the Launder & Spaulding (1974) k-ε turbulence model and validated against experimental data from Bulzan et al (1987) and Laats & Frishman (1970) the conditions of which were a close match to the initial conditions of the two-fluid model. The two-fluid
model assumes a very high mass fraction. The authors investigated the effect of the various
turbulent dispersive terms in the model and the impact on the solution with and without them.
These terms included Reynolds stresses, turbulent diffusion and turbophoresis, the latter of
which describes the migration of particles from areas of high turbulence to low turbulence.
Since the turbulence in jets is decidedly not homogeneous this term ought to have a significant
impact on the dispersion of the particles. The authors show that turbophoresis has an effect in
areas where there is a turbulence gradient, however the Reynolds stresses are found to be the
dominant mechanism on the distribution of particles. It should also be noted that the use of a
two-equation model for the continuous phase is also likely to provide inaccuracies due to the
anisotropic nature of the turbulent jet, inaccuracies which will be inherited by the particles. A
more recent study by Kartushinsky et al (2014) used a similar method and compared the impact
of high/low particle concentration with high/low densities on the characteristics of the
continuous phase. The turbulent mechanisms included in this model were more numerous than
previous studies and include the effects of turbulent wakes from larger particles and the
modulating effects of smaller particles. The authors found that for higher particle loading the jet
had a lower rate of spreading which was in alignment with experimental data from Crowe
(2000) and Michaelides (2006). They concluded that this was due to the modulating effect of
particles on the velocity fluctuations being augmented by the presence of more particles.
Specifically concerning wakes, smaller particles are shown to concentrate within large scale
turbulence structure such as vortices produced from wakes or jets entering stagnant fluid. Their
relative velocity gradually decreases as the distance from the centre of such structures is
increased. Larger particles however, tend to only occupy the outer region of these vortices and
possess a significant radial component when entering the core region of these structures.
Therefore, through centrifugal forces, these structures produce a significant dispersion of larger
particles and tend to trap smaller particles until they dissipate.

The Eulerian-Lagrangian technique treats the continuous phase in an Eulerian manner, whilst
solving the equations of motion for individual point particles on a moving frame of reference.
This implies that a frame of reference moves with the particle through the stationary frame of
reference occupied by the continuous phase. Typically, the Eulerian-Lagrangian approach is
limited to dilute particulate systems, although exceptions do exist (Apte et al, 2003).
Furthermore, estimation errors can be incurred if inappropriate assumptions are made regarding
particle motion through the continuous phase (Fox, 2012 and Subramaniam, 2013). Some
numerical simplification can be achieved by adopting the point-volume formulation in which
the particle characteristics such as mass, heat transfer and surface stresses are condensed and
averaged across the particle and represented by a single point. Alternatively, the resolved-
volume formation can be used which considers the actual boundary of the particle and the
resultant wake of the particle in the flow. This method is usually limited to a low to moderate
number of particles due to the necessity for describing the spatial and temporal scales associated with the movement of the particle through the flow. The computational requirement for this method to accurately represent real engineering flows with typical mass fractions would be extreme to say the least. A real weakness of the Lagrangian model was highlighted by Fox (2012) in a review of Eulerian-Lagrangian methods stating the approximations involved in the calculation of the particle motion can lead to errors. If the movement of the particles are coupled to the fluid, the erroneous particle behaviour will be transferred to the fluid phase degrading the accuracy of the solution even further. This statistical error was actually illustrated by Passalacqua & Fox (2013). Loth (2000) suggests using LES to simulate the fluid will be beneficial as it will capture the large scale turbulence structures which realistically influence the behaviour of the particles which an averaged solution might not capture. Armenio et al (1999) and Miller & Bellan (2000) investigated the sensitivity of particle behaviour to the SGS model and found that incorrect representation of the SGS stresses and velocity fluctuations led to serious inaccuracies. This is in-line with Boivin et al (2000) who states that due to this sensitivity, such studies must be substantiated against experimental or DNS data. Almeida & Jaberi (2008) conducted a study which evaluated the overall performance of a particle-laden turbulent round jet using LES using a Lagrangian method. Their results were compared against some limited data obtained from an experimental study by Gillandt et al (2001) and showed that alignment was very poor when the SGS model was neglected and a representative particle size distribution was not used. Further analysis using the LES gave anticipated results for different particle sizes based on the theories already discussed in the experimental section on multi-phase studies. This suggests that with two-way coupling and correct representation of the SGS stresses, particle-laden jets can be simulated accurately. Breuer & Alletto (2012) conducted a study using LES with two and four-way coupling to handle higher particle loaded systems for a turbulent combustion jet. They chose to use LES due to its capability to simulate turbulent eddies which results in a much more realistic continuous phase that the particles can interact with.

The particle kinetic equilibrium is represented by the Stokes number. The definition of Stokes number can vary dependent upon the ratio which correctly represents the type of flow in question. For instance, Eq. (2.1) is the typical definition of Stokes number with regards to the particle response time and the local fluid integral time scale:

\[ St = \frac{\tau_p U_b}{D} \]  

where \( D \) is the pipe or jet nozzle diameter, \( U_b \) is the bulk velocity. The fluid response time, \( \tau_p \), represents the time taken for the particle to respond to specified level of an instantaneous velocity fluctuation.
The response time is defined as Eq (2.2):

\[ \tau_p = \frac{\rho_p d_p^2}{18 \mu} \]  (2.2)

where \( \rho_p \) is the particle density, \( d_p \) is the diameter of the particle and \( \mu \) is the viscosity of the continuous phase. In summary, a small Stokes number represents a particle which is more likely to follow the streamlines of the continuous phase; when particularly low Stokes numbers are experienced, the particle will almost act as a tracer for the flow. High mass loadings of particles with smaller Stokes number have a significant influence on the flow through turbulence modulation and velocity fluctuation dampening compared to single-phase flow. Using DNS predictions, Squires & Eaton (1991) showed particles with smaller Stokes numbers tended to move towards regions of high strain rate. According to Balachandar & Eaton (2010) the Eulerian-Eulerian approach is best suited in this case. For higher Stokes numbers, the nature of the particle is such that turbulent structures are unlikely to influence the particle trajectory by much. Larger particles tend to ignore the streamlines of the fluid and have little effect on the turbulence unless their relative velocities are large. In this event, large particles can leave a wake behind them which actually results in an augmentation of the turbulence (Loth, 2000 and Crowe, 2000). Furthermore, the Stokes number also gives an indication of the turbulent dispersion of the particle as a higher Stokes number is less likely to result in a well dispersed multi-phase system.

The treatment of particles at walls is an area of difficulty in CFD due to the number of variables involved in influencing the outcome. Particle interaction at the wall is governed by hydrodynamic forces and collision forces. The former constitutes a function of the fluid and particle distance to the wall concerning pressure effects and velocity gradients. Collision forces are the forces involved in the contact of the particle on the surface. The coefficient of restitution, \( C_R \), is an empirical correlation between incident and resultant particle velocity and angle. A correlation can be empirically developed to determine the resultant velocity and trajectory of a particle material ‘a’ colliding with a surface of material ‘b’. The correlations are a function of density, smoothness and elasticity, however through empirical methods one can obtain a relationship between the incident angle and velocity to provide the \( C_R \). Whilst there may be other variables that influence the resultant normal and tangential velocity as a particle rebounds off a wall, the empirical data attempts to capture this within the coefficients that it produces, similar to the argument of Odar & Hamilton (1964). One particular study by Grant & Tabakoff (1975) provided a fairly standard correlation for glass particles impacting on a stainless steel surface resulting in a \( C_R \) defined as Eq. (2.3):
\[ C_{R,n} = \frac{U_{al}}{U_{a2}} = 1.0 - 0.4159\alpha_1 + 0.4994\alpha_1^2 - 0.292\alpha_1^3 \]
\[ C_{R,t} = \frac{U_{al}}{U_{a2}} = 1.0 - 2.12\alpha_1 + 3.0775\alpha_1^2 - 1.1\alpha_1^3 \]  \hspace{1cm} (2.3)

where \( C_{R,n} \) denotes the coefficient in the wall normal direction and \( C_{R,t} \) is the wall parallel direction. \( \alpha_1 \) is the incident angle of the particle on the wall. This has been successfully applied in the past by Njobuenwu et al (2012) for simulations involving particle interactions with a wall in a channel flow and should be suitable for the present work.

When considering four-way coupling, particle reflections become particularly significant. Rychkov & Milosheivich (1998) performed numerical studies looking at particle density distribution in an impinging jet with and without consideration of reflected particles. The resultant distribution clearly showed that particles reflecting off the surface heavily influenced particles within the stagnation zone, creating a particle density much closer to the impingement plate. The authors also found in two-way coupled studies that particles >10\( \mu \)m had negligible effect on the continuous phase. Further work regarding particle behaviour at the wall was conducted by Ziskind et al (2002a & 2002b) who looked at modelling particle re-suspension using the previously discussed empirical models by Reeks & Hall (2001). They found that particle re-suspension could be improved by pulsation of jets, a conclusion which was shared by Tsubokura et al (2003) and potentially poses an avenue for future work.
3.1 Fundamentals of fluid-phase modelling

Prior to discussing the specifics of the methodologies used in the present research, a brief overview of the governing equations of computational fluid dynamics is provided, along with some fundamental assumptions that must be made in order to solve them. The governing equations of fluid dynamics represent long-established statements based on the conservation laws of physics. These include the conservation of mass, momentum (Newton’s second law) and energy (first law of thermodynamics). They are generally known as the Navier-Stokes equations after George Stokes and Louis Navier derived them.

The conservation of mass can be derived by considering a control volume. The net mass flow rate across all surfaces of this control volume must result in the rate of accumulation of mass. For a compressible or incompressible fluid, Eq. (3.1) shows the changes in the flowrate of mass in written in Cartesian tensor notation where the first term represents the rate of accumulation of mass.

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

(3.1)

The momentum and energy conservation laws concern the changes of properties for a fluid particle over time, \( t \). Newton’s second law states that the rate of change of momentum of an object (in this case the fluid particle) is equal to the sum of the forces acting upon it. This is expressed as Eq. (3.2) for the \( i \)-component with a compressible fluid.

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_i)}{\partial x_i} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ii}}{\partial x_i} + S_{Mi}
\]

(3.2)

Forces acting upon the fluid particle are primarily pressure and viscous forces, however additional body forces, \( S_{Mi} \), such as gravity or centrifugal forces can also be included when situations arise in which they are necessary. In Eq. (3.2) subscript \( l \) represents the dummy summation index.
For completeness the energy equation is derived from the first law of thermodynamics which states that the rate of change of internal energy of a fluid particle is equal to the rate of heat addition (or subtraction depending on the temperature gradient) plus the rate of work done on the fluid particle. The heat flux through a fluid particle is three dimensional (x, y and z). The net rate of heat transfer in each dimension is considered to be the rate of heat into the $x_i$ face and out of the $x_{i+1}$ face. The rate of work done on the object is equal to the product of the surface force and the velocity component perpendicular to the plane in question. Overall, the energy equation is expressed as Eq. (3.3):

$$
\frac{\partial}{\partial t} (\rho e) + \frac{\partial}{\partial x_j} (\rho u_j e) = -p \frac{\partial u_j}{\partial x_j} + \frac{\partial}{\partial x_j} \left( k \frac{\partial T}{\partial x_j} \right) + \tau_{ij} \frac{\partial u_i}{\partial x_j} + S_E
$$

(3.3)

where $e$ is the total energy and $T$ is the temperature. For incompressible flows the energy equation is primarily of interest when heat transfer situations are being considered. As stated throughout Chapter 2, heat transfer properties are not considered in the present research and therefore the energy equation is of little further interest.

The governing equations describe the evolution of the instantaneous quantities of fluid motion. They contain terms such as the viscous stresses, $\tau_{ij}$, which are defined as Eq. (3.4):

$$
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \text{div} \, u \delta_{ij}
$$

(3.4)

The stress terms are substituted into Eq. (3.2) and (3.3) to form the full versions of the Navier-Stokes equations. Solving these equations for turbulent flows is extremely computationally demanding and remains impractical for most engineering applications. Engineering practices required a method in which such flows can be modelled in a shorter time frame. The Reynolds-Averaged Navier-Stokes (RANS) equations are time averaged versions of Eq. (3.1), (3.2) and (3.3), because they do not solve the instantaneous turbulence values and small scale turbulence structures in space or time. Despite significant computational developments in the last three decades and it is still largely impractical to model turbulent flows directly from the Navier-Stokes equations, hence why RANS is still heavily relied upon in industry.
3.1.1 Time-averaging the Navier-Stokes equations

The basis of the Reynolds Averaged Navier-Stokes (RANS) equations is to develop a time averaged set of equations to define the flow. By time-averaging we are reducing the computational requirements of both memory and time-related limitations to reach converged solutions. This is achieved by breaking a flow property, \( \varphi \), down into a mean, \( \overline{\varphi} \), and a fluctuating component, \( \varphi' \), yielding Eq. (3.5):

\[
\varphi = \overline{\varphi} + \varphi'
\]

The statistical mean of the flow property is defined by Eq. (3.6):

\[
\overline{\varphi} = \lim_{\Delta t \to \infty} \frac{1}{\Delta t} \int_{t}^{t+\Delta t} \varphi(t) \, dt
\]

The averaging period, \( \Delta t \), must be significantly greater than the timescale associated with the largest velocity fluctuation and averaged over a reasonably long time. The time average of the fluctuations is by definition equal to zero. In order to gain statistical information on the size of the fluctuations, and through this the scale of the turbulence, the root-mean-square (r.m.s) of the fluctuations is used:

\[
\varphi_{rms} = \sqrt{\langle \varphi'^2 \rangle}
\]

The kinetic energy, \( k \), associated with the turbulent velocity fluctuations is defined by Eq. (3.8):

\[
k = \frac{1}{2} (u'^2 + v'^2 + w'^2)
\]

These definitions can be used to develop some rules discussed by Versteeg & Malalasekera (1995). Following these rules we arrive with the time-averaged versions of the continuity equation – Eq. (3.9) and the momentum equations – Eq. (3.10):

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

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u_i}{\partial x_j} - \rho u_i u_j \right) + S_{vi}
\]

The process of time averaging removes information concerning the state of the flow and the instantaneous velocity fluctuations. Therefore we now have unknown terms in the equation set.
which must be modelled in order to close the equations and allow us to solve it. Turbulence models are used to close the RANS equations by modelling the additional Reynolds stress terms, $\rho u' u'$. 

With the RANS equations in place the next step is to look into the ways in which these equations are solved in the present research. There are a number of different approaches to these equations, and several are investigated in the present work. Ranging from basic models to complex simulation techniques, the research here hopes to investigate the performance of different methods for predicting impinging jet flows with the underlying fundamentals as stated above.

### 3.2 Fluent RANS

To begin a comparison between academic fluid dynamic codes and industrial modelling methods, appropriate commercial CFD software had to be chosen. Ansys Workbench is a commercial package widely used in industry and contains the Ansys Fluent CFD code. National Nuclear Laboratory among many others rely heavily on Ansys Fluent in their simulation and modelling work and therefore it seems logical that Fluent represents commercial software in the current research.

Within Ansys Fluent there are a number of turbulence models and simulation approaches that one may take. They range from very basic, laminar models to somewhat complex and intricate simulation techniques. In order to obtain a good coverage of the RANS methods that Fluent offers, three turbulence models have been selected based on their complexity and ability to handle impinging flows. Firstly, a realisable $k-\varepsilon$ two-equation model has been chosen as a foundation for the work. This basic turbulence model is very often applied to industrial applications due to its robustness and rapid computation time. It also provides a good starting point as the most basic turbulence model within the present work. The second and third turbulence models investigated with Fluent are Reynolds stress turbulence models (RSTM) with respective linear and non-linear variations to the pressure-strain correlation. These models contain an additional five transport equations for flows modelled in 2D and seven for 3D flows. Calculation of the individual stresses allows RSTM’s to better accommodate streamline curvature, swirling flows and rapid changes in strain rate.
It is anticipated that the results might show a gradual improvement in the predictions as one progress through the turbulence models. This chapter will go into some detail describing these turbulence models defining the computational domain employed within Fluent.

3.2.1 Realisable \( k\)-\( \varepsilon \) model

The \( k\)-\( \varepsilon \) model is a two-equation turbulence model which solves the two transport equations for turbulent kinetic energy, \( k \), and dissipation rate, \( \varepsilon \). The \( k\)-\( \varepsilon \) model is a popular turbulence model designed to be robust and give a reasonable prediction for simple shear flows. The degree of accuracy of said answer will vary considerably dependent upon the type of flow system being studied. As it only solves two transport equations, the turbulence model is relatively fast in terms of computation time which makes it a useful tool for gaining a very early understanding about a particular flow geometry. It is a semi-empirical model based upon physical and dimensional considerations with model constants being optimised experimentally. Primarily for these reasons, the \( k\)-\( \varepsilon \) model is used very often in industry.

The \( k\)-\( \varepsilon \) model is based on the assumption that the flow is fully turbulent and the effects of molecular viscosity are negligible. Therefore, the basic \( k\)-\( \varepsilon \) model is only suitable for simple, fully-turbulent flows. Over time, modifications of the \( k\)-\( \varepsilon \) model have been developed to accommodate different flow features and improve the accuracy of the system. The realisable \( k\)-\( \varepsilon \) model builds upon the standard and RNG \( k\)-\( \varepsilon \) models by modifying the transport equation for the dissipation rate, \( \varepsilon \), and using an alternative formulation for the turbulent viscosity, \( \mu_t \). Realisability implies that the model applies mathematical constraints on the Reynolds stresses to prevent non-physical results. In practice this has shown to improve predictions significantly compared with the standard \( k\)-\( \varepsilon \) model and in many cases better than the RNG \( k\)-\( \varepsilon \) model where strong streamline curvature is present (i.e. impinging jets).

The transport equations for \( k \) and \( \varepsilon \) and the related terms for the realisable \( k\)-\( \varepsilon \) model are given by Ansys (2011) by Eq. (3.11) and (3.12):

\[
\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial k}{\partial x_i} \right] - \rho \varepsilon + P_k + G_b + S_k \tag{3.11}
\]

\[
\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + \rho C_\varepsilon S \varepsilon
- \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}} + C_{1\varepsilon} \frac{\varepsilon}{k} C_\varepsilon G_b + S_\varepsilon \tag{3.12}
\]
The terms for turbulent kinetic energy production, $P_k$, buoyancy, $G_b$, and the mean strain rate, $S$, are defined shortly. $C$ and $\sigma$ terms are constants and defined at the end of this section. The realisable $k$-$\varepsilon$ model differs in some ways from the standard $k$-$\varepsilon$ model, but is also similar in some respects. Eq. (3.11) is the transport equation for the turbulent kinetic energy, $k$, which is defined as Eq. (3.12).

Modelling turbulence in this manner allows us to take into account the anisotropy of the turbulence to some extent. Turbulence is a 3-dimensional phenomenon which must be accounted for in complex flow geometries. This is the fundamental disadvantage of the two-equation approach which often leads to poor predictions when validated against experimental data. The additional terms in the transport equations are contributions from turbulent production – Eq. (3.13) which requires modelling to allow Eq. (3.11) to be closed.

$$P_k = -\rho \partial_k \dot{u}_j \frac{\partial \dot{u}_j}{\partial x_i}$$

(3.13)

The production of turbulent kinetic energy, $P_k$, is calculated using the gradients of the mean velocity and is often found in two-equation turbulence models. Although buoyancy does not play a role in the current calculations, it is included in Eq. (3.11) and (3.12) so is defined here for clarity:

$$G_b = g_i \frac{\mu_i}{\rho \Pr_t} \frac{\partial \rho}{\partial x_i}$$

(3.14)

The term representing the mean strain rate, $S$, is defined as:

$$S = \sqrt{2S_y S_y}$$

(3.15)

where

$$S_y = \frac{1}{2} \left( \frac{\partial \dot{u}_i}{\partial x_i} + \frac{\partial \dot{u}_j}{\partial x_j} \right)$$

The Reynolds stress terms which appear in Eq. (3.13) are modelled using an extended Boussinesq relationship which is defined by Eq. (3.16)

$$\bar{u}_i \bar{u}_j = \frac{2}{3} k \delta_{ij} - \nu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$$

(3.16)

where $\nu$ is the kinematic turbulent viscosity and $\delta_{ij}$ is the Kronecker delta.
The turbulent viscosity is defined as:

$$\mu_t = \rho \nu_t = \rho C_\mu \frac{k^2}{\varepsilon}$$

(3.17)

where, in the standard \(k-\varepsilon\) model \(C_\mu\) is assigned a constant value which strongly influences the performance of the turbulence model. This constant has been the root of many problems for CFD users. It is considered another limiting factor of two-equation models. When certain conditions are met it can lead to negative values for the normal stresses which by definition is incorrect. These conditions are typically given as:

$$\frac{k}{\varepsilon} \frac{\partial U}{\partial x} > \frac{1}{3C_\mu} \approx 3.7$$

(3.18)

In the realisable \(k-\varepsilon\) model \(C_\mu\) is no longer constant but modelled as shown by Eq. (3.19)

$$C_\mu = \frac{1}{A_0 + A_3 \frac{kS_0}{\varepsilon}}$$

(3.19)

where

$$A_0 = 4.04; \quad A_3 = \sqrt{6} \cos \phi; \quad S_0 = \sqrt{S_{ij}S_{ij} + \Omega_g \Omega_{ij}^2}; \quad \phi = \frac{1}{3} \cos^{-1} \left( \sqrt{6} \frac{S_{ij}S_{kj}S_{ki}}{\left( \sqrt{S_{ij}S_{ij}} \right)^3} \right)$$

A variable \(C_\mu\) ensures positive normal stresses and inequality for the shear stresses when Eq. (3.18) is met as suggested by Reynolds (1987) who noted that \(C_\mu\) does vary depending on the flow’s homogeneity. \(\Omega_{ij}\) is a function of the mean rate of rotation tensor, \(\tilde{\Omega}_{ij}\) viewed in the moving reference frame of the angular velocity, \(\omega_k\), and \(\varepsilon\) and is defined as:

$$\tilde{\Omega}_{ij} = (\overline{\Omega}_{ij} - \varepsilon_{ij}\omega_k) - 2\varepsilon_{ijk}\omega_k$$

(3.20)

where further definitions and derivations can be found in Ansys Fluent Theory Guide (2010).

In summary, \(C_\mu\) is now a function of the mean strain and rotation rates, the angular velocity of the system rotation, \(k\) and \(\varepsilon\), which lends itself to systems which have high streamline curvature.

The turbulent kinetic energy dissipation transport equation is given as Eq. (3.12) and similar to that used in the standard \(k-\varepsilon\) model. However, the \(C_f\) term is no longer constant but computed from the following:

$$C_f = \max \left[ 0.43, \frac{\eta}{\eta + 5} \right]; \quad \eta = S \frac{k}{\varepsilon}$$

where

$$S = \frac{k^2}{\varepsilon}$$

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This ensures that the production term can be moderated in regions where the mean strain rate is high. The remaining constants for Eq. Eq. (3.11) and (3.12) are \( C_{1c} = 1.44, \ C_2 = 1.9, \ \sigma_k = 1.0 \) and \( \sigma_e = 1.2 \). As the buoyancy term is neglected, \( C_{3c} = 0 \).

### 3.2.2 Reynolds stress turbulence model

Leaving behind the eddy-viscosity hypothesis, the Reynolds stress models solve the transport equations for each of the Reynolds stresses making them more elaborate and better suited to complex flow systems. The Reynolds stress turbulence models or second moment closures used within Fluent contain input from many different authors who have proposed various modifications to bring predictions closer to reality. The Reynolds stress transport equation is shown by Eq. (3.21) and is closed by modelling a number of other terms that appear in it:

\[
\frac{\partial}{\partial t} \left( \rho \epsilon \right) + \frac{\partial}{\partial x_i} \left( \rho \frac{\partial \epsilon}{\partial x_i} \right) = \frac{\partial}{\partial x_i} \left[ \left( \mu + \mu_t \right) \frac{\partial \epsilon}{\partial x_i} \right] C_{\epsilon} \frac{1}{2} \left[ S_{ii} + C_{\epsilon 3}S_{ii} \right] \frac{\epsilon}{k} - C_{\epsilon 3} \frac{\epsilon^2}{k} + S_{\epsilon}
\]

(3.22)

Terms I and II correspond to the rate of change of Reynolds stresses and the convective influence upon them. Terms III and IV represent the turbulent and molecular diffusion of the Reynolds stress. Term V is the production of stress and VI the turbulence due to buoyancy effects. Term VII is the pressure-strain correlation and is a very challenging term that requires suitably complex modelling to ensure it does not give non-physical results. Terms VIII and IX

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are the dissipation rate and stress production due to system rotation terms respectively. Of these terms, III, VI, VII and VIII contain unknown correlations and require modelling whilst the remaining terms do not.

In modelling term III, Fluent uses a simplified scalar turbulent diffusivity which improves the stability of the calculation as shown by Lien & Leschziner (1994). The scalar turbulent diffusion is modelled as Eq. (3.23):

\[
D_{T,i,j} = \frac{\partial}{\partial x_k} \left( \mu_i \frac{\partial u'_i u'_j}{\sigma_k} \right) \tag{3.23}
\]

where the turbulent viscosity is obtained from Eq. (3.17).

Term VI constitutes the effects of buoyancy on the Reynolds stresses and requires a model. As the current setup is isothermal this term is not included in the actual calculation but has been left in Eq. (3.21) for completeness. However, a study by Yuan, Liburdy & Wang (1987) shows that the buoyancy term can have a significant impact on impinging jets when temperature gradients are present, particularly on their heat transfer properties. Studies which are not isothermal must include this term.

In the pressure-strain correlation the turbulent kinetic energy, \( k \), is obtained from Eq. (3.8) by taking the trace of the Reynolds stress tensor. The turbulent energy dissipation Eq. (3.22) takes the constants as \( \sigma_k = 1.0 \), \( C_{\varepsilon 1} = 1.44 \), \( C_{\varepsilon 2} = 1.92 \) and \( C_{\varepsilon 3} \) is determined based upon the gravity vector. The dissipation rate tensor is calculated from Eq. (3.24):

\[
\varepsilon = \frac{2}{3} \delta_{ij} \varepsilon \tag{3.24}
\]

Ansys Fluent also solves the transport equation for \( k \) defined as Eq. (3.25) to obtain the boundary conditions for the Reynolds stress. The equation is essentially the same as for the standard \( k-\varepsilon \) turbulence model or a variant of the realisable \( k-\varepsilon \) turbulence model, Eq. (3.11) where \( \sigma_k = 0.82 \).

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_k}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + \frac{1}{2} \left( P_k + G_k \right) - \rho \varepsilon (1 + 2M_t^2) + S_k \tag{3.25}
\]

where \( G_{b,ij} \) within Eq. (3.25) has been defined by Eq. (3.14) and \( M_t \) is the turbulent Mach number defined as:

\[
M_t = \sqrt{\frac{k}{a^2}} \tag{3.26}
\]
where $a$ is the speed of sound.

Modelling the pressure-strain correlation, $\phi_{ij}$, is considered pivotal to the precision and accuracy to which turbulence models can achieve. There are two approaches to modelling this term in Ansys Fluent and both of these are investigated in the present research. The linear and quadratic pressure-strain models are discussed in the following sub-sections.

### 3.2.2.1 Linear pressure-strain model

The linear model for the pressure-strain correlation term, $\phi_{ij}$, is the classical approach developed by Gibson & Launder (1978), taking the form of Eq. (3.27)

$$\phi_{ij} = \phi_{ij,1} + \phi_{ij,2} + \phi_{ij,w}$$  (3.27)

where

$$\phi_{ij,1} = -C_1 \rho \left[ \frac{e}{k} \left( \frac{u_i u_j}{u_j} - \frac{2}{3} \delta_{ij} k \right) \right]$$  (3.28)

Eq. (3.28) is the slow pressure-strain term, where $C_1 = 1.8$ and is responsible for returning the stresses towards an isotropic state in the absence of any generation terms. The second term, $\phi_{ij,2}$, is the rapid pressure-strain term and is used to transfer a portion of energy based on opposing the anisotropy of the generation terms.

$$\phi_{ij,2} = -C_2 \left[ \left( P_{k,j} + F_{ij} + \frac{5}{6} G_{b,ij} - C_{ij} \right) - \frac{2}{3} \delta_{ij} \left( P + \frac{5}{6} G - C \right) \right]$$  (3.29)

where $C_2 = 0.6$, $P = \frac{1}{2} P_{kk}$, $G = \frac{1}{2} G_{kk}$ and $C = \frac{1}{2} C_{kk}$ ensure that $\phi_{ij,2}$ is traceless whilst $P_{k,j}$ and $G_{b,ij}$ have been previously defined in Eq. (3.13) and (3.14) respectively and $F_{ij}$ and $C_{ij}$ are the stress production by system rotation and the convection terms defined in Eq. (3.21).

The wall reflection term, $\phi_{ij,w}$, is responsible for controlling the redistribution of the Reynolds stresses near the wall. As the flow approaches the surface, the stresses are dampened, whilst the wall-normal components are dampened more than the wall-parallel stresses.

The term is modelled as Eq. (3.30):
\[ \phi_{ij,w} = C'_1 \varepsilon \left( \frac{u_k' u_m' n_k n_m \delta_{ij} - 3}{2} \frac{u_j' u_k' n_j n_k - 3}{2} \right) C k^{3/2} \frac{\varepsilon y}{C} + C'_2 \left( \phi_{kn,2} n_k n_m \delta_{ij} - 3 \phi_{jk,2} n_j n_k - 3 \right) \frac{C k^{3/2}}{\varepsilon y} \]  

(3.30)

where \( C'_1 = 0.5, \ C'_2 = 0.3, \) \( n_k \) is the \( x_k \) component of the unit normal to the wall, \( y \) is the normal distance to the wall and \( C_\ell = C_\mu^{3/4}/\kappa \) where \( C_\mu = 0.09 \) and \( \kappa = 0.4187 \) (von Kármán constant).

This linear formulation is designed to accommodate simple shear flows where the main generation is in the streamwise stress component, making the \( \phi_{ij,w} \) a reasonable estimate for small corrections. However, this presents a problem for an impinging jet where the principal stress generation is in the wall normal direction, up to the impingement plate. It has been reported (Craft et al, 1993) that this term dramatically fails in such flows around regions where normal straining is dominant (i.e. in the stagnation region of the impinging jet). At further radial distances, the system reverts to what might be considered a simple shear flow and the wall reflection term should perform as intended and produce reasonable results. With such an approach it is extremely difficult to model this varying behaviour at the wall. More recently there have been modifications to the pressure-strain to try and alleviate the poor predictive capabilities of this formulation in stagnating flows by implementing a non-linear variation of the pressure-strain correlation. The linear form of the correlation is selected by default in Ansys Fluent and must be manually changed to use the alternative.

### 3.2.2.2 Non-linear pressure-strain model

Ansys Fluent has recognised the limitations of the linear pressure-strain models for more complex flow systems. A quadratic pressure-strain model proposed by Speziale, Sarkar & Gatski (1991) has been included and is investigated in the present research. The quadratic pressure-strain correlation is reported to be better suited to more complex flow systems as a result of the non-linearity of the wall correction term. The \( \phi_{ij} \) term in the non-linear form is given by Eq. (3.31):

\[
\begin{align*}
\phi_{ij} & = - \left(C_1 \rho \varepsilon + C'_1 P b_{ij} + C_2 \rho \varepsilon \left( b_{ij} + b_{ij} - \frac{1}{3} b_{mm} b_{mm} \delta_{ij} \right) + \left(C_3 - C'_1 \sqrt{b_{ij} b_{ij}}\right) \rho k S_{ij}\right) \\
& + C_4 \rho k \left(b_{ik} S_{ik} + b_{ik} S_{ik} - \frac{2}{3} b_{mm} S_{mm} \delta_{ij}\right) + C_5 \rho k \left(b_{ik} \Omega_{ik} + b_{ik} \Omega_{ik}\right)
\end{align*}
\]  

(3.31)
where

\[
b_{ij} = -\left( -
\frac{u_i u_j + \frac{2}{3} k \delta_{ij}}{2k}\right) \tag{3.32}
\]

and

\[
\Omega_{ij} = \frac{1}{2} \left( \frac{\partial \overline{u_i}}{\partial x_j} - \frac{\partial \overline{u_j}}{\partial x_i} \right) \tag{3.33}
\]

The constants in the equations are \( C_1 = 3.4, C_1^* = 1.8, C_2 = 4.2, C_3 = 0.8, C_3^* = 1.3, C_4 = 1.25, C_5 = 0.4 \). The quadratic pressure-strain model does not use a \( \phi_{ij,w} \) term to account for additional wall-reflection effects. Instead it is assumed that the non-linear handling of the Reynolds stresses in the wall region should improve the solution accuracy, at least in the stagnation region. Fluent limits the wall boundary condition treatment options available when the quadratic pressure-strain model is specified; therefore, the differences in these need also be considered when comparing the linear and non-linear RSTM techniques.

### 3.2.3 Numerical solution and computational domain

All numerical modelling is known to be sensitive to the computational domain or mesh that is used. The commercial software Gambit has been used to develop a series of meshes to investigate sensitivity of the Fluent simulations to the computational mesh. In the 2D jet height case, three meshes were generated with an increasing number of nodes. The intent was to determine a suitable grid resolution which did not influence the converged solution. Table 3.1
shows the grid resolutions for the three sensitivity studies for the 2D jet height and the remaining 6 and 10D jet height domains.

<table>
<thead>
<tr>
<th>Grid Number</th>
<th>Jet height</th>
<th>Number of grid cells</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$N_x$</td>
<td>$N_y$</td>
</tr>
<tr>
<td>Grid I</td>
<td>2D</td>
<td>100</td>
<td>240</td>
</tr>
<tr>
<td>Grid II</td>
<td>2D</td>
<td>210</td>
<td>260</td>
</tr>
<tr>
<td>Grid III</td>
<td>2D</td>
<td>260</td>
<td>300</td>
</tr>
<tr>
<td>Grid IV</td>
<td>6D</td>
<td>570</td>
<td>260</td>
</tr>
<tr>
<td>Grid V</td>
<td>10D</td>
<td>940</td>
<td>260</td>
</tr>
</tbody>
</table>

Table 3.1 – Fluent grid details for 2, 6 and 10D jet heights

Non-uniform meshes were generated with a higher density of nodes along the impingement wall and the shear boundary between the jet and the stagnant fluid as demonstrated by Figure 3.2. To save computational run time, 2D axisymmetric meshes were generated. The default boundary conditions within Ansys Fluent were sufficient to closely represent the experimental conditions without the necessity to add custom boundary conditions or user defined functions (UDFs). The boundary conditions applied to the computational domain are summarised in Figure 3.1 and the details are discussed in this section.

**Velocity inlet**

The velocity inlet in Fluent is a fairly straightforward boundary condition in which the user specifies the velocity vectors at the inlet cells along with any turbulence statistics. The pressure is calculated based on the computed static pressure to maintain a constant flowrate into the domain. In the present study, fully developed pipe-flow profiles have been obtained and applied at the jet inlet to replicate experimental conditions. This was achieved by modelling a 4m long straight pipe in Fluent and interpolating the velocity and turbulence profile near the outlet over the jet nozzle. A number of pipe flow simulations were run, with the same turbulence models as used in the impinging jet simulations, in order to provide consistent inlet conditions for each case. The profiles were compared with experimental data from Laufer
(1953), Browne & Dinkelacker (1995) and den Toonder & Nieuwstadt (1997) and found to be in very good alignment. A Reynolds number of 23,000 corresponds to a bulk velocity, $U_b$, of $13.4 \text{ m/s}$, given the present geometry dimensions and fluid properties.

**Pressure inlet**

The pressure inlet (or constant pressure boundary) has been specified along the top open boundary which is to act in lieu of an entrainment boundary. The experimental conditions of Cooper et al (1993) had a large open space above the impingement plate and the jet nozzle. However, it is inefficient to mesh this area of stagnant fluid since only small amounts will be entrained. The pressure inlet allows fluid to leave or enter the domain driven by the specified gauge pressure and local turbulence statistics. The normal-to-boundary velocity is obtained from continuity. Conditions within the domain will determine whether fluid is entering or leaving the domain. A zero gradient condition is applied when fluid enters or leaves the domain, as the quantities will be small, this will not have a large impact on the bulk of the fluid. It is desired to remove this boundary from the area of interest of the flow and the jet nozzle to ensure it does not influence the areas of interest. Within Fluent, it was fairly straightforward to create an offset between the jet nozzle and the pressure inlet boundary to minimise the impact that the upper boundary may have upon the solution.

**Pressure outlet**

Determining the static pressure at the pressure outlet is similar to that of the pressure inlet. The local fluid statistics and local static pressure are used to determine the pressure at the outlet boundary and allow fluid to leave the domain with minimal impact on the upstream flow prediction. The pressure can be fixed by the user as a guage pressure, although this may not reflect an appropriate pressure value at the boundary and result in pressure reflections back along the radial wall jet. It is desired to keep this boundary as far as possible from the area of interest (the stagnation region). This way the boundary will only have a small if not negligible effect on the fluid statistics.

**Symmetry axis**

The axis of symmetry lies along the centre-line of the domain. About this axis the domain is implicitly rotated by $360^\circ$ removing the need to model full 3D flows. Standard conditions at a
symmetry axis are typically no scalar flux or fluid flow across the boundary, and typically the normal velocities are set to zero. All other fluid properties which lie along the boundary take the value of the nearest nodes within the domain (zero gradient).

Wall boundary

All wall boundary types in Fluent use a no-slip basis, where the velocity and turbulent statistics are set to zero at the wall. The use of a wall function avoids the necessity to resolve the near-wall viscous layer. There are a number of near wall functions available within Fluent. The non-equilibrium wall function was applied with the $k-\varepsilon$ model. This wall function used local wall statistics to determine which function to use and is a two-layer method which assumes a viscous sub-layer and a fully turbulent layer.

The mean velocity is handled according to Launder & Spalding (1974), sensitised to the pressure gradient by Eq. (3.34) and (3.35):

$$\frac{\bar{u} C_{\mu}^{1/4} k^{1/2}}{\tau_w / \rho} = \frac{1}{\kappa} \ln \left( \frac{E^* \rho C_{\mu}^{1/4} k^{1/2} y}{\mu} \right)$$

(3.34)

where $\kappa$ is the von Kármán constant ($= 0.4187$), $E^*$ is an empirical constant ($= 9.793$). $\bar{u}$ is the time-averaged velocity at a point above the wall such that $\left( k^{1/2}/\nu \right)$ at the same point is much greater than unity. In Ansys Fluent, the velocity at this point is defined by:

$$\bar{u} = -u - \frac{1}{2} \frac{dp}{dx} \left[ \frac{y_v}{\rho \kappa \sqrt{\kappa}} \ln \left( \frac{y}{y_v} \right) + \frac{y - y_v}{\rho \kappa \sqrt{\kappa}} \frac{y_v^2}{\mu} \right]$$

(3.35)

where $y_v$ is the physical thickness of the viscous sub-layer defined by Eq. (3.36):

$$y_v = \frac{11.225 \mu}{\rho C_{\mu}^{1/4} k_p^{1/2}}$$

(3.36)

This concept can then be used to compute the turbulent kinetic energy generation in the near wall cell. The variation of turbulent shear stress, turbulent kinetic energy, and dissipation rate across the near-wall cell are assumed as the following simple forms:

$$\tau_i = \begin{cases} 0, & y < y_v \\ \tau_w, & y > y_v \end{cases} \quad k = \begin{cases} \left( \frac{y}{y_v} \right)^2, & y < y_v \\ k_p, & y > y_v \end{cases} \quad \varepsilon = \begin{cases} \frac{2v_k}{y^2}, & y < y_v \\ \frac{k^{3/2}}{C_i y}, & y > y_v \end{cases}$$

(3.37)
where \( k_p \) is the turbulent kinetic energy at the first near-wall node, \( C_{\mu}^{\ast} = \kappa C_{\mu}^{-3/4} \).

Using these assumed profiles, cell-averaged approximations for the turbulent kinetic energy generation, \( P_{k}^{\ast} \), and the dissipation rate, \( \varepsilon^{\ast} \), can be obtained within the viscous sub-layer. \( P_{k}^{\ast} \) is determined using Eq. (3.38):

\[
P_{k}^{\ast} = \frac{1}{y_n} \int_{0}^{y_n} \tau_i \frac{\partial U}{\partial y} dy = \frac{1}{k y_n} \rho C_{\mu}^{\ast} k_{p}^{1/2} \ln \left( \frac{y_n}{y_v} \right) \quad (3.38)
\]

and \( \varepsilon^{\ast} \) Eq. (3.39):

\[
\varepsilon^{\ast} = \frac{1}{y_n} \int_{0}^{y_n} \varepsilon dy = \frac{1}{y_n} \left[ \frac{2\nu}{\kappa y_n} + \frac{k_{p}^{1/2}}{C_{\mu}^{\ast}} \ln \left( \frac{y_n}{y_v} \right) \right] k_{p} \quad (3.39)
\]

where \( y_n \) is the height of the first cell. It is clear from the conditions of Eq. (3.37) that when in the viscous sub-layer Eq. (3.38) is zero. The proportions of the viscous sub-layer and the fully turbulent layer determine the kinetic energy budget in the near wall region. Within an impinging jet there is a considerable variation in the thickness of the viscous sub-layer from the stagnation region to the outer reaches of the radial wall jet. This can be considered a function of the pressure gradients across the impingement plate. The non-equilibrium wall function takes into account some of these variations and uses the most appropriate treatment for the kinetic energy at that point. The standard wall function would neglect this difference which would lead to poorer predictions near the wall, which makes it unsuitable for complex flows with impingement.

When using the RSTM, Ansys Fluent requires conditions for the individual Reynolds stresses as well as the dissipation rate at the wall. These can either be input directly or calculated from the turbulent intensity and characteristic length (either input directly or calculated from the mesh spacing). The values are calculated using a local co-ordinate system where \( t, b \) and \( n \) are the tangential, normal and binormal co-ordinates respectively the relations shown by Eq. (3.40):

\[
\frac{u_{t}^{\ast 2}}{k} = 1.098; \quad \frac{u_{n}^{\ast 2}}{k} = 0.247; \quad \frac{u_{b}^{\ast 2}}{k} = 0.655; \quad \frac{u_{t} u_{n}^{\prime}}{k} = 0.255 \quad (3.40)
\]

where \( u_{t} \) is the tangential velocity, \( u_{n} \) is the normal velocity and \( u_{b} \) is the binormal velocity and \( k \) is obtained from the transport equation, Eq. (3.25) with the cell-averaged generation and dissipation rate terms outline above the Reynolds stress anisotropies are fixed at the wall. The values given in Eq. (3.40) are the result of local equilibrium forms of the Reynolds stress equations with transport terms omitted and using the log-law to approximate the shear strain which is assumed to be the only strain (Launder & Sandham, 2002). Ansys Fluent also allows the Reynolds stresses at the wall to be fixed based on the friction velocity and the normal
stresses in a similar group of equations although this has not been investigated in the present work.

3.3 STREAM RANS

The original STREAM code was developed by Lien & Leschziner (1994) at the University of Manchester, UK. They developed a computational procedure for modelling turbulent flows in complex geometries based on a structured finite volume framework. Velocity is decomposed in Cartesian components and all flow variables and statistics are stored at the same set of nodes. The code uses an iterative solution algorithm to reach a converged solution with the assistance of the SIMPLE pressure correction scheme from Patankar & Spalding (1970). Convection effects are approximated using the MUSCL scheme by van Leer (1979). A number of two-equation and second moment closure turbulence models were initially added to suit a range of high and low Reynolds number flows. Additional turbulence models have since been added to the code including non-linear variations and other developmental schemes. The STREAM code has been used to demonstrate that with improved correlations and appropriate physics for complex geometries, RANS methods can still provide good predictions for complex flows. Similar to the Fluent work, multiple turbulence models have been chosen to model an impinging jet to gain a good representation of the turbulence models available within STREAM. The turbulence models selected were a non-linear \( k-\varepsilon \) turbulence model developed by Shih, et al (1995) and a high Reynolds number RSTM, based on the Gibson & Launder form described above, but with a wall reflection term developed by Craft & Launder (1992).

3.3.1 Non-linear \( k-\varepsilon \) model

The limitations of the standard \( k-\varepsilon \) model have motivated a number of authors to develop non-linear \( k-\varepsilon \) models in an attempt to find a more accurate relationship between the Reynolds stresses and the mean flow statistics than the Boussinesq hypothesis. Shih et al (1995) developed a non-linear \( k-\varepsilon \) model looking to overcome the difficulties when modelling the dissipation rate term in complex engineering geometries. The turbulence model was derived from the constitutive relations for the Reynolds stresses developed by Pope (1978), Yoshizawa (1984) and Rubinstein & Barton (1990). This constitutive relation relies upon the assumption that the Reynolds stresses are dependent only on the mean velocity gradients and the turbulence can be characterised by \( k \) and \( \varepsilon \). Shih et al have tuned the general form of the constitutive
relation to include the effects of rapid rotation using rapid distortion theory (RDT) using the
studies of Reynolds (1987) and Coleman & Mansour (1991). Furthermore, the authors made
the relation realisable, using a functional form of $C_\mu$ to ensure that under certain strain fields the
model would not give non-physical stress fields (such as negative normal Reynolds stresses).
Reynolds (1987) and Coleman & Mansour (1991) showed that rapid rotation has no effect on
isotropic turbulence which provided a constraint for the development of the model. Since this
approach adopts the Boussinesq hypothesis to explicitly define the Reynolds stresses (without
needing to solve the individual transport equations for them) it is sometimes referred to as an
graphic model.

The stress-strain relation is written as Eq. (3.41):

$$\overline{u_i u_j} = \frac{2}{3} k \delta_{ij} - C_\mu \frac{k^2}{\varepsilon} - 2S_{ij}^* + 2C_2 \frac{k^3}{\varepsilon^3} \left(-S_{ik}^* \Omega_{kj}^* + \Omega_{ik}^* S_{kj}^*\right)$$  \hspace{1cm} (3.41)

where $C_\mu$ is a non-constant relationship identical to that used in Fluent, Eq. (3.19) where the
empirical constant $A_0 = 6.5$. Applying the constraint of Eq. (3.18) to (3.41) gives an equation
for the value of $C_2$ as Eq. (3.42):

$$C_2 = \sqrt{1 - 9C_\mu^2 \left(\frac{S^* k}{\varepsilon}\right)^2}$$

$$C_0 + 6 \frac{S^* k \Omega^* k}{\varepsilon \varepsilon}$$  \hspace{1cm} (3.42)

where the constant $C_0 = 1.0$, is computed using the product of the eddy viscosity and the mean
strain-rate tensor. The full derivation of Eq. (3.41) is not presented here but can be found in the
literature (Shih, Zhu & Lumley, 1995) along with application of the model to some challenging
geometries. No additional transport equations are required, which saves on computational
resources and does not diminish the fast computing time associated with two-equation models.

The benefit of this model over other $k$-$\varepsilon$ models is that the effective eddy viscosity is anisotropic
which is closer to reality. Furthermore, the effects of mean rotation on the Reynolds stresses are
also taken into account which agrees with RDT results. This is important for complex
domains where anisotropy and rotating shear forces are experienced. The equations for the
turbulent kinetic energy and dissipation rate are defined similarly to the standard $k$-$\varepsilon$ model as
Eq. (3.43) and (3.44):

$$\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho \overline{u_i k})}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu + \mu_t}{\sigma_k}\right) \frac{\partial k}{\partial x_i} - \rho \overline{u_i u_j} \frac{\partial u_j}{\partial x_i} - \rho \varepsilon$$  \hspace{1cm} (3.43)
\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} - \rho C_{\varepsilon 1} \varepsilon \frac{\partial u_j}{\partial x_i} - \rho C_{\varepsilon 2} \varepsilon^2 \frac{\partial u_j}{\partial x_i} \quad (3.44)
\]

The coefficient in Eq. (3.43) is \( \sigma_k = 1.0 \) whilst Eq. (3.44) are given as \( C_{\varepsilon 1} = 1.44 \), \( C_{\varepsilon 2} = 1.92 \), \( \sigma_\varepsilon = 1.3 \).

The authors of this model have applied this model to rotating homogeneous flows, back-facing steps and confined jets with considerable success. It has been adopted by other studies as a benchmark for non-linear \( k-\varepsilon \) models capable of predicting complex geometries within a reasonable tolerance of accuracy. The model has demonstrated that with the constraints of RDT and realisability the correct effect of rotation on the Reynolds stresses are captured as well as producing non-negative Reynolds stresses in anisotropic flows. Finally, whilst these improvements over existing (at the time of writing) models were significant it came with little extra cost to robustness or computational resources.

### 3.3.2 High Reynolds number RSTM with wall reflection

The Reynolds stress model used with the STREAM RANS code is a high Reynolds RSTM, based on the linear Gibson-Launder version described in Section 3.2.2 with reflection term developed by Craft et al (1993) at University of Manchester. This wall reflection term was designed with impinging jets in mind and therefore, the wall reflection term is more carefully optimised for flow impinging normally to a wall. The transport equations for the Reynolds stresses and energy dissipation rate are given by Eq. (3.45) and (3.46) respectively:

\[
\frac{\partial \left( \overline{u_i^' u_j^'} \right)}{\partial t} + \frac{\partial}{\partial x_k} \left( u_k \overline{u_i^' u_j^'} \right) = \left[ \frac{\overline{u_i^' u_k^'} + \overline{u_j^' u_k^'}}{\varepsilon} \right] \frac{\partial \varepsilon}{\partial x_k} - \frac{2}{3} \varepsilon \frac{\partial \delta_j^g}{\partial x_k} + p \left( \delta_j^g \varepsilon + \delta_k^g u_j^' \right)
\]

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_k} \left( \mu \delta_k^g + C_{\varepsilon 1} \frac{\overline{u_i^' u_k^'}}{\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_k} + \rho \varepsilon \frac{\partial u_j}{\partial x_i} \delta_j^g - \rho \varepsilon \frac{\partial u_j}{\partial x_i} \delta_j^g \quad (3.46)
\]

Essentially, the transport equations shown above remain largely unchanged from those stated in the Fluent section with some small exceptions. The main modification is made to the wall
reflection part of the pressure-strain correlation, $\phi_{ij}$, in Eq. (3.45). This term is again split into the parts of (3.47) below.

$$\phi_{ij} = \phi_{ij,1} + \phi_{ij,2} + \phi_{ij,w}$$  \hspace{1cm} (3.47)

The slow, rapid and wall related terms in Eq. (3.47) are defined by Eq. (3.48) to (3.51)

$$\phi_{ij,1} = -C_1 \frac{\varepsilon}{k} \left( \overline{u_i' u_j'} - \frac{2}{3} k \delta_{ij} \right)$$  \hspace{1cm} (3.48)

Eq. (3.48) represents the interaction between the fluctuating components.

$$\phi_{ij,2} = -C_2 \left( P_{ij} - \frac{1}{3} P k \delta_{ij} \right)$$  \hspace{1cm} (3.49)

Eq. (3.49) is the interaction between the fluctuating velocities and the main flow by linear relation to the mean velocity gradients. $P_k$ is the production of the normal stress and has been defined by Eq. (3.13).

$$\phi_{ij,w1} = C_{w1} \frac{\varepsilon}{k} \left( \overline{u_i' u_j'} - \frac{3}{2} u_i u_j n_k n_l - \frac{3}{2} u_j u_i n_k n_l \right) f_y$$  \hspace{1cm} (3.50)

$$\phi_{ij,w2} = -C_{w2} \frac{\partial U_j}{\partial x_m} u_i' u_j' \left( \delta_{ij} - 3n_k n_l \right) f_y$$

$$- C_{w2} k a_{lm} \frac{\partial U_k}{\partial x_m} n_l n_m \delta_j - \frac{3}{2} \frac{\partial U_i}{\partial x_m} n_j n_l - \frac{3}{2} \frac{\partial U_j}{\partial x_m} n_i n_l \right) f_y$$

$$+ C_{w2} k \frac{\partial U_i}{\partial x_m} n_l n_m \left( n_k n_l - \frac{1}{3} \delta_{ij} \right) f_y$$  \hspace{1cm} (3.51)

Eq. (3.50) and (3.51) are the modified wall reflection terms by Craft & Launder (1992), where:

$$f_y = k^{3/2} / (C_1 \varepsilon y)$$  \hspace{1cm} (3.52)

These terms have been the root of many challenges for complex geometries when using the RSTM. They are responsible for redistributing the Reynolds stresses in the vicinity of the wall and reducing (or augmenting) the effects of $\phi_{ij,1}$ and $\phi_{ij,2}$. Craft & Launder (1992) noted that despite current proposals for the pressure-strain correlation term, very few were successful in modelling stagnation flows. The constants used throughout this RSTM are listed in Table 3.2.
### 3.3.3 Numerical solution and computational domain

The setup of the computational domain is very similar to that already described in Section 3.2.3 and illustrated by Figure 3.1, with some small variations for specific boundary conditions. These will be discussed in this section.

The computational mesh was created with a bespoke code modified by the present author to produce meshes of similar composition to those described in Section 3.2.3. Grid independence studies were carried out to determine that the shape and node distribution did not influence the predictions of the STREAM RANS. Table 3.3 shows the grid resolutions used throughout the STREAM RANS predictions.

<table>
<thead>
<tr>
<th>Grid Number</th>
<th>Jet height</th>
<th>Number of grid cells</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$N_x$</td>
<td>$N_y$</td>
</tr>
<tr>
<td>Grid I</td>
<td>2D</td>
<td>125</td>
<td>200</td>
</tr>
<tr>
<td>Grid II</td>
<td>2D</td>
<td>150</td>
<td>250</td>
</tr>
<tr>
<td>Grid III</td>
<td>2D</td>
<td>200</td>
<td>300</td>
</tr>
<tr>
<td>Grid IV</td>
<td>6D</td>
<td>270</td>
<td>250</td>
</tr>
<tr>
<td>Grid V</td>
<td>10D</td>
<td>400</td>
<td>250</td>
</tr>
</tbody>
</table>

Table 3.3 – STREAM grid details for 2, 6 and 10D jet heights

As with the Fluent meshes, nodes were concentrated around areas of anticipated high turbulence, shear layers and streamline curvature.

![Figure 3.3 – Computational domain used with STREAM for the 2D jet height](image-url)
Inlet conditions & Outflow boundary

As in the Ansys Fluent calculations, fully-developed pipe flow profiles were applied at the jet inlet. In this case they were obtained using the BOFFIN RANS code with straight pipe of sufficient length to reach a fully developed profile. Velocity and turbulence statistics were taken from near the outlet of the straight pipe and interpolated over the jet nozzle. The profiles corresponded well with experimental data and those obtained from Fluent. The outflow boundary uses the exact same conditions as described in section 3.2.3.

Wall boundary conditions

The STREAM code has two wall treatments available: A low-Reynolds model and a wall function. The low-Reynolds number model is based on the work Menter (1994) and requires a high resolution mesh at the wall and is intended for low Reynolds number flows. In the present work, wall functions have been used, and the standard form of these is identical to that described in Section 3.2.3.

Unlike the Fluent case, in STREAM a short interior section of the pipe was meshed and modelled. The pipe ‘wall’ has a finite thickness corresponding to two cells, and the same wall-function treatment was used along these as the impingement plate. Two cells was considered a thick enough wall to be representative of the unknown pipe wall thickness used in the experiment. The impact of this small geometrical difference is not expected to be large at the jet discharge heights studied here, and so results can sensibly be compared with those obtained from Fluent.
Entrainment boundary conditions

The entrainment boundary conditions were implemented in the STREAM code by the present author. They reflect the method used by Craft et al (1993) to ensure the upper boundary has a minimal impact on the solution.

Axial velocity component, \( \frac{\partial V}{\partial y} = 0 \)

Radial velocity component, \[
\begin{cases}
V < 0 \text{ (inflow)}: & U = 0 \\
V > 0 \text{ (outflow)}: & \frac{\partial U}{\partial y} = 0
\end{cases}
\]

Normal and shear stresses, \( \overline{u^2} = \overline{v^2} = \frac{2}{3}k, \overline{uv} = 0 \)

Pressure, \( P = 0 \) \hspace{1cm} (3.53)

Where \( i \) and \( j \) correspond to the axial and radial components, \( n \) and \( n+1 \) correspond to first cell inside the boundary and the final node outside the boundary respectively. The axial velocity component is relatively small in comparison to the velocities in the stagnation region and the radial wall jet. The zero gradient condition on fluid entering and leaving the domain at this point should not have a noticeable effect on the area of interest. The radial (or parallel) velocity component is set to zero when entering the domain and zero gradient if leaving. For the turbulence a zero gradient condition is applied when the flow is leaving the domain and a low turbulence level is specified for fluid entering the domain, with an isotropic stress distribution based on \( k \).

3.4 BOFFIN LES

LES uses filtered governing equations to calculate the time-dependent, three-dimensional, large-scale eddy structures of a turbulent flow. As these large scale turbulence structures are simulated directly, their full contribution to the flow is captured. Smaller turbulent structures are modelled using a simple sub-grid scale model. The use of a very simple model for the sub-grid scale stresses is generally assumed to have less impact than using such a model in RANS, since the smaller scales have much less impact on the velocity and turbulence statistics. Furthermore, these eddies are considered to be more isotropic than the larger ones. Thus LES can produce superior predictions which align better with experimental or real data. The filtering
technique used can vary, but all generate additional terms for the governing equations which must be modelled to close them. This chapter aims to describe the governing equations and the filtering techniques employed in the BOFFIN LES code and used in this research. Furthermore, the computational domain and boundary conditions are discussed in Section 3.4.2.

3.4.1 Governing equations and sub-grid scale model

The basis of LES is obtaining a set of governing equations which describe the large scale turbulence structures. This is achieved by filtering the instantaneous quantities in the flow using an appropriate filtering operation. The filtering operation is defined according to Eq. (3.54):

$$\bar{f}(x,t) = \int \int G(x-x',\Delta)f(x,t)dx'$$  \hspace{1cm} (3.54)

where the filtered quantity is denoted by an overbar and $G(x,\Delta)$ is the filtering function characterised by a length scale, $\Delta$. The length scale is typically related to the computational mesh and in the present work is defined as Eq. (3.55) so as to support non-uniform meshes.

$$\Delta = \left(\Delta_i\Delta_j\Delta_k\right)^{1/3}$$  \hspace{1cm} (3.55)

where $\Delta_i\Delta_j\Delta_k$ are the node spacings at a certain point of the mesh in the $i$, $j$ and $k$ directions. As the axisymmetric jet requires 3-dimensional resolution, it is important that the filter width is a function of all 3 Cartesian directions. In terms of wave number, $\kappa$, (inverse wavelength) the instantaneous variables can be written as the products of Fourier transforms, denoted by the hat above the symbol. The larger turbulence scales are associated with low wave numbers, whilst smaller turbulence scales having increasing wave numbers. This provides a means to separate the different scales of turbulence using a filtering function.

There are a number of different filter functions available, with various advantages and disadvantages, such as the sharp cut-off, Gaussian and top-hat filters. The latter is employed within the BOFFIN LES according to Germano (1992) and is defined by Eq. (3.56):

$$G(x-x',\Delta) = \begin{cases} 
\frac{1}{\Delta_i\Delta_j\Delta_k} & \text{if } x_i-x'_i < \frac{\Delta}{2} \\
0 & \text{otherwise.} 
\end{cases}$$  \hspace{1cm} (3.56)

A problem noted by Zhou et al (1989) was that averaged quantities produced by spatial filtering and spatial differentiation do not commute for non-uniform meshes. Developments by di Mare
& Jones (2003) determined these errors to be very minor against the dissipative nature of the turbulent kinetic energy and variances of the small scale turbulence, so these errors can be ignored here.

Applying the filtering decomposition of Eq. (3.54) to the continuity and Navier-Stokes equations will yield Eq. (3.57) and (3.58) respectively:

\[
\begin{align*}
\frac{\partial \overline{u_i}}{\partial t} + \sum_{j=1}^{n} \frac{\partial \overline{u_i} \overline{u_j}}{\partial x_j} &+ \frac{1}{\rho} \frac{\partial \tau_{ij}}{\partial x_j} - \nu \frac{\partial^2 \overline{u_i}}{\partial x_j \partial x_j} = 0 \\
\frac{\partial \overline{u_i}}{\partial x_j} & = 0 
\end{align*}
\]  

(3.57)

These equations are then used to calculate the large scale turbulence structures of the flow which carry amounts of energy significant to govern the behaviour of the fluid. The linear nature of the continuity equation Eq. (3.57) leaves it largely unchanged. In Eq. (3.58) the impact of the smaller scales are captured by the SGS stress tensor, \( \tau_{ij} \), this is subsequently defined as Eq. (3.59):

\[
\tau_{ij} = \overline{u_i u_j} - \overline{u_i} \overline{u_j} 
\]

(3.59)

The dynamic model which Smagorinsky (1967) developed captures the backscatter and shows the small but important influence of the small scale turbulence on the larger scales. The SGS stress tensors must be modelled before filtered Eq. (3.58) can be closed. The BOFFIN LES code uses the dynamic model of Germano et al (1991), implemented using the approximate localisation procedure of Piomelli & Liu (1994) with modifications proposed by the studies of di Mare & Jones (2003). The smaller turbulence scales can be considered isotropic far more readily than the larger scales of turbulence; therefore a simple formulation using the eddy-viscosity hypothesis is not unreasonable. The SGS stresses are thus modelled as:

\[
\tau_{ij} = -2 \left( C \Delta \right)^2 \overline{S} \overline{S}_{ij} 
\]

(3.60)

where

\[
\overline{S} = \sqrt{2\overline{S}_{ij} \overline{S}_{ij}} ; \quad \overline{S}_{ij} = \frac{1}{2} \left( \frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) 
\]

(3.61)

The superscript, \( a \), represents the anisotropic or large scale quantities, and the model parameter, \( C \), must be estimated. The dynamic Smagorinsky model estimates \( C \) by using a second filtering
operation to Eq. (3.58) and filtered quantities are denoted by a tilde. The resultant SGS stresses in this second filtered field are given by:

\[ T_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j \]  

(3.62)

The difference between Eq. (3.59) and (3.62):

\[ L_{ij} = T_{ij} - \tilde{T}_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j \]  

(3.63)

is known as Germano's identity and features only the resolved (large-scale) quantities, therefore can be evaluated. A relationship is required between the model constants \( \bar{C}_1 \) and \( \bar{C}_2 \) for the first and second filtering operations respectively. This relationship will rely on the hypothesis that the cut-off length falls inside the inertial sub range such that Eq. (3.64) might be assumed:

\[ C^2 = C^2 \left( \bar{f} \right) \]  

(3.64)

As such a hypothesis is unlikely to be particularly accurate in near-wall or low Reynolds number flows, the model constants can be expected to differ significantly between filter levels. The largest deviation will be in areas of weakly resolved strain tensors. Based on this, di Mare & Jones (2003) proposed a first order expansion of the scale-dependent expression for \( C \) using a length scale and a velocity scale to account for the discrepancy:

\[ C^2 \left( \bar{f} \right) = C^2 \left( \bar{f} \right) \left( 1 + \frac{\varepsilon}{2\sqrt{2} \Delta^2 \bar{S} \bar{S}^2} \right) \]  

(3.65)

In Eq. (3.65), the dissipation term is modelled simply by \( \varepsilon \approx v^2/l \) using one velocity scale, \( v \), and one length scale, \( l \), which is assumed \( \Delta \equiv l \). Eq. (3.65) is based on the assumption that the scale invariance will fall within an inertial sub-range. When this is true, the dissipation provided by the model should represent the entire dissipation present in the flow. At the high Reynolds number limit the dissipation is represented only by the aforementioned velocity and length scales which forces the assumption that the turbulence can be characterised by just \( v \) and \( l \). A measure of scale preserving conditions can thus be obtained when one looks at the ratio of \( \varepsilon \) and \( \Delta^2 \| \bar{S} \|^3 \). Eq. (3.65) represents a first order expansion of the other scale dependent expressions for \( C \) such as that of Porte-Agel et al (2000). Combining Eq. (3.63) and (3.65) and contracting both sides yields Eq. (3.66):
\[
C^2 = \frac{2\sqrt{2} (C^2 \Delta)^2 \left[ S_{ij} \left( \bar{S}^u_{ij} - L_{ij} \bar{S}^u_{ij} \right) \right]}{\varepsilon + 2\sqrt{2} \Delta^{-2} \left[ S_{ij} \right]} (3.66)
\]

where \( C^2 \) is given an initial estimate based on the field of \( C^2 \) and subsequently takes the value of the previous timestep for \( C^2 \). From Eq. (3.66) a simple relationship for \( C^2 \) is acquired which yields smooth and conditioned behaviour from the model and ensures the resolved strain tends to zero as \( C^2 \) tends to zero, whilst \( C^2 \) remains bounded. Eq. (3.66) is a least square method and therefore requires no averaging and produces maximum values for \( C^2 \) which are similar in magnitude to the estimates of Lilly (1967). However, Eq. (3.66) does not prevent the appearance of negative values of the model parameter which can lead to instabilities in the calculation. Such values are automatically set to zero and negative values for the SGS viscosity are also set to zero to improve stability. The cost of this improved stability is that there is no backscatter available when these values are set to zero.

### 3.4.2 Numerical solution and computational domain

It is well known that the stability of LES is very sensitive to the initial conditions it is supplied with. The final solution is also highly dependent upon the turbulent boundary conditions that are specified in the computational model. Furthermore, areas of high strain need sufficient resolution to correctly predict the turbulent structures in those regions. The present work with LES involves the use of several boundary conditions including an inlet with instantaneous velocity generator, outlet, wall and entrainment boundaries.

The BOFFIN LES uses a finite volume approach, integrating the Navier-Stokes equation over the computational mesh. All spatial derivatives with the exception of the convective term are approximated using a standard second order central difference scheme. To reduce error or non-physical values the total variation diminishing (TVD) scheme by Orszag & Patterson (1972) is used. The pressure and velocity field are coupled using the SIMPLE scheme by Patankar & Spalding (1972). As with the STREAM code, BOFFIN uses a collocated storage arrangement with fourth-order pressure smoothing by Rhie & Chow (1983) to prevent oscillatory errors forming in the pressure field. The timestep is based on the Courant number which must lie between 0.1 and 0.3 else the solution is prone to deteriorate. The convergence of the solution is sensitive to the Courant number which in physical terms is the number of cells a fluid particle will pass through in one timestep. By ensuring the timestep is such that the Courant number is
kept between these values, one improves the stability of the calculation. Time advancement is achieved through an implicit Gear method for all terms such as that used by Temmerman et al (2003).

The computational mesh in Figure 3.6 shows the node distribution used for the 2D jet height with the LES BOFFIN. It was generated by mapping a square mesh to a circle, which results in a cylindrical mesh with a non-uniform distribution of nodes in the radial direction.

**Inlet conditions & instantaneous velocity generator**

To align the computation better with the conditions in the experiment, time-varying velocity profile to simulate fully developed turbulent pipe flow is applied to the jet nozzle. Based on the work of Lund et al (1998), Klein et al (2003) and di Mare et al (2006) an instantaneous velocity generator is used to specify a time-dependent approximation to fully developed pipe flow profile at the inlet. Using RANS data of a fully developed pipe flow, the mean values,
Reynolds stresses, length and time scales can be used to generate artificial velocity fluctuations within certain statistical constraints.

The RANS data for a fully developed pipe flow was generated using a periodic straight pipe flow with the RANS BOFFIN code – a Reynolds averaged version of the LES BOFFIN used in the current work that was developed by Jones (1991). The calculation was initialised with a uniform inlet velocity of 13.4m$^{-1}$ corresponding to a Reynolds number of 23,000 and run until a fully developed profile was obtained.

Three randomly fluctuating signals with means of zero and variance of unity are filtered to correlate the supplied mean fully developed pipe profile in space and time. These correlated values are then transformed into a velocity fluctuation by multiplying them by an amplitude tensor. The amplitude tensor is obtained through the process developed by Lund et al (1998) which uses the Reynolds stresses at the same location. This ensures a more representative value for the fluctuations based on the Reynolds stresses rather than a simple random number generator. The velocity fluctuations are then added to the mean velocity giving the artificial instantaneous values for the velocity at a certain timestep. This process is repeated every specified number of timesteps to give an instantaneous fully developed pipe flow field at the jet nozzle.

Wall boundary conditions

The wall boundary conditions in impinging jets are difficult problems to overcome. The variation of the turbulence and boundary layer along the impingement plate is such that the thickness of the viscous sub-layer varies considerably from the stagnation region to the outer reaches of the radial wall jet. If the no-slip wall condition is to be used the $y^+ < 1$ condition must be met along the entirety of the impingement plate. This requires an extremely small grid spacing for the first node in the stagnation region, although it can gradually increase as the radial wall jet develops. Furthermore, in order to preserve numerical accuracy, the growth rate of cells from the wall must not be high, resulting in a very large number of cells to accurately resolve the flow behaviour near to the wall.

For impinging jets of high Reynolds numbers a full resolution of the viscous sub-layer is not feasible and approximate boundary conditions are adopted. In the LES BOFFIN code a generalised version of the Grötzbach-Schumann formulation is used (Schumann, 1975 and Grötzbach, 1987). This approach assumes that the instantaneous velocity parallel to the wall coincides with the shear stress at the same location in time. The mean wall shear stress is computed from the logarithmic law of the wall in an iterative fashion:
\[ \tau_{w,0} = \frac{\overline{\tau} \left( x, \Delta y, z, t \right)}{\overline{w} \left( x, \Delta y, z, t \right)} \langle \tau_w \rangle \]  
\[ \tau_{u,0} = \frac{\overline{\tau} \left( x, \Delta y, z, t \right)}{\overline{u} \left( x, \Delta y, z, t \right)} \langle \tau_u \rangle \]  

where \( u \) and \( w \) denote spanwise and tangential directions, all values are to be filtered and \( \langle \cdot \rangle \) brackets denote terms to be ensemble averaged. Wall normal values of velocity, \( v \), in the \( y \)-direction are equal to zero.

\[ v \big|_{y=0} = 0 \]

The ensemble averaged wall shear stress, \( \langle \tau_{w,0} \rangle \), is computed from the law of the wall according to Werner & Wengle (1993):

\[ u^+ = \frac{\langle \overline{\tau} \left( x, \Delta y, z, t \right) \rangle}{u_T} = y^+ \quad 0 \leq y^+ \leq 11.81 \]  

where the value of 11.81 was found to be the upper limit of the time-averaged values of \( y^+ \) adjacent to the wall in their study, thus the linear law of the wall was sufficient. For \( y^+ \) above this value:

\[ \langle \overline{u} \left( x, \Delta y, z, t \right) \rangle = \frac{u_T}{k} \ln y^+ + B \quad 11.81 < y^+ < 1000 \]

where superscript \( + \) values and the friction velocity, \( u_T \), are defined as:

\[ u^+ = \frac{u}{u_T} \quad y^+ = \frac{yu_T}{v} \quad u_T = \sqrt{\tau_w / \rho} \]

respectively and \( k \) is the von Kármán constant (= 0.4187) and \( B = 5.5 \) (Hassan & Barsamian, 2001; di Mare & Jones, 2001; Tang et al, 2004).

**Entrainment boundary**

The entrainment boundary has been implemented by the present author in essentially the same way as in the STREAM code. Following Eq. (3.53) one can replace the averaged terms with instantaneous quantities. It must be assumed at this stage that similarly with the RANS
predictions, the prescribed entrainment boundary is far away enough such that it has little effect on the stagnation region or the radial wall jet.

**Outflow boundary**

The outflow boundary condition used in BOFFIN is the same as that used within STREAM and Ansys Fluent.
Chapter 4  Multi-phase methodology

This chapter looks at the methodologies used in the present research to predict particle trajectories and the overall dispersion of particles in impinging jets. With the continuous-phase solution, the distribution of particles can be investigated through the use of particle trackers either in parallel with the calculation or separately once a converged solution has been reached. Various models are used throughout the research including academically developed codes and industrially used CFD codes such as Ansys Fluent.

Prior to describing the specifics of each model used, an overview of the fundamentals of particle motion is provided. Section 4.1 intends to develop the particle equation of motion up to the point at which the various methods differ. The following parts will then describe how the equations shown in Section 4.1 are used.
4.1 Fundamentals of the particle equation of motion

The first step in simulating discrete particles moving through a continuous flow field using an
Eulerian-Lagrange approach is to define the particle equation of motion. These equations
describe the inertia and external forces acting on the particle as it moves through the fluid flow
field. Depending on the solver and the form of the final equation, thousands of iterations may
be necessary over thousands of particles to obtain smooth statistical averages. The particle
equation of motion often found in the literature is a modified version of Maxey & Riley (1983)
with the $i$th component of a particle’s velocity governed by, Eq. (4.1):

$$
\rho_p \frac{du_{p,i}}{dt} = \rho_f \frac{Du_{f,i}}{Dt} + \left( \rho_p - \rho_f \right) g_i - \frac{3\nu \rho_f}{4d_p^2} \left( u_{p,i} - u_{f,i} - \frac{d_p^2}{6} \nabla^2 u_{f,i} \right)
$$

The particle and fluid quantities are represented by $p$ and $f$ subscripts respectively for clarity.
Derivatives concerning the particle are written $d/dt$ whilst fluid derivatives are shown as $D/Dt$.
Eq (4.1) is the full equation of motion for a single particle that is often referred to in the
literature although not all terms are necessarily relevant in the present study. For completeness
each term is defined here.

The first term, $I$, represents the inertia of the particle to follow the flow of the continuous phase.
Particles with higher inertia are less likely to follow the streamline path of the fluid. The second
term, $II$, represents the pressure gradient term which arises from the difference in fluid
acceleration relative to the undisturbed fluid. Term $III$ is the buoyancy term and includes the
effects of gravity, $g_i$. The fourth term, $IV$, constitutes the steady state drag force of the fluid
acting on the particle. Term $V$ is the added mass which is the force developed as the result of the
relative difference between the acceleration of the particle and the fluid. As the particle
moves through the fluid, it must displace some volume of fluid as it moves through it; this term
represents this effect as a volume of fluid that moves with the particle. Finally, the sixth term,
VI, is known as the **Bassett history** term and is associated with turbulence developed in the wake of the particle as it moves through the fluid.

The fundamental assumption of Eq. (4.1) and the Lagrangian approach is that the discrete phase occupies a low enough volume fraction that particle-particle interactions can be neglected. Therefore a particle can be assumed to have complete freedom in its motion. The terms in Eq. (4.1) proportional to \(d^2_p \nabla^2 u_{f,j}\) are known as the Faxen terms and account for the non-uniformity of the velocity of the flow. Faxen’s law is a correction to the Stokes terms which accounts for the friction on spherical particles in viscous fluids. When the relative velocity between the fluid and the particle is close to zero, the Faxen terms tend to zero, affecting the drag, added mass and Bassett history terms. Such conditions tend to mean the particle is closely following the fluid velocity, a phenomenon which occurs when the particle size is smaller than the Kolmogorov scale. However, when heavier/larger particles are encountered the Faxen terms need to be considered, else the non-uniformity will not be captured and the accuracy of the solution may suffer; that is the streamline curvature around the particle is neglected. The particles in the current study have been found to be smaller than the Kolmogorov scale, \(\eta\), where \(\eta \equiv \nu^3 / \epsilon\) and \(d_p < \eta\) as well as the ratio of fluid density to solid-phase density was such that it reasonably permits the exclusion of the Faxen terms. Several empirical coefficients are also added in this formulation which permits the use of Eq. (4.1) with the flow system of interest here. So for spherical, non-rotating and non-colliding particles and dividing all terms by the mass, \(m_p = \rho_p V_p\), of a particle we reach a simpler form of the equation of motion for the particles.

\[
\frac{du_{p,i}}{dt} = \beta \frac{Du_{f,j}}{Dt} + (1 - \beta) g_i - \frac{3\beta}{4d_p} C_D \left(u_{p,i} - u_{f,i}\right) \left[u_{p,i} - u_{f,i}\right] \\
- \frac{\beta}{2} C_A \frac{d}{dt} \left(u_{p,i} - u_{f,i}\right) - \frac{9\beta}{2d_p} \sqrt{\frac{\nu}{\pi}} C_H \left[ \int_0^t \frac{1}{\sqrt{t - \tau}} d\tau \left(u_{p,i} - u_{f,i}\right) \right] d\tau
\]  

(4.2)

Eq. (4.2) is the version of Berlemont et al (1990), where \(\beta\) is the ratio of fluid to particle density. With the Faxen terms removed, the effects of streamline curvature are no longer captured. However the \(C_D\), \(C_A\) and \(C_H\) coefficients for the drag, added mass and history terms respectively are introduced. These coefficients have been derived through experiments and studies for various particulate systems to make the equation of motion valid for higher Reynolds number flows. Eq. (4.2) is now semi-empirical.
The coefficients are taken as:

\[ C_D = \frac{24}{\text{Re}_p} f_D, \quad C_A = 2.1 - \frac{0.132 \text{Ac}^2}{(1+0.12 \text{Ac}^3)}, \quad C_H = 0.48 - \frac{0.5 \text{Ac}^3}{(1+\text{Ac}^3)} \] \quad (4.3)

Where \( f_D \) is an empirical drag correction factor. The forms of \( C_A \) and \( C_H \) are those of Odar & Hamilton (1964) with the acceleration number, \( \text{Ac} \), and the particle Reynolds number, \( \text{Re}_p \), defined as:

\[ \text{Ac} = \frac{1}{d_p} \left| \frac{d}{dt} \left( u_p - u_f \right) \right|^2 \] \quad (4.4)

and

\[ \text{Re}_p = \frac{\rho d_p \left| u_p - u_f \right|}{\mu} \] \quad (4.5)

### 4.1.1 Simplified equation of motion

Vojir & Michaelides (1994) investigated the sensitivity of the terms in Eq. (4.2) under different conditions. It was found that when the fluid-to-particle density ratio was less than 0.002 the Bassett history term could be neglected without significant effects on the resultant particle motion. In the studies of Hurn (2006), who used Michaelides (1992) version of Eq. (4.2) for a free jet, he determined that the history term had very little effect. This is significant due to the dramatic increase in computation time this term alone causes. Run times up for ten times the duration of equivalent calculations without the history terms are experienced. Considering that the ratio of densities is much less than those of Hurn (2006):

\[ \beta = \frac{\rho_{f,\text{air}}}{\rho_{p,\text{glass}}} = \frac{1.2}{2500} = 0.00048 \]

The history term can be neglected with this assumption whilst the continuous phase is air.

Multi-phase studies such as Clift et al (1978), Burry & Bergeles (1993), Vojir & Michaelides (1994) Michaelides (1997) and Crowe et al (1995) have shown that when \( \rho_f \ll \rho_p \) the inertia and drag forces dominate the remaining terms. Hence, in gas-solid calculations it is common to
also remove the added mass and pressure effect terms which reduces the particle equation of motion to Eq. (4.6):

\[
\frac{du_{p,i}}{dt} = -\frac{3}{4d_p} \beta C_D \left( u_{p,i} - u_{f,i} \right) \left| u_{p,i} - u_{f,i} \right| + (1 - \beta) g_i + F_{x,i}
\]  

(4.6)

Additional forces, \( F_x \), such as Saffman, \( F_L \), and Magnus (Lun, 2000) lift have been considered in the studies mentioned above, although their contribution remains small compared to the drag term. The Saffman term accounts for lift due to shear forces in the flow. When the flow undergoes shear, high velocity gradients induce pressure differences on the surface of the particle which causes lift. The common expression for the Saffman lift is defined by Eq. (4.7):

\[
F_{L,i} = \frac{2\beta K \sqrt{\nu S_{ij}}}{d_p \left( S_{ik} S_{kj} \right)^{0.25}} \left( u_{f,j} - u_{p,j} \right)
\]  

(4.7)

where \( K = 2.594 \) is a constant coefficient by Saffman (1965) and \( S_{ij} \) is the strain rate tensor, defined in Section 3.2.1. This form of the lift force is intended for small particle Reynolds numbers, typically less than the square root of the fluid Reynolds number based on the shear field and is intended for use with submicron particles. Magnus lift accounts for lift generated due to the rotation of the particle. As such effects are not considered in the present work, it is not investigated further.

Solving Eq. (4.6) will yield the velocity which can then be used to track the particle’s trajectory defined by Eq. (4.8)

\[
\frac{dx_i}{dt} = u_{p,i}
\]  

(4.8)

The simplified particle equation of motion does not consider two-way coupling, which requires a momentum exchange term with the fluid.

**4.1.2 Drag coefficient**

The drag term in Eq. (4.2) represents the acceleration or deceleration of a particle in a fluid flow when \( u_f > u_p \) or \( u_f < u_p \) respectively. The drag coefficient, \( C_D \), which studies, reviewed by Lareo et al (1997), have attempted to characterise, is an empirical coefficient to account for the discrepancies found when using the equation of motion. In reality it is not possible to separate the forces into drag, added mass and Basset history components however, it is argued that the
coefficients that have been determined from studies such as that of Odar & Hamilton (1964) are obtained from experimental observation and therefore originate in physically real multi-phase flows. Furthermore, the improvement often seen with the drag coefficient cannot be denied, as discussed by Michaelides (1997). Figure 4.1 illustrates the variation of the complete $C_D$ term as a function of particle Reynolds number:

![Figure 4.1 – Drag coefficients for a smooth solid sphere at various Reₚ for incompressible flow](image)

Repeated here for convenience is the common definition of the drag coefficient.

$$ C_D = \frac{24}{\text{Re}_p} f_D $$  \hspace{1cm} (4.9)

The correction factor, $f_D$, for the drag coefficient is obtained from Figure 4.1 to relate the drag to the particle Reynolds number. Brenn et al (2003) reviewed the following most common equations for $f_D$ that are given as:

\begin{align*}
 f_D &= 1 & \text{Re}_p &\leq 0.2 \\
 f_D &= \left(1 + 0.1 \text{Re}_p^{0.99}\right) & 0.2 < \text{Re}_p &\leq 2 \\
 f_D &= \left(1 + 0.11 \text{Re}_p^{0.81}\right) & 2 < \text{Re}_p &\leq 21 \\
 f_D &= \left(1 + 0.189 \text{Re}_p^{0.632}\right) & 21 < \text{Re}_p &\leq 200 \\
 f_D &= \left(1 + 0.15 \text{Re}_p^{0.687}\right) & 200 < \text{Re}_p &\leq 1000 \\
 f_D &= 0.44 \times \text{Re}_p / 24 & 1000 < \text{Re}_p &\leq 3 \times 10^5 \\
 f_D &= 0.1 \times \text{Re}_p / 24 & \text{Re}_p &> 3 \times 10^5
\end{align*}  \hspace{1cm} (4.10)
Based on a recent review by Barati et al (2014) and the work of Clift et al (1978) \( f_D \) for the region \( 200 < \text{Re}_p \leq 1000 \) is frequently employed as it encompasses the majority of gas-solid flows. These factors are only suitable for spherical particles. For non-spherical particles other correlations such as those developed by Haider & Levenspiel (1989) can be used, although investigation of particle shape is beyond the scope of the current work.

### 4.1.3 Particle-wall interaction

The present research considers smooth surfaces and hard spherical particles. This means that particle deformation does not occur upon collision with a surface. The particle collides with a surface when its position is \( d_p/2 \) from the surface. When the particle collides it loses momentum before rebounding back into the domain. In the current research, experimental values for the coefficient of restitution, \( C_R \) have been used. From experimental studies measurements of the normal and tangential coefficients of restitution are obtained as polynomial functions of the form

\[
C_{R,n} = \frac{u_{n,2}}{u_{n,1}} = a_n + b_n \alpha^2 + c_n \alpha^3 + d_n \alpha^4 + \ldots
\]

\[
C_{R,t} = \frac{u_{t,2}}{u_{t,1}} = a_t + b_t \alpha^2 + c_t \alpha^3 + d_t \alpha^4 + \ldots
\]

(4.11)

where \( \alpha \) is the particle angle of incidence and the coefficients \( a_n, b_n, c_n, d_n \) and \( a_t, b_t, c_t, d_t \) are dependent on the particle and surface properties and determined by experimental analysis. The values used in the present work are those of Grant & Tabakoff (1975):

\[
C_{R,n} = 0.993 - 1.76 \alpha^2 + 1.56 \alpha^3 - 0.49 \alpha^4
\]

\[
C_{R,t} = 0.988 - 1.66 \alpha^2 + 2.1 \alpha^3 - 0.67 \alpha^4
\]

(4.12)

These coefficients correspond to spherical high silica sand particles impacting a smooth steel surface. These experimental conditions are suitably close enough to the current computational setup to permit their use. The resultant velocity after collision with the wall is then given by Eqs. (4.13), (4.14) and (4.15):

\[
u_{n,2} = -C_{R,n} u_{n,1}
\]

(4.13)

\[
u_{t,2} = C_{R,t} u_{t,1}
\]

(4.14)
\[ u_{s,2} = C_{R,s}u_{s,1} \]  

where \( u_{s,1} \) and \( u_{s,2} \) correspond to the initial and resultant velocity in the third dimension for full 3-dimensional simulations (LES).

### 4.2 Fluent: Discrete phase modelling

#### 4.2.1 Integral time

Ansys Fluent predicts the trajectory of a discrete particle by stepwise integration of the particle equation of motion – Eq. (4.6) – over a specific time scale. The particle trajectories are computed based on a fixed continuous-phase and use a Lagrangian frame of reference for the particle. The integral time scale used to determine the trajectory of the particle is defined by the time spent in turbulent motion along the particle path. In the present research the integral time becomes the fluid Lagrangian integral time, or the lifetime of a characteristic eddy, since particles are anticipated to move with the fluid. This is defined as:

\[ \Delta t_L = 0.3 \frac{k}{\varepsilon} \]  

when using the RSTM. The value of 0.3 can vary depending upon the turbulence model being used and is the source of some difficulty when setting up this model. A value of 0.15 is used when the \( k-\varepsilon \) turbulence model is used. These values originate from Daly & Harlow (1970). As \( k \) increases, the scale of turbulence increases, as one should expect. The discrete random walk model uses a random variation about \( \Delta t_L \) to determine the characteristic lifetime of the eddy as:

\[ \tau_e = -\Delta t_L \ln(\xi) \]  

where \( \xi \) is a random number between 0 and 1. Assuming a large enough number of particles is used, the directionality and chaotic effects of turbulence can be captured by the particle dispersion. The particle is assumed to interact with the fluid phase eddy for the duration of Eq. (4.17) at which point a new value for \( \Delta t_L \) is needed. The larger this value is, the fewer times this calculation must be done, which can potentially lose the influence of the smaller turbulent features but result in slightly faster computation times.
4.2.2 Discretisation scheme

Solving the equation of motion, Eq. (4.6), in Ansys Fluent can be approached in a number of ways. Trapezoidal discretisation, Analytical and Runge-Kutta schemes are available.

In the \textit{trapezoidal discretisation scheme} the relative velocity between fluid and particle is taken as the average values over two time-steps. This changes the explicit equation for the new particle velocity and location.

The \textit{Analytical discretisation scheme} has been chosen in the present work. Integrating Eq. (4.6) and Eq. (4.8) over small time steps using the analytical discretisation scheme yields the form of Eq. (4.18) and Eq. (4.19) for the new velocity and location at the end of the timestep:

\begin{equation}
\begin{aligned}
u_{p,i}^{n+1} &= \nu_{p,i}^n + \exp^{\frac{-\Delta t}{\tau_p}} \left( \nu_{p,i}^n - \nu_{f,i}^n \right) - \tau_p^* \left( \exp^{\frac{-\Delta t}{\tau_p}} - 1 \right) g_i \\
\end{aligned}
\end{equation}

\begin{equation}
\begin{aligned}
x_{p,i}^{n+1} &= x_{p,i}^n + \Delta t \left( \nu_{f,i}^n + \tau_p^* g_i \right) + \tau_p^* \left( 1 - \exp^{\frac{-\Delta t}{\tau_p}} \right) \left( \nu_{p,i}^n - \nu_{f,i}^n - \tau_p^* g_i \right) \\
\end{aligned}
\end{equation}

In these equations the superscript \( n \) denotes velocities and locations at the previous time step. No additional forces are considered in the particle equations with Fluent. The particle response time, \( \tau_p \), contains the drag coefficient in this format hence it is denoted \( \tau_p^* \) and defined as Eq. (4.20):

\begin{equation}
\beta_p^* D_a = \frac{18 \mu}{\rho_p} \frac{d_p^2}{C_D^*} 
\end{equation}

without the drag coefficient in the particle response time equation, it is simply referred to as \( \tau_p \). Ansys Fluent uses the drag coefficient law for smooth spherical particles by Morsi & Alexander (1972) defined by Eq. (4.21) which differs from the definition stated previously as Eq. (4.3) hence the superscript *:

\begin{equation}
C_D^* = a_1 + \frac{a_2}{Re} + \frac{a_3}{Re^2} 
\end{equation}

where the constants \( a_1, a_2 \) and \( a_3 \) apply over several ranges of Reynolds numbers and are dynamically chosen to suit the local Reynolds number. The values of these constants are given in Table 4.1.
<table>
<thead>
<tr>
<th>Range</th>
<th>$a_1$</th>
<th>$a_2$</th>
<th>$a_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0 &lt; \text{Re} &lt; 0.1$</td>
<td>0</td>
<td>24</td>
<td>0</td>
</tr>
<tr>
<td>$0.1 &lt; \text{Re} &lt; 1$</td>
<td>3.69</td>
<td>22.73</td>
<td>0.0903</td>
</tr>
<tr>
<td>$1 &lt; \text{Re} &lt; 10$</td>
<td>1.222</td>
<td>29.1667</td>
<td>-3.8889</td>
</tr>
<tr>
<td>$10 &lt; \text{Re} &lt; 100$</td>
<td>0.6167</td>
<td>46.5</td>
<td>-116.67</td>
</tr>
<tr>
<td>$100 &lt; \text{Re} &lt; 1000$</td>
<td>0.3644</td>
<td>98.33</td>
<td>-2778</td>
</tr>
<tr>
<td>$1000 &lt; \text{Re} &lt; 5000$</td>
<td>0.357</td>
<td>148.62</td>
<td>-47500</td>
</tr>
<tr>
<td>$5000 &lt; \text{Re} &lt; 10000$</td>
<td>0.46</td>
<td>-490.546</td>
<td>578700</td>
</tr>
<tr>
<td>$\text{Re} \geq 10000$</td>
<td>0.5191</td>
<td>-1662.5</td>
<td>5416700</td>
</tr>
</tbody>
</table>

Table 4.1 – Constant values by Morsi & Alexander (1972) used with the drag coefficient equation in Fluent

Iteratively solving these equations gives a particle trajectory profile from which velocity and turbulent statistics can be measured. The time step should be sufficiently small to achieve a good resolution of the particle movement through the domain.

The Runge-Kutta method by Cash & Karp (1990) is also available within Fluent. This well established method for numerical integration includes a family of formulae of increasing order which determine the error margins as the calculation progresses. This process ensures the error is controlled to within a very small tolerance whilst the particle equation of motion is being solved.

Particle starting location is specified by the type of distribution. A uniform distribution over the surface of the inlet has been specified for the calculations with Fluent. They have been prescribed an initial velocity equal to the bulk velocity of the fluid as this is the requirement for the surface injection of particles in Fluent. There is no particle size distribution and particle diameter is fixed (no reaction or agglomeration). Table 4.2 summarises the particle characteristics used in the Fluent predictions.

<table>
<thead>
<tr>
<th>Particle diameter, $d_p$</th>
<th>Bulk velocity, $U_b$</th>
<th>Density, $\rho_p$</th>
<th>Stokes number, $\text{St}$</th>
<th>Particle Reynolds number, $\text{Re}_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20µm</td>
<td>13.4 m/s</td>
<td>2500 kg/m³</td>
<td>1.4</td>
<td>13.5</td>
</tr>
<tr>
<td>40µm</td>
<td>13.4 m/s</td>
<td>2500 kg/m³</td>
<td>5.8</td>
<td>27.0</td>
</tr>
</tbody>
</table>

Table 4.2 – Summary of the particle characteristics used for predictions within Fluent.

These particle characteristics correspond to a very simple and ideal multi-phase system. From idealised setups such as these, the behaviour of the equations of motion and the random walk model can be analysed without too many additional factors to consider.
4.2.3 Discrete random walk model

Within Ansys Fluent there are two ways of modelling the turbulent dispersion of particles: the cloud model and the discrete random walk (DRW) model. Whilst the former has its uses in some circumstances in the present work it is limited. Engineering applications very often exhibit specific particle characteristics which are extremely difficult to characterise. Hence the particle properties (such as shape, roughness, rheology etc...) are often simplified to basic spherical particles, unbinding and elastic collisions. With such simplification, the physics is easier to implement and thus calculation times are decreased. With the addition of UDFs (user defined functions) in Fluent, CFD users can capture interesting particle phenomena, although this requires detailed knowledge of particle properties which are not always known. In the nuclear industry, where sampling and characterisation experiments are extremely difficult, it is standard to use simulants or simplified particles which can show the general or governing behaviour of particles in certain systems. These can later be compared to predictions of particles with different properties to see what impact different features have on the solution.

The cloud model obtains a mean trajectory from a particle inlet point into the domain and attributes a ‘cloud’ of particles about it. The cloud is represented by a probability density function Gaussian distribution to model the dispersion using statistical methods. Due to the lack of applicability and poor preliminary results using this model it was not used further in this work.

Modelling turbulent dispersion using DRW has the advantage of providing ‘instantaneous’ particle locations as the simulation progresses. For a representative number of particles these can then be averaged to develop mean velocity and turbulent velocity fluctuating profiles for the particles. To solve the equation of motion for the velocity of the particle and thus solve the particle trajectory, instantaneous velocities are required. As the solution has been generated with RANS turbulence models, all values for the velocity are averaged, thus an artificial instantaneous value must be used. The approach to generate artificial instantaneous velocities is essential to the reliability of the physics. The fluctuations must account for the local turbulence. The values of the artificial instantaneous velocity are sampled from a Gaussian distribution of either \( \sqrt{(2/3)k} \) in the case of \( k-\varepsilon \) or \( k-\omega \) models or from the Reynolds stresses if an RSTM is used. The former requires an assumption of isotropy whilst if the RSTM is used the velocity fluctuations take into account the directionality of the turbulence and hence the anisotropy of the Reynolds stresses, Eq. (4.22):

\[
\mathbf{u}_i = \bar{\xi} \sqrt{\bar{u}_i^2}
\]

(4.22)
where $\xi$ represents a normally distributed random number which obeys a Gaussian probability distribution. The distribution of $\xi$ could not be tested as it is built within the Fluent source code. Many commercial codes do not release the source code or allow it to be altered in any form.

### 4.3 Stream: Lagrangian particle tracker

#### 4.3.1 Michaelides particle equation of motion

For the single-phase predictions from the Stream code the particle trajectories are solved with a post-processing calculation using the Rely particle tracking code. The calculation is one-way coupled; therefore the tracker reads a fully converged (and averaged) solution from the Stream code and introduces particles. The Rely code has two options for the particle equation of motion. The first is a simplified equation, which only considers the drag force on the particle. When using the simplified equation, the calculation time is reduced dramatically. The second is the Michaelides (1992) version of Eq. (4.2) which uses a Laplace transform to provide an explicit equation for the relative velocity, $w_i$, thus reducing the computational time required due to the integral term. The resultant expression is defined by Eq. (4.23):

$$
\frac{d^2 w_i}{dt^2} + \lambda \left( 2C_D - \beta \frac{p\lambda C_H^2}{2} \right) \frac{dw_i}{dt} + \lambda^2 C_D^2 w_i = \lambda (1-\beta) \frac{d^2 u_{f,i}}{dt^2} - \lambda^2 (1-\beta) C_D \frac{du_{f,i}}{dt} + \lambda^2 (1-\beta) C_H \sqrt{\frac{9}{2\pi t}} \beta \left[ (1-\beta) \frac{du_{f,i}}{dt} - \lambda (1-\beta) G_i \right] + \lambda^3 C_D (1-\beta) G_i
$$

(4.23)

The coefficients $C_D$ and $C_H$ have already been stated previously - Eq.(4.3). The coefficients are those established experimentally by Odar & Hamilton (1964) and have since been verified by Tsuji et al (1991). They have also been used in the form of Eq. (4.23) for an axisymmetric jet by Hurn & Fairweather (2008). Note the absence of the added mass term, hence $C_A$ is not required. The initial acceleration is given by Eq. (4.24):

$$
\frac{dw_i}{dt} = -\lambda (1-\beta) \frac{du_{f,i}}{dt} + \lambda (1-\beta) G_i
$$

(4.24)
where the relative velocity, \( w_i = u_{f,i} - u_{p,i} \), \( \lambda = 1/(1 + 0.5 \beta) \) and \( G_i = g \tau_p / U_0 \). As previously stated, in the present work the Basset history term is also neglected, hence Eq. (4.23) reduces to Eq. (4.25):

\[
\frac{d^2 w_i}{dt^2} + \lambda 2 C_D \frac{dw_i}{dt} + \lambda^2 C_D^2 w_i = \lambda (1 - \beta) \frac{d^2 u_{f,i}}{dt^2} - \lambda^2 (1 - \beta) C_D \frac{du_{f,i}}{dt} + \lambda^2 C_D (1 - \beta) G_i
\]

(4.25)

Eq. (4.25) is now explicit in \( w_i \) and contains the second order differential of the fluid velocity. Despite this there is no need for an iterative approach to solving the history term as with Eq.(4.2). However, the equation needs to be solved many times for many particles to obtain statistically smooth averaged results. Using the coefficient, \( C_D \), makes Eq. (4.25) semi-empirical in nature and therefore additional forces cannot be added, such as Saffman lift. Arguably Saffman lift is only relevant for submicron particles which would make its impact in the present work negligible. Magnus lift force is another which accounts for the rotation of particles. Particle rotation has not been considered in the present work. Such effects were considered beyond the scope of this work and would require in-depth knowledge of the particle characteristics and mechanics.

### 4.3.2 Discretisation scheme and integral time

The equation of motion given above is solved using a fourth order Runge-Kutta method for second order differential equations. When applied to Eq. (4.25) this is given by Stroud (1990) as:

\[
k_1 = \frac{1}{2} \Delta t^2 f \left\{ t_n^*, w_n^*, \frac{dw_n}{dt} \right\} = \frac{1}{2} \Delta t^2 \frac{d^2 w_n}{dt^2}
\]

\[
k_2 = \frac{1}{2} \Delta t^2 f \left\{ t_n^* + \frac{1}{2} \Delta t^*, w_n^* + \frac{1}{2} \Delta t^* \frac{dw_n}{dt} + \frac{1}{4} k_1, \frac{dw_n}{dt} + \frac{k_1}{\Delta t^*} \right\}
\]

\[
k_3 = \frac{1}{2} \Delta t^2 f \left\{ t_n^* + \frac{1}{2} \Delta t^*, w_n^* + \frac{1}{2} \Delta t^* \frac{dw_n}{dt} + \frac{1}{4} k_1, \frac{dw_n}{dt} + \frac{k_2}{\Delta t^*} \right\}
\]

\[
k_4 = \frac{1}{2} \Delta t^2 f \left\{ t_n^* + \Delta t^*, w_n^* + \Delta t^* \frac{dw_n}{dt} + k_3, \frac{dw_n}{dt} + \frac{2k_3}{\Delta t^*} \right\}
\]

(4.26)
Using these definitions, \( P \) and \( Q \) can be determined:

\[
P = \frac{1}{3} (k_1 + k_2 + k_3)
\]

\[
Q = \frac{1}{3} (k_1 + 2k_2 + 2k_3 + k_4)
\]  

(4.27)

and finally:

\[
t^{*,n+1} = t^{*,n} + \Delta t^*
\]

\[
w_i^{n+1} = w_i^n + \Delta t^* \frac{dw_i^n}{dt} + P
\]

\[
\frac{d w_i^{n+1}}{dt} = \frac{d w_i^n}{dt} + \frac{Q}{\Delta t^*}
\]  

(4.28)

The superscripts \( n \) and \( n+1 \) represent the values at the beginning and the end of the calculation time-step respectively. \( \Delta t^* \) is the time-step used for the fluid particles and is kept below \( 0.1 \tau_p \). This has been shown to be sufficient to capture the motion of the particle by Macinnes & Bracco (1992). The initial condition \( w_i^n \) is known as its derivative is found using Eq.(4.24).

### 4.3.3 Particle dispersion model

Much like the DRW model used with Fluent, instantaneous velocities are needed to solve the particle equation of motion. The particle tracker generates random velocity fluctuations to create an instantaneous velocity field around the particle. To obtain these values the Burry & Bergeles (1993) method is used. Developed from the work of Zhou & Leschziner (1991) the model is designed to account for the time-based correlation of fluctuating velocities of the fluid. This covers the directionality of the turbulence and the anisotropy of the Reynolds stresses. Similar to the Berlemont (1990) form the correlation function is simplified and does not need to retain the fluctuating values of previous timesteps to account for the Basset history term. A study by MacInnes & Braco (1992) observed that the more complex approach did not present much improvement when compared against experimental data and was not worth the added computation time and cost. The model used is described in detail here.

The fluid and discrete particle velocity fluctuation at the particle position can be related to the previous fluctuations by Eq. (4.29) and (4.30) respectively:

\[
\dot{u}_{f,t} = \{ \beta \} \dot{u}_{f,t-\delta t} + d_t
\]

(4.29)
\[ u'_{p,t} = \{\gamma\} u'_{f,t} + e_t \]  

where \(\{\beta\}\) accounts for the influence of the velocity fluctuation at the previous time step/location, \(\{\gamma\}\) the effects arising from the departure of the discrete particle from the fluid particle and the second terms in both equations represent the randomness of the turbulence during \(\delta t\) and at \(t\) respectively.

Multiplying Eq. (4.29) and (4.30) by the transpose of \(u'_{f,t-\delta t}\) and \(u'_{f,t}\) respectively and time averaging gives:

\[
\overline{u'_{f,t} u'^T_{f,t-\delta t}} = (\{\beta\} u'_{f,t-\delta t} + d_t) u'^T_{f,t-\delta t} \equiv \{C\} \tag{4.31}
\]

\[
\overline{u'_{p,t} u'^T_{f,t}} = (\{\gamma\} u'_{f,t} + e_t) u'^T_{f,t} \equiv \{D\} \tag{4.32}
\]

The right hand side become:

\[
(\{\beta\} u'_{f,t-\delta t} + d_t) u'^T_{f,t-\delta t} = \{\beta\} u'_{f,t-\delta t} u'^T_{f,t-\delta t} + d_t u'^T_{f,t-\delta t} = \{\beta\} \text{cov}_{u'_{f,t-\delta t}} + 0 \tag{4.33}
\]

\[
(\{\gamma\} u'_{f,t} + e_t) u'^T_{f,t} = \{\gamma\} u'_{f,t} u'^T_{f,t} + e_t u'^T_{f,t} = \{\gamma\} \text{cov}_{u'_{f,t}} + 0 \tag{4.34}
\]

The final terms in Eq. (4.33) and (4.34) become zero as \(d_t\) has no correlation with fluctuations from the previous time step and \(e_t\) has no correlation with the fluctuation at the fluid particle position at time \(t\). In these equations, \(\text{cov}\) refers to a covariance matrix. These matrices for the respective equations are:

\[
\{\text{cov}\}_{u'_{f,t-\delta t}} = \overline{u'_{f,t-\delta t} u'^T_{f,t-\delta t}} = \begin{pmatrix}
\overline{u_1^2} & \overline{u_1 u_2} & \overline{u_1 u_3} \\
\overline{u_2 u_1} & \overline{u_2^2} & \overline{u_2 u_3} \\
\overline{u_3 u_1} & \overline{u_3 u_2} & \overline{u_3^2}
\end{pmatrix}_{t-\delta t} \tag{4.35}
\]

\[
\{\text{cov}\}_{u'_{f,t}} = \overline{u'_{f,t} u'^T_{f,t}} = \begin{pmatrix}
\overline{u_1^2} & \overline{u_1 u_2} & \overline{u_1 u_3} \\
\overline{u_2 u_1} & \overline{u_2^2} & \overline{u_2 u_3} \\
\overline{u_3 u_1} & \overline{u_3 u_2} & \overline{u_3^2}
\end{pmatrix}_t \tag{4.36}
\]
These matrices can be evaluated using the time averaged values for the Reynolds and shear stresses obtained in the single-phase solution with the RANS Stream code. Combining Eqs. (4.31) and (4.33) then Eq. (4.32) and (4.34) gives:

\[
\{C\} = \{\beta\}\{\text{cov}\}_{t_{ij}} \Rightarrow \{\beta\} = \{C\}\{\text{cov}\}_{t_{ij}}^{-1}
\]

(4.37)

\[
\{D\} = \{\gamma\}\{\text{cov}\}_{t_{ij}} \Rightarrow \{\gamma\} = \{D\}\{\text{cov}\}_{t_{ij}}^{-1}
\]

(4.38)

Directional, temporal and spatial correlation coefficients must now be defined for Eqs. (4.37) and (4.38). The common approach used for approximating the coefficients (generally denoted, \( R \)) is the Frenkiel function – Eq. (4.39) and (4.40). This is what enables the model to perform under anisotropic turbulent conditions. The directional and temporal correlation can be defined as (with no summation in \( i \) and \( j \) for the following):

\[
R_{ij} = \frac{u_{i,j}u_{i,j-\delta}}{u_{i,j-\delta}u_{i,j}} = \exp \left[ -\frac{\delta t}{(m^2 + 1)\tau_{L,ij}} \right] \cos \left[ \frac{m\delta t}{(m^2 + 1)\tau_{L,ij}} \right]
\]

(4.39)

and for the spatial correlation (also no summation in \( i \) and \( j \)):

\[
R_{ij} = \frac{u_{p,i}u_{p,j}}{u_{p,i}u_{p,j}} = \exp \left[ -\frac{r}{(m^2 + 1)L_{E,ij}} \right] \cos \left[ \frac{mr}{(m^2 + 1)L_{E,ij}} \right]
\]

(4.40)

In Eq. (4.39) \( \tau_L \) is the Lagrangian time scale and \( m \) is a parameter which determines the number of negative loops in the correlation function. This is related to the type of flow being modelled, where isotropic conditions use \( m = 0 \). When \( m \) is nonzero, the set of functions described herein are used. Picart et al (1986) expand upon the value of \( m \) and state that it is considered a closure constant, the value of which should be obtained from experiments. However, they also note that its value must be less than 3.644 to avoid negative dispersion coefficients. In the present work, it is assigned the recommended value, \( m = 1 \) (Calabresse & Middleman, 1979; Gouesbet et al, 1984). The denominator on the left hand side of both Eq. (4.39) and (4.40) is known from the RANS solution. \( \tau_{L,ij} \) and \( L_{E,ij} \) are defined by Eqs. (4.41) and (4.42) respectively:

\[
\tau_{L,ij} = C_L \frac{u_i^2 + u_j^2}{2\varepsilon}
\]

(4.41)

\[
L_{E,ij} = C_{\varepsilon} \tau_{L,ij} \sqrt{\frac{u_i^2 + u_j^2}{2}}
\]

(4.42)
where \( i, j = 1, 2, 3 \) and \( u_1, u_2, u_3 = u, v, w \) and \( i \neq j \). In this case, it does not imply summation notation. \( C_2 \) is taken as 0.2 for turbulent flows (including jets) and \( C_{ij} \) is a constant dependent upon the turbulence field and scale though usually taken as 1. The definitions of \( \tau_{L,ij} \) and \( L_{E,ij} \) are the primary difference between the Berry & Bergeles (1993) model and Zhou & Leschziner’s (1991, 1996 and 1997) model. This approach normalise the velocity correlations with the corresponding Reynolds stress, whilst Zhou & Leschziner’s model normalised the velocity correlations by the r.m.s velocities in the directions of \( i \) and \( j \). In the case of the latter it is not surprising to get negative values for the Lagrangian cross time-scales, hence the method of Berry & Bergeles has been adopted. With these equations we can now calculate the matrices \( \{\beta\} \) and \( \{\gamma\} \) from Eq. (4.37) and (4.38) leaving \( d \) and \( e \) to be determined.

We can obtain the values for \( d \) and \( e \) by a similar process to that outlined already. Rearranging Eq. (4.29) and (4.30) for \( d \) and \( e \) gives Eq.

\[
d_t = u'_{f,j} - \{\beta\} u'_{f,j-\delta t} \tag{4.43}
\]

\[
e_t = u'_{p,j} = \{\gamma\} u'_{f,j} \tag{4.44}
\]

Multiplying Eq. (4.43) and (4.44) by their respective transposes and time averaging similarly to Eq. (4.35) and (4.36).

\[
\overline{d_t d_t^T} = \{\text{cov}\}_d \tag{4.45}
\]

\[
\overline{e_t e_t^T} = \{\text{cov}\}_e \tag{4.46}
\]

and

\[
(u'_{f,j} - \{\beta\} u'_{f,j-\delta t})(u'^T_{f,j} - \{\beta\} u'^T_{f,j-\delta t}) = u'_{f,j} u'^T_{f,j} - u'_{f,j} u'^T_{f,j-\delta t} \{\beta\}^T - \{\beta\} u'_{f,j-\delta t} u'^T_{f,j} + \{\beta\} u'_{f,j-\delta t} u'^T_{f,j-\delta t} \{\beta\}^T \tag{4.47}
\]

\[
(u'_{p,j} - \{\gamma\} u'_{f,j})(u'^T_{p,j} - \{\gamma\} u'^T_{f,j}) = u'_{p,j} u'^T_{p,j} - u'_{p,j} u'^T_{f,j} \{\gamma\}^T - \{\gamma\} u'_{f,j} u'^T_{p,j} + \{\gamma\} u'_{f,j} u'^T_{f,j} \{\gamma\}^T \tag{4.48}
\]

Combining Eq. (4.45) and (4.47) and Eq. (4.46) and (4.48) with our definitions for \( \{C\} \) and \( \{D\} \) the following equations can be written:
\[
\{\text{cov}\}_d = \{\text{cov}\}_{w_{ij}} - \{\text{cov}\}_{w_{ij}} \{C\}^T - \{C\} \{\text{cov}\}_{w_{ij}} \{\beta\}^T + \{\text{cov}\}_{w_{ij}} \{\beta\}^T
\]
\[
= \{\text{cov}\}_{w_{ij}} - \{\beta\} \{C\}^T
\]
(4.49)

\[
\{\text{cov}\}_e = \{\text{cov}\}_{w_{ij}} - \{\gamma\} \{D\}^T - \{D\} \{\text{cov}\}_{w_{ij}} \{\gamma\}^T + \{\text{cov}\}_{w_{ij}} \{\gamma\}^T
\]
\[
= \{\text{cov}\}_{w_{ij}} - \{\gamma\} \{D\}^T
\]
(4.50)

All the terms on the right hand sides of Eq. (4.49) and (4.50) are known which allows us to calculate the vectors \(d_t\) and \(e_t\). These are constructed to perform as a Gaussian conditional probability density function shown by Eq. (4.51):

\[
P(d_t) = \frac{1}{(2\pi)^{N/2}|\text{cov}_{d_t}|^{1/2}} \exp \left\{ -\frac{1}{2} (d_t)^T \{\text{cov}\}_{d_t}^{-1} (d_t) \right\}
\]
(4.51)

where \(N\) is the number of dimensions under consideration. In the present work for the Stream RANS and following Rely particle tracking, the calculation is solved in 2 dimensions. Considering \(Z\), a set of random variables with independent standard normal distribution, Eq. (4.51) may be written as:

\[
d_t = \{b\} Z
\]
(4.52)

where the components of \( \{b\} \) are correlated and can be found by multiplying Eq. (4.52) with the transpose of \(d_t\) then time averaging. The components of the resultant matrix are given as follows:

\[
b_{11} = \sqrt{d_{11}^2}
\]
\[
b_{12} = 0
\]
\[
b_{13} = 0
\]
\[
b_{21} = \frac{(d_{11}d_{12})}{b_{11}}
\]
\[
b_{22} = \frac{(d_{12}^2 - b_{21}^2)}{b_{21}}
\]
\[
b_{23} = 0
\]
(4.53)

\[
b_{31} = \frac{(d_{11}d_{13})}{b_{11}}
\]
\[
b_{32} = \frac{(d_{12}d_{13} - b_{21}b_{13})}{b_{22}}
\]
\[
b_{33} = \frac{(d_{13}^2 - b_{31}^2 - b_{32}^2)}{b_{22}}
\]

(4.53)

The cross correlations needed for the above set of equations can be determined from the elements of Eq. (4.49). Exactly the same method is used to determine \(e_t\):

\[
e_t = \{s\} Z
\]
(4.54)

where the elements of \( \{s\} \) are shown in Eq. (4.55) and the cross correlations required are obtained from Eq. (4.50).
With this definition, all that is required for solutions to Eqs. (4.29) and (4.30) is to obtain the fluctuating velocity for the particle.

### 4.3.4 Random numbers & Gaussian distribution implementation

What is important in any stochastic process including the one outlined above is the generation of random numbers. It is near impossible to create a number generator that is truly random, although one can ensure that the pattern does not repeat for a large enough number of calls to prevent noticeable signs of bias. The random number generator used in the present thesis is that of Press et al (1992) and uses real numbers between 0 and 1.0 as inputs. It does not repeat for at least 14 million calls. The random number generator has been tested for 100,000 calls where the normalised results are displayed in Figure 4.2.

![Figure 4.2 - Results from test of random number generator](image)

The implementation of this method has been evaluated and tested for free jets by Hurn (2006). The random number is used with an approximation for the inverse normal distribution function. The function was proposed by Acklam (2002) and is based on rational approximations. Hurn (2006) reported relative errors of less than $1.15 \times 10^{-9}$ in testing it for 100,000 results. The Gaussian distribution was sampled using a uniform random variant. This is used as an input to
the inverse normal distribution function to obtain a value for the standard normal deviation (Z).
In the present work this was tested for 100,000 results and the samples are displayed in Figure 4.3

![Sampled Gaussian distribution](image)

Figure 4.3 – Sampled Gaussian distribution

The bars in Figure 4.3 represent normalised sampled frequency of $Z$ whilst the solid line indicates the theoretical Gaussian distribution. It is clear from this illustration that the agreement is excellent and reflects what Hurn (2006) determined in his preliminary studies.

### 4.4 Boffin: Lagrangian particle tracker

The Boffin Lagrangian particle tracker uses a semi-analytical method similar to the one outlined in Section 4.2. Eq. (4.6) and (4.8) are integrated over time-steps small enough to resolve the particle relaxation time and fluid velocity constant. The time-step is divided into smaller subintervals at which the particle position, velocity and angular velocity are calculated. Between each subinterval it must assumed that the drag coefficient remains constant. For this to be valid the subintervals of time must be sufficiently small, for instance, 50% of the particle relaxation time and the integral time scale of turbulence. This lowers the risk of numerical instabilities.

The particle integration time step is:

$$
\Delta t_L = \min \left( \frac{\Delta x}{u_p}, \tau_p, \tau_v, \tau_r \right)
$$

(4.56)
where $\Delta x$ is the minimal distance across a computational cell, $\tau_e$ and $\tau_p$ have been previously defined (Eqs. (4.17) and (4.20) respectively). Boffin also considers the transit time, $\tau_r$, in the magnitude of the time-step. It is determined from the linearised form of the particle momentum equation (Gosman & Ioannides, 1981; Naik & Bryden, 1999) Eq. (4.57):

$$\tau_r = -\tau_p \ln \left(1 - \frac{C_L}{\tau_p [\bar{u}_{f,i} - \bar{u}_{p,i}]} \right)$$  \hspace{1cm} (4.57)

Unlike Fluent, the Boffin LPT relates $C_L$ to the turbulence through:

$$C_L = C_{\mu}^{3/4} \frac{k^{3/2}}{\varepsilon}$$  \hspace{1cm} (4.58)

The values of $k$ and $\varepsilon$ are assumed constant for the duration of the time-step.

The integration of Eq. (4.6) and (4.8) gives us the analytical equations for the velocity and particle position as shown by Brenn et al. (2003)

$$u_{p,i}^{n+1} = u_{p,i}^n + \left(u_{p,i}^n - u_{f,i}^n\right) \exp \left(\frac{-\Delta t}{\tau_p}\right) + \frac{3}{4} \beta \tau_p \left(1 - \exp \left(\frac{-\Delta t}{\tau_l}\right)\right) \left\{(1 - \beta) g_i, \right.$$  

$$+ \left(u_{p,i}^n - u_{f,i}^n\right) \left\{\frac{\omega_{p,y}^n - 1}{2} \frac{\partial u_{f,i}^n}{\partial z} - \frac{\partial u_{f,k}^n}{\partial x}\right\} - \left(u_{p,i}^n - u_{f,i}^n\right) \left\{\frac{\omega_{p,z}^n - 1}{2} \frac{\partial u_{f,i}^n}{\partial y} - \frac{\partial u_{f,i}^n}{\partial y}\right\}\right\}$$  \hspace{1cm} (4.59)

$$x_{p,i}^{n+1} = x_{p,i}^n + \frac{1}{2} \left(u_{p,i}^{n+1} + u_{p,i}^n\right) \Delta t_L$$  \hspace{1cm} (4.60)

The moment of inertia of a spherical particle, $I_p$, is the rotational inertia integrated over the shape of the particle, for a sphere defined as:

$$I_p = 0.1 \rho_p V_p d_p^2$$  \hspace{1cm} (4.61)

This definition changes as the shape of the particle varies, however, the present work does not investigate different particle shapes other than a solid sphere. The torque, $T_{p,i}$, acting on a particle is found by differentiating the angular momentum w.r.t time and is:

$$T_{p,i} = I_p \frac{d\omega_{p,i}}{dt}$$  \hspace{1cm} (4.62)
The angular velocity is obtained through integration of Eq. (4.62) and extended by Brenn et al (2003) to a second-order equation, containing an exponential term that was shown to further improve its reliability:

$$\omega_{p,i}^{n+1} = \frac{1}{2} \nabla \times \bar{u}_{i,j}^{n+1} + \left( \omega_{p,i}^n - \frac{1}{2} \nabla \times \bar{u}_{f,i} \right) \exp \left\{ - \frac{60 \rho_f \mu_f}{\rho_p d_p^2 \Delta t_L} \right\}$$  (4.63)

Note that superscript $n$ indicates the value at the start of the subinterval and $n+1$ indicates the value at the end of the subinterval for Eq. (4.59) and (4.60). The instantaneous velocities required are obtained directly from the LES, without the need to generate synthetic turbulent velocity fluctuations as required in the RANS solution schemes.
Chapter 5  Fluent RANS results

5.1 Grid and particle number independence

It is important to establish that the final prediction is independent of the computational mesh. This is achieved with grid-independence studies. Although RANS predictions are slightly less sensitive to the computational mesh than LES, it is still a necessary requirement. This section demonstrates that the computational mesh has not influenced the predictions. Differences between data sets can then be attributed directly to the turbulence models that generated them and the results can be considered mesh independent.

Three meshes were used and classified as coarse, intermediate and fine with increasing number of cells in each. The specific details of each classification of mesh are shown in Table 3.1.

Figure 5.1 – (a-d) Grid independence profiles at 9D from centre line for (a) velocity magnitude, (b) r.m.s turbulent velocity normal-to-wall, (c) r.m.s turbulent velocity parallel-to-wall and (d) shear stress where (solid) coarse mesh, (dashed) intermediate, (dotted) fine mesh

Figure 5.1(a) shows a velocity magnitude profile at a radial distance of 9D (close to the outlet of the domain). The profile indicates that the results from all three meshes are in close agreement, with only a slight deviation for the coarse mesh. Figure 5.1(b-d) shows the turbulent r.m.s and
shear stresses at the same radial distance. These turbulent quantities are more sensitive to changes in the mesh and as such are a better indicator of grid independence. From all profiles shown in Figure 5.1 it is clearly concluded that by the intermediate mesh, grid independence has been reached. Additional nodes do not appear to make any difference to the velocity or turbulence profiles.

Since there is little to gain by using more computational cells than necessary, the intermediate mesh is taken forward for the single-phase and multi-phase models. This ensures that the computational resources are used as efficiently as possible, avoiding unnecessarily long computational times.

Figure 5.2 – Particle mean and r.m.s turbulent velocity profiles at 9D from centreline for (triangle) 40k particles and (circle) 80k particles

Particle number independence was achieved by steadily increasing the number of particles introduced into the simulation. Once the averaged profiles of the particle variables stopped changing, it could be assumed that the solution was no longer particle number dependent. Figure 5.2(a-c) shows the velocity magnitude and turbulent quantities at a radial distance of 9D for two total particle numbers. This demonstrates particle independence between 40 and 80 thousand particles specified at the inlet. In the majority of cases presented in this thesis, the number of particles was many times greater than this to remove any doubt concerning particle independence. Furthermore, particle distribution is not even throughout the domain. In certain regions, particularly just above the jet, particle numbers are low. Therefore, for smooth statistical averaging of particle data in the region above the radial wall jet, the total number of particles must be increased significantly above that required for smooth statistical averages within the wall jet.
5.2 Single-phase predictions

The plots within this section account for the continuous phase predictions for three different jet heights. The methods used have been described in Chapter 3 and the resultant predictions of each approach are discussed herein. The results have been compared with experimental data to provide validation. By validating the predictions this thesis provides a useful series of plots with which the performance of the realisable $k$-$\varepsilon$ model, linear RSTM and non-linear RSTM turbulence models can be established.

5.2.1 2D jet height

The shortest jet height offers the chance to compare the turbulence models when impingement occurs within the potential core. For this type of the jet there is no fully developed jet region and it can be difficult to distinguish the different regions of the jet. Figure 5.3 shows the development of the velocity magnitude along the centreline of the jet. The profiles convincingly reflect what has been observed in previous studies. A constant velocity along the centreline indicates the presence of the potential core, unaffected by the wall and not yet decayed by the entrainment of the surrounding quiescent fluid.

![Figure 5.3 – Velocity magnitude along the centreline of the jet](image)

Along the centreline, the fluid remains largely unaffected by the shear or Reynolds stresses and is primarily influenced by pressure reflections from the wall. There is a slight decrease in the axial velocity along the centreline and this is due to the use of a fully developed profile at the jet nozzle as opposed to a flat velocity profile. Narayanan et al (2004) and Birch et al (2005) also found this to be the case when applying a fully developed profile at the jet nozzle. The effect of this is clearer at greater jet heights and will be discussed in more detail in the following section.
The RSTM profiles show identical velocity predictions along the centreline because the mean velocity is only affected by the pressure reflections. The influence of the wall can be seen to begin at around 1.0D from the wall by a sharp reduction in the velocity magnitude. This finding is in line with other studies such as Beltaos & Rajaratnam (1974), Cooper et al (1993), Craft et al (1993) and Shademan (2013). However, this does not give us a good indication regarding the overall performance of turbulence models. Figure 5.4 to 5.7 shows profiles of the mean velocity and Reynolds stresses across the radial jet at selected radial positions, compared with experimental data. These profiles are perhaps more indicative of the turbulence model performance, and particularly at the smaller radial locations will reflect the nature of the flow around the stagnation region.

Figure 5.4 demonstrates reasonable alignment of the velocity magnitude predictions with experimental data from Cooper et al (1993). If one were to use only Figure 5.4 to determine the relative performance of each turbulence model, one might conclude that the \( k-\varepsilon \) model gives better alignment with experimental data. Indeed, both the RSTMs do poorly predict the near wall velocity maxima whilst the \( k-\varepsilon \) model predicts it reasonably well. All three models appear to predict greater levels of entrainment at larger radial distances, shown by Figure 5.4(c). This can be seen by increased velocity values towards the outer wall jet region (for \( y/D \) greater than around 0.15D), compared to the measurements. This can be attributed to elevated levels of turbulent mixing, as shall be explained. The acceleration of the radial wall jet appears to have been accurately captured by all three turbulence models with the peak velocity occurring around 1D and decelerating at \( x/D > 1 \), which is in agreement with the observations of Xu & Hangan (2008).

Whilst velocity data is extremely useful to visualise an impinging jet, it only provides indirect evidence when investigating the performance of turbulence models. The r.m.s of the turbulent velocity fluctuations give direction information on the normal Reynolds stresses. As can
initially be seen from Figure 5.5 and 5.6 all three turbulence models used overpredict the magnitude of the turbulent velocity fluctuations. The overprediction is greatest close to the stagnation region, an observation which is in line with previous studies (Craft et al, 1993).

The poor predictions close to the centreline are expected due to the complex nature of the flow around the region of irrotational straining. The deflection of the jet requires a suitable redistribution of energy from a dominantly axial direction to an axisymmetric radial direction. The linear nature of the eddy-viscosity-based stress-strain relationship limits the ability of the $k$-$\varepsilon$ model to accurately predict the normal stresses in this area. In the irrotational region, it is the product of normal Reynolds stresses and mean strains that contribute to the turbulent kinetic energy generation rate, and the misrepresentation of the normal stresses consequently leads to a significant over-prediction of (or in some locations non-physical) turbulence levels.

In the case of the RSTMs, the poor alignment with experimental data can, in part, be attributed to the handling of the pressure-strain correlation. This deficiency was previously highlighted by Craft et al (1993) as the modelling process of $\phi_{ij,w}$ as described in Chapter 3, Eq. (3.30). The $\phi_{ij,2}$ term is responsible for transferring a portion of the energy generated from the stream-wise velocity fluctuations to the planes perpendicular to the mean velocity. In the case of a stagnation flow, this is the radial and azimuth directions. To moderate the effects of this
process near the wall, $\phi_{ij,w}$ is included. In the most widely-used models for this process it essentially reduces the strength of $\phi_{ij,2}$ close to the wall. In simple shear flows, this process is acceptable and helps maintain a small value of the normal-to-wall Reynolds stress component. However, in stagnation flows the result of this $\phi_{ij,w}$ model is to reduce the transfer of energy from $\sqrt{\overline{u'^2}}$ to the radial and azimuthal planes. The primary stress generator is now in the axial direction, hence the action of $\phi_{ij,w}$ leads to a dramatic over-prediction of the r.m.s velocity fluctuations normal-to-wall which, is reflected in Figure 5.5(a-d) and the turbulent kinetic energy.

![Figure 5.6](image_url)  
**Figure 5.6** – (a-c) r.m.s turbulent velocity fluctuations parallel-to-wall at radial stations (a) 0.5D, (b) 1D and (c) 2.5D from centreline

![Figure 5.7](image_url)  
**Figure 5.7** – (a-c) Shear stress at radial stations (a) 0.5D, (b) 1D and (c) 2.5D from centreline

As the radial wall jet develops, the flow returns to a shear-dominated system. The modelling adopted for the $\phi_{ij,2}$ process is now better suited to this type of flowfield configuration, although the over-prediction of turbulence energy near the stagnation line still has a detrimental effect on the results at further radial distances. Indeed, Figure 5.5 and 5.6 show gradual improvement as the flow develops radially, albeit only slightly. Figure 5.6 illustrates the development of the r.m.s radial velocity fluctuations. It shows a similar trend as Figure 5.5, resulting in a slight
under-prediction at greater radial distances whilst all turbulence models over-predict the fluctuations in the outer part of the jet as a result of the higher turbulence upstream which has lead to too much spreading of the jet (as mentioned earlier).

It is the poor predictions of the r.m.s velocity fluctuations which result in the over-prediction of the shear stresses, shown in Figure 5.7. The elevated shear stress levels indicate a higher degree of mixing in the shear layer between the radial wall jet and the ambient fluid. This promotes the expansion of the radial wall jet which is seen in Figure 5.4(c). If a superior prediction were to be obtained in the stagnation region for the r.m.s velocity fluctuations, then this might improve the entirety of the prediction.

5.2.2 6D jet height

When the jet height is increased, a different classification of impinging jet is observed. As discussed in Chapter 2, Beltaos & Rajaratnam (1974) state that a jet height of 6D represents an impinging jet in which the potential core has just reached maximum penetration into the domain. At this point the surrounding ambient fluid has eroded the potential core to the centreline. The 6D jet height was selected to evaluate if this transitional class of impinging jet has an impact on the resulting radial wall jet near the stagnation region.

Figure 5.8 shows the centreline velocity for the 6D jet height. Similar to the 2D jet height case, the potential core is characterised by only a small decrease in the axial velocity. Many studies of free jets show this velocity to be constant along the centreline of the jet. This is usually due to the use of a flat or top-hat velocity profile at the jet nozzle. In a top hat case, a very small shear layer exists at the edge of the jet which grows as the jet develops and has a constant, flat velocity profile across the width of the nozzle. With an impinging jet, a shear layer already exists, the width of which is dependent upon the turbulence model used and the straight pipe geometry. The difference between the fully developed profile and that of a top-hat profile will undoubtedly produce a different height at which the mixing layers to reach the centreline.

When the jet becomes in range of the influence of the wall, \( y/D < 1 \), there is a sharp drop in the velocity. We can see that the increase in height adds few additional features to the centreline velocity other than a longer profile showing the centreline-velocity remain unchanged in the potential core.
Figure 5.8 – Velocity magnitude along the centreline of the jet

Perhaps more interesting is the impact the larger jet height has upon the resultant radial wall jet. The shortfalls of the turbulence models discussed in the previous section are magnified for the greater jet height, producing over-predicted values for the r.m.s velocity fluctuations. Particularly in the stagnation region the difference between experimental and predicted data is several times larger than in the 2D jet height case. At greater radial distances, the peak stress levels demonstrate acceptable agreement with the experimental data; however, the width of the radial wall jet is much greater than the experiment due to the elevated turbulence and hence mixing upstream near the stagnation region.

Figure 5.9 – (a-c) r.m.s turbulent velocity fluctuations normal-to-wall at radial stations (a) 0.5D, (b) 1.5D and (c) 3D from centreline

In the 6D jet height case, the developing jet must travel a greater distance before impingement. This allows more time for mixing between the developing jet and the ambient fluid surrounding the jet which spreads the jet to a greater radial distance. The result is a flatter velocity profile and larger turbulence levels reaching the stagnation region. The ultimate effect of this leads to a
greater rate of jet spreading in the radial wall jet which aligns well with the observations of Shademan (2013).

![Figure 5.10](image1)

Figure 5.10 – (a-c) r.m.s turbulent velocity fluctuations parallel-to-wall at radial stations (a) 0.5D, (b) 1.5D and (c) 3D from centreline

The poor predictions of the r.m.s give the velocity and shear stresses little hope of aligning with experimental data. Indeed, the velocity magnitude shown in Figure 5.11 is negatively affected by the poor turbulence predictions, resulting in worse alignment than the 2D jet case. Comparing Figure 5.11(a) against Figure 5.4(a) for the 2D jet height, one can judge that the axial velocity prior to impingement is diminished for the greater jet height. This ought to be anticipated as the jet has had further to travel and axial velocity within the mixing layer of the developing jet will deteriorate unlike within the potential core. This manifests itself as a curved profile along x/D = 0.5 as opposed to the near constant velocity profile for the 2D case.

![Figure 5.11](image2)

Figure 5.11 – (a-c) Velocity magnitude at radial stations (a) 0.5D, (b) 1.5D and (c) 3D from centreline

Once more, the poor r.m.s predictions lead to elevated levels of shear stresses observed in Figure 5.12. The experimental data at 0.5D was not reported by Cooper et al due to difficulties in differentiating the separate components in what was an extremely turbulent stagnation region.
This also impacts the velocity magnitude as can be seen at the greater radial distances, a wider radial wall jet is predicted than the experiment. With larger values of the r.m.s axial velocity fluctuations the associated error is correspondingly larger, which reflects even more poorly on the downstream properties of the impinging jet.

![Image](image.png)  
*Figure 5.12 – (a-b) Shear stress at radial stations (a) 1.5 and (b) 3D from centreline*

All three turbulence models perform poorly at this jet height, arguably more so than for the 2D jet height. Selecting a turbulence model to continue with the multi-phase studies at this point is therefore difficult. Considering the overall alignment of the predicted data with the experiments and considering the ease of obtaining the desired data from Fluent, the quadratic RSTM has been chosen to move forward with. Whilst there is little to choose between the turbulence models, it is believed that the quadratic RSTM is also the most likely to give favourable predictions for a variety of engineering flows. First however, a final data set is presented for the 10D jet height.

### 5.2.3 10D jet height

The 10D jet height is the first example of an impinging jet which demonstrates all three of the sub-regions described in Chapter 2. Very few studies consider jet heights up to 10D, possibly because the developing jet can be replicated by a free jet or the radial wall jet is of less interest at this offset. Also, as stated previously, many studies concern heat transfer with impinging jets and a jet height of 10D would present a poor configuration for heat transfer. In the current case it is desired to show the turbulence models’ ability to predict all three regions of the developing jet region as well as compare with radial wall jet data from Cooper et al (1993). Figure 5.13 shows the centreline velocity and indicates the different regions. As identified in the previous two cases, the slowly diminishing centreline velocity indicates the potential core using the fully
developed profile. There are more complex fluid mechanics going on in this regime than with a top-hat profile. The shear stress profile at the jet nozzle from the straight pipe ensures that there are shear forces acting on the centreline the moment it enters the domain, albeit small. This causes a very small gradual diminution in the centreline velocity. In Figure 5.13, the height above the plate where $1 < y/D < 4$, the shear layers between the developing jet and the ambient fluid have fully penetrated to the centreline and begin to reduce the centreline velocity at a much faster rate as can be seen in Figure 5.13. The shear forces in the mixing layer of the jet are much larger than those within the fully developed profile specified at the nozzle.

The fully developed region shows a gradual decline in the centreline velocity due to the adjacent shear layers. Furthermore, there are now some notable differences between the RSTMs. As the shear forces are calculated using different equations, the results differ. The non-linear RSTM shows the onset of significant centreline decay slightly later than the linear RSTM. It is perhaps easier to make out from the $k$-$\varepsilon$ model results where each regime starts and ends.

This form of jet was analysed in a much smaller amount of detail by Cooper et al (1993), mainly due to the difficulty in obtaining statistically smooth hot-wire velocimetry data. Figure 5.14 shows the r.m.s parallel-to-wall velocity fluctuation profiles from close to the stagnation region to the further reaches of the radial wall jet. It is clear that all three turbulence models follow the same pattern as in the earlier geometries discussed in this chapter so far. Figure 5.14(a) also highlights the inability of the models to produce the near wall maxima close to the stagnation region. As the radial wall jet develops, the turbulence models begin to align slightly better with the experimental data. This agrees with earlier observations where the wall reflection term is better suited to shear-dominated wall bounded flows.

![Figure 5.13 – Velocity magnitude along the centreline of the jet](image-url)
The radial wall jet is considerably weaker in the 10D jet than the two preceding jet heights investigated. This is intuitive given the increased distance the jet must travel prior to impingement. As much more of the fluid momentum is dissipated into the surrounding fluid, this results in a substantially weaker radial wall jet.

Since there is no additional experimental data to validate the turbulence models it is difficult to draw very definite conclusions as to how the turbulence models have performed at the 10 jet height. Furthermore, given the performance observed at the 2D and 6D jet heights, drawing conclusions regarding the fundamental effects of increasing the jet height seems futile. Analysis of the 10D jet height with Fluent is therefore not taken beyond Figure 5.13 and 5.14, and the inclusion of this case is primarily for the completeness of the data set.
5.3 Multi-phase predictions

Studies considering multi-phase impinging jets are few and far between at present. There is very little experimental data which can be used to validate particle models and turbulence models. In the current research, the effect of particle size has been investigated using the same codes as in the single-phase methodologies: Fluent, STREAM and BOFFIN. This chapter looks at the velocity and r.m.s velocity fluctuations of particles for different jet heights and two particle sizes, using the fluid dynamic turbulence models in Fluent, as described in the earlier parts of the chapter. The influence of the jet height on the turbulent field provides an interesting opportunity to see if the particles also respond to the change.

5.3.1 2D jet height

The continuous phase for the 2D jet height is the same as that shown in Section 5.2.1 using the quadratic (non-linear) RSTM. As the simulations are not two-way coupled, the continuous phase profiles do not change with the addition of particles. Though this may seem like a backwards step, the primary interest here is to see the how the various particle trackers respond to differing particle sizes and geometries.

Particles are characterised by the Stokes number, St:

\[
St = \frac{\tau_p U_b}{D}
\]  

where \( u_b \) is the bulk velocity of the fluid, \( \tau_p \) the particle response time and \( D \) the pipe diameter, in the present research taken as the jet nozzle diameter. The particle response time has been previously defined as Eq. (4.20). The Stokes number is a dimensionless number which provides a useful value that indicates a particle’s tendency to follow the streamlines and to respond to fluctuations of the fluid. A particle with Stokes number less than one will follow fluid streamlines very closely, whilst a particle with Stokes number greater than one will be slow to respond to changes in the flow direction, and so can be expected to follow a different path to the fluid streamlines. The greater the Stokes number, the more significant this effect.

The particles under observation here have been summarised in Table 4.2. In the present setup, the Stokes numbers 1.4 and 5.8 correspond to the 20µm and 40µm particle diameters respectively. We can see then, that by the definition of the Stokes number, neither of these particles are expected to follow the fluid perfectly as they are both above 1. However, it is
anticipated that the smaller of the two should follow the flow more closely than the larger particles. In an impinging jet, one of the most important manifestations of these fluid and particle path differences is the rebounding of particles from the surface in the stagnation region. Where the fluid phase deflects in the radial directions as it comes under the influence of the wall, the particle may have sufficient inertia to overcome this quick change of direction. In this event the particle will continue its path normal to the wall and collide with the surface. The magnitude of the particle’s post-collision velocity, and thus the rebound height, is governed by the coefficient of restitution. The relationship considers the incident angle, particle and surface material properties and initial velocity.

Figure 5.15 – (a-d) Velocity magnitude at radial stations (a) 0.5D, (b) 1D, (c) 2D and (d) 4D from the centreline

Figure 5.15 shows the velocity magnitude of the particles and continuous phase. The stagnation region is characterised by deflection, deceleration and rebounding particles followed by radial acceleration and/or re-entrainment in the radial wall jet. Figure 5.15(a) shows the velocity magnitude of particles at a radial distance of 0.5D, effectively along the shear layer between the developing jet and the ambient fluid. As they approach the wall, the smaller particles decelerate and are mostly deflected, following the fluid streamlines as it nears the impingement plate, although with some particles colliding with the surface and rebounding. Close to the impingement surface, the 20μm particles are shown to have a higher velocity than the 40μm particles. This is because the smaller particles are more readily accelerated in the radial
direction than the larger particles, an observation which agrees with Yoshida et al (1990). The 40\(\mu\)m particles have a much higher inertia and, therefore, overcome the change in direction of the fluid as they approach the surface and collide, head-on, with the wall at a much higher velocity than the smaller particles. The resultant rebound is significantly higher than that for the smaller particles and the effects can be seen in Figure 5.15(a-b) as an increase in velocity around \(y/D = 0.4\). The rebounding particles either re-enter the radial wall jet from above through gravity or are slowly accelerated radially. The differences in the particle accelerations can be correlated to the residence time in the stagnation region, where larger particles have longer residence times which is in line with the observations of Yoshida et al (1990).

Figure 5.15(c-d) suggests that the particles are actually moving faster than the fluid in the radial wall jet. This is the result of the particles’ inertia as the radial wall jet slows down. The fluid slows down as a result of momentum conservation as it entrains the ambient fluid above the radial wall jet causing the wall jet to grow and the peak velocity to diminish. This gradual deceleration is not immediately mirrored by the particles, which slow down when the relative velocity is larger.

Figure 5.16 – (a-d) r.m.s turbulent velocity fluctuations normal-to-wall at radial stations (a) 0.5D, (b) 1D, (c) 2D and (d) 4D from the centreline

What is perhaps surprising from Figure 5.16(a) is that the r.m.s velocity fluctuations remain quite small for the rebounding particles, the velocity of which is predominantly in the axial
direction. What is more understandable is that the larger particles are less prone to responding to the fluctuations of the fluid than the smaller particles, and therefore exhibit the lower r.m.s velocity values. This is true for all profiles in Figure 5.16 with the slight exception of Figure 5.16(b) where in the region of 0.3 < \( y/D < 0.5 \) the wall jet shows the larger particles actually have higher levels of turbulent velocity fluctuations than the smaller particles. It is suspected that this is due to the larger particles re-entering the radial wall jet by entrainment as the particles pass through the free shear layer. Since the height of rebound is much greater for the large particles than for the smaller ones, they will re-enter the radial wall jet at a greater \( x/D \).

Figure 5.17 – (a-d) r.m.s turbulent velocity fluctuations parallel-to-wall at radial stations (a) 0.5D, (b) 1D, (c) 2D and (d) 4D from the centreline

Figure 5.17(a-d) suggests that the particles have higher parallel-to-wall velocity fluctuations in the upper region of the radial wall jet. Whilst the rebounding particles may contribute to this, it is primarily due to the shear forces acting between the radial wall jet and the ambient fluid above it. Furthermore, the shear forces generated as a result of the particles’ acceleration out of the stagnation region also contribute to the turbulence. By Figure 5.17(c-d) the radial wall jet is considered almost if not fully developed and the particles assume a qualitative alignment with the fluctuations of the fluid velocity. Both sets of particles reach a state which nears a uniform profile of turbulence by \( x/D = 4D \), with the smaller particles appearing to reach this state before the bigger particles.
5.3.2 6D jet height

Increasing the jet height further, one can expect there to be a greater amount of particle dispersion prior to impingement as the jet has more time to develop. Particles within the mixing layer of the developing jet will decelerate slowly with the fluid whilst particles along which remain in the potential core will retain their velocity until they enter the stagnation region. Figure 5.18 shows the velocity magnitude in the radial wall jet at this jet height:

![Figure 5.18 - (a-d) Velocity magnitude at radial stations (a) 0.5D, (b) 1D, (c) 2D and (d) 4D from the centreline](image)

Figure 5.18(a) suggests that the particles do not bounce off the impingement surface as fiercely as in the 2D jet height case by the absence of a significant peak in the velocity profile above the impingement plate. The same pattern of the 2D jet is observed throughout, with the smaller particles more readily accelerating into the radial wall jet. The greater level of dispersion in the developing jet region makes obtaining statistically smooth averages extremely difficult, particularly in the upper regions of the radial wall jet. For every 1000 particles prescribed at the inlet, only a few may pass through this region, therefore requiring huge numbers of particles for smooth averages to be obtained in the upper region of the radial wall jet. Hence, Figure 5.18(a-b) shows non-smooth data points at higher $y/D$ which are redacted from later figures.
The velocity profiles for both particle sizes are closer to the continuous phase in the 6D jet than the 2D jet at this stage. If one considers the Stokes number definition, it is clear that at lower velocities the particle has a lower St. Therefore, at lower velocities, particles will align more closely to the continuous phase. In the 6D jet, the gradual loss of axial momentum with the fluid causes the particles outside the potential core to slow down also. This means that particles are more likely to follow the fluid in these slower moving regions. The difference between the behaviour of the different particle sizes can still be seen, although it is smaller in this case than in the 2D jet case.

![Graphs](image)

Figure 5.19 – (a-d) r.m.s turbulent velocity fluctuations normal-to-wall at radial stations (a) 0.5D, (b) 1D, (c) 2D and (d) 4D

The lack of sensitivity of both sets of particles to the axial fluid velocity fluctuations is quite striking in Figure 5.19(a-b). At a 2D jet height, the particles showed a small, but not insignificant, trend to follow the fluid. For the current jet height, the discrete random walk model does not appear to reflect the continuous phase velocity fluctuations around the stagnation region at all. The components of the particle velocity fluctuations are obtained by applying a Gaussian distribution to the square root of the appropriate Reynolds stress. The instantaneous velocity is used for the duration of the particle time-step, defined by Eq. (4.17) in section 4.2. In an impinging jet, this time-step might not be short enough to capture the rapidly changing turbulent properties in the stagnation region. The discrete random walk model might
therefore not be ideal for use with complex geometries where the turbulent eddy sizes may vary significantly.

The limitations of the continuous phase predictions are inherited by the particle predictions. If continuous phase predictions can be produced which align better with real data then the resultant particle distribution, velocity and turbulence quantities would also be closer to reality. When real flows are evaluated, one must consider the effects that large and small scale turbulences might have on the overall behaviour of particles. Anderson & Longmire (1995) investigated the effects of such turbulent eddies and vortices in free and impinging jets and found that particle distribution was significantly altered by the presence of these turbulent structures. With RANS methods, these turbulences are not represented instantaneously and therefore will be different than they would in a real multi-phase system. As these artificial fluctuating turbulence values are based upon random number generation, the assumptions and shortfalls of these methods are inherited by the behaviour of the particle, which is very likely to be different in a real multi-phase system. Therefore the reliability of the continuous phase and its origin must be factored in to the performance of multi-phase models.

![Continuous phase predictions](image)

Figure 5.20 – (a-d) r.m.s turbulent velocity fluctuations parallel-to-wall at radial stations (a) 0.5D, (b) 1D, (c) 2D and (d) 4D

Figure 5.20(a-d) shows the velocity fluctuations parallel to the wall. Particle data now shows better qualitative alignment with the continuous phase, which one might expect based on the
Stokes numbers. At greater radial distances in the far field, the particle fluctuations (both wall-normal and parallel) are close to matching those of the fluid. In this sense, a similar pattern is observed for the 2D jet height.

5.3.3 6D jet height with axial wall

The effect of placing an outer wall at the furthest radial boundary in place of an outflow is investigated in this section. Experimentalists conducting flow measurements in tanks, for instance, usually assume that this boundary is suitably far away from the stagnation region to have no effect. However, the HAS tanks, which the present research has constantly in mind, have impinging jets located around the edge of the vessel, close to such an outer wall, and the current geometry is therefore also industrially relevant. The objective is to observe the resultant secondary wall jet and whether this has any impact on the original radial wall jet as it approaches the axial wall. What is perhaps interesting is whether this ‘bounded’ jet will respond in a similar way to a ‘confined’ jet in which the entrainment boundary is replaced by a wall. Fairweather & Hargrave (2002) and Hadziabdic & Hanjalic (2008) have found that in a confined jet, a non-negligible recirculation current occurs which can have implications for particle suspension and particularly particle deposition. This feature is the primary focus of this section whilst considering the implications the addition has on the radial wall jet behaviour.

Figure 5.21 – (a-b) Velocity magnitude at radial stations (a) 4D and (b) 6D from centreline

The velocity magnitude shown in Figure 5.21(a-b) shows the profiles at greater radial distances leading up to the outer wall than have so far been considered. The profiles around the stagnation region were found to be identical to those in Section 5.3.2 and have not been presented here. A better look at profiles around the stagnation region with the outflow replaced by a wall is provided in Section 6.2.3. In Figure 5.21(a) and (b) the profiles are 6D and 4D
away from the outer wall respectively. It is clear that whilst there is little impact on the continuous phase, the behaviour of the particles has changed significantly. To aid the description of the particle behaviour the vector plot of the continuous phase has been presented as Figure 5.22.

![Figure 5.22 – Vector plot of continuous phase velocity magnitude for 6D jet height with axial wall at the radial boundary](image)

Analysing the velocity vectors shown in Figure 5.22, a clear re-circulation zone appears that the particles follow to varying extents. The centre of this recirculation flow occurs at point A in Figure 5.22. The scale and location of this recirculation zone is governed by the strength of the axial wall jet and the shear layers along the boundary with the ambient fluid. These in turn are affected by the strength of the radial wall jet and the distance from the centreline at which the axial wall is placed. When the velocity of the entraining fluid moving adjacent to the axial wall jet is overcome by the downward moving fluid, being drawn toward the radial wall jet, the flow reverses creating the recirculation zone. The fluid velocity vectors show clear entrainment streamlines into both wall jets. At point B the fluid is entraining directly into the axial wall jet. At point C the fluid is entraining into the radial wall jet before it undergoes its secondary impingement against the axial wall. It is important to note that the radial velocity at point B is much less than the axial velocity at point C. This has implications for the particle distribution which would suggest that smaller particles may be more likely to re-enter both axial and radial wall jets whilst larger particles might only re-enter the radial wall jet due to their inertia. The simple result of this is that larger particles have an even longer residence time in the domain as a result of this.

Gravity also plays an important role in the recirculation of particles close to the axial wall. When particles of both sizes leave the axial wall jet their axial momentum is eventually reversed due to the gravity force thus, particles travel down towards the impingement plate. The gravity term is greater for larger particles therefore; larger particles reach a higher velocity as they fall back down towards the impingement plate. From Figure 5.21 this manifests itself as a steady
increase in the velocity magnitude above the jet half-width. As particles re-enter the radial wall jet, the velocity component acting perpendicularly away from the wall slows the axial component of the particle’s momentum and the particle is gradually accelerated radially again.

![Figure 5.23 – (a-b) Velocity magnitude at axial stations close to the outer axial wall (a) 2D and (b) 3D above impingement plate](image)

The main difference between the behaviour of the particle sizes arises in the axial wall jet that develops vertically along the outer wall. The smaller particles are quickly entrained in the axial wall jet after the secondary impingement and carried away by the moving fluid. The larger particles are slower to accelerate, particularly acting against gravity, and tend to leave the axial wall jet and enter the ambient fluid around \(x/D < 8\). These freely moving particles are carried by a small recirculation current back towards the centreline of the jet. The larger particles are then re-entrained into the radial wall jet sooner than the smaller particles due to the greater influence of gravity upon them, and their smaller tendency to follow the recirculation current. This is why we see the increase in velocity in Figure 5.21(b) for the larger particle size only. Smaller particles which do manage to leave the axial wall jet are dispersed by the streamlines mentioned previously from Figure 5.22. Additionally there are streamlines which carry particles back towards the centreline where they begin to re-entrain into the radial wall jet around \(x/D \approx 4\) - Figure 5.21(a).

The r.m.s turbulent velocity fluctuations serve to reflect what has already been established from the velocity profiles above. When compared to the 6D jet without the outer wall, the increase in turbulent fluctuations noticeable, particularly for the larger particle size. The elevated turbulent velocity fluctuations arise as the particles re-enter the radial wall jet shear layer with a higher axial component of velocity due to gravity. Although this process would account mainly for increases in the wall-normal velocity component, it is suspected that the process of axial deceleration and radial acceleration all within the shear layer causes significant increase in the turbulence levels of both components.
The turbulent velocity fluctuations of both sets of particles in the axial wall jet show that after the secondary impingement there is very little energy left in the jet. This is particularly true for the larger particles which are much slower to respond to fluctuations in the fluid; it can be seen
that the scale of the particle velocity fluctuations in the axial jet is 10 times less than that in the radial jet.

![Figure 5.27](image)

**Figure 5.27** – (a-b) r.m.s turbulent velocity fluctuations normal-to-wall at axial stations close to the outer axial wall (a) 2D and (b) 3D above impingement plate

Because there is little data to validate these observations it is difficult to conclude definitively whether the DRW has accurately portrayed the effects of the outer wall. Comparing with observations of other studies, however, suggests that there are similarities between the behaviour of the present bounded jet, and that of a confined impinging jet, as one might expect.

### 5.4 Concluding remarks

The single and multi-phase data presented in this chapter has provided a foundation for the industrial component of this thesis. Fluent is a commercial CFD software which is very often used in industry, and therefore, the results obtained with it can be considered representative of the quality of results that one might get in industry. In many cases, these may be satisfactory and meet the standards required for modelling fluids and multi-phase systems. However, it has been shown that, for even the more advanced two-equation and second moment closure models, flows in complex engineering geometries are poorly predicted. Alignment with experimental data for the single-phase has been used to validate the performance of these models in an impinging jet flow and varying jet heights. Around the stagnation region are some of the more complex flow features associated with the impinging jet. This is the region in which the quantitative alignment of the prediction with experimental data tended to be worse for all three turbulence models. The limitations of the turbulence models which were the underlying cause behind this have been identified in the chapter. Some regions, such as the developed radial wall jet are better predicted than others, although this tended to be when the flow characteristics happen to coincide with specific conditions for which the models were originally designed.
However, these regions were notably marred by the poor predictions upstream in the stagnation region. If better predictions within Fluent are to be obtained then various improvements or options must be added to the available turbulence models to allow them more flexibility to predict more complex impinging jet flows.

The multi-phase predictions in Section 5.3 have not been validated with experimental data as there is a definite lack of available data. Whilst it can be said that there needs to be more experimental multi-phase impinging jet studies published, sadly a definitive conclusion about the performance of the DRW model cannot be provided. However, the behaviour of the particles have been analysed and the effect of increasing the jet height and particle size has been considered. Increasing the jet height produces a greater degree of particle distribution across the developing jet and produces a faster growing radial wall jet. Particles were found to rebound less fiercely at higher jet heights due to the loss of momentum as particles enter the slower moving and more developed mixing region of the impinging jet. The addition of the axial wall in place of the outflow created a noticeable recirculation zone which dispersed particles of different sizes to different regions of the domain. Finally, the quality of the multi-phase prediction is governed primarily by the quality of the continuous phase prediction. Without suitable turbulence models for the fluid the particle predictions have little hope of achieving realistic velocity and turbulence statistics. This emphasises the importance of ensuring accurate continuous phase predictions can be obtained.
Chapter 6  STREAM RANS results

6.1 Single-phase predictions

The turbulence models used in this chapter are all contained in the academic code STREAM developed at the University of Manchester. The turbulence models themselves are the work of several authors from various institutions who, through studies and publications showed that their developments can provide significant improvements over other existing turbulence models, although in some cases the benefits may be limited to particular classes of flows, and in others they may be more wide-ranging. Validation with experimental data of particular cases typically has been used to show how their modifications have improved their alignment with physical data, and so a similar approach is used here, to assess their performance in the class of impinging flows of interest to the present study.

By comparing STREAM results with those from Fluent the potential benefits of using academic codes can be evaluated. The plots shown in this chapter are identical to those presented in Chapter 5 for the equivalent Fluent turbulence models. The key differences are highlighted with explanations as to why certain models have performed better than others. Furthermore, it is important to note that STREAM is not a commercial code, but one used principally in a research environment. Therefore its use and implementation in the following predictions requires extensive modifications to several subroutines of the code in order to set up and match the cases used with Fluent.

There are two turbulence models within STREAM that have been investigated. The first is a non-linear, realisable $k$-$\varepsilon$ model by Shih et al (1995) which has been shown to provide some improvement for stagnating flows and geometries typically found in engineering such as a back-facing step and a pipe expansion. The key modifications made by Shih et al (1995) were a new dissipation rate equation based on the dynamic equation of the mean square vorticity fluctuations in highly turbulent regions and a realisable eddy-viscosity formulation. By accounting for these changes, the turbulence model is expected to better predict systems with high Reynolds numbers and prevent non-physical turbulence statistics generating in regions of high strain.

The second turbulence model is the RSTM of Gibson & Launder (1978) with modifications to the wall reflection term by Craft & Launder (1992). The modifications have been made to the stress-strain correlation, specifically with impinging jets in mind. As the RSTM excels in
simple, shear dominated flows which tend to run parallel to a wall, the standard wall reflection
term is heavily based on maintaining the axial component. The modifications change the
redistribution of stresses in the axial direction to the radial direction so that a more
representative redistribution of energy is predicted which one should anticipate in an impinging jet
where the axial component is the primary strain generator.

6.1.1 2D jet height

Calculations using two turbulence models from STREAM were performed for the smallest jet
height with a closely matched setup to that used in Fluent. The radial wall jet velocity profiles,
r.m.s turbulent velocity fluctuations (wall-normal and wall parallel) and the shear stresses are
shown in Figure 6.1 to 6.4 respectively. A cross comparison can be made by comparing these
plots with their equivalent (Figures 5.4 to 5.7) in Section 5.2.1.

![Figure 6.1 – (a-c) Velocity magnitude at radial stations (a) 0.5D, (b) 1D and (c) 2.5D from
centreline](image)

The velocity profiles in the radial wall jet give the initial impression that both turbulence models
have performed well. Both turbulence models show good agreement with experimental data at
the measured radial distances. The alignment of the velocities in the stagnation region is
perhaps unsurprising as this region is predominantly determined by the non-uniform pressure
field, and to a lesser extent the Reynolds stresses. However, away from this region the Shih et
al \( k-\varepsilon \) model predicts a decay rate of the radial velocity slightly larger than shown by the
experiment. This is first noticeable in Figure 6.1(b) as a lower peak value of \( U_{mag} \) in the radial
wall jet. The RSTM with wall reflection term by Craft et al, shows excellent alignment with
data, particularly in the stagnation region and at \( r/D = 1 \). Figure 6.1(c) shows this alignment to
lessen slightly at greater radial distances. This was also observed by Craft et al (1993) who
identified the problem as high levels of mixing in the radial wall jet. Despite these small
differences, the growth rate of the radial wall jet is predicted with a reasonable degree of accuracy throughout.

These observations are indicative that both of these turbulence models (or at least some of the modifications included within them) were designed with jets in mind. Whilst the immediate near-wall behaviour of the jet is not under particular scrutiny in the current work, the wall functions employed within the STREAM code appear to have performed well, despite the varying thickness of the viscous sub-layer along the impingement plate. At the very least it can be said that the wall function has not had a detrimental impact on the radial wall jet away from the immediate wall vicinity.

A wider impression as to the performance of the turbulence models is shown by Figure 6.2 and Figure 6.3. The r.m.s velocity fluctuation profiles are plotted at several radial distances. The r.m.s velocity fluctuations in the stagnation region are once again over-predicted by the $k$-$\varepsilon$ model, although not as dramatically as the realisable $k$-$\varepsilon$ model in Fluent. The developments introduced into this model by Shih et al were primarily based around improving the prediction in the mixing layer of a free jet, amongst other geometries, which does not have a direct impact upon the prediction in the stagnation region of an impinging jet, although as suggested by these results, some improvement is brought about by them. Regions in which shear-dominated mixing occurs, such as the shear layers between the jet and the ambient fluid, are well predicted by the $k$-$\varepsilon$ scheme.

![Figure 6.2 – (a-c) r.m.s turbulent velocity fluctuations normal-to-wall at radial stations (a) 0.5D, (b) 1D and (c) 2.5D from centreline](image)

The dynamic definition of $C_{mu}$ (Eq. 3.17) has a direct effect on the turbulent viscosity. The high strain rate which reduces $C_{mu}$ lowers the turbulent viscosity. This in turn reduces the return to anisotropy for the normal stresses ultimately leading to a lower production of turbulent kinetic energy levels. Ultimately this reduces the anisotropy between the normal stresses from which the velocity fluctuations are drawn. Hence the over-prediction of $\overline{u'^2}$ is less than that seen in
Section 5.2. The non-linear terms from the Shih et al \( k-\varepsilon \) model depend upon the vorticity which does not contribute significantly in the impingement region and therefore does not appear to offer a huge improvement. Whilst the improvements were not observed to be better than those of Suga et al (1996), the improvement with this simple modification is still notable. In the case of Suga et al (1996), the scheme included a greater variety of non-linear elements which contribute more in various complex flow geometries and therefore can offer further improvements.

![Graphs](image-url)

Figure 6.3 – (a-c) r.m.s turbulent velocity fluctuations parallel-to-wall at radial stations (a) 0.5D, (b) 1D and (c) 2.5D from centreline

This observation indicates that complex geometries such as impinging jets cannot be accurately modelled with a linear eddy-viscosity formulation such as the one used in Fluent. Furthermore, many non-linear versions of \( k-\varepsilon \) models are not adapted to capture the effects of streamline curvature such as the Shih et al (1995) \( k-\varepsilon \) model, which is important in the region where the incoming jet flow is turned to flow parallel to the plate. However, there is hope for more complex non-linear eddy-viscosity models when more elements of the production and dissipation terms are non-linearised. This serves to highlight the importance of selecting the correct turbulence model when using CFD to help design and optimise such flow geometries.

The normal stresses are far better predicted by the RSTM with wall reflection modifications. As a result of the modifications, the turbulence model is far more adapted to redistributing the stresses within the stagnation region which is reflected in Figure 6.2 and 6.3. Both near wall and the upper region of the radial wall jet are both in very good alignment with experimental data. What is also interesting to note is that at greater radial distances from the centreline, the predictions continue to be in good agreement. The modifications were expected to slightly reduce the ability of the model in this region as the flow becomes shear-dominated however; it appears that the improvements in the stagnation region are propagated downstream and actually improve the prediction rather than worsen it.
As one starts to move away from the stagnation region, the development of the shear stresses plays an important role in the development of the radial wall jet as it becomes a shear dominated flow. The shear levels are an indication of the degree of mixing that occurs and thus the growth rate of the wall jet. A similar conclusion was drawn by Suga et al who stated that the eddy-viscosity formulation they used was central to obtaining reasonable physical agreement for impinging jets as well as a wide variety of other complex engineering applications. Therefore, it is anticipated that shear predictions for the scheme by Shih et al will not provide substantially improved results over the realisable \( k-\varepsilon \) model from Fluent.

The shear stress profiles shown in Figure 6.4(a-c) show an improvement over the predictions from Fluent. Whilst neither turbulence model aligns perfectly with the experimental data, the RSTM is at least always qualitatively aligned and quantitatively better than the \( k-\varepsilon \) model shown here and all three turbulence models in section 5.2. This improvement is quite significant in terms of the usefulness of the turbulence model for the design and optimisation of impinging jet flows, which will be discussed later in Section 6.1.2.

6.1.2 6D jet height

Increasing the jet height offers a different category of impinging jet, the features of which have already been discussed in Section 5.2.2. The velocity magnitude, r.m.s velocity fluctuations and shear stresses are shown by Figure 6.5 to 6.9.

Increasing the jet height appears to have relatively little impact on the pattern seen from the previous jet height in terms of predicting the velocity magnitude. The level of mixing, indicated by the reduction of the peak velocity in the radial wall jet and a thicker wall jet, is higher at the increased jet height as one might expect, due to the greater development of the incoming jet.
before it impinges and is turned into the radial wall jet. The RSTM with wall reflection term seems to outperform the $k-\varepsilon$ model again, whilst both turbulence models shown here show much better agreement with experimental data than those reported earlier in the Fluent chapter.

![Graph](image)

**Figure 6.5** - (a-c) Velocity magnitude at radial stations (a) 0.5D, (b) 1.5D and (c) 3D from centreline

Considering that increasing the jet height does not change the fact that the primary stress generator in the impingement region is the wall normal Reynolds stress component it is not surprising that the RSTM with wall reflection term continues to do well across different jet heights. To better see this effect and indeed, the performance of both turbulence models, Figure 6.6 and 6.7 show the r.m.s turbulent velocity fluctuations for wall normal and wall parallel components respectively.

![Graph](image)

**Figure 6.6** – (a-c) r.m.s turbulent velocity fluctuations normal-to-wall at radial stations (a) 0.5D, (b) 1.5D and (c) 3D from centreline

Obtaining the correct distribution of stresses in the stagnation region is a well-known problem that was particularly well highlighted by the models used with Fluent in Section 5.2 and by authors Craft et al (1993), Suga et al (1996), Shademan (2013) and Wang et al (2014). Within stress transport models, the standard Gibson & Launder scheme for the pressure-strain
correlation, $\phi_{ij}$, represses the re-distributive action of $\phi_{ij,2}$, through $\phi_{ij,w2}$. In simple shear flows, this serves to keep a small level of the wall-normal stress which is reasonable. In the stagnation region however, this is the primary stress generator and the repression of $\phi_{ij,2}$, leads to elevated levels of the wall-normal stress which is seen throughout the RSTM so far.

(a) (b) (c)

Figure 6.7 – (a-c) r.m.s turbulent velocity fluctuations parallel-to-wall at radial stations (a) 0.5D, (b) 1.5D and (c) 3D from centreline

The modified pressure-strain correlation, $\phi_{ij}$, in the current RSTM addresses this issue of excessive levels of the turbulent stresses in the stagnation region. The wall correction term is designed such that the terms involving the Reynolds stresses, wall normal vector and mean strains will give the same behaviour as the standard Gibson & Launder form in a wall-parallel flow, but to also reduce the wall-normal stress component in an impinging flow. Thus a greater proportion of the wall normal velocity fluctuations can be redistributed to the other components and bring levels of $\overline{u^2}$ closer to physically realistic values. Better agreement with the r.m.s velocity fluctuations in the stagnation region, leads to a better turbulence generation rates, and consequently an improved behaviour as the shear-dominated radial wall jet begins to develop. This was the rationale of Craft et al (1993) with their modification to the $\phi_{ij,w2}$ term. Indeed the results show an improvement over the $k-\varepsilon$ model as when the flow becomes shear dominated, the action of the modified $\phi_{ij,w2}$, is to returns to its original purpose which maintains a small wall-normal Reynolds stress component.

The improvement of the current turbulence model’s ability to predict the shear stresses over those used in Fluent is very significant. Both jet heights that have been validated thus far in this Chapter have shown that the predicted shear stress profiles align far better with experimental data than those models used within Fluent. Shear stress data can be correlated to sediment bed erosion and particle re-suspension. In simple systems, where inter-particle forces are considered negligible, the shear stresses of the fluid are directly responsible for the re-suspension of particles (Reeks et al, 2001). The design and optimisation of HAS tanks at Sellafield needs models capable of predicting such turbulence profiles with excellent reliability and confidence.
Factors such as jet height, nozzle diameter, Reynolds number and incident angle of the jet will produce different velocity and turbulence fields.

Computational predictions such as these can be used to help co-ordinate experiments. When conducting experiments it is highly beneficial to have only a few decisive variables to investigate due to the challenging nature of physically setting up equipment. With reliable computational modelling, these variables can be selected based on predictions made before experiments can begin which saves a great deal of time and expense. Thus far in the present research, the models readily available in Fluent have failed to match the performance of those developed and implement in the academic research code STREAM.

In support of Fluent, and the methods generally adopted in industry, the difficulty and effort (measured by time taken) to set up the flow geometries thus far is greatly increased for STREAM. Ansys Fluent has an extremely intuitive GUI which speeds the process of meshing and setting up the calculation, although in certain cases this time saving might need to be balanced against limitations in the accuracy of flow predictions inherent with some of the models available.

6.1.3 10D jet height and the effects of jet height

Finally, the 10D jet height represents the final single-phase run with both turbulence models in this Chapter. Once again, limited experimental data is available for validation purposes, although the velocity and remaining turbulence statistics are presented in Figure 6.9 to 6.12 to help illustrate the effects of a 10D jet height on the radial wall jet compared with the previously studied 2 and 6D jet heights.
Figure 6.9 – (a-d) r.m.s turbulent velocity fluctuations parallel-to-wall at radial stations (a) 0.5D, (b) 1.5D, (c) 4D and (d) 6D from centreline

The parallel to wall r.m.s velocity fluctuations show both models performing to a similar level of agreement with the experimental data. Both turbulence models appear to fail to accurately predict the near wall maxima of $\bar{u}^2$ in the vicinity of the stagnation region seen in Figure 6.9(a-b). The predicted peak is offset from the impingement plate by approximately 0.1D. This result is highlighted by showing the profile in Figure 6.9(a-b) at greater $y/D$, across the jet width. Cooper et al (1993) reported it was difficult to ascertain the wall-normal and wall-parallel directions close to the stagnation region and therefore difficulties in the experimental measuring methods cannot be ruled out as to the cause of the discrepancy.

As the 10D jet height has a fully developed jet flow (i.e. the mixing layer has penetrated to the jet axis) prior to impingement, this means that flow in the stagnation region is more turbulent and slower moving than previous jet heights. As the slower moving fluid impinges, the fluid is forced to slow down and redistribute its momentum radially. The shear forces induced from the radial acceleration of the fluid cause an initial increase in the parallel to wall velocity fluctuations. The effect of this appears to be difficult for both turbulence models to capture in the stagnation region at this jet height.
The effects of jet height on the resultant radial wall jet can be observed by considering the individual plots presented so far in Chapter 6 and the following plots for velocity magnitude, r.m.s velocity fluctuations normal to the wall and shear stresses, shown in Figure 6.10 to 3.12.

![Graphs of velocity magnitude](image)

Figure 6.10 – (a-d) Velocity magnitude at radial stations (a) 0.5D, (b) 1.5D (c) 4D and (d) 6D from centreline

The velocity magnitude of the 10D jet is presented above. The velocity profile taken at 0.5D does not show the near wall increase below y/D > 0.2 as it did in the 2D and 6D jet height cases. There is a small plateau and then a very minor near wall peak. Due to a wider impingement, the momentum of the fluid prior to impingement is much smaller hence a significantly weaker radial wall jet is seen. The radial component of the velocity along the developing jet is higher than previous jet heights which may also contribute to the elevated velocity above y/D > 0.2. There is only a slight increase in the growth rate of the radial wall jet in terms of the jet half width as the jet height is increased. The jet half width is defined as the height, y/2, above the surface at which U_{max}/2 occurs. Note that the RSTM with wall reflection term predicts that the velocity in the stagnation region will be greater than that predicted by the k-ε model. This can, in part, be attributed to the levels of mixing anticipated by both turbulence models, which is reflected in the normal to wall r.m.s velocity fluctuations in Figure 6.11 and to a lesser extent the parallel to wall r.m.s velocity fluctuations in Figure 6.9. A higher turbulent velocity fluctuation implies a greater level of mixing which is seen for the k-ε model.
As the jet height is increased there appears to be a slight increase in the wall normal velocity fluctuations, captured by the STREAM RSTM version only. This trend occurs due to a greater degree of mixing and entrainment of ambient fluid which suggests higher levels of turbulence. This observation aligns with Cooper et al (1993) who also observed a similar trend in their experiments.

The profiles in Figure 6.9 to 6.12 extend to 6D, which demonstrates the behaviour of the radial wall jet at greater radial distances. It is clear that initially there is an increase in the velocity fluctuations both normal and parallel to the wall. This is due to the initially thin although steep gradient shear layers associated with the initial radial wall jet development. Eventually a point is reached where the jet becomes thicker and the shear gradient becomes lower, causing the turbulent velocity fluctuations begin to decline. This also corresponds to a gradual diminishment of the shear stresses shown in Figure 6.12(a-d). Eventually a uniform turbulence distribution is achieved from above the viscous sub-layer to the height of the velocity maxima in the radial wall jet.
The deterioration of the shear stress is as one might expect. As the radial wall jet extends radially, the entrainment of more fluid into the jet will result in the jet losing energy and lowering the turbulence levels. This is a good indication that at greater radial positions the jet has less potential to resuspend particles from the surface.

If, to a first approximation, the particle re-suspension could be directly correlated to the shear stress then it is possible to consider the effects of jet height on the effectiveness of particle re-suspension. Of the three jet heights considered thus far in the present work, the 6D jet height appears to have peak values for the shear stresses in Figure 6.8, and would thus be expected to perform best in terms of particle re-suspension. This in-part is likely due to impingement occurring towards the peak of what is left of the potential core from the fully developed profile, whereas the other two cases considered here impinge within or well beyond the potential core. The elevated levels of turbulence expected in the stagnation region also correspond with improved heat transfer characteristics of impinging jets.
6.2 Multi-phase predictions

The multi-phase post-process calculations performed with the Rely code using the single-phase flow field from the STREAM RSTM are presented in this chapter. The purpose is two-fold: firstly to observe and analyse the differences between the predictions herein with those obtained in Fluent and secondly to look at the behaviour of an additional particle size.

6.2.1 2D jet height

Using the Rely particle tracking code for post-processing particles on to the continuous phase velocity and turbulence field, a series of predictions have been made for the behaviour of particles of various sizes. The resultant profiles of results from several particle sizes (and those of the continuous phase, for comparison) are presented here. The velocity magnitude of three particle sizes and the continuous phase is shown in Figure 6.13(a-c).

![Figure 6.13](image)

Figure 6.13 – (a-c) Velocity magnitude at radial stations (a) 1D, (b) 2D and (c) 3D from centreline

Observing the profiles in Figure 6.13 a distinct difference can be seen between the predictions with the Rely particle tracker and those from Fluent in Figure 5.15. The most notable difference (or lack thereof) is between the 20µm and 40µm particles. The Fluent DRW model predicted a difference in the magnitude of these particle velocities whereas the Rely code predicts that the difference is negligible and the effects of particle size are only apparent once the particles are ten times larger than the smaller particle size tested here. The Rely code uses the Michaelides definition of the particle equation of motion as explained in Section 4.2. The two smaller particles are shown to be more disposed to follow the streamlines of the continuous phase. This is indicated by particle data aligning very closely with the continuous phase. The larger
particles are less so, and the effect of the rebound on the impingement surface can be seen in Figure 6.13(a) as a raised velocity magnitude from \( y/D > 0.3 \) for the 200\( \mu \)m particles. When the radial wall jet reaches 3D from the centreline, Figure 6.13(c), the fluid has lost much of its momentum to the ambient fluid and therefore slows down. With slower moving fluid, the particles more readily align with the streamlines, which is what we see here. The rapid alignment of all three particle sizes is particularly surprising considering the differences predicted by Fluent. The DRW model did not show similar velocity or r.m.s fluctuating velocity profiles between particles until 4D from the centreline. Even at 4D, there is some slight discrepancy near to the wall. Using the Rely particle tracker, the particles have already aligned with the fluid by 1D.

![Figure 6.13](a) (b) (c)

Figure 6.14 – (a-c) r.m.s turbulent velocity fluctuations normal-to-wall at radial stations (a) 1D, (b) 2D and (c) 3D from centreline

The normal-to-wall velocity fluctuations of all particle sizes (shown in Figure 6.14) align closely with the continuous phase as one would expect considering the velocity magnitude plots. Once again the exception of the 200\( \mu \)m particles at \( x/D = 1 \) suggests that they are experiencing more turbulent behaviour than the other particle sizes, although not by a great amount. This is indicative of rebounded particles quickly re-entering the radial wall jet. Velocity fluctuations above the radial wall jet, for all three particle sizes are somewhat higher than the continuous phase. This is likely due to particles re-entering or escaping the radial wall jet as it develops radially. By Figure 6.14(c) the radial wall jet has grown beyond \( y/D > 0.6 \) and the normal r.m.s turbulent velocity fluctuations have diminished somewhat.
The particles have begun to reach a steady state, in-line with the streamlines of the fluid as the result of deceleration of the fluid. The parallel-to-wall r.m.s velocity fluctuations are given by Figure 6.15(a-c). All particle sizes initially show slight to considerable deviation from the continuous phase parallel-to-wall velocity fluctuations. The differences in the bulk of the radial wall jet seen in Figure 6.15(a-b) can be attributed to the acceleration of the particles away from the stagnation zone. The gradual diminishment of the parallel to wall velocity fluctuations as one moves away from the centreline brings the particles closer in-line with the continuous phase. As the radial wall jet loses energy by dissipation to the surrounding fluid, it ceases to accelerate and begins to decelerate, lessening the fluctuations further. The larger particles respond to this change much slower than the smaller particles which is expected due to the Stokes effect. At greater radial distances, the trend of velocity fluctuation diminishment simply continues with the 200µm particles’ profile getting closer to those of the continuous phase. However, such is the response of the particle size, that the 200µm particles do not actually fully align with the continuous phase before reaching the end of the domain and being deleted.

The re-entry or escape of particles from the radial wall jet is once again reflected by a small increase in the velocity fluctuations at $y/D > 0.4$ within Figure 6.15(a & b). This feature occurs at $y/D > 0.6$ in Figure 6.15(c), because of the wider jet at this radial distance. As very few particles appear to escape and re-enter, it is extremely difficult to obtain statistically smooth data in this region.

What can be gathered from these plots is that when using the Rely particle tracker, the effect of particle size has a much lower impact on the behaviour compared to the predictions within Fluent. Only significant increases in particle size appear to produce observable differences. In the work of Zhao et al (2012), who looked at the effect of Stokes number on particle slip velocity in wall-bounded turbulent flows, the differences achieved when increasing Stokes
number were small for Stokes numbers of 1 and 5 compared to the differences from even greater Stokes number. The particle slip velocity was also aided by the dampening of the fluid velocity. In the radial wall jet, even at the peak velocity, 2D from the centreline, the local Stokes numbers for 20 and 40µm particles were found to be 0.9 and 3.4 respectively. One would anticipate some deviation from the fluid for the larger particle in this case, however the smaller particle at \( St < 1 \), should be acting as a tracer. Using the discrete random walk model in Fluent, the former case is observed for both sets of particles, whilst the 20 and 40µm particles act almost as tracers when using the Rely code. Based on the findings of Zhao et al, it might be reasonable at this stage to state that the differences predicted by Fluent between particle sizes were too large and the differences with Rely were too small.

6.2.2 6D jet height

With a 6D jet height the developing jet has further to travel in which it can entrain more of the surrounding fluid and particles can reach a greater level of dispersion in the radial direction. As a consequence of this spreading particles are already fairly dispersed throughout the jet at the point of impingement. Because of its greater jet development, the mixing region of the 6D jet is much wider than that in the 2D jet. Particles located within this mixing region are generally slower moving than particles which have remained in the potential core. This is because smaller particles with lower inertia are more likely to be dragged outwards into the mixing region and ultimately lose axial momentum due to the drag coefficient, \( C_D \). The 200µm particles have sufficient inertia to overcome these small radial components of the velocity and therefore tend to remain essentially in the centre of the developing jet. This also implies that the larger particles will remain in the faster moving region of the developing jet, around the potential core.

Anderson & Longmire (1995) also made this observation stating that larger particle sizes actually tended towards the centreline whilst smaller particles were more evenly dispersed.

Because differences in the particle velocity profiles extend out to greater radial distances in the 6D jet height case than in the previous 2D case, the results are shown out to 8D. This will help show the gradual alignment and continued diminishme of the turbulence that was described towards the end of Section 6.2.1.

The velocity magnitude presented in Figure 6.16(a-d) generally reflects what has been shown for the impinging jets studied thus far. It is unusual that by 4D, Figure 6.16(d), the velocity of the larger particles remains noticeably higher than the continuous phase although, the qualitative alignment in the shape of the profile seems reasonable, and the other particle sizes show velocity profiles that closely match those of the fluid. The reason for the difference seen in the
largest particle profiles is that the axial growth of the radial wall jet reduces the velocity magnitude of the fluid quite quickly. Evidently when using the Michaelides’ equation of motion, a 200µm particle does not react very quickly to the decreasing fluid velocity as a result of its own inertia. To create a significant change in velocity, via its drag, the relative velocity difference between particle and fluid must be higher than it is here.

Figure 6.16 – (a-d) Velocity magnitude at radial stations (a) 1D, (b) 2D, (c) 4D and (d) 8D from centreline

The r.m.s turbulent velocity fluctuations in Figure 6.17 and 6.18 follow a similar trend to those in the 2D jet height. Once again the normal to wall r.m.s turbulent velocity fluctuations are very closely followed by the particles off the plate to a height of 0.6 < \( y/D \). The profiles do not show the small increase in turbulent velocity fluctuations at the shear boundary between the wall jet and the ambient fluid as the wall jet grows beyond at \( y/D = 0.6 \) in this case, and so the jet edge lies beyond the extent of the graphs presented here. Comparing Figure 6.17(a) with Figure 6.14(a) from the 2D jet height, one can see a difference in the upper region of the plot. Despite being 1D from the centreline Figure 6.17(a) is actually partly situated within the stagnation region due to the increased level of spreading in the developing jet region. Figure 6.17(b) shows the r.m.s normal velocity fluctuations as the jet leaves the stagnation region and Figure 6.17(c-d) the diminishment of the normal to wall component of turbulence.
Figure 6.17 – (a-d) r.m.s turbulent velocity fluctuations normal-to-wall at radial stations (a) 1D, (b) 2D, (c) 4D and (d) 8D from centreline

Figure 6.18 – (a-d) r.m.s turbulent velocity fluctuations parallel-to-wall at radial stations (a) 1D, (b) 2D, (c) 4D and (d) 8D from centreline
The parallel-to-wall r.m.s fluctuating velocity component follows a similar trend to that of 2D case, with the addition of the enlarged stagnation region just described. The peaks of the wall-parallel r.m.s velocity fluctuations in Figure 6.18(a-b) are at a similar height to those of the 2D jet, however the particles are more detached from the continuous phase at the 6D jet height. The r.m.s fluctuating velocity profile is much flatter for the 6D jet, which suggests that the rate of radial jet growth is greater than that of the 2D jet. A faster rate of radial growth implies that the dissipation of momentum from the radial wall jet to the ambient fluid is greater, driven by higher levels of turbulence. This appears to result in a peak in the velocity fluctuations about \( y/D \approx 0.1 \) above the continuous phase peak.

### 6.2.3 6D jet height with axial wall

The outflow boundary condition at the furthest radial boundary has been replaced with a wall perpendicular to the impingement plate. This configuration of impinging jet is considered a bounded jet as described in Chapter 3, this is representative of what would be found in a HAS tank; it has similarities with, but also some important differences from, a confined jet in which the upper boundary would be specified as a wall instead of an entrainment boundary. The near and far field velocity and turbulence profiles have been presented in what can be considered a bounded jet. In the current chapter the plots also include the 200\( \mu \)m particles to increase the range of Stokes numbers studied so a greater difference can be seen. Particle data is obtained through the Rely particle tracker and the continuous phase once again is that which was predicted by the RSTM with modified wall reflection term with STREAM. The effect of the axial wall is observed by comparing these plots with those in Section 6.2.2 in both the near and far field radial wall jet.

The velocity magnitude is presented for the near and far field radial wall jet, then at 2D and 3D above the impingement plate, close to the axial wall in Figure 6.19 and 6.20 respectively. Similarly with the predictions of the jet heights considered thus far with the Rely particle tracker, there is very little difference between the profiles from the two smaller particle sizes and only the significantly larger particles shows much sign of detachment from the fluid.
The inertia of the larger particles is sufficient to keep the particles moving ahead of the continuous phase as it slows down. The similarity of Figure 6.19(d) with that of Figure 6.16(d) suggests that the axial wall does not dampen the approaching fluid significantly at these locations. This may be because the fluid and particles are moving at such a lower velocity that pressure reflections and the presence of the wall do not come into effect until much closer to the wall than $x/D = 8$. The lack of a second maximum above the radial wall jet suggests that the particles are not re-circulating as they did in the Fluent predictions, or at least not re-entering the radial wall jet with any particularly high velocity at the profiles considered in Figure 6.19. Predictions from Fluent indicated that particles were re-entraining up to 4D from the centreline or higher in the case of the 40µm particle. Since the behaviour of the particles investigated so far in this case show that they follow the fluid almost completely it is not surprising that the 20 and 40µm particles are simply carried out of the domain by the bulk of the fluid as it moves up the axial wall without much deviation. It is possible that the simplified form of Michaelides equation of motion, Eq. 4.25, which does not contain an added mass or Basset history term does not capture the subtler turbulent features that the equation of motion Fluent uses does, which may become more important as the velocity diminishes. As the relative velocity decreases, smaller contributions which may have been considered insignificant before may no longer be so. However, in the defence of the method used, all the simulations presented thus far have a
density ratio of $4.8\times10^{-4}$. Shirolkar (1996) states that the history term can be neglected where the density ratio is less than $5\times10^{-3}$ and Vojir & Michaelides (1994) give a figure of $2\times10^{-3}$. The latter, however, state that for incompressible jet flows the history term may not be insignificant. Nevertheless, Hurn (2006) found that for small particles, the Basset history term made very little change to the velocity or turbulence profiles in a free jet, and it might therefore seem unlikely that the exclusion of the Basset history term has had a negative impact on the predictions presented here. What is more, Hurn found the inclusion of the Basset history term increased the computational run times by a factor of 10, whilst producing virtually no change in the results.

The velocity magnitude profiles close to the axial wall indicates a similar trend to that shown for the same setup within Fluent. The smaller particles follow the streamlines of the fluid to the extent that there is minimal recirculation of particles back towards the radial wall jet. The larger particles more readily fall out of the axial wall jet and, under gravity, accelerate downwards towards the radial wall jet where they are re-entrained. Evidence of this can be seen in Figure 6.20(a & b) where the re-circulating particles are actually moving faster than the axial wall jet. What is surprising is that this is not reflected in the radial wall jet profiles. Comparing Figure 6.20 with 5.22 one can see two distinct differences. Firstly the re-circulating particles have differing velocities. Whilst this varies with particle size, the 200µm particles which are not carried out of the domain have nearly twice the velocity magnitude outside the axial wall jet as those within it. Secondly, this maxima occurs at 8D from the centreline in Figure 6.20 and at 5D from the centreline in Figure 5.22. Both methods include the gravity term in their calculation of the particle velocity. It can be assumed that in the ambient fluid outside either the radial or axial wall jets, the gravity term is the dominant term which affects the particle velocity. The gravity term in question increases with particle diameter through the response time (Eq. 4.20). Therefore, the impact of the gravitational acceleration on the larger particles will be

Figure 6.20 – (a-b) Velocity magnitude at axial stations close to the outer axial wall (a) 2D and (b) 3D above impingement plate
much higher than that for the smaller particles investigated in Fluent. What we see then, in the present case, is particles re-entraining into the radial wall jet at \( x/D > 8 \) or even immediate re-entrainment into the axial wall jet.

The turbulence statistics shown are near identical to those presented for the 6D jet height. Even at greater radial distances the velocity fluctuations remain largely unchanged despite the presence of the axial wall. Whilst this contrasts radically with the predictions made with Fluent, it is not for different reasons to those already stated. As particles are no longer re-entering the radial wall jet at locations \( x/D < 8 \), there is no reason why the turbulent velocity fluctuations are likely to change in this region. In reality, the predictions from the Rely particle tracker would suggest that the particles are carried much further by the fluid, even at lower velocities, up the axial wall and dispersed into the ambient fluid well above \( y/D > 6 \). This is discussed in more detail shortly.

The turbulent velocity fluctuations are severely dampened as the particles move up the axial wall after the secondary impingement. Whilst all three particles sizes show qualitative alignment with the shape of the r.m.s profiles of the fluid, it is interesting to see that they are approximately half the strength. As the axial jet is much weaker and acting against gravity, the acceleration of the particles is much slower which results in less turbulent velocity fluctuations.
With little difference between the data sets for each particle, the particle size can be said to have little effect on the fluctuations at such low velocities and turbulence levels.

Figure 6.22 – (a-b) r.m.s turbulent velocity fluctuations normal-to-wall at different axial stations close to the outer axial wall (a) 2D and (b) 3D above impingement plate

Figure 6.23 – (a-c) r.m.s turbulent velocity fluctuations parallel-to-wall at different radial stations (a) 1D, (b) 2D and (c) 4D from centreline

The parallel-to-wall velocity fluctuations in Figure 6.23 are very similar to those for the unbounded 6D jet height case. Observing the same deviations between the different particle size profiles allows us to conclude from these predictions that the presence of the axial wall does not affect the radial wall jet, regardless of particle size. This implies that when bounded jets are applied to re-suspension applications, the presence of the wall should not dramatically
affect the velocity and turbulence statistics in the radial wall jet and therefore the resultant clearance area. This is assuming the axial wall is at a distance $x/D > 10D$ from the centreline and is perpendicular to the initial impingement plate. Many additional factors may change this conclusion and could dramatically alter the particle behaviour seen in the predictions. For instance, if the axial wall was placed much closer to the centreline, where the radial wall jet is still accelerating, or has more momentum, the reflections are likely to be much stronger and reflect back along the radial wall jet. However, this remains to be seen as such a prediction has not been performed within the present, or other, studies.

![Figure 6.24](image.png)

Figure 6.24 – (a-b) r.m.s turbulent velocity fluctuations parallel-to-wall at different axial stations close to outer axial wall (a) 2D and (b) 3D above impingement plate

What is perhaps not completely obvious from the plots presented here is the impact that the rising particles might have once they finally settle. The predictions with the Rely particle tracker suggest that the two smaller particle sizes are carried higher up the domain than the larger particle size before falling from the axial wall jet, which suggests they may distribute across a wider area. In the simulation, however, the particles are deleted once they leave the domain, which is not high enough for the particles to reach the location where they would fall from the jet, and so this effect is not captured and would require an extensive domain height above the jet for it to be observed. As the axial wall jet develops and loses momentum the gravitational force will overcome the inertial force and the particles will begin to descend back towards the impingement plate. When considering the industrial application, a situation such as this is desired, as it suggests the device could be used to maintain particles in suspension once they have lifted off the base of the tank. The difference between Fluent and the Rely particle tracker predictions is somewhat concerning as the implication of one prediction is quite different from the other, particularly when trying to design and optimise process equipment. However, without experimental data structured for validation purposes it is difficult to determine which of these methods is closer to reality and therefore which is better used to aid in the design and optimisation process.
One of the weaknesses of the Lagrangian-Eulerian method of discrete phase modelling is the necessary requirement of a finite residence time for the particle in the domain. The method does not perform well when particles settle, remain in the domain for a prolonged length of time or there is not a clearly defined inlet and outlet for the particles. Normally, the maximum number of time-steps simulated is chosen to be sufficient to ensure that under normal circumstances the particles have enough time to traverse through the domain and out of the appropriate boundary. However, in cases where a re-circulation current is present, the particle may become trapped or enters a region of stagnant fluid from which it cannot regain sufficient momentum to exit the domain within the maximum number of time-steps. Beyond this maximum number, the particle is deleted wherever it may be. The re-circulation in the present geometry is not strong enough to cause a large number of particles to remain in the domain for an unmanageable amount of time, and the above potential problem is therefore not of great concern. When considering more specific geometries and process specific systems, such as an impinging jet pulse for instance, where particles will become re-suspended then ultimately settle, other techniques are best used. For future studies more focused on particle settling and deposition an Eulerian-Eulerian method may be better suited.

6.3 Concluding remarks

Presented so far are two different approaches to CFD modelling. The first being the commercial CFD software Ansys Fluent and the second being an academically developed and peer reviewed code that is modified each time to suit the geometry being studied. Results produced with Ansys Fluent were in very poor alignment with experimental data which reflects negatively on RANS methods for predicting the fluid streamlines in complex engineering geometries. However, when the academic code STREAM was used, not all turbulence models were found to be in poor agreement. The plots in Section 6.1 have shown that certain RANS techniques can produce good alignment with experimental data when the turbulence models have been developed to suit more complex engineering problems can produce much better flow field data. The $k$-$\varepsilon$ model by Shih et al showed a minor improve over the realisable $k$-$\varepsilon$ model in Fluent, although the fundamental assumptions of the eddy-viscosity hypothesis limit the ability of this model to predict the correct levels of turbulence in the stagnation region, which ultimately degrades the downstream regions of the flow. The modifications to the wall reflection term by Craft et al (1993) allowed the Gibson & Launder RSTM to greatly improvement the prediction in the stagnation region. The improvement to the turbulence predictions in this region were translated downstream which improved the alignment with experimental data in those regions too.
Essentially this shows that RANS methods can be used to predict more complex engineering flows, however, additional development and terms are needed to ensure that the predictions are close enough to reality. Commercial codes need to adopt more advanced turbulence models or more options within existing ones which can cater to certain types of flows. With better turbulence models, the reliability of commercial codes can be improved significantly which ultimately leads to more trust in CFD by its users. Better predictions leads to fewer inaccuracies made on the empirical side of the process of designing and optimising which can produce better results in a shorter space of time.

Following on from the improvements of the turbulence models and quickly re-iterating what was concluded in Section 5.4: with a better continuous phase prediction a more realistic particle-phase prediction can be expected. The Rely particle tracker has predicted that the particles will behave differently from Fluent’s DRW model. It is difficult to definitively conclude which method produces the most accurate results without experimental results to validate against. At this stage, only reasonable and intuitive assumptions regarding the differences can be made. Comparing the response of one particle size to another, shows that increasing the diameter of the particle size by 20µm would not make a great deal of difference when considering the Stokes number effects. The effects of particle size have been investigated by other authors in simpler flow geometries and found that significant effects do not really occur until the Stokes number exceeds 100.

In the present study of impinging jets it was found to be difficult to assign a specific Stokes number to the whole flow. Whilst this may be acceptable in channel or pipe flow, in an impinging jet there are many different features of the flow in which the Stokes number will change dramatically. A local Stokes number was therefore found to be necessary to recognise what behaviour was expected in different regions of the flow.

To fully appreciate which method provided the most accurate particle predictions, experimental data is needed. This emphasises the need for well-defined experimental data in more complex geometries such as impinging jets which modellers can use to validate against. In the following chapter, a recently obtained experimental data set is compared with the discrete phase models studied so far. Furthermore, the benefits of using large eddy simulation can be observed and the effect of particles in an instantaneous velocity field can be compared against the methods used thus far.
Chapter 7 Multi-phase validation and LES results

7.1 6D jet height (McKendrick, 2014)

As has been stipulated throughout this thesis, the lack of experimental data for multi-phase impinging jets has been a limiting factor on validating the models used for multi-phase predictions. A recent multi-phase experimental data set by McKendrick (2014) obtained using PIV has been published and presents an opportunity to validate some of the models used thus far. A separate geometry and flow configuration matching that of the McKendrick experiment. A jet height of 6D was used with a 4mm jet nozzle, meaning that although the domain was physically smaller, the node distribution did not have to be adjusted. The Reynolds number was used was 10,000, less than half that of Cooper et al (1993) and the continuous phase was water as opposed to air. A fully-developed turbulent inflow for water at the new bulk velocity of 2.5m/s was interpolated at the jet nozzle along with the corresponding turbulent energy profile. As with previous multi-phase predictions a converged single-phase solution was obtained first using the quadratic RSTM from Fluent and the RSTM with wall reflection term from STREAM. The particles were then added in a post-process calculation using the DRW model within Fluent and the Rely particle tracker in STREAM. The predictions were once again, one-way coupled. It is anticipated that some discrepancy might be observed between the continuous phase of the experiment and the prediction due to the influence of particles. Only in a two-way simulation might these differences be accounted for in the prediction. Therefore, an experimental data set using particles of mean diameter, $d_p = 67.5\mu m$ with low enough volume fraction to justify a one-way coupled calculation, was selected to help match the experiment and simulation as much as possible. As with previous chapters, the velocity and turbulent quantities are presented for both continuous- and multi-phases. Whilst plotting the continuous phase and particles provides an opportunity to observe the behaviour of particles in different regions of the flow and the effects of varying jet height, with experimental data the performance of the models can be discussed as well. The differences between the DRW model and the STREAM/Rely particle tracker have already been discussed and with the use of experimental data validation can be used to determine which one is closest to reality. As a final note, it should also be added that only one particle size could be presented, as the experiment did not feature enough particles to reach reasonably smooth, meaningful averages.
The velocity magnitude at 1D away from the jet nozzle is shown in Figure 7.1 for the particles (left) and the continuous phase (right). At this distance it is unlikely that the jet should have expanded or changed significantly from the profile specified at the jet nozzle therefore, the difference between the continuous phase CFD predictions and the experimental predictions are most likely incurred as a result of differing inlet conditions.

The predicted data from Fluent and STREAM/Rely for the continuous phase and the particles are almost the same in the developing jet region. The agreement between both RSTM’s is reassuring that the discrepancy is not due to a convergence or setup error. Both methods show the particles following the velocity and turbulent quantities of the continuous phase very closely. However, it is clear from Figure 7.1 that there is a significant difference between computed predictions and the experimental results. At 1D away from the jet nozzle, the profile across the developing jet should strongly resemble that of the inlet profile that was specified as not enough distance has passed for the shear boundary layers to reach a width large enough to begin eroding the centreline velocity of the jet. Based on this observation, the computational predictions appear to agree in principle with the experimental work of Myszko (1997) and the computations of Souris et al (2002) in this region whilst the data of McKendrick seem to contradict this by rapidly changing the observed profile. The inlet profile interpolated across the jet nozzle of all jets in the current work is that of a fully-developed straight pipe flow using the same turbulence model that was used for the subsequent impinging jet simulation. This corresponded to the declared experimental conditions that state a straight pipe of suitable length to ensure a fully-developed profile was used. The fully-developed profile interpolated across the jet nozzle was in good agreement with straight pipe profile experimental data from Laufer (1953), Browne & Dinkelacker (1995) and den Toonder & Nieuwstadt (1997). It is possible that the experimental conditions were not as intended due to vibrations in the pipe up to the jet.
nozzle or perhaps an underestimation of the length of pipe required for a fully-developed profile. Alternatively the presence of particles is having a major dampening effect on the developing jet which causes a rapid deceleration of the continuous phase velocity in the developing jet when the jet enters the domain. As the simulations are one-way coupled, the effect of particles on the continuous phase is not captured which means the jet is free to develop as it would without the particles. The r.m.s velocity fluctuations appear to be augmented by the presence of particles in the experiment, where the particles respond closely to the axial fluctuations yet appear to respond much less so to the radial fluctuations than the predicted profiles suggest. Overall, the discrepancy is suspected to be an amalgamation of the above factors and therefore must be accounted for in the observations of the resulting radial wall jet.

The experimental profiles of turbulent velocity fluctuations suggest that significant shear layers have been generated very early in the development of the jet. This can be correlated to an enhancement of the mixing layer between the jet and the surrounding ambient fluid. Not only does this manifest itself as an elevated rate of decay to the potential core in the developing jet, but also it increases the rate at which the developing jet expands radially. This is indicated in Figure 7.2 and 7.3 by essentially non-zero values closer to $x/D = 1$ and helps explain the wider velocity magnitude profile in Figure 7.1.

![Figure 7.2 – (left-right) r.m.s turbulent axial velocity fluctuations in developing jet region, 5D above the impingement plate where (left) and (right) are as Figure 7.1](image)

Figure 7.2 – (left-right) r.m.s turbulent axial velocity fluctuations in developing jet region, 5D above the impingement plate where (left) and (right) are as Figure 7.1.

The turbulence levels of the continuous phase are shown on the right hand side of Figure 7.2 and 7.3. The peak in the turbulent fluctuations represents the centre of the mixing layer in the developing jet. The location of this peak in the experimental jet is closer to the centreline which suggests the jet has a narrower potential core. This indicates that the mixing layer predicted by both Fluent and STREAM models is not as wide as the experiment shows after 1D from the jet nozzle. Therefore, the development of the radial component of the velocity will increase at a
slower rate and the jet will spread less prior to impingement. It is interesting to note that the turbulent velocity fluctuations are quantitatively better predicted by the STREAM/Rely method than Fluent.

![Graph showing r.m.s turbulent radial velocity fluctuations](image)

Figure 7.3 – (left-right) r.m.s turbulent radial velocity fluctuations in developing jet region, 5D above the impingement plate where (left) and (right) are as Figure 7.1

From the developing jet profiles presented, the experiment shows the particles lagging behind the continuous phase by quite a large margin with the exception of the axial velocity fluctuations. The Stokes number in the developing jet region is the maximum it will be throughout the whole flow system as the velocity of the fluid exiting the jet nozzle is at its peak; it is therefore surprising to see such a velocity slip here. The r.m.s axial velocity fluctuations show the particles aligning with the continuous phase fairly well for both experimental and computational results. However, the experimental r.m.s radial velocity fluctuations show a rather larger difference between the particulate and continuous phase. The radial velocity fluctuations are notably smaller in this region which, would mean the relative velocity between the two would be very small. Therefore, the inertia is sufficient to overcome these small velocity fluctuations, but not to overcome the larger fluctuations in the axial direction. Both Fluent DRW and Rely particle tracker predict that the particles will follow the turbulent quantities of the fluid closely. When considering the Stokes number effect in these problems, it is important to recognise that it will change from one region to another. Using the velocity field, a contour plot of the Stokes number has been calculated and is shown in Figure 7.4.
It is understandable that where the Stokes number is highest will be where the fluid and particle will have the greatest degree of detachment. This does seem to fit the current case where the highest Stokes number is in the region of the upper developing jet. However, the Stokes number is less than one, which also indicates that there should be very little detachment between the two phases. Whilst the computations predict this behaviour, the experimental data does not, as shown in Figure 7.1 to 7.3.

In the stagnation region, as has been seen thus far, the Stokes number is less important. Due to the rapid change of direction of the flow as it comes into range of the impingement plate the particles are likely to impact and rebound due to their inertia and the degree to which this occurs is dependent upon the magnitude of their inertia. It has been shown in the previous studies, the majority of particles between 40µm and 100µm rebound off the surface and are eventually swept away by the radial wall jet. The residence time the particle has in the stagnation region is then correlated with the acceleration of the particle into the radial wall jet which is a function of the Stokes number. Figure 7.5 shows the velocity magnitude of the particles and the continuous phase in the radial wall jet.

The experimental data shows a slightly higher degree of radial expansion at 1D from the jet nozzle which seems reasonable considering the elevated r.m.s turbulent velocity fluctuations in Figure 7.2 and 7.3 of the continuous phase.
The continuous phase velocity is over-predicted at 1D from the centreline compared to the experiment. This is strange as the velocity was well predicted for the experiments of Cooper et al (1993). It is possible that in the stagnation region, the presence of particles slows the radial acceleration of the fluid. This behaviour was not predicted by the computational methods due to the one-way coupling. The particles from the Rely particle tracker are reasonably well aligned with experimental data. Fluent’s RSTM model over-predicts the velocity of continuous phase which gives an already poorly predicted velocity field for the particles.

The coefficient of restitution used with STREAM is that which was used in the previous studies. A suitable relation could not be found for the glass in water so the original was carried over into these simulations. Studies by Gondret et al (1999 & 2002) and Joseph et al (2001) investigated
the coefficient of restitution as a function of the Stokes number. The Stokes number, itself a function of the viscosity of the fluid, was found to show a fairly consistent correlation with the coefficient of restitution. The dissipation of the kinetic energy of the particle in water by viscous forces as it nears the wall differs from a particle in air. As the simulation in the present chapter uses air instead of water it is important to consider whether this will have a detrimental impact on the results. The study by Gondret et al (2002) in particular indicates that the resultant coefficient of restitution is constant above a critical Stokes number. This applies to particles in both air and water which, in the current study, have Stokes numbers well above this value and therefore the change from air to water should make little difference. It should be noted that the aforementioned authors define the elastohydrodynamic Stokes number, $St_e$, as:

$$St_e = \left( \frac{1}{9} \right) \frac{\rho_p}{\rho_f} Re$$  

(7.1)

At a distance of 2D from the centreline, the agreement is much improved for both Fluent and STREAM/Rely with the best agreement being from the STREAM/Rely combination. At this distance from the centreline, the fluid and particles should have reached their peak velocity and begin decelerating as the radial distance increases further as with the Cooper et al single-phase case. However, whilst the continuous phase predictions at 5D from the centreline show the velocity magnitude to have roughly halved over the 3D separation between the profiles, the experiment actually suggests that the continuous phase and particles have accelerated. It seems strange that the experiment would suggest that the radial wall jet does not begin to decelerate until $x/D > 5$, which is a much higher value than that observed for the jet of Cooper et al (1993). This contradicts the early findings of Xu & Hangan (2008) who observed that for a range of Reynolds numbers (23,000 to 190,000) the radial velocity peaked at 1.1D and ~0.03D above the impingement plate. The computational predictions, however, are in agreement with this observation.

The growth of the radial wall jet is a good measure as to the performance of the turbulence model. The jet half-width is reasonably well predicted by both models and this is then reflected for the particles. Both computational approaches show overall reasonably good qualitative alignment with experimental data, at least in terms of the velocity magnitude. When compared with the gaseous impinging jets studies in the previous chapters, the absolute turbulence levels are considerably lower. Therefore, the error around the stagnation region is not quite as quite as spectacular as seen in Section 5.2. With slightly more manageable levels of turbulence, the degree of mixing which occurs in the radial wall jet is also lower, resulting in a more appropriate growth rate of the radial wall jet. This is not to say that the quadratic RSTM used within Fluent does not over-predict the velocity fluctuations in the stagnation region, which it
The RSTM with modified wall reflection term once again achieves a much better prediction when aligned with experimental data.

At 1D from the centreline shown in Figure 7.6(a), the STREAM RSTM continuous phase turbulent velocity fluctuations normal-to-wall does not predict a sharp peak very close to the wall, but a stretched out profile which is otherwise quantitatively realistic. Fluent RSTM overpredicts the fluctuations at 1D and 2D similarly to the gaseous impinging jets of Cooper et al (1993). At 5D from the centreline where the flow has become shear-dominated, Figure 7.6(c) shows both STREAM and Fluent give similar results which lie close to the experimental data. The radial wall jet at this stage has lost much of its momentum and appears to have a much flatter profile although the experiment still shows a short peak close to the wall it is not predicted by either turbulence model.

Figure 7.6 – (a-c) r.m.s turbulent velocity fluctuations normal-to-wall at radial stations (a) 1D, (b) 2D and (c) 5D from centreline where (left) and (right) are as Figure 7.1
The particles remain close to the fluid phase throughout the whole jet with better alignment being for the Rely particle tracker. The experiment observes the particles responding quickly to the fluctuations of the fluid which is observed more so for the Rely particle tracker, particularly around the stagnation region. Here the Fluent DRW does not perform so well as a result of the continuous phase prediction. The Stokes number in this region, Figure 7.4, of the jet is substantially lower than in the developing jet region where the fluid is moving much faster and turbulence levels are high. It is to be expected then that the particles will not detach from the fluid by a large amount. By 5D the particles radial wall jet has lost much of its momentum and the particles adopt very flat profile close to, but irrespective of the continuous phase. At this stage the predicted particle data from the Rely particle tracker lies very close to the experimental data.

Figure 7.7 – (a-c) r.m.s turbulent velocity fluctuations parallel-to-wall at radial stations (a) 1D, (b) 2D and (c) 5D from centreline where (left) and (right) are as Figure 7.1
The experimental parallel-to-wall turbulent velocity fluctuations for the particles are shown in Figure 7.7(a-c) and show a lesser response to the fluctuations of the fluid with detachment being strongest at greater radial distances. At 1D from the centreline, in Figure 7.7(a), particles near the wall are accelerating in the radial direction which generates turbulence. Away from the wall it is possible that the slower moving particles which are not in the bulk of the radial wall jet actually have a dampening effect on the turbulence and reduce it. The predicted continuous phase does not account for this an overprediction in the upper region of the radial wall jet is observed. The development of the continuous phase shows a very similar trend to that of Figure 7.6. The turbulent fluctuations in the stagnation region are over-predicted again by the Fluent RSTM due to the pressure-strain correlation but quantitatively well predicted by the STREAM RSTM. The particles from the Rely particle tracker closely follow the streamlines of the fluid which results in only reasonable quantitative alignment.

7.2 LES BOFFIN

7.2.1 Single-phase results & discussion

In this chapter, large eddy simulation has been used to predict a 3-dimensional 2D jet height. LES is considered to be the next step in terms of complexity for computational modelling after RANS. As the jet has been simulated in 3 dimensions (as opposed to 2D, axisymmetric) a significantly higher number of nodes is required in addition to a much greater node density along the wall. This means that the computational time for the LES predictions take substantially more time to reach a fully converged solution. The computational mesh is therefore under a lot of scrutiny in the current simulation and as to the effect it has on the prediction as well as the performance of the code itself.

Due to the underlying fundamentals of LES, the prediction is anticipated to show far more realistic velocity and turbulence quantities than those shown for RANS methods so far. With the exception of DNS, LES predictions should provide the most realistic predictions of a complex engineering flow. This is because LES is able to capture the large scale turbulence structures such as vortices and temporary recirculation zones that make up the often overlooked features of the impinging jet. These features are not observed in time-averaged solutions such as RANS methods yet play a significant role in the turbulence field. Furthermore, in multi-phase simulations, these large-scale turbulent structures can dramatically alter the behaviour of particles and thus affect the final solution. The experimental observation of Landreth & Adrian
(1990) and Yoshida et al (1990) have shown these structures governing the particle distribution in the developing jet and radial wall jet. In these regions, this highly influences the velocity and turbulence of the continuous phase and the particles. Tsubokura et al (2003) accurately modelled such turbulent structures in a pulsating jet using an earlier version of the LES code to the one used in the current work. However, the jet in question used an excited inlet which forced the large turbulent structures to generate at a more regular frequency so they could be reliably observed.

The mean velocity profiles are presented in Figure 7.8 within the stagnation region and the radial wall jet. The profiles show reasonably good alignment with experimental data at all locations however, there are a few discrepancies which need explaining. The predictions are very sensitive to the computational mesh and the distribution of nodes in particular areas such as boundary layers and the wall. Near the wall, the nodes must be sufficient to capture the near-wall fluid behaviour directly, without the use of a wall function. Similarly, in areas of high shear, a high concentration of nodes ensures that the distance between nodes is small enough to better capture the interaction of the shear layers. At 0.5D from the centreline, the velocity magnitude is reasonably well predicted particularly at the wall, although at $y/D > 0.1$ the velocity is slightly over-predicted. At this location in the domain, the radial component is becoming more dominant than the axial component. The LES predicts that the jet should begin accelerating radially at a slightly greater height off the impingement plate. This appears as an elevated velocity away from the wall which peaks at around $y/D = 0.3$ and its discrepancy from the experiment is primarily due to the computational mesh, as shall be discussed shortly.

Outside the stagnation region, the radial wall jet is accelerating and by Figure 7.8(c) should be decelerating. The magnitude of the radial wall jet is in very close agreement with the experiment although the qualitative alignment above the radial wall jet leaves something to be desired. At 1D, Figure 7.8(b) the wall jet does not have the sharp peak the experiment shows and away from the wall, the jet has not grown into the ambient fluid as rapidly as the experiment shows. It is believed that is due to the nature of the Cartesian coordinate system that was used to mesh the impinging jet geometry. The LES prediction shown here appears to show certain features of a plane or slot jet, as well as an axisymmetric jet. These features were briefly discussed in section 2.1 but are re-iterated here for convenience. The differences between a plane and a round jet are clear by observing the radial wall jet. In the stagnation region of a plane jet, the distribution of the fluid is along a single plane, whilst an axisymmetric jet redirects the jet 360°. The level of turbulence in the radial wall jet away from the centreline is thus much lower in an axisymmetric jet. A plane jet however, has high levels of turbulence which result in a wider wall jet with a faster rate of growth into the ambient fluid above it. At the inlet, the node spacing had to be sufficient to allow the interpolation of a round inlet.
Without huge numbers of nodes concentrated along the edge of the jet nozzle, a flat edge along the x and y axis of the jet is inevitable. This flat edge to the ‘round’ nozzle appears to have had an effect on the radial wall jet near the stagnation region by introducing certain traits of a plane jet. This manifests itself as a flatter peak velocity in the developing radial wall jet and a lower rate of radial jet growth into the above ambient fluid. These are both characteristics of plane jets noted by Rajaratnam (1976). By 2.5D from the centreline, the radial wall jet aligns more closely with the experimental data.

The r.m.s velocity fluctuations parallel and normal-to-wall are presented in Figure 7.9 and 7.10 respectively. In the LES, the fluctuations are not based on the Boussinesq hypothesis, but are taken as the actual difference between the instantaneous velocity and the local mean velocity. This is a more accurate representation of the turbulence than the approach of the RANS methods used thus far due to the lack of the eddy-viscosity assumption for the turbulence scales which arguably affect the flow. The quality of the predictions close to the wall is in excellent agreement with the experiment. This is an indication that the number of nodes close to the wall was sufficient to capture the near-wall behaviour. In order to attain this behaviour, a significant number of nodes were required in the near-wall region. Ultimately, this limited the number of nodes available for the rest of the domain and resulted in the slight discrepancy away from the wall, the upper region of the radial wall jet. In the stagnation region, a slight under prediction transitioning to an over prediction as the radial wall jet develops. Due to memory limitations, only so many nodes could be used which contributed to the aforementioned problems around the jet nozzle. Rhea et al (2009) studied impinging jets also with RANS and LES and too found difficulty with the node distribution in LES, this time in the near wall region which had an insufficient number of nodes for a good prediction.

Figure 7.8 – (a-c) Velocity magnitude at radial stations (a) 0.5D, (b) 1D and (c) 2.5D from the centreline
The parallel-to-wall r.m.s velocity fluctuations are qualitatively better than the RANS predictions. This is particularly impressive considering that LES BOFFIN has no specific pressure reflection term and is not designed with an impinging jet in mind, unlike the RANS turbulence model from STREAM. The linear and quadratic RSTM both also had special wall reflection terms built within the code. The LES BOFFIN has been designed so that it is a generic code that can be confidently applied to any geometry and provide realistic predictions which should align very well with experimental data. Hadziabdic (2006) used LES to model confined impinging jets and determined that the pressure reflection effects are automatically captured with LES. Without the need for special terms, LES is an extremely powerful tool for simulating complex engineering flows and obtaining realistic, physical data for assisting design and optimisation of process equipment.

(a) (b) (c)

Figure 7.9 – (a-c) r.m.s turbulent velocity fluctuations parallel-to-wall at radial stations (a) 0.5D, (b) 1D and (c) 2.5D from centreline

(a) (b) (c)

Figure 7.10 – (a-c) r.m.s turbulent velocity fluctuations normal-to-wall at radial stations (a) 0.5D, (b) 1D and (c) 2.5D from centreline
The normal-to-wall velocity fluctuations are predicted well for all radial distances and are inline with experimental data. The predictions are also well predicted for the RSTM with modified wall reflection term; however, the near wall turbulence is better predicted by the LES. Contrasting the applicability of the LES with that of the RSTM in STREAM, one can argue that the RSTM is suited to impinging flows whereas the LES is suited to impinging and non-impinging flows, although the modified wall reflection term greatly improves the predictions in the stagnation region as has been shown thus far.

Contrasting the LES with the RSTM in STREAM specifically, one can further add that the somewhat bespoke wall reflection term is only relevant to impinging flows and that its use may degrade the solution where it is not applicable, just as the standard wall reflection term does within Fluent. Although the improvements greatly improve the prediction in the stagnation region, the solution downstream is slightly deteriorated for the reasons discussed in Chapter 6. Therefore, when considering geometries in which many different flow features occur the RSTM with wall reflection term may produce unrealistic predictions of the flow field. With LES this is not necessarily the case, although as problems get more complex greater numbers of nodes are required. Therefore, in some ways LES can be considered as a more versatile method than RANS although this versatility comes at the cost of high sensitivity to the computational mesh and node distribution as well as the inlet and boundary conditions specified.

Following on from this comment, the inlet conditions used in the LES are a series of generated, instantaneous, turbulent velocity profiles to more appropriately represent an instantaneous velocity flow at the inlet. Compared with the fully-developed, time-averaged solution from the RSTM this is the closest the computation can get to matching the initial experimental conditions. Applying this inlet condition also assists with the stability of the simulation, which can sometimes be an issue when generic or unrealistic inlet conditions are specified.
Through the overall promising alignment of the turbulent velocity fluctuations with the experimental data and the positive factors which contribute towards the superior predictions, the shear stresses are also in reasonable alignment with experimental data. The shear stresses are presented in Figure 7.11 and are a marked improvement from the predictions seen thus far. An amalgamation of the reasons stated so far are behind the reasons why the shear stresses are mostly predicted well. With an improvement to the shear stress predictions, the re-suspension characteristics of the jet can be investigated with more confidence. Only in very simplified systems can the shear stress be directly related to the ability of particle re-suspension. However, regardless of complexity, the shear stress is still a crucial factor in determining this characteristic of a jet and it can therefore be used to help draw valuable data regarding impinging jets in such operations as the HAS tanks. The under-prediction in the stagnation region is due to the corresponding under prediction in of the parallel-to-wall turbulent velocity profiles.

At greater distances away from the centreline, the results would be anticipated to align better with experimental data than RANS methods due to the formation of large turbulent eddies off the radial wall jet. As the radial wall jet loses momentum, the radial component of the velocity diminishes which weakens the wall jet and increases the likelihood that random chaotic turbulent structures might spring from the radial wall jet into the ambient fluid above. These structures contribute real turbulence statistics to the radial wall jet which might otherwise not be captured by RANS methods.

### 7.2.2 Multi-phase results & discussion

In this section, particles are added to a series of instantaneous velocity fields from the LES predictions outlined above. Once a fully converged, single-phase solution for the 2D jet height had been obtained from the LES a separate subroutine was activated to begin writing instantaneous velocity fields every 5th iteration. A total of 10,000 instantaneous, 3-dimensional profiles were written for the velocity which was considered sufficient to represent the turbulent nature of the fluid. The simulations were once again one-way coupled and used the Brenn et al (2003) equation of particle motion contained within the Rely particle tracker. Unlike the STREAM/Rely multi-phase computations, the instantaneous velocity is not based on a random number generator, but the actual instantaneous velocity at the particle location predicted by the LES. This velocity is used with the equation of particle motion for five timesteps. The particle’s position is advanced and a new instantaneous velocity profile is loaded. After 50,000 timesteps, the instantaneous profiles are cycled round and begin again at profile number one.
As the instantaneous velocity is read at the particle’s location, it is extremely unlikely that subsequent particles will see the same velocity field as a previous particle. The particles are inserted at the jet nozzle and evenly distributed across the nodes of the inlet. This aligns with the previously studied methods used with STREAM/Rely and Fluent DRW model.

The purpose of this exercise is to observe whether the real turbulence field and large scale structures help the particles to respond in a more realistic way to the velocity they are seeing. As the turbulence is more representative than the artificial fluctuating component generated within the Fluent DRW model and the STREAM/Rely, it is anticipated that the particles will behave closely to that expected from its Stokes number. The reality of the particles seeing this physically more realistic velocity field is that many times more particles are required to observe statistically smooth averages. Therefore, in the interests of time and computations, only the velocity has been presented. Turbulent velocity fluctuations are available; however, they can take upwards of 50,000 particles to appear statistically smooth and at the time of writing, do not show meaningful trends. As has been highlighted previously, the velocity components are slightly less sensitive and therefore do not take as long to produce meaningful plots. Those presented in Figure 7.12 and 7.13 have been observed to show meaningful alignment with the continuous phase and so are discussed here.

![Graph](image_url)

Figure 7.12 – (a-b) Velocity magnitude in developing jet region at (a) 1.5D and (b) 1D above the impingement plate

The particles in the developing jet continue to show the behaviour which was observed in the Fluent DRW and the STREAM/Rely particle tracker. In the developing jet, the particles quickly gain sufficient momentum from the fast-moving fluid to maintain strong alignment with the continuous phase. Particles are shown to spread from the bulk of the developing jet into the surrounding ambient fluid where their inertia is usually sufficient to bring them to the impingement plate before they reach a substantial radial distance. Despite the offset of the nozzle being only 2D in this case as opposed to 6D which has been presented thus far in the thesis for multi-phase, the particles are travelling at roughly the same velocity prior to the point
of impingement. Indeed, the number of particles travelling close to the bulk velocity is larger in
the 2D jet than the 6D as the mixing layer has had little chance to entrain ambient fluid and
disperse the momentum across the developing jet. Therefore, more particles are seen hitting the
surface with velocity close to that of the bulk of the fluid, which implies that more particles are
likely to rebound and less will be swept away by the radial wall jet prior to impact. The inertia
of the 40\(\mu\)m particles has been shown thus far to be sufficient to overcome the change of
direction of the flow towards the radial direction. Particles rebounding off that surface,
ultimately re-enter the radial wall jet from above.

Figure 7.13 – (a-c) Velocity magnitude at radial stations (a) 0.5D, (b) 2D and (c) 4D from
centreline

The radial wall jet profiles show that the particles are initially following the fluid streamlines
closely. Along the edge of the developing jet, Figure 7.13(a) the particles are simply carried
along and ignore the radial components of the velocity. The rebounding particles are captured
by the velocity magnitude plot by a slight elevation to the velocity above \(y/D > 0.2\). By 2D
from the centreline, the particles appear to still be accelerating, which is in-line more with the
predictions of the DRW model than the STREAM/Rely particle tracker. The latter showed
particles acting almost as tracers. In Figure 7.13(b), the particle data in the upper region of the
jet has been redacted as there were simply too few particles to present sensible data.

At a greater radial distance 4D from the centreline; the particles have finally reached the
velocity of the fluid shown by the alignment of both phases. This completes the trend shown by
both other particle tracking methods presented already. As the Stokes number is a function of
the fluid velocity, it is expected that as the fluid velocity decreases, the Stokes number also
decreases. Therefore, considered on the basis of the Stokes number effect, we observe the
correct behaviour of the particle as the relative velocity between the fluid and the particle
diminishes.
7.3 Concluding remarks

When compared to experimental data, it was found that the Fluent DRW model performed to an acceptable level although it was greatly hindered by the continuous phase prediction. The principle particle behaviour that one might expect from a particle size which has a Stokes number greater than one was observed, although there were some discrepancies. The main problem, appeared that as the particle entered regions of slower moving fluid where the local Stokes number should have also been lower it did not align well with the continuous phase. In comparison, the STREAM/Rely combination provided equally, if not better predictions of the particle behaviour which aligned very well with experimental data. The vastly superior single-phase prediction from the RSTM within STREAM contributed a lot to this improvement and better alignment with the experimental data. The Rely particle tracker was then able to use this flow field and apply the appropriate particle behaviour to it. The alignment with particulate and continuous phase experimental data was poor in the developing jet region; however, the unusual velocity and turbulence profile of the continuous phase leads one to conclude that the initial conditions at the inlet may not have been the same. The alignment was best when the flow was in a region which could be considered fully-developed such as the further radial distances of the radial wall jet. The STREAM/Rely particles showed a substantial propensity for following the streamlines of the fluid. Considering the local Stokes number contour plot presented, this should seem a more appropriate particle behaviour by following the Stokes number effect.

The adjustment from air to water did not appear to have much of an impact on the simulation overall other than a corresponding lower bulk velocity and lower turbulence levels. The characteristics of both jets were found to be the same, with similar rates of radial wall jet growth and turbulence dissipation. The coefficient of restitution was also found to perform well, despite originally being established in air. The relation of the coefficient of restitution to the Stokes number showed that above a particular Stokes number, the coefficient would not change. As the Stokes numbers for the Cooper et al and McKendrick studies were reasonably similar, the particles and the surface were the same, the coefficient of restitution was found to be suitable for both.

Large eddy simulation proved to be a very powerful tool for predicting impinging jet flow fields. Based on the geometry that was studied, the LES predicted a very realistic radial wall jet. The profiles observed were in reasonable alignment with experimental data. The importance of appropriate node distribution was highlighted throughout the analysis. The velocity and turbulence data above the radial wall jet was occasionally not in good agreement with experimental data. This was primarily due to the low concentration of nodes around the jet
nozzle which did not allow for a perfectly round inlet. Therefore, the radial wall jet showed traits of a plane or slot jet rather than a round, axisymmetric jet. The near wall behaviour was captured very well due to the high concentration of nodes along the impingement plate and did not require any wall treatment to approximate the viscous sub-layer along the wall.

When particles were added to the continuous phase solution from the LES, the behaviour of the particles closely matched that which was anticipated based on the local Stokes number. The simulation was able to demonstrate the impact of the particle inertia, the slow acceleration of the 40µm particle as it enters the radial wall jet and the gradual alignment with the fluid as the relative velocity diminishes.

From these studies, LES can be highly recommended for complex engineering flows, provided the computational mesh is sufficiently refined and the user has the luxury of time and computational capacity. The computational time to reach a fully-developed solution was found to be 10-20 times longer than for any RANS method, even whilst running a parallel code. What this brings to bear, is that which was pointed out at the start of this thesis: in many industrial, engineering situations a compromise must be reached. With RANS and LES methods studied so far, that compromise is between the quality of the solution and the time available in which it can be achieved.
Chapter 8  Conclusions & further work

8.1 Conclusions

The work undertaken in this thesis has been to present and compare the available methods of modelling and simulation for an industrially relevant geometry. Three codes were chosen based on their use in industry and academia: Ansys Fluent, RANS STREAM and LES BOFFIN. Ansys Fluent was chosen to represent a code that is frequently used in industry to obtain solutions for an enormous range of engineering problems and geometries. One particular question this thesis sought to answer was whether the often simplified turbulence models built into Fluent were capable of predicting complex flow geometries such as impinging jets. The streamline curvature and irrotational normal straining of impinging jets make them particularly difficult for eddy-viscosity models to correctly predict the turbulence levels within the stagnation region, which leads to problems elsewhere in the domain. The effects of jet height were also investigated on the resultant velocity and turbulence field, the effects of which have connotations for the re-suspension traits of the jet which are relevant to the industrial application. Finally, the behaviour of particles was considered by implementing one-way coupled methods with the fully developed flow field at two jet heights.

The realisable $k$-$\varepsilon$ model, a linear and non-linear RSTM within Fluent were used to analyse the capabilities of some simple and slightly more complex turbulence models. Three jet heights were chosen to represent different categories of impinging jet. The solutions were validated with matching experimental data from Cooper et al (1993) and the degree of alignment indicated the performance of the turbulence model and the quality of the solution. It was found that for all three turbulence models, the turbulence quantities in the stagnation region were overpredicted, even for the quadratic stress-strain correlation RSTM. The poor prediction in the stagnation region, ultimately had an impact on the downstream flow and affected the resultant radial wall jet which these turbulence models should be able to predict without too much discrepancy. The poor performance of the latter model was surprising as it was implemented into Fluent specifically with this kind of flow in mind. The linear $k$-$\varepsilon$ and remaining RSTM were selected to demonstrate more basic turbulence models and thus highlight the importance of selecting the right turbulence model for the problem at hand.
These predictions were then compared with equivalent simulations from an academically developed RANS code called STREAM. A realisable, non-linear $k$-$\varepsilon$ model and a RSTM with modified wall reflection term were used within the STREAM code. The latter having been developed by Craft (1992) with impinging jets in mind, aimed to improve upon the turbulence re-distribution in the stagnation region which would lead to an improvement of the geometry overall. The predictions indeed, did show this to be the case making it far superior to any of the turbulence models used with Fluent. Whilst the $k$-$\varepsilon$ model from Shih et al (1995) repeated the earlier turbulence discrepancies from Fluent, the model was able to recover very quickly and provide better alignment in the developed radial wall jet. The cubic relation for the stress-strain relation also assisted in this case with the Shih et al model.

Finally, the LES BOFFIN code was used to simulate a 2D jet height and compare it with the predictions of the STREAM turbulence models. LES, being the next logical step in terms of complexity from the RANS methods investigated so far, was anticipated to improve upon the predictions of the RSTM with modified wall reflection. Indeed, the results showed that LES is very capable of predicting such a flow in a complex geometry without the need for modified terms which may (or may not) be better suited to particular types of flow. The only downside with the LES that was firmly established was the necessity to have an extremely high number of nodes, particularly in highly turbulent and boundary regions. As the LES solves for the instantaneous quantities and does not time-average, the jet is not considered axisymmetric and therefore the full 3-dimensional geometry must be solved. The large turbulent structures that are captured by the LES have a significant impact on the turbulence field and are very influential on the particle distribution. By capturing the large-scale turbulence structures, assumptions regarding turbulence intensity and dissipation are removed and replaced with the explicit solution of those structures.

With the validated, fully-converged, single-phase solutions of the impinging jets at 2D and 6D jet heights, different multi-phase models were used to analyse the behaviour of particles inserted into the jet nozzle. The discrete random walk (DRW) model within Fluent was chosen over the cloud model as it was found to be more appropriate to represent the individual particles and average the velocity and turbulence statistics. The Rely particle tracker was used with the single-phase solution from the RSTM with wall reflection term. The results indicated quite a large difference between 20µm and 40µm particles for the DRW model, which is surprising considering the difference in Stokes number is not very great. The Rely particle tracker predicted that the 20µm and 40µm particles would respond very quickly to the fluid streamlines and showed very little difference. Because of this, a 200µm particle was added to observe the behaviour of a much larger particle. A difference in the velocity and turbulence statistics were subsequently seen. The inertia of the larger particles in each technique was sufficient to
overcome the change in direction of the fluid as it approaches the impingement plate. This causes the larger particles to rebound from the surface and enter the radial wall jet from above. From the DRW model, the acceleration of the 40µm particles was less than that of the 20µm particles which means that the larger particles have a longer residence time in the stagnation region. This was not the case in the Rely particle tracker which demonstrated both 20µm and 40 µm particles behaving the same and the residence time not increasing until a particle of 200µm was added. As there was no experimental data to validate against, it was difficult to establish which method was most realistic. This has implications for the distribution of particles in industrially relevant impinging jets, such as when jets are fired periodically. The resultant particle size distribution will lean towards larger particles closer to the stagnation region and smaller particles will be carried further by the flow. When a radial wall was situated in place of an outflow, a recirculation current was induced. This recirculation showed smaller particles travelling back to within diameters of the stagnation region, whilst the larger particles were shown to fall out of the axial wall jet much sooner and re-enter the radial wall jet after travelling only 2 or 3 diameters back towards the centreline. Eventually, most particles were carried beyond the upper boundary of the domain and removed, suggesting that at a radial distance of 10D from the centreline, a 6D jet height is still sufficient to lift particles into the bulk of suspension. The conditions of the simulation were then adjusted to match the experimental conditions of McKendrick (2014).

When matching the conditions of the McKendrick experiment, a 67.5µm particle was used at a Reynolds number of 10,000. Despite a differing profile in the developing jet region, the experiment showed that the particles responded very closely to the velocity and turbulent fluctuations of the fluid which was captured well by the Rely particle tracker and also by the DRW model. The main difference was found to be from the continuous phase profile. As the velocity and turbulence flow field was not well predicted by the quadratic RSTM from Fluent, the particles were already starting from a poor alignment with the data. The response of the particles was predicted best by the Michaelides equation of particle motion used within the Rely particle tracker, as particles not only aligned well with data, but also showed the same behaviour as was seen in the experiment. Of particular note, was at greater radial distances the particles maintained enough momentum once the radial wall jet began to decelerate due to the dissipation of the momentum into the ambient fluid. Particles appeared to be moving slightly faster than the fluid they were surrounded by. What could not be captured, was the influence of the particles on the fluid. A two-way coupled approach would be necessary to see such effects and is discussed in the next section.

What has been established through the simulations and cases summarised above, is that the turbulence models within Fluent are not capable of accurately predicting complex engineering
flows such as the impinging jets situated in HAS tanks. The resultant continuous phase velocity and turbulence field does not align well with experimental data and the inclusion of particles inherits this poor accuracy. Additional options which help optimise the turbulence models towards specific engineering geometries ought to be included in Fluent to ensure that the best available method is applied. With less emphasis on generic and one-size-fits-all turbulence models, more accurate and realistic predictions can be obtained. Presented in this thesis has been the RSTM with modified wall reflection term. This has been shown to greatly improve upon the abilities of the basic Gibson & Launder RSTM to predict impinging jets which produces velocity and turbulent quantities that align very close with real, physical data from experiments. Improving the quality of the turbulence models, automatically helps the discrete phase models by providing them with more realistic velocity and turbulence statistics.

Finally, although limited runs were able to be completed during the course of this thesis, the LES prediction showed that LES is well suited to predicting complex engineering geometries without the need for modification to particular terms or corrections. Companies and industries which heavily rely on CFD now have huge computational resources at their disposal and simply lack the codes or expertise to use LES. It appears from the experience and findings of the author that LES is the next logical step that industry ought to take when modelling and simulating process equipment. With modifications to particularly sensitive terms in the RANS methods, realistic predictions can be obtained which may provide an excellent precursor to more refined LES solutions.

8.2 Suggestions for further work

Throughout this thesis a range of computational modelling techniques have been investigated over a number of impinging jet configurations and with validation against available experimental data, the performance of these techniques has been analysed and discussed. The time intensive nature of this has limited other areas that the research might have expanded upon and leaves room for the continuation of the work.

The $k-\varepsilon$ turbulence model by Shih et al (1995) was more recently superseded by a two-equation model by Suga et al (1996) which is much better suited to impinging jet flows. It was regrettable that this turbulence model was not available at the time of the research within the STREAM code. It would be interesting to compare the predictions of the cubic $k-\varepsilon$ model by Suga et al with the turbulence models already considered to the predictions of the other turbulence model to determine whether a realistic solution of a stagnating flow is indeed possible with the two-equation model. This may affect the discussion and conclusions that have
been drawn in the thesis, particularly concerning the predictive ability of RANS turbulence models to accurately represent the velocity and turbulence field of impinging jets without bespoke formulations. The quick runtime for a converged solution coupled with the robust nature of two-equation models makes them extremely useful for gaining an initial insight into the flow.

The number of jet height cases considered using LES was limited to just one jet height. This was due to time constraints and also the limitations of the available memory at hand. If a 6D jet height was to be considered, a huge amount of nodes would be required this would necessitate more computational memory to store the appropriate arrays. However, LES has been shown to provide superior solutions given the correct computational mesh and therefore it is considered an important avenue of future work that the remaining jet configurations are studied using LES and the subsequent multi-phase solutions are attempted.

Given the improvement that LES can offer, it was discussed that additional jet configuration variables also be considered simply to observe their effect on the flow field. Fixing features such as the jet height and bulk velocity and adjusting other jet variables such as the angle of incidence, jet nozzle diameter or the distance from the centreline to the axial wall are all configurations that are of industrial relevance and interest. With LES and the improvements made to the turbulence field, it would also be interesting to see the re-suspension effects of particles from a bed. The implementation of this can range from very simple to highly complex. In the simple case which uses the current particle tracking methods presented in this thesis, particles might be inserted at the impingement plate with zero velocity and ultimately swept away by the radial wall jet with a behaviour relative to the properties of the wall jet. It should be understood however, that this is merely a starting point for future simulations which may have to adopt an Eulerian-Eulerian approach to represent significant volume fractions of particles which might remain in the domain for the entire duration of the simulation.

So far, the influence of the single-phase on the particles has been shown. However, in reality the particles can also have a significant influence on the fluid. This can be represented in computational fluid dynamics by two or four-way coupling. Should such a system be implemented then a very powerful tool for observing multi-phase flows is available for investigating the real, physical effects of multi-phase impinging jets. With successful validation against experimental data then further complexity might be considered such as the effect of particle shape, agglomeration, rheological properties of the particles etc… This tool would be able to simulate very closely the actual behaviour of the impinging jets in the HAS tanks, for which the current thesis is aimed at.
To necessitate this progression towards better modelling and simulation of a multi-phase impinging jet, more experimental data is required. In the two-way coupled case, data is needed for the continuous phase and the particles simultaneously. This is known to be a difficult task by experimentalists although recent work by McKendrick (2014) and Vickers (2015) have shown PIV to be a very effective method of obtaining such data. Attaining such data would allow the validation of two-way coupled simulations for impinging jets, leading to the optimisation and development of the code so that superior predictions can be achieved.

Ultimately, for any developed scheme or code to be useful to industry it must have a wide range of applicability; therefore in order to test the limits of a particular method (such as LES) it is important to consider radically different geometries and compare the degree of alignment with experimental data. The robust nature of the code is also an important factor, however the cost must be weighed against the complexity and thus the reliability of the solution to align with real, physical data.
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