Using large eddy simulation to model buoyancy-driven natural ventilation

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Using Large Eddy Simulation to Model Buoyancy-Driven Natural Ventilation

Supervisors

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Prof. J.J. McGuirk (Dept. of Aeronautical and Automotive Engineering)
Abstract

A major current focus in the building industry is how to incorporate low-energy strategies into building design in order to meet the carbon emission targets set out in Part L of the UK Building Regulations (DTLR, 2000). Natural ventilation provides a potential means of achieving this whilst also potentially improving indoor air quality. Due to the small driving forces responsible for natural ventilation relative to mechanical driven systems, some form of airflow modelling is often useful at the design stage. Designers require a method which offers the potential to deliver high levels of detail with sufficient accuracy at acceptable cost. Over recent decades, this role is increasingly played by computer simulations, in particular, Computational Fluid Dynamics (CFD).

The performance of one such CFD technique known as Large Eddy Simulation (LES) is investigated for modelling buoyancy-driven natural ventilation. LES was applied to a test case in which two, unequal heat sources are used to drive the flow, then to a test case in which multiple steady states were reported and finally to a realistic auditorium building. This study reports on the performance of LES (Smagorinsky SGS model) against conventional RANS/URANS (RNG k-ε turbulence model) in modelling buoyancy-driven naturally ventilated enclosures by comparing their results with theoretical and experimental data. An $L/\Delta > 12$ ratio was used for mesh generation in LES while mesh independence analysis was carried out for RANS/URANS studies.

For the twin plume test case the height of the temperature interface was predicted and compared with theory using LES and RANS. Results showed a 12% and 18.4% discrepancy respectively. The merging height, volume flow rates and nature of the two plumes agreed closely with theoretical predictions. LES analysis of the pressure isosurfaces demonstrated the interaction phenomena of the two plumes, the coherent structures and the behaviour of the interface. Spectral analysis of the
vertical velocity predicted by LES obeyed the -5/3 power law which is a characteristic of high Reynolds number fully developed turbulence.

For the second test case both LES and URANS were able to capture multiple steady states for the second test case however URANS was unable to capture unsteadiness in its steady state period (i.e. URANS solution converged to a RANS solution). LES was also able to accurately predict steady state temperatures (0.15% discrepancy) relative to URANS (1.42% discrepancy) and the time to reach steady state temperatures, giving confidence that LES has potential for modelling this important class of flows.

The last test case exposed an inherent weakness of RANS/URANS to smear out details of the flow which could have design consequences which LES was able to capture. For example, inaccurate location of the temperature interface, inaccurate plume structures, absence of vortex structures, thermal dissatisfaction of occupants due to sensation of draughts, residence time of fluid in the domain which can be important in smoke evacuation design or artificial fog design for on-stage performances.

In all three cases the RANS/URANS method consistently over predicts temperatures in the enclosures. The last test case also helped elucidate the accuracy-cost trade-off of using the LES approach.

It was seen that opting for an LES approach would increase the computational time by a factor of 10 and that a cluster of ~100 parallel processors would be required to run LES on real building geometries.

Considerable insight has been gained concerning the LES approach to model buoyancy-driven natural ventilation. As well as demonstrating that LES has the potential to accurately predict the fluid dynamics occurring in a naturally ventilated building, this research contributes to bridging the gap between researchers and practitioners by taking the knowledge gained from the research community and applying it to the typical challenging problems a practitioner is likely to face on a day to day basis and providing confidence and modelling guidelines as a consequence.
Acknowledgements

First and foremost, I thank Allah (God) for endowing me with health, patience, knowledge to complete this work.

There are really just so many people I would like to thank for helping me over these past years. I would like to express my deepest gratitude to my supervisors, Prof Malcolm Cook and Prof Jim McGuirk for all their guidance, support and encouragement during this work. I also thank them for all the financial support, particularly in the latter stages of my research. Many thanks go, too, to Dr Ibrahim Abdallah, Dr Tong Yang, Rehan Yousaf, Ben Hardcastle and ANSYS support team who made so many helpful suggestions as I carried out CFD simulations in this research. Dr Mahroo Eftekhar and Helen Newbold were very helpful with general PhD related issues. The funding for this PhD research provided by Loughborough University is greatly acknowledged.

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Contents

Chapter 1. Introduction ........................................................................................................... 1
  1.1. Background ................................................................................................................ 1
  1.2. Natural Ventilation .................................................................................................. 1
  1.3. Computational Fluid Dynamics (CFD) ..................................................................... 4
  1.4. Research aims and objectives ................................................................................... 6
  1.5. Thesis structure ......................................................................................................... 6

Chapter 2. Turbulence ........................................................................................................... 9
  2.1. Introduction ............................................................................................................... 9
  2.2. Energy cascade ......................................................................................................... 9
  2.3. Turbulence modelling .............................................................................................. 11
     2.3.1. Introduction ....................................................................................................... 11
     2.3.2. Reynolds-Averaged Navier Stokes equations ...................................................... 12
     2.3.3. Buoyancy calculation ........................................................................................ 14
     2.3.4. RANS based turbulence models ......................................................................... 15
     2.3.5. URANS ............................................................................................................. 18
     2.3.6. Large Eddy Simulation ...................................................................................... 18
     2.3.7. Detached Eddy Simulation ............................................................................... 23

Chapter 3. Previous work on wind and buoyancy driven natural ventilation ................... 24
  3.1. Introduction ............................................................................................................... 24
  3.2. Role of experiments in understanding natural ventilation .......................................... 27
  3.3. Use of CFD in building ventilation analysis ............................................................... 37
  3.4. Steady State Analysis using CFD ............................................................................. 42
     3.4.1. Reynolds-Averaged Navier Stokes (RANS) equations ........................................ 42
  3.5. Time dependent flows .............................................................................................. 49
     3.5.1. Unsteady RANS (URANS) ................................................................................. 50
3.5.2. Large Eddy Simulation (LES) ............................................................... 54
3.5.3. Detached Eddy Simulation (DES) ......................................................... 65
3.6. Summary ..................................................................................................... 66

Chapter 4. Methodology ...................................................................................... 68

4.1. Introduction ................................................................................................. 68
4.2. CFD codes .................................................................................................. 68
4.2.1. PHOENICS software ............................................................................ 69
4.2.2. ANSYS software .................................................................................. 70
4.3. Investigative strategy ................................................................................... 70
4.3.1. A preliminary test case ......................................................................... 71
4.3.2. Benchmark 1 test case ......................................................................... 73
4.3.3. Benchmark 2 test case ......................................................................... 74
4.3.4. Benchmark 3 test case ......................................................................... 76
4.4. Numerical method ....................................................................................... 77
4.5. Time step selection ..................................................................................... 77
4.5.1. Time step selection for RANS/URANS ................................................. 77
4.5.2. Time step selection for LES .................................................................. 78
4.6. Boundary conditions ................................................................................... 80
4.6.1. Solid wall boundaries ............................................................................ 81
4.6.2. Openings or Inflow/Outflow boundaries ................................................ 83
4.6.3. Solver Control and choice of convection discretisation scheme ........... 84
4.6.4. Domain initialisation .............................................................................. 85
4.6.5. Heat sources ........................................................................................... 85
4.6.6. Output control ....................................................................................... 86
4.7. Mesh selection methodology ...................................................................... 86
4.8. Parallel processing computations ................................................................. 89
4.9. Summary ..................................................................................................... 92
Chapter 5. Preliminary test case

5.1. Introduction

5.2. Background

5.3. The situation considered and associated theory

5.4. CFD modelling assumptions

5.4.1. Computational domain

5.4.2. Numerical solver

5.4.3. Grid refinement

5.4.4. Plume flow rate estimation

5.5. Results

5.5.1. Illustrative flow field results

5.5.2. Comparisons with experiments

5.6. Summary

Chapter 6. Benchmark 1: LES of twin thermal plumes

6.1. Introduction

6.2. The flow problem considered and associated theory

6.3. Computational methodology

6.3.1. The computational domain and mesh generation

6.3.2. LES software package and boundary conditions

6.3.3. LES numerical details

6.4. CFD results

6.4.1. Determining Statistical Stationarity

6.4.2. Mean flow field and interface height

6.4.3. Instantaneous flow field

6.4.4. Plume merge height

6.4.5. Ventilation flow rate

6.4.6. Vortex structures
Chapter 7. Benchmark 2: Buoyant flow in an enclosure with ceiling vent stacks and lower openings – multiple solutions ......................................................................................................................... 129

7.1. Introduction ............................................................................................................. 129
7.2. Background ............................................................................................................. 129
7.3. Numerical details .................................................................................................... 133
7.3.1. Computational geometry and mesh ................................................................. 133
7.3.2. Boundary conditions ........................................................................................ 135
7.3.3. The URANS and LES approach ...................................................................... 136
7.4. Methodology ........................................................................................................... 136
7.4.1. Regime B .......................................................................................................... 137
7.4.2. Regime A and C .............................................................................................. 137
7.5. Results .................................................................................................................... 137
7.6. Steady state solution ............................................................................................. 137
7.7. Multiple steady states ........................................................................................... 139
7.8. Comparison with analytical model ........................................................................ 142
7.9. Summary ................................................................................................................ 144

Chapter 8. Benchmark 3: URANS and LES practicality assessed on an auditorium test case ........................................................................................................................................ 147

8.1. Introduction ............................................................................................................. 147
8.2. Background ............................................................................................................. 148
8.3. Numerical procedure ............................................................................................. 148
8.3.1. Computational mesh and domain ................................................................. 148
8.3.2. Boundary conditions ........................................................................................ 151
8.3.3. URANS and LES numerical details ................................................................. 152
8.4. CFD results ............................................................................................................. 154
8.4.1. Instantaneous temperature field ........................................................................ 154
8.4.2. Statistically steady state ................................................................. 157
8.4.3. Velocity streamlines .................................................................... 161
8.4.4. Flow rate through the enclosure .................................................. 163
8.4.5. Fourier analysis ............................................................................ 164
8.5. Summary .......................................................................................... 167

Chapter 9. Summary, conclusions and future work .................................. 169
9.1. Research strategy ............................................................................. 169
9.2. Conclusions from benchmark test cases .......................................... 170
9.2.1. Benchmark 1 ................................................................................ 170
9.2.2. Benchmark 2 ................................................................................ 171
9.2.3. Benchmark 3 ................................................................................ 171
9.3. Contribution to knowledge ............................................................... 172
9.4. Limitations of the research ............................................................... 174

List of contributions ................................................................................ 187

List of Figures

FIGURE 1.1: AN EXAMPLE OF A NATURALLY VENTILATED BUILDING SHOWING A TYPICAL
ATRIUM ASSISTED BUOYANCY DRIVEN FLOW (SOURCE: CIBSE AM10 (2005) EDITED) . 2
FIGURE 1.2: THE LANCASTER LIBRARY, COVENTRY UNIVERSITY (LEFT) CFD ANALYSIS OF
THE BUILDING DURING DESIGN STAGE (RIGHT) (COOK, 2012) ..................................... 4
FIGURE 1.3: CASE STUDY OF NURSING LIBRARY BUILDING AND ITS INDOOR CFD ANALYSIS BY
HAJDUKIEWICZ ET AL. (2013) .................................................................................. 5
FIGURE 1.4: THESIS STRUCTURE FLOW CHART ...................................................... 8
FIGURE 2.1: ENERGY SPECTRUM ........................................................................ 10
FIGURE 2.2: SCHEMATIC REPRESENTATION OF TURBULENT MOTION (LEFT) AND THE TIME
DEPENDENCE OF A VELOCITY COMPONENT AT A POINT (RIGHT) (SOURCE: FERZIGER AND
PERIC (2002)) ..................................................................................................... 19
FIGURE 3.1: CROSS SECTION OF THE PROPOSED DESIGN BY BAHADORI (1985) ........ 26
FIGURE 3.2: Sketch of the development of stratified environment due to a heat source, showing the motions in the plume and environment, and the corresponding temperature profiles at two times (source: Baines and Turner (1968)). Where, \( F_0 \) is the buoyancy strength of the heat source, \( z \) is the height from the heat sources, \( T_1 \) and \( T_2 \) are the temperatures at interface 1 and 2 respectively, \( W \) is the plume width, \( \rho \) is the density of the plume and \( \rho_0 \) is the density of the environment .............................................. 27

FIGURE 3.3: Steady displacement flow with an internal horizontal line source. The internal stratification after time \( t = (a) 10, (b) 30, (c) 90 \) and \( (d) 240s \). Note the rising of the interface with time. (After Linden et al. 1990) .............. 28

FIGURE 3.4: Plume-plume interaction for (a) axisymmetric plume (b) plane plume (after Pera and Gebhart (1975)) ................................................................. 30

FIGURE 3.5: The situation considered by Hunt and Linden i.e. wind and buoyancy forces assist one another (source: (Hunt and Linden, 2001)) ................... 31

FIGURE 3.6: Schematic of the laboratory setup used by Hunt and Linden (source: (Hunt and Linden, 2001)) ................................................................. 31

FIGURE 3.7: Schematic showing two plumes merging in the far field and the virtual origin of the merged plumes (Kaye and Linden (2004)) ...................... 32

FIGURE 3.8: Schematic of three layer stratification due to buoyancies of different strengths for (a) co-flowing plumes (b) opposing plumes (Linden and Kaye (2006)) ................................................................. 33

FIGURE 3.9: Schematics of a confined descending plume colliding with the horizontal surface, spreading out radially and then rising up the sidewalls and overturning (Kaye and Hunt (2007)) ......................................................... 34

FIGURE 3.10: Schematics of three steady state ventilation regimes (a) regime A (b) regime B and (c) regime C (Chenvidyakarn and Woods (2005)) .............. 35

FIGURE 3.11: Ventilation performance in buildings predicated by different models in 2007 (Chen (2009)) ................................................................. 36

FIGURE 3.12: Six in-room flow configurations investigated by Ayad (1999) (1) cross ventilation, (2) cross ventilation with large exit openings, (3) cross ventilation with two exit openings, (4) ventilation with exit openings at adjacent walls, (5) ventilation with openings at far ends of adjacent walls with normal wind and (6) ventilation with openings at far ends adjacent walls with 30° incidence wind ................................................................. 40
FIGURE 3.13: Ventilation profiles over a plane at a height of 2.3m (Méndez et al. (2008))......................................................................................................................... 41

FIGURE 3.14: CFD analysis by Cook et al. (2003) velocity profile (left) and temperature profile (right) inside the enclosure ................................................. 43

FIGURE 3.15: Airflow patterns for the cases modelled by Asfour and Gadi (2007) .......................................................................................................................... 44

FIGURE 3.16: Predicted velocity and temperature profiles for an unventilated atrium (A,B) and a ventilated atrium (C,D) by Ji et al. (2007) ......................... 46

FIGURE 3.17: CFD predictions of buoyancy-driven natural ventilation in an atrium by Gan (2010) ....................................................................................... 47

FIGURE 3.18: Temperature visualization under different ambient conditions Liu et al. (2009) .......................................................................................................... 48

FIGURE 3.19: Tundish flow features: (A) basic structure (B) instantaneous streamlines in the numerical solution (Schwarze and Obermeier, 2006)...... 52

FIGURE 3.20: Comparison of time averaged temperature contours produced by URANS and DES on surface of the manikin (Deevy et al. (2008))........... 53

FIGURE 3.21: Side view of the (A) temperature and (B) velocity fields showing thermal plume rising in the centre of the room, cooler ambient air entering through the lower vents and warm air escaping through the upper vents (Kaye et al. (2009))............................................................................................................. 54

FIGURE 3.22: Measured and LES data comparison for (A) single-sided, windward ventilation, (B) single-sided, leeward ventilation and (C) cross ventilation (Jiang et al. (2003)) ........................................................................................................ 56

FIGURE 3.23: Velocity distribution around the buildings at 3m height from the ground with (A) wind from northwest direction and (B) a variable wind direction from north to west and a mean direction from northwest (Jiang and Chen (2002)) .................................................................................................................. 58

FIGURE 3.24: Turbulent kinetic energy distribution predicted by LES and experiment (Hu et al. (2008)) ................................................................................. 59

FIGURE 3.25: Time averaged velocity vectors (A) standard k-ε turbulence model (b) RNG k-ε turbulence model (c) realizable k-ε turbulence model (d) RNG based sub-grid scale turbulence model (e) Smagorinsky-Lilly sub-grid turbulence model and (f) experimental data (after Tutar and Oguz (2002))60
FIGURE 5.5: Velocity profile of a plume representing the Gaussian and "top-hat" profiles (source: Cook, 1998) ................................................................. 101

FIGURE 5.6: Velocity vector plot representing the flow directions inside the enclosure .............................................................................................. 102

FIGURE 5.7: Velocity contours on a plane perpendicular to the heat sources (x-y plane, z=2.5m), showing the coalescence of the two plumes using the RNG K-ε turbulence model. ............................................................... 103

FIGURE 5.8: Temperature stratification inside the enclosure showing the two fluid layers separated by a horizontal interface (x-y plane, z=2.5m) using the RNG K-ε turbulence model. ............................................................... 103

FIGURE 5.9: Prediction of the plume flow rate using the K-ε turbulence model compared with the flow rate measurements for two merging plumes for buoyancy flux ratio $\Psi = 0.45$. The red cross indicates a change in gradient indicating the merge height. .............................................................................. 104

FIGURE 5.10: Prediction of the plume flow rate using the RNG K-ε turbulence model compared with the flow rate measurements for two merging plumes for buoyancy flux ratio $\Psi = 0.45$. The red cross indicates a change in gradient indicating the merge height. .............................................................................. 105

FIGURE 6.1: Three layer stratification for non-interacting plumes .................. 108

FIGURE 6.2: Computational domain ........................................................................ 110

FIGURE 6.3: L/Δ plot for designed mesh for BM1 LES simulations; (left) front view and (right) top view ................................................................. 111

FIGURE 6.4: Snapshot of the transient values of flow through the enclosure at each opening to illustrate period of start-up, buffer and transient statistics ........................................................................................................ 113

FIGURE 6.5: Mean temperature contours predicted by LES (x-y plane, z=0.5m) for $\Psi = 0.5$ .............................................................................. 114

FIGURE 6.6: Mean temperature contours predicted by RANS (RNG K-ε) (x-y plane, z=0.5m) for $\Psi = 0.5$ ................................................................. 115

FIGURE 6.7: Vertical temperature profile comparing theoretical and predicted temperature interface heights in the domain. The vertical profile is plotted on a vertical line located at (x=0.1, z=0.1) ......................................................... 116

FIGURE 6.8: Slope of the temperature curve predicted by LES ......................... 117
Figure 6.9: Instantaneous temperature contours on an X-Y plane for $\psi = 0.5$, (Z=0.5) and at times (a) T1=0.5sec, (b) T2=2sec, (c) T3=3sec, (d) T4=10sec .... 118

Figure 6.10: Instantaneous temperature contours over vertical planes. X-Y plane, Z=0.5 (left) Y-Z plane x=0.5, (right) ................................................................. 119

Figure 6.11: Instantaneous W velocity normalised by max value of velocity $V_m$ plotted along Y-axis ................................................................. 121

Figure 6.12: Merging Gaussian profiles of the two plumes for $\psi = 0.5$ ........ 121

Figure 6.13: Variation of plume flow rates with height above the heat source ........................................................................................................ 123

Figure 6.14: Instantaneous pressure isosurface ($P=-0.028\text{Pa}$) at time $=150s$ and coloured by velocity .............................................................................. 124

Figure 6.15: Temperature isosurface ($T=27^\circ\text{C}$) at time $=150s$ and coloured by velocity ........................................................................................................ 125

Figure 6.16: Power spectral density of the vertical velocity at $X, Y, Z = 0.5, 0.3, 0.0$ ........................................................................................................ 126

Figure 7.1: Scaled down model of the room used by Chenvidyakarn and Woods (2005) in laboratory experiments ......................................................... 130

Figure 7.2: Schematics of the three steady state ventilation regimes reported by Chenvidyakarn and Woods: (a) Ventilation Regime A; (b) ventilation regime B; (c) ventilation regime C (after Chenvidyakarn and Woods (2005)) .............................................................................. 131

Figure 7.3: Relationship between the dimensionless room temperature, $\theta$ and the dimensionless time to converge to equilibrium $\tau$ (after Chenvidyakarn & Woods (2005)) ................................................................. 133

Figure 7.4: Computational domain ........................................................................ 134

Figure 7.5: L/\Delta plot of the mesh used for BM2 LES predictions .................... 135

Figure 7.6: Snapshot of the evolution of dynamical values of instantaneous temperature within the domain using LES .......................................................... 136

Figure 7.7: Comparison of the time to adjust to steady state as predicted by URANS, LES and the theory ................................................................. 138

Figure 7.8: Relationship between the dimensionless room temperature, $\Theta$, and the dimensionless time to converge to equilibrium, $\tau$ ........................................ 139
FIGURE 7.9: Temperature plot at $t = 320s$ on a plane midway through the domain using URANS illustrating (a) Regime A, (b) Regime B and (c) Regime C (dotted black lines representing an interface) ........................................................ 141
FIGURE 7.10: Temperature plot at $t = 320s$ on a plane midway through the domain using LES illustrating (a) Regime A, (b) Regime B and (c) Regime C ............ 141
FIGURE 7.11: Instantaneous temperature plots of the taller stack of the building during the switch from Regime C to Regime: (a) $T = T_{SS,C}$, (b) $T = T_{SS,B} + 190.05s$, (c) $T = T_{SS,B} + 198.05s$ and (d) $T = T_{SS,B}$ .............................................. 142
FIGURE 7.12: Comparison between theory (dotted lines) and URANS predictions (marker points) of dimensionless room temperature, $T^*_in$ with changes in area of bottom opening, $A^*_3/A^*_1$ (dotted lines show theory) ................................. 143
FIGURE 7.13: Comparison between theory (dotted lines) and LES predictions (marker points) of dimensionless room temperature, $T^*_in$ with changes in area of bottom opening, $A^*_3/A^*_1$ (dotted lines show theory) .............................................. 144
FIGURE 8.1: The Lichfield Garrick Auditorium with the Studio space and stairwells blurred out. ................................................................................ 148
FIGURE 8.2: Auditorium model built in ICEM CFX ................................................. 149
FIGURE 8.3: L/Δ plot for the mesh constructed for LES, BM3 test case .......... 151
FIGURE 8.4: Monitor points. Location of point 1 $(x,y,z = 5,12,7.5)$ and 2 $(x,y,z = 23,11,7.5)$ shown in red whilst others in green .............................................. 152
FIGURE 8.5: Dynamic temperature plot for two points (using URANS approach) .................................................................................................................. 153
FIGURE 8.6: Dynamic temperature plot for two points using LES approach ..... 154
FIGURE 8.7: Instantaneous temperature plots using URANS and LES predictions at time $t =$ (a) $15s$ (b) $35s$ (c) $55s$ (d) $100s$ and (e) $200s$. .................................................. 156
FIGURE 8.8: Instantaneous temperature contours at statistically steady state for URANS and LES at $t=320s$................................................................................. 158
FIGURE 8.9: Velocity plots for BM3 test case using URANS and LES at $t=320s$ ......................................................................................................................... 159
FIGURE 8.10: Time averaged temperature plots over the statistically steady state for BM3 test case using URANS and LES ................................................. 160
FIGURE 8.11: Streamline plots (colored by velocity) using URANS and LES .... 162
FIGURE 8.12: Air change per hour plotted against time for URANS and LES .... 163
FIGURE 8.13: LOCATION OF THE THREE POINTS WHERE FFT STATISTICS ANALYSED. (X,Y,Z) OF (A) POINT 1 (5,10,7.5) (B) POINT 2 (12,6,7.5) AND (C) POINT 3 (22,4,7.5) ........ 164

FIGURE 8.14: POWER SPECTRAL DENSITY OF THE VERTICAL VELOCITY AT POINT 1, 2 AND 3 .............................................................................................................................................. 166

FIGURE 8.15: INSTANTANEOUS VELOCITY V PLOTTED AGAINST TIME FOR POINT 1, 2 AND 3 WITH THE HORIZONTAL DASHED LINES SHOWING STATISTICALLY STEADY STATE PERIODS .............................................................................................................................................. 166

List of Tables

TABLE 5-1: GRID MESH SETTINGS AND RESULTING VOLUMETRIC FLOWS ....................... 99
TABLE 5-2: PERCENTAGE DISCREPANCIES BETWEEN CFD PREDICTIONS AND EXPERIMENTAL DATA ......................................................................................................................... 105
TABLE 6-1: SUMMARY TABLE OF COMPARISONS WITH COMMENTS ...................... 128
TABLE 7-1: SUMMARY TABLE OF COMPARISONS WITH COMMENTS ...................... 146
TABLE 8-1: DIMENSIONS OF IMPORTANT FEATURES OF THE AUDITORIUM MODEL FOR BENCHMARK 3 ......................................................................................................................... 150
TABLE 8-2: HEAT LOADS USED IN CFD SIMULATIONS .................................................. 151
TABLE 8-3: SUMMARY TABLE OF COMPARISONS WITH COMMENTS ...................... 168
Nomenclature

\( A^* \) effective opening area (m²)

\( \text{ACH} \) air changes per hour (-)

\( a_b \) area of the lower opening (m²)

\( a_t \) area of the upper opening (m²)

\( B \) buoyancy strength (m⁴/s⁴)

\( b_G \) Gaussian plume width (m)

\( b_T \) top-hat plume width (m)

\( C_d \) coefficient of discharge (-)

\( C_e \) coefficient of expansion (-)

\( C_p \) specific heat capacity (J/kg K)

\( C_s \) Smagorinsky constant

\( CFL \) Courant number (-)

\( \hat{F}_n \) buoyancy flux in plume \( n \) (m⁴/s⁴)

\( f \) loss coefficient (-)

\( G_r' \) specific buoyancy in the plume (m/s²)

\( g \) acceleration due to gravity (m/s²)

\( G \) filter convolution kernel

\( H \) total height of computational domain (m)

\( H e_T \) top-hat enthalpy (J/kg)

\( H e_G \) Gaussian value for enthalpy (J/kg)

\( H_h \) heat gains from occupants & equipment (W)

\( h \) mean interface height (m)

\( k_t \) time-mean total turbulence kinetic energy (J)

\( k_{\text{res}} \) resolved turbulence kinetic energy (J)

\( k_{\text{SGS}} \) SGS kinetic energy (J)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>k\textsubscript{RANS}</td>
<td>RANS predicted turbulence energy (J)</td>
</tr>
<tr>
<td>S</td>
<td>Strain rate (-)</td>
</tr>
<tr>
<td>Re\textsubscript{t}</td>
<td>turbulent Reynolds number (-)</td>
</tr>
<tr>
<td>L</td>
<td>integral turbulent length scale (m)</td>
</tr>
<tr>
<td>l\textsubscript{SGS}</td>
<td>SGS length scale (m)</td>
</tr>
<tr>
<td>M</td>
<td>volume flux (m\textsuperscript{3}/s)</td>
</tr>
<tr>
<td>P</td>
<td>pressure (Pa)</td>
</tr>
<tr>
<td>Pe</td>
<td>Peclet number (-)</td>
</tr>
<tr>
<td>Pr\textsubscript{SGS}</td>
<td>SGS Prandtl number (-)</td>
</tr>
<tr>
<td>Pr\textsubscript{T}</td>
<td>Turbulent Prandtl number (-)</td>
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<tr>
<td>q</td>
<td>heat source strength (W)</td>
</tr>
<tr>
<td>\bar{q}\textsubscript{i}</td>
<td>time-mean molecular heat flux (W)</td>
</tr>
<tr>
<td>q\textsubscript{w}</td>
<td>heat flux across a wall (W)</td>
</tr>
<tr>
<td>Q</td>
<td>volume flux (m\textsuperscript{3}/s m\textsuperscript{2})</td>
</tr>
<tr>
<td>Q\textsuperscript{*}</td>
<td>non-dimensional volume flow rate (-)</td>
</tr>
<tr>
<td>T</td>
<td>temperature (C)</td>
</tr>
<tr>
<td>T\textsubscript{E}</td>
<td>the exterior ambient temperature (\degree C)</td>
</tr>
<tr>
<td>T\textsubscript{in,ss}</td>
<td>indoor temperature at steady state (\degree C)</td>
</tr>
<tr>
<td>T\textsuperscript{*}\textsubscript{in,ss}</td>
<td>dimensionless temperature (-)</td>
</tr>
<tr>
<td>T\textsubscript{ref}</td>
<td>reference temperature (\degree C)</td>
</tr>
<tr>
<td>t\textsubscript{s}</td>
<td>dimensional timescale to converge to equilibrium (s)</td>
</tr>
<tr>
<td>u</td>
<td>velocity along x-axis (m/s)</td>
</tr>
<tr>
<td>U\textsubscript{n}</td>
<td>normal velocity (m/s)</td>
</tr>
<tr>
<td>u\textsuperscript{'}</td>
<td>turbulence intensity (m/s)</td>
</tr>
<tr>
<td>u\textsubscript{SGS}</td>
<td>subgrid velocity scale (m/s)</td>
</tr>
<tr>
<td>u\textsuperscript{*}</td>
<td>near wall velocity (m/s)</td>
</tr>
<tr>
<td>u\textsubscript{\tau}</td>
<td>friction velocity (m/s)</td>
</tr>
</tbody>
</table>
\( \bar{u} \): velocity tangent to the wall at a distance \( \Delta y \) (m/s)

Vol: local cell volume (m³)

\( v \): velocity along y-axis (m/s)

\( V \): volume of the room (m³)

\( v \): linear velocity (m/s)

\( V_m \): mean velocity along plume-axis (m/s)

\( V_G \): Gaussian velocity (m/s)

\( V_T \): top-hat velocity (m/s)

\( w \): velocity along z-axis (m/s)

\( x,y,z \): Cartesian coordinates (m)

\( x_0 \): heat source separation (m)

\( y_v \): distance of the virtual origin below heat source (m)

\( y^+ \): dimensionless distance from the wall (-)

\( z_m \): plume merge height (m)

\( \alpha_G \): Gaussian plume entrainment coefficient (-)

\( \alpha_T \): normalised plume entrainment coefficient (-)

\( \alpha \): plume entrainment coefficient (-)

\( \beta \): coefficient of thermal expansion (-)

\( \alpha^* \): volumetric expansion constant (1/K)

\( \beta^* \): heat loss air exchange parameter (m³/s)

\( \Delta P_{loss} \): pressure loss across the opening (Pa)

\( \Delta t \): time step size (s)

\( \Delta x \): filter width (m)

\( \Delta \): grid size (m)

\( \varepsilon \): turbulent energy dissipation per unit mass (m²/s³)

\( \varepsilon_{RANS} \): RANS predicted dissipation rate (m²/s³)

\( \varepsilon_{LES} \): LES estimated dissipation rate (m²/s³)
\begin{itemize}
    \item $\varepsilon'$: perturbation in interface height (-)
    \item $\rho$: density (kg/m$^3$)
    \item $\rho_{\text{ref}}$: constant reference density (kg/m$^3$)
    \item $\lambda$: fluid thermal conductivity (W/m·K)
    \item $\xi$: normalised interface height (h/H) (-)
    \item $\xi'$: normalised interface height with virtual origin correction (-)
    \item $\xi_v$: normalised distance of virtual origin below source (-)
    \item $\psi$: buoyancy flux ratio (-)
    \item $\varphi$: any fluctuating variable (-)
    \item $\gamma^*$: wind air change parameter (m$^3$/s)
    \item $\theta$: dimensionless room temperature (-)
    \item $\tau$: dimensionless time (-)
    \item $\bar{\tau}_\omega$: time-mean wall shear stress (Pa)
    \item $\eta$: Kolmogorov length scale (m)
    \item $\nu$: kinematic fluid viscosity (m$^2$/s)
    \item $\mu_t$: turbulent eddy viscosity (Pa·s)
    \item $\mu_{\text{SGS}}$: SGS eddy viscosity (Pa·s)
\end{itemize}
Chapter 1. Introduction

“For, usually and fitly, the presence of an introduction is held to imply that there is something of consequence and importance to be introduced” – Arthur Machen

1.1. Background
Since early times mankind has used shelter for protection, from both wild and inhospitable weather conditions. Over time the aim shifted to providing comfortable conditions for living and working purposes as humans started to spend more time indoors. An important part of this provision is ventilation which is the process of supplying, removing and circulating air inside enclosures. Today people spend up to 90% of their time indoors (EPA, 2008). Post the industrial revolution, the use of air-conditioning in buildings increased rapidly in order to provide comfortable indoor conditions specifically in terms of prevailing temperatures (Penz, 1983). However, growing concerns regarding energy efficiency in the latter part of the 20th and early 21st centuries has focused attention on the impact buildings have on carbon dioxide emissions. In the UK and other EU countries, buildings consume 40-50% of the primary energy (CIBSE, 2003). The UK government has set a goal of reducing the emissions of greenhouse gases by 80% by the year 2050 under the Kyoto Protocol (DTI, 2003). This has led to more stringent building regulations and, as a result, it has become common practice for energy efficient strategies to be incorporated into modern low energy building design. Natural ventilation is one such energy efficient strategy.

1.2. Natural Ventilation
Natural ventilation takes advantage of the readily available resources of wind and thermal energy. Although these resources are free (renewable), controlling them can be difficult in order to regulate internal prevailing conditions. This is because only
small temperature differences are typically available and the direction and speed of winds are variable and difficult to predict. On hot and windless days natural ventilation may not be able to meet comfort criteria (Linden, 1999). Better knowledge of natural ventilation and improvement of design guidelines would have a significant effect on the optimal implementation of natural ventilation. Figure 1.1 shows a typical layout of a naturally ventilated building.

During the operation of a building that incorporates natural ventilation a worst case scenario might arise on a hot and windless day. On such a day ventilation is driven by buoyancy forces. Buoyancy-driven natural ventilation harnesses the buoyancy forces associated with the temperature differences between interior and exterior environments to drive airflow through a building. Thus, focusing research on this worst case scenario has clear benefits e.g. meeting thermal comfort criteria and avoiding CO₂ build up in the building.

Buildings that incorporate natural ventilation are often highly innovative in their design, for example the Lanchester library (Coventry University, UK), whose lightwells penetrate the heart of the building to provide ventilation. Other examples are the Queens Building (De Montfort University, UK), ventilated by stacks, the Mode-Gakuen Spiral Towers (Nagoya, Japan) which corkscrews 36 storeys high,
and the pointed Russia tower (Moscow, Russia) which is amongst the tallest buildings in the world and is naturally ventilated. All these buildings differ significantly in their design from conventional buildings and thus conventional design guidelines become limited in addressing design issues. Thus, some form of air flow modelling is desirable at the design stage in order to examine questions such as:

- will the proposed ventilation strategy deliver the required levels of fresh air and meet the thermal comfort criteria?
- in what ways would design modifications help in improving the ventilation strategy?

Cook et al. (2003a) inform us that:

“there is, in general, a need to understand how the air flow rates, temperatures and general comfort conditions within a space are affected by the geometry of the enclosure, the size and location of the ventilation openings, the distribution of the heating (or cooling) sources and the driving force produced by the wind.”

In general there are three approaches to modelling natural ventilation (Cook et al. (2003a)): analytical, empirical/experimental and computer simulation.

Allocca et al. (2003) have noted that empirical models are usually developed from a combination of analytical solutions and experimental data. These are simple and straightforward to use for designers, however they do not account for the impact of building forms, surroundings, and interior spaces on the ventilation performance of a building (Jiang and Chen, 2003).

Experimental measurements and computer simulations on the other hand can allow for such effects. Katayama et al. (1992), however, concluded that whilst experimental measurements do give realistic information about natural ventilation, these are often expensive to acquire and time consuming. Jiang and Chen (2002) outline how wind-tunnel and full-scale measurements are still the most common approaches used to understand natural ventilation. To study buoyancy-driven natural ventilation, however, it is hard for scaled wind tunnel models to generate the correct ratios of buoyancy to inertia effects (i.e. high-Grashof numbers) to assume they are genuinely analogous to full-scale situations (Jiang and Chen, 2003). There is little
doubt that experimental methods are an expensive option both in operation time and equipment costs. Furthermore, experimental measurements may not provide the sufficient detail everywhere throughout the flow domain of interest that is necessary for complete understanding of the mechanism of natural ventilation, such as small scale flow structures, and unsteady coherent structures within thermal plumes.

Due to the highly innovative designs of naturally ventilated buildings as previously discussed, designers require a method which offers the potential to deliver high levels of flow detail with sufficient accuracy at low cost. This is the role increasingly played by computer simulations over the last few decades making use of the technical discipline known as Computational Fluid Dynamics.

1.3. Computational Fluid Dynamics (CFD)

Computational Fluid Dynamics (CFD) is a numerical technique that solves the partial differential equations for the conservation of mass, momentum, energy, if necessary chemical species concentrations and supplementary quantities that are chosen to characterise the turbulent nature of the flow. Full volumetric field distributions of pressure, temperature, velocity, concentrations of water vapour and contaminants and turbulence parameters in both indoor and outdoor spaces can be predicted using CFD (Chen, 2009). Figure 1.2 and Figure 1.3 provide illustrations of CFD analysis used to understand practical natural ventilation building problems.

Figure 1.2: The Lancaster library, Coventry University (left) CFD analysis of the building during design stage (right) (Cook, 2012)
In spite of decades of development in turbulence modelling, computer capacity, computer speed and reduced cost, ‘steady state’ CFD analysis is still the type of numerical modelling approach most frequently adopted for natural ventilation analysis. CFD also has the added benefit of producing much more informative results than experimental procedures as data collection limitations in CFD are much more flexible. Results from CFD are usually validated by comparing them with experimental data. However, turbulence modelling is still a fundamental problem in CFD after more than 50 years of research (Tennekes and Lumley, 1972; Wilcox, 1993). In the last decade or so more accurate turbulence modelling techniques, which explicitly account for unsteady turbulent processes, have become more computationally affordable. The most promising example of this is the so-called Large Eddy Simulation (LES) technique. It is important to assess the potential of such new CFD approaches for application to buoyancy-driven naturally ventilated buildings. In the author’s view this has to date not been comprehensively studied and thus a gap in research exists which needs to be investigated and this forms the motivation for the present research.

Figure 1.3: Case study of nursing library building and its indoor CFD analysis by Hajdukiewicz et al. (2013)
1.4. Research aims and objectives

The aim of the current research was therefore to assess the performance of the LES technique in modelling buoyancy-driven natural ventilation and compare its performance to conventional CFD techniques. Results from both these techniques are validated against theoretical models and experimental data.

The high level objectives of the project are as follows:

- Use LES to model buoyancy-driven natural ventilation in a simple geometry (but still relevant to the application area of interest) for which the flow phenomena are well understood and well documented
- Apply LES to more realistic benchmark problems (of increasing complexity) for buoyancy-driven natural ventilation flows
- Compile guidelines for users of LES wishing to model buoyancy-driven natural ventilation
- Establish the trade-off between the physical accuracy and cost of LES with respect to conventional CFD

1.5. Thesis structure

The first half of the thesis is divided as follows. Chapter 2 introduces the phenomenon of turbulence and defines key CFD techniques as well as some basic aspects of the typical experimental modelling technique of salt bath modelling. Chapter 3 reviews previous research carried out on natural ventilation design and the different approaches used for modelling natural ventilation. This chapter also identifies the research gap, describes the basic research problem to be addressed and the perceived strengths and weaknesses of LES in predicting natural ventilation flows. The methodology of the numerical approach finally adopted is presented in Chapter 4.

The second half of the thesis presents the results of all simulations performed. Chapter 5 presents results for a preliminary natural ventilation test case involving twin merging buoyant flows carried out using the PHOENICS software (CHAM, 2009) and only using conventional steady state turbulence modelling to build up the author’s understanding of CFD mesh generation, convergence, boundary conditions etc. This chapter also illustrates how the choice of turbulence model affects airflows
predictions. Chapter 6 reports both conventional turbulence model predictions and LES simulations of a similar twin buoyant plume flow in a naturally ventilated enclosure. Because this problem was considered using different turbulence model approaches it is referred to in this work as the “Benchmark 1” test case. Benchmark 2 test case comprises the more complex flow of an open plan office space with two unequal length stacks, and is also analysed with both conventional turbulence modelling and LES in Chapter 7 with results compared with experimental data. The specific aim of this test case was to compare the performance of both techniques in capturing multiple steady states in natural ventilation. Chapter 8 extends the assessment of performance of conventional and advanced turbulence modelling to prediction of flow dynamics of a practical problem i.e. a real theatre building. Finally, in Chapter 9 a summary of the work is given and conclusions drawn. Limitations of the work and recommendations for future work are also presented. The thesis structure is summarized in the following flow chart.
Figure 1.4: Thesis structure flow chart
Chapter 2. Turbulence

“I am an old man now, and when I die and go to heaven I would like to be enlightened on two subjects: quantum electrodynamics and turbulence. And I am rather optimistic about the former” – Sir Horace Lamb

2.1. Introduction

In nature and in most engineering flows fluid motion is normally turbulent. Turbulence is perhaps to be considered undesirable in machines in which fluid flow occurs, since more energy has to be provided to sustain a turbulent than a non-turbulent flow. On the other hand turbulence is in some applications desirable as it substantially increases the rate of mixing and heat or mass transfer. Although we intuitively know what it is, a satisfactory definition of turbulence is still elusive. One characteristic is that it is unavoidable in flows at high Reynolds number (Re) due to inherent instability of boundary layers and free shear layers. A general way of defining a turbulent flow is that all flow variables behave in a permanently unsteady chaotic manner and are always 3D in nature.

2.2. Energy cascade

One crucial characteristic of high Re turbulent flow is the appearance of a broad spectrum of vortices of different sizes. The turbulent field is a superposition of large, small and medium 3D vortices also known as ‘eddies’. The size and strength (kinetic energy) of these eddies can be considered representative of the length scale and velocity scale characteristic of each eddy. The large scale eddies are limited in size by the characteristic dimension of the mean flow with a characteristic size referred to as the integral length scale, $L$. The smallest scales of turbulence are the inner scales or more commonly known as the Kolmogorov scales $\eta$. These eddies have a
relationship with turbulent energy dissipation, \( \varepsilon \) and kinematic fluid viscosity, \( \nu \) given by:

\[
\eta \equiv \left( \frac{\nu^3}{\varepsilon} \right)^{1/4}
\]  

where, for a so-called high Re equilibrium cascade, the magnitude of \( \varepsilon \) may be related to large scale turbulence intensity (\( u' \)) and length scale (\( L \)) as:

\[
\varepsilon \approx \frac{u'^3}{L}
\]

Eddies smaller than \( \eta \) do not exist since any fluctuating energy transferred to them is instantly dissipated into heat by \( \nu \). This behaviour is more clearly described as an energy cascade. The idea is that large eddies (which gain their kinetic energy by vortical interactions with the mean statistically steady flow) transfer their energy into slightly smaller eddies by a process of vortex stretching; these in turn transfer it to even smaller eddies until the energy reaches the smallest length scale \( \eta \) where it is dissipated into heat through viscosity. Figure 2.1 illustrates the energy spectrum of a typical high Re turbulent flow.

Figure 2.1: Energy spectrum
The horizontal axis shows the eddy frequency (f). The frequency range (f is proportional to the reciprocal of the eddy size since \( f \approx \frac{\text{eddy velocity scale}}{\text{eddy length scale}} \)) contains a peak associated with the integral length scale (size of energy containing eddies) at the flow field point in question. An energy cascade from larger to smaller eddies due to vortex stretching in which energy is conserved can also be identified, which at high Reynolds numbers follows a theoretical -5/3 slope in an inertial sub range. A cut off then occurs at length scales approaching the Kolmogorov scale \( \eta \) with the energy falling steeply to negligible values due to viscous dissipation.

In order to resolve numerically the dynamics of the smallest scales, very fine meshes need to be employed with a spatial resolution of the order of the Kolmogorov scale \( \eta \). This so-called Direct Numerical Simulation (DNS) approach results in extremely high computational power and time requirements which also rapidly get worse as Reynolds number increases. Due to this limitation DNS is not a practical approach for applied CFD and various forms of averaging or filtering are adopted so that some (or all) aspects of unsteady turbulence are removed from the numerically resolved flow. In order to account for these excluded effects of turbulence on the numerical solution various approaches to turbulence modelling have been developed and these are reviewed next.

2.3. Turbulence modelling

2.3.1. Introduction

The instantaneous Navier Stokes equations apply to the flow of any Newtonian fluid. However, finding analytical solutions to these for most flows of relevance to engineering is not possible. Researchers have had to turn to a numerical and model-based approach given the cost of DNS as noted earlier. There are two possible approaches. The first – and oldest – solves the so-called Reynolds Averaged Navier-Stokes (RANS) equations and is described and reviewed next. The second – only perhaps 30 years old – is the Large Eddy Simulation (LES) approach. Finally, the high computational cost of LES (although much less than DNS) has created in the last decade a search for possible hybrid RANS/LES methods; one such technique is reviewed to close this chapter – Detached Eddy Simulation (DES).
2.3.2. Reynolds-Averaged Navier Stokes equations

The application of one of the following averaging processes to the Navier Stokes equations yields the Reynolds-Averaged Navier Stokes (RANS) equations. In a statistically steady flow, all instantaneous quantities can be decomposed into time-averaged and fluctuating components:

\[ u_i(x_i, t) = \bar{u}_i(x_i) + u_i'(x_i, t) \]  

where,

\[ \bar{u}_i(x_i) = \lim_{T \to \infty} \frac{1}{T} \int_0^T u_i(x_i, t) dt \]  

is known as time averaging. Here \( T^* \) represents the averaging interval and \( t \) is the time. Ensemble averaging on the other hand is used for cases where the flow is statistically non-stationary, and in this case the mean quantity is defined as:

\[ \bar{u}_i(x_i, t) = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} u_i(x_i, t) \]  

where \( N \) represents an imagined multiple repetition of the flow starting from the same initial conditions.

Note that in statistically stationary flows, the mean is independent of time, whereas for ensemble averaging the mean still depends on time. The former is usually referred to as a RANS approach and the latter as URANS (Unsteady RANS).

For incompressible flows density does not depend on pressure; in buoyant flows, local fluid density may still depend on local temperature or species concentration, but, as explained below, it is an accepted and accurate practice to ignore density variations except in the gravitational term. Thus, initially, density may be assumed constant in space and time in all other terms and the averaged continuity, momentum and energy equations can be written (in Cartesian coordinates):

\[ \frac{\partial (\rho \bar{u}_i)}{\partial x_i} = 0 \]  

and,
\[
\frac{\partial}{\partial t} (\rho \overline{u_i}) + \frac{\partial}{\partial x_j} \left( \rho \overline{u_i u_j} + \rho \overline{u_i u_j} \right) = - \frac{\partial \overline{p}}{\partial x_i} + \frac{\partial \overline{\tau_{ij}}}{\partial x_j} + \Delta \rho g_i \tag{2-7}
\]

where \( \Delta \rho \) is the difference between local density and a reference density \( \rho_{ref} \) (\( \rho \) in all other terms is set to \( \rho_{ref} \)). Also \( \overline{\rho u_i u_j} \) are the Reynolds stresses, \( \overline{\tau_{ij}} \) are the time-mean viscous stress tensor components and \( g_i \) is the gravitational acceleration.

Similarly, for conditions typical of natural ventilation, the energy equation (1\textsuperscript{st} law of thermodynamics) may be written:

\[
\frac{\partial \overline{\rho T}}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho \overline{u_i T} + \rho \overline{u_i T} \right) = - \frac{\partial \overline{q_i}}{\partial x_i} \tag{2-8}
\]

where,

\[
\overline{q_i} = - \frac{\lambda}{C_p} \frac{\partial T}{\partial x_i} \tag{2-9}
\]

where \( \overline{q_i} \) is the time-mean molecular heat flux (\( \lambda, C_p \) are fluid thermal conductivity and specific heat respectively), and \( \rho \overline{u_i T} \) are the turbulent heat fluxes.

The appearance of the Reynolds stresses and turbulent heat fluxes in these equations means the set of equations is not closed. This is therefore known as the closure problem. Thus, approximations are introduced into the equations via a turbulence model. An eddy-viscosity model is the most commonly used turbulence model in RANS CFD and models the Reynolds stresses as follows (\( \mu_t \) is the eddy viscosity):

\[
-\rho \overline{u_i u_j} = \mu_t \left( \frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) - \frac{2}{3} \rho \delta_j \tag{2-10}
\]

The heat fluxes are modelled by analogy (\( Pr_T \) is the turbulent Prandtl number for heat transfer):

\[
-\rho \overline{u_i T'} = \frac{\mu_t}{Pr_T} \frac{\partial \overline{T}}{\partial x_j} \tag{2-11}
\]

where, \( k \) is the turbulent kinetic energy given by:
The most popular two-equation eddy viscosity model is the high Reynolds number k-\(\varepsilon\) model (Lauder and Spalding, 1974) which uses the following expression to determine \(\mu_t\):

\[
\mu_t = C_{\mu} \rho \frac{k^2}{\varepsilon}
\]  

2-13

Here, \(C_{\mu}\) is an empirical dimensionless constant which has to be calibrated as part of the model derivation, and has a value of 0.09 for the \(k-\varepsilon\) model; \(\varepsilon\) is the turbulence energy dissipation rate; model equations to determine \(k\) and \(\varepsilon\) are given below.

2.3.3. Buoyancy calculation

For calculations involving buoyancy, a source term is present in the vertical momentum (\(v\)) equation of equation 2-7:

\[
S_{v,\text{buoy}} = -(\Delta \rho)g
\]  

2-14

The density term \(\Delta \rho\) (the difference between local density and a constant reference density \(\rho_{\text{ref}}\)) is evaluated using the Boussinesq approach which will be discussed below. The hydrostatic gradient due to the reference density in the momentum equation is excluded when buoyancy is activated. The modified pressure \(p\) appearing in the momentum equation 2-7 is called “motion pressure” as it is purely responsible for driving the flow. The reference density is related to absolute static pressure as follows:

\[
p_{\text{abs}} = p + p_{\text{ref}} + \rho_{\text{ref}} g_i (r_i - r_{\text{ref}})
\]  

2-15

where, \(r_{\text{ref}}\) is a reference location within the flow domain.

2.3.3.1. Boussinesq assumption

As noted above, in buoyancy-driven flows, if the density variations in space and time are small, these can be ignored in all terms except for the body force in the vertical momentum equation. This is known as the Boussinesq assumption. In the current study to execute buoyancy calculations the Boussinesq assumption has been
employed. For the buoyancy source term and where buoyancy is driven by
temperature differences:

$$\Delta \rho = -\rho_{ref} \beta (T - T_{ref})$$  \hspace{1cm} 2-16

where \( T_{ref} \) is a reference temperature and \( \beta \) is the thermal expansion coefficient (a
fluid property):

$$\beta = -\frac{1}{\rho_{ref}} \frac{\partial \rho}{\partial T}$$  \hspace{1cm} 2-17

2.3.4. RANS based turbulence models

Two-equation models are the most common type of RANS based turbulence model. Chen (2009) suggests the most popular two-equation models are the high Re standard k-\( \epsilon \) model (Launder and Spalding, 1974) and the RNG k-\( \epsilon \) model (Yakhot et

2.3.4.1. k-\( \epsilon \) model

The k-\( \epsilon \) model includes two extra transport equations to represent the turbulent
properties of the flow. This makes it possible to account for transport effects of the
flow like convection and diffusion on turbulence properties. The first variable is the
turbulent kinetic energy, \( k \), which characterises the local energy characteristics of
turbulence \( (k^{1/2} \) represents the velocity scale of turbulent mixing processes); the
second transported variable is the turbulent dissipation, \( \epsilon \), which can be used to
characterise the length scale of the turbulent eddies (on dimensional analysis
grounds, a turbulence length scale may be calculated from \( k^{3/2}/ \epsilon \)). The Launder and
Spalding formulation of the k-\( \epsilon \) model is typically called the ‘standard high Re k-\( \epsilon \)
model’. The transport equations for this model are as follows:

For turbulent kinetic energy, \( k \):

$$\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k \bar{u}_i) = \frac{\partial}{\partial x_j} \left[ \mu + \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right] + P_k + P_b - \rho \epsilon$$  \hspace{1cm} 2-18

For turbulent dissipation, \( \epsilon \):
\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho \varepsilon \bar{u}_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \frac{\varepsilon}{k} (C_{1\varepsilon} P_k + C_{1\varepsilon} P_b - C_{2\varepsilon} \rho \varepsilon)
\]

Turbulent or eddy viscosity is modeled as:

\[
\mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon}
\]

Production of \( k \) is determined by:

\[
P_k = -\rho u_i u_j \frac{\partial \bar{\tau}_{ij}}{\partial x_i}
\]

\[
P_k = \mu_t S^2
\]

where \( S \) is the modulus of the mean rate of strain tensor:

\[
S \equiv \sqrt{2S_{ij}S_{ij}}
\]

The source/sink term for \( k \) due to buoyancy is calculated by:

\[
P_b = -\frac{\mu_t}{Pr_t} \beta g_i \frac{\partial \bar{T}}{\partial x_i}
\]

where \( Pr_t \) is the turbulent Prandtl number (a dimensional number defined as the ratio of viscous diffusion rate and thermal diffusion rate).

The calibrated model constants accepted for use in the standard \( k-\varepsilon \) model are:

\( C_{1\varepsilon} = 1.44, C_{2\varepsilon} = 1.92, C_{\mu} = 0.09, \sigma_k = 1.0, \sigma_\varepsilon = 1.3 \) and \( Pr_t = 0.9 \).

2.3.4.2. **RNG \( k-\varepsilon \) model**

A mathematical technique called the “Renormalization Group (RNG)” method was developed by Yakhot et al. (1992) and used to formulate the RNG-based \( k-\varepsilon \) turbulence model. In this technique the smaller eddies are eliminated and their mean effect on the remaining larger eddies is replaced by increasing the viscosity via a simple iterative procedure. This helps in damping out the smaller eddies.
resulting equation is rescaled through an iterative process until two successive iterations match closely. It has been observed and commented in literature (see Chapter 3) that the RNG k-ε model is more responsive to streamline curvature, high strain rate and buoyancy than the standard k-ε model.

The transport equations for turbulence properties are the same as those for the standard k-ε model, however the model constants differ with constant $C_{2\varepsilon}$ becoming $C^*_{2\varepsilon}$, $C_{1\varepsilon}$ being replaced by the function $C_{1\varepsilon\text{RNG}}$ and $C_\mu$ with $C_{\mu\text{RNG}}$.

The transport equation for turbulent dissipation, $\varepsilon$ becomes:

$$
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho \varepsilon \bar{u}_i) = \frac{\partial}{\partial x_j} \left[ \mu \frac{\partial \varepsilon}{\partial x_j} \right] + \frac{\varepsilon}{k} \left( C_{1\varepsilon\text{RNG}} P_k + C_{1\varepsilon\text{RNG}} P_b - C^*_{2\varepsilon} \rho \varepsilon \right)
$$

where

$$
C_{1\varepsilon\text{RNG}} = 1.42 - f_n
$$

$$
C^*_{2\varepsilon} = C_{2\varepsilon} + C_{\mu\text{RNG}} \eta^2 f_n
$$

Also,

$$
f_n = \frac{\eta \left( 1 - \frac{\eta}{\eta_0} \right)}{(1 + \beta_{\text{RNG}} \eta^3)}
$$

and

$$
\eta = \frac{P_k}{\sqrt{C_{\mu\text{RNG}} \rho \varepsilon}}
$$

The turbulent viscosity is calculated in the same manner as with the standard k-ε model.

Model constants:
\[ C_{1\varepsilon} = 1.42 \, , \, C_{2\varepsilon} = 1.68 \, , \, C_{\mu RNG} = 0.0845 \, , \, \sigma_k = 0.7194 \, , \, \sigma_\varepsilon = 0.7194 \, , \, \eta_o = 4.38 \, \text{and} \, \beta_{RNG} = 0.012 \]

In all the above differential transport equations (2-7, 2-8, 2-18, 2-19, 2-25), the unsteady term \( \frac{\partial}{\partial t} \) has been included. For steady RANS solutions, these terms are of course omitted.

### 2.3.5. URANS

URANS modelling is appropriate when it is believed that there is some physical process (or some unsteady boundary conditions) which can introduce long term periodic oscillations in a turbulent flow. In this case, ensemble averaging must be used since the mean flow never becomes truly steady, and the unsteady term is used to capture the periodic oscillation. The steady RANS modelling approach is retained for the Reynolds stresses which are assumed to be de-coupled from the unsteady periodic oscillations. The \( \frac{\partial}{\partial t} \) term in all transport equations are of course retained when solving in URANS mode.

### 2.3.6. Large Eddy Simulation

Due to the adoption of an averaging procedure for all scales of turbulent motions (the integrals in equations 2-4 and 2-5 extend to \( \infty \)), the RANS approach can significantly reduce computational time but at the loss of including the instantaneous dynamics of any turbulent motions. However, if it is believed that inclusion of at least some of the unsteady motions may be important then the Large Eddy Simulation (LES) approach can provide an alternative option and improve the predictive accuracy (compared to RANS) and still reduce computational time (compared to DNS).

LES uses low pass spatial filtering of the flow field intended to remove a range of small scales from the solution to the Navier-Stokes equations. As discussed earlier, in any turbulent flow there exist large scale eddies which depend strongly on the boundaries and nature of the flow. These are eddies which, because they contain most of the kinetic energy (see Figure 2.1), are mainly responsible for the increased transport of mass, momentum and temperature by turbulence. Smaller scale eddies which are caused by the interactions of large scale eddies only dissipate the fluctuations and consequently affect the mean flow only to a small extent. These characteristics have led to an approach in which small scales that are not captured
by the numerical mesh are removed (filtered) from the description of the flow during the simulation process. The flow field structures that are greater than the filter size (i.e. are captured by the numerical grid) are calculated using spatially filtered Navier-Stokes equations, while the effects of eddies smaller than the filter size on the numerically resolved flow are modelled. This gives LES the potential to provide more accurate simulations than RANS though admittedly with higher computational costs. However, this computational time is much less compared to DNS since the smaller scales are not resolved and the computational time should also not depend too much on flow Reynolds number.

LES models were first developed and utilised by Smagorinsky (1963), Lilly (1962) and Deardoff (1970). The formalism of the filter function as used today was introduced by Leonard (1974) which was reviewed by Ferziger et al. (1977). The filtering was later generalised by Germano (1992). This makes LES CFD spatially filtered while RANS CFD is temporally (or ensemble) filtered.

“Practical” LES has been described in different manners. Pope (2000) suggests -well resolved- LES as being a “practical” simulation in which 80% of the fluctuating turbulent energy is resolved numerically accurately. Ferziger (1977) suggested that in LES the scales of motion resolved should be down to the Taylor microscale, which is the largest length scale at which fluid viscosity significantly affects the dynamics of the turbulent eddies. Figure 2.2 illustrates schematically the difference between LES and DNS.

![Figure 2.2: Schematic representation of turbulent motion (left) and the time dependence of a velocity component at a point (right) (source: Ferziger and Peric (2002))](image)
LES is based on four basic steps (Veloudis, 2006):

1. A spatial filtering operation is defined, where the velocity is decomposed into the sum of the filtered (or resolved) component and the subgrid scale (SGS) non-resolved component.

   \[ u(x_i, t) = \bar{u}(x_i, t) + u'(x_i, t) \quad \text{2-30} \]

   Here, \( \bar{u}(x_i, t) \) characterizes the dynamics of the resolved eddies and \( u'(x_i, t) \) represents the small non-resolved eddies.

2. The Navier Stokes equations are filtered to derive the equations for \( \bar{u}(x_i, t) \). The LES equations of motion contain the SGS stress tensor due to the SGS motions.

3. The unknown value of this stress tensor is modelled via an SGS model.

4. The large scale motions are thus simulated by solving for \( \bar{u}(x_i, t) \) using the filtered and SGS modelled equations.

To carry out the filtering procedure a filter is required. Suppose this filter is applied to any instantaneous field \( \varphi(x_i, t) \) where \( \varphi \) can be any fluctuating variable (pressure, velocity, temperature):

\[ \bar{\varphi}(x_i, t) = \int_{-\infty}^{+\infty} \varphi(\xi_i, t) G(x_i - \xi_i) d^3\xi_i \quad \text{2-31} \]

where \( G \) is the filter convolution kernel (a mathematical operation on two functions producing a third modified function) and is characteristic of the filter applied. This can be written symbolically as:

\[ \bar{\varphi} = G \ast \varphi \quad \text{2-32} \]

The three filters proposed for spatial filtering in LES are the Box, Gaussian and Sharp spectral filter (Pope, 2000) although the majority of LES CFD now uses the Box filter. The Box filter is appropriate for use in finite volume based CFD and is defined as follows:

In physical space (in 1D for simplification) the filter kernel is given by:

\[ G(x - \xi) = \begin{cases} \frac{1}{\Delta}, & |x - \xi| \leq \Delta/2 \\ 0, & \text{otherwise} \end{cases} \quad \text{2-33} \]
A 3D version of this can easily be defined (see Sagaut (2005)).

2.3.6.1. Filtered LES equations

The filtered continuity, momentum and temperature equations thus become:

\[ \frac{\partial \rho \tilde{u}_i}{\partial x_i} = 0 \quad 2-34 \]

\[ \frac{\partial \rho \tilde{u}_i}{\partial t} + \frac{\partial \rho \tilde{u}_j \tilde{u}_i}{\partial x_j} = -\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial \tilde{\tau}_{ij}}{\partial x_j} - \frac{\partial \tilde{\tau}_{ij}'}{\partial x_j} + \Delta \tilde{p} g_i \quad 2-35 \]

\[ \frac{\partial \rho \tilde{T}}{\partial t} + \frac{\partial (\rho \tilde{u}_i \tilde{T})}{\partial x_i} = -\frac{\partial \tilde{q}_i}{\partial x_i} - \frac{\partial \tilde{q}_i'}{\partial x_i} \quad 2-36 \]

where, \( \tilde{p} \) is the spatially filtered pressure field. The term \( \tilde{\tau}_{ij}' \) is the subgrid residual scale stress tensor formulated by Leonard (1974):

\[ \tilde{\tau}_{ij}' = \rho \tilde{u}_i \tilde{u}_j - \rho \tilde{u}_i \tilde{u}_j \quad 2-37 \]

And the subgrid heat flux is:

\[ q_i' = \rho \tilde{u}_i \tilde{T} - \rho \tilde{u}_i \tilde{T} \quad 2-38 \]

Using a set of boundary conditions for the filtered primitive variables and a model for the SGS stress and heat flux term the equations above can be solved numerically to produce \( \tilde{p}(x_i, t), \tilde{u}_i(x_i, t) \) and \( \tilde{T}(x_i, t) \). Thus both boundary conditions and the SGS model play a vital role in the stability and accuracy of the LES simulations.

2.3.6.2. Smagorinsky SGS model

Smagorinsky (1963) developed the first SGS model although Lilly (1962) was using variants of this already. Since then a wide variety of SGS models have been developed notable of which is the Dynamic model developed by Germano (1996). Additionally, many RANS based turbulence models have been modified and employed as SGS models. However, these varieties are less robust and more sensitive to the mesh employed when compared to the Smagorinsky model (Ferziger, 1996). The Smagorinsky model is thus by far the most commonly used SGS model.
Veloudis, 2006). Thus for this study the SGS model selected was that proposed by Smagorinsky (1963).

The SGS viscosity $\mu_{SGS}$ can be expressed as:

$$\mu_{SGS} \propto \rho \times l_{SGS} \times u_{SGS}$$

where, $l_{SGS}$ is the SGS length scale (usually referred as proportional to the grid size: $\Delta=(Vol)^{1/3}$ where Vol is the local cell volume, i.e $l_{SGS} = C_s \Delta$ where $C_s$ is the Smagorinsky constant) and $u_{SGS}$ is the subgrid velocity scale.

The SGS velocity scale can be expressed on dimensional grounds as:

$$u_{SGS} = C_s \Delta |\vec{S}|$$

where,

$$|\vec{S}| = (2S_{ij}S_{ij})^{1/2}$$

Thus the Smagorinsky model for the SGS viscosity becomes:

$$\mu_{SGS} = \rho (C_s \Delta)^2 |\vec{S}|$$

$C_s$ is not a universal constant and its value changes depending on the type of flow; however a value of 0.1 is usually used and is thus adopted in this work.

Thus, the SGS model to calculate the stress $\tau_{ij}^r$ is:

$$\tau_{ij}^r = -2\mu_{SGS} \bar{S}_{ij} + \frac{1}{3} \tau_{ii}^r \delta_{ij} = -\mu_{SGS} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) + \frac{1}{3} \tau_{ii}^r \delta_{ij}$$

and the SGS heat flux $q_i^r$ is calculated by:

$$q_i^r = -\frac{\mu_{SGS}}{Pr_{SGS}} \frac{\partial \bar{T}}{\partial x_i}$$

The SGS Prandtl number $Pr_{SGS}$ (which is the LES analog of the turbulent Prandtl number) is obtained by applying the dynamic procedure originally proposed by Germano (Germano et al., 1996) to the SGS flux. Here $Pr_{SGS} = 0.85$. 
2.3.7. Detached Eddy Simulation

The wide range of spatial and temporal scales encountered, especially in near wall regions, makes it necessary to use very fine LES meshes as well as long simulation times; this in turn results in high computational effort to obtain good quantitative solutions. This difficulty of using LES in near-wall regions has led to the development of hybrid models that combine the best aspects of RANS and LES in a single technique. This idea has emerged from the observations of the close similarity of RANS equations (2-6, 2-7 and 2-8) to LES equations (2-34, 2-35 and 2-36). Detached Eddy Simulation (DES) is one such technique which proposes to treat near wall regions in a RANS-like manner, and treats the rest of the flow in an LES manner. The method works by the turbulence model switching to an SGS formulation in regions where the mesh is judged fine enough for LES, otherwise a RANS turbulence formulation is used. In general regions near solid boundaries or where an estimate of local turbulence length scale (from the RANS turbulence model) is less than the local grid dimension are assigned to a RANS mode of solution. In addition to switching the details of turbulence closure between RANS ($\mu_t$) and LES ($\mu_{SGS}$), it is also important to select appropriate discretisation practices for RANS and LES regions. In LES it is very important that convection discretisation method is non-dissipative to enable capture of the energy conserving cascade described earlier. Thus, in the RANS regions some form of upwind differencing is often used but in the LES regions central differencing is always adopted.

For the present problem it has been decided not to explore at this stage the performance of the DES approach to turbulence modelling. This is for two reasons. Firstly, as noted above, the main benefits of the DES approach are observed to occur when modelling flows with strong wall influences. For natural ventilation flows, which are considered to be dominated by turbulent problems in the free shear regions on the edges of entraining buoyant plumes, DES is unlikely to offer much advantage. Secondly, it is considered better to concentrate on ‘pure’ LES until a clear picture has emerged fully of how the LES approach performs in natural ventilation buoyancy dominated flows.
Chapter 3. Previous work on wind and buoyancy driven natural ventilation

“A bad review is even less important than whether it is raining in Patagonia” – Iris Murdoch

3.1. Introduction

In service and non-residential buildings nearly 68% of the total energy is attributed to HVAC systems (Orme, 2001). Natural ventilation has recently become popular because of the need to introduce energy efficiency, sustainability measures and also because recent developments in control systems have enabled natural ventilation to satisfy occupant thermal comfort and indoor air quality criteria. If not applicable by itself, natural ventilation can be part of a hybrid ventilation strategy. Over the last two decades, new design methods based on improved understanding of natural ventilation have been developed.

Comprehensive guidelines for overall natural ventilation design are available for designers to consult during the design process (e.g. (Allard and Santamouris, 1998; Jackman, 1999; CIBSE, 2005).

The potential of natural ventilation as a viable design strategy has been described by Allard and Santamouris (1998). In their book they also discuss the appropriate use, design and dimensioning of a natural ventilation strategy such as inlet openings and stacks. They also stress the need for an integrated design approach and additionally advise on how to overcome barrier to natural ventilation such as sizing and placement of openings. CIBSE (1997) provides guidelines for engineers in the application of natural ventilation in non-domestic buildings. The publication deals
with developing design strategies, review of the ventilation components and how they should be integrated in the overall process of natural ventilation design and finally the design calculations directed towards the building services engineers. It serves as a good introduction to natural ventilation design. Li et al. (1999) provides a critical literature review and recent developments in the analysis methods of natural and hybrid ventilation. Their paper also reviews challenging issues such as 'multiple solutions' to air flow analysis.

In addition to the general guidelines for natural ventilation cited above, extensive research has been carried out on the individual components of natural ventilation. Guidelines for designing the envelopes (e.g. sizing and positioning of openings in isolated and connected spaces) of natural ventilated buildings were presented by Etheridge (2002). He provided these guidelines in the form of non-dimensional graphs which were generated from theoretical models and experimental data. He suggests such graphs are easy and quick to use, have wide application and accuracy. For example, the use of pressure coefficients for quantifying the surface pressure on buildings generated by wind. The surface pressure can be described by coefficients which are independent of wind speed, if the wind direction and building environment is the same. Thus the need for dimensional pressure data at each wind speed of interest is made redundant.

Bahadori (1985) provided guidelines on a proposed improved wind tower design for natural ventilation. The improvements consisted of one-way dampers at the tower head, long clay conduits in the stacks acting as energy storage material and evaporative cooling of air by wetting of the clay conduits (Figure 3.1). Under the same climatic conditions the new design delivered higher flow rates into the building. The tower design was also claimed to have the capability of evaporative cooling of the air which can then be used on summer nights for cooling down the building mass.
An atrium - a common feature of many modern naturally ventilated buildings - has been investigated by Holford and Hunt (2003). Atria can be used to produce large temperature gradients and thus act as an outflow path for stale air inside buildings. A theoretical model is presented that predicts the steady state stack-driven displacement flow. With this model they identify the extreme condition where the atrium does not provide any significant enhancement to the flow. They also suggest that atria can play a significant role only if the upper opening in the storey is of "intermediate size" whilst the lower opening is sufficiently small.
Apart from these general guidelines for natural ventilation, extensive research has been carried out using experiments to more fully understand natural ventilation performance.

### 3.2. Role of experiments in understanding natural ventilation

The term ‘filling box’ (characteristic setup of fluid flow through scaled-down models of buildings in water) was first coined by Baines and Turner (1968) who considered the effect on the indoor environment in an enclosure of a small source of buoyancy (Figure 3.2). A main assumption they made was that the entrainment into the turbulent buoyant jet region increased in a proportional rate to local upward velocity. Theory was presented for filling a box with a plume and validated using salt bath experiments that suggested that a stable temperature gradient was formed. The filling box model introduced in their paper (Baines and Turner, 1968) was later taken up by other researchers.

![Figure 3.2: Sketch of the development of stratified environment due to a heat source, showing the motions in the plume and environment, and the corresponding temperature profiles at two times (source: Baines and Turner (1968)). Where, \( F_0 \) is the buoyancy strength of the heat source, \( z \) is the height from the heat sources, \( t_1 \) and \( t_2 \) are the temperatures at interface 1 and 2 respectively, \( w \) is the plume width, \( \rho \) is the density of the plume and \( \rho_o \) is the density of the environment.](image)

Another pioneering work in understanding the fluid mechanics of natural ventilation inside buildings is that of Linden et al. (1990). In their paper they elucidate that the steady state stratification which develops in a space is a result of solely the position and size of openings and the position and nature of the heat sources. This is true for
both displacement and mixing flows which were studied theoretically with results subsequently compared with laboratory experiments. These laboratory experiments were undertaken in a large reservoir of fresh water in which a small scale model of the building made of perspex was suspended (Figure 3.3). Holes were drilled into the model to act as openings which can be blocked if needed with plugs. Buoyancy-driven flows were created by introducing brine (denser than fresh water) into the perspex models. The denser brine plume thus descends driving fluid through the model and resulting in an exchange with the external ambient fluid. Transient and steady state behaviours were then investigated for different configurations of openings. This method of experimentation is known as ‘salt bath modelling’. The effects of point, line and vertically distributed sources were also studied.

Figure 3.3: Steady displacement flow with an internal horizontal line source. The internal stratification after time $t= (a) 10$, (b) 30, (c) 90 and (d) 240s. Note the rising of the interface with time. (after Linden et al. 1990)
With the aim of providing designers with rules and intuition on how air moves through a building Linden (1999) carried out further research. He investigated two modes of ventilation i.e. mixing ventilation, in which the interior temperature is approximately uniform, and displacement ventilation, where strong stratification exists. He examined these buoyancy-driven flows and the effects of wind on them. He concluded that wind effects appear to be dominant on the basis of pressure variations from windward to leeward and top to bottom of a building. However, the effects of wind were diminished by closing down vents. He explained that it is the internal stratification that determines the flow patterns in most cases.

Cross ventilation was investigated by Katayama et al. (1992) using full-scale measurements and wind tunnel tests of apartment houses. They concluded that wind tunnel tests could simulate cross ventilation accurately, also providing an experimental technique that can be utilized to design better cross ventilation in apartment buildings.

Plumes are an important feature of buoyancy driven natural ventilation systems. Pera and Gebhart (1975) investigated the interaction of laminar thermal natural convection plumes generated by line and concentrated heat sources. Experimental investigations were carried out using the Mach-Zehnder interferometer. It was found that plane plumes interact more strongly compared to axisymmetric plumes at the same separation distance (Figure 3.4). Numerous types of plume entrainment interference were investigated for which a successful model was formulated. The volume flux of the plume was defined by the location of the interface because the total discharge into the environment has been entrained at this level. Baines (1983) carried out experiments to verify this relation.
Hunt and Linden (2001) examined ventilation in an enclosure with a buoyancy source and an external wind (Figure 3.5 and Figure 3.6). Salt bath experiments were carried out to determine the parameters that govern the ventilation under such conditions. The results from the laboratory experiments were then compared with theory. They reported an increased rate of ventilation with increase in the pressure difference between windward and leeward openings. Two-layer stratification was observed for a range of wind speeds. They also elucidated that the steady height of the interface depended upon both the Froude number and the dimensionless area of openings ($A^*/H^2$).
Transient buoyancy driven natural ventilation flow was examined by Kaye and Hunt (2004). Turbulent plumes introduced into the enclosure play the role of buoyancy source/s. They presented a theoretical model to predict the strength of stratification and volume flow rate through the openings in the enclosure as a function of time. Salt bath modelling was used to validate their formulation. They reported the timescale for the flow to reach steady state as depending on the box height $H$, cross sectional area $S$, effective opening area $A^*$ and the strength, number and distribution of the heat sources.
Kaye and Linden (2004) investigated the interaction of axisymmetric thermal plumes in a buoyancy driven natural ventilated enclosure, by developing a theoretical model and comparing this with salt bath experiment results. They defined the point of coalescence of two plumes as that point where only a single peak appears in the horizontal buoyancy profile Figure 3.7 and a prediction was made for this height. Far field calculations were made for the virtual origin of the merged single plume. This was compared with dye attenuation technique experiments and showed good agreement.

Interaction of turbulent plumes in a ventilated enclosure has also been investigated by Linden and Kaye (2006). They suggested that previous models for buoyancy driven natural ventilation were based on simplifications with respect to the heat sources and did not take into account plume-plume interaction. They used salt bath modelling techniques to investigate co-flowing coalescing plumes in close proximity to one another and two opposing plumes colliding in a ventilated space (Figure 3.8). They presented models to predict the interface height depending on where the co-flowing plumes merge. They stressed the need to model heat sources accurately to
predict the ventilation system performance. This is even more important in a tall, high occupancy, naturally ventilated space.

Figure 3.8: Schematic of three layer stratification due to buoyancies of different strengths for (a) co-flowing plumes (b) opposing plumes (Linden and Kaye (2006))

Kaye et al. (2010) examined the role of diffusivity (molecular or turbulent) on the steady-state stratification in a ventilated filling box. Previous studies with a filling box assumed that diffusion plays no role in development of the ambient buoyancy stratification. They suggested that with an increase in enclosure cross section and for the interface to remain sharp the amount of fluid that must be entrained into the plume must be high while diffusion is a slow process. Thus a diffused interface is expected. However with increase in the source buoyancy flux the interface thickness decreases. They presented two models to predict the interface thickness as a function of enclosure height, base area, composite vent area, plume buoyancy flux and buoyancy diffusivity. The models agree favourably with results based on previous reported data.

The phenomenon of overturning in an enclosure due to a turbulent plume was examined theoretically and experimentally (using salt bath modelling) by Kaye and Hunt (2007). The buoyant flow that travels up the side walls is termed the initial penetration depth ($h$) and was defined as a function of the box radius ($R$) and height ($H$) (Figure 3.9). The problem was simplified to finding $\eta=h/H$ as a function of aspect ratio $\Phi=R/H$. Two regimes were observed: when the plume outflow was adjusting
toward a pure gravity current on impact with the vertical wall, $\eta \sim \Phi^{1/3}$, but when the outflow was fully developed before/or on impact, $\eta \sim \text{Const.}$

![Figure 3.9: Schematics of a confined descending plume colliding with the horizontal surface, spreading out radially and then rising up the sidewalls and overturning (Kaye and Hunt (2007))](image)

Recently, researchers have been attracted by the phenomenon of multiple steady states in naturally ventilated enclosures. Chenvidyakarn and Woods (2005) investigated an occupied open plan office which was naturally ventilated via two stacks and a low level opening. Occupants at the floor level act as the buoyancy force to drive the flow through the building. They reported the occurrence of three steady state displacement ventilation regimes (Figure 3.10). In the first regime, warm air exits through the taller stack while ambient air is drawn in through the shorter stack and through the lower openings (regime A). In the second regime, warm air exits through both stacks whilst drawing air in through the lower openings (regime B). Finally in the third regime, ambient air is drawn in through the taller stack and lower openings whilst the warm air exits through the shorter stack (regime C). A quantitative model was developed describing the indoor temperatures for the three steady states and compared successfully with laboratory experiments. Their model showed that the ventilation regime was dependent on the geometry of the room.
(height of the room, and stack and opening sizes). According to Chenvidyakarn and Woods, the heat source had no effect on the regimes.

Yuan and Glicksman (2007) suggested that multiple steady states exist in natural ventilated systems in combined buoyancy and wind driven mode. For small disturbances various steady states can be stable but the system can flip from one steady state to another if sufficiently strong perturbation is applied. The analysis was carried out with two types of perturbations i.e. fluctuations in heat source strength and variation in wind strength. The minimum perturbation time and minimum perturbation magnitude parameters were defined which helped to find the robustness of a given steady state. These were successfully used to validate the results of another research.

Yuan and Glicksman (2008) suggested a single zone with combined wind and buoyancy can exhibit three steady states. Two of these (wind dominated downward
and buoyancy dominated upward) are mathematically stable while the third is unstable even to infinitesimal disturbance. They used a dynamical system method in this study which they proposed could help designers avoid the complexities of multiple steady states by careful choice of relevant parameters.

Li et al. (2001) reported multiple solutions for flow rate in a naturally ventilated enclosure under certain conditions. This was induced by non-linear interactions between wind and buoyancy forces. In their paper they showed that for even simple systems natural ventilation flows can be quite complex. They investigated three cases experimentally (using salt bath models) where they observed for a certain range of parameters, multiple solutions for flow rate could exist.

Finally Chen (2009) has reviewed the methods used to predict ventilation performance of buildings. In his review he found that analytical and empirical models have made minimal contributions to literature in recent years. Small-scale and full-scale model experiments were mainly used to generate data in order to validate numerical models. Ventilation performance in entire buildings was being predicted by improving multi-zone models. Coarse grid CFD was replacing zonal models with limited applicability. Chen found that 70 percent of the literature found was contributed by CFD models. The main applications of CFD were on indoor air quality, natural ventilation, and stratified ventilation as these were difficult to assess with other models (Figure 3.11).

![Figure 3.11: Ventilation performance in buildings predicted by different models in 2007 (Chen (2009))](image)
From the previous discussion it is clear that natural ventilation has been under active study over the past few decades. New computer design tools and the incorporation of modern control strategies are sought to make natural ventilation as reliable as mechanical ventilation when properly designed and operated (Li and Heiselberg, 2003). During the design stage of a building some form of air flow and modelling is viewed as desirable in order to predict and/or improve the design of the proposed ventilation strategy (Cook et al., 2003b). The application of CFD to ventilation analysis is now reviewed in more detail.

3.3. Use of CFD in building ventilation analysis

The use of CFD in buoyancy/wind-driven naturally ventilated enclosures is not without its difficulties. Fracastoro and Perino (1999) have explained that non-trivial difficulties are faced when modelling even simple geometries. Li et al. (1999) warn that CFD simulations can be more time consuming to establish and execute than multi-zone methods. They also explain that the combined effect of wind and buoyancy further causes difficulties as this gives rise to unstable flow modes and consequently stronger non-linearity in the phenomenon. This means that for the same set of boundary conditions there can be several possibilities of air flow pattern within the space, or the pattern can even oscillate between one solution and another. Fracastoro et al. (2002) gave an overview of the use of CFD by saying that even though CFD codes can yield plentiful information regarding a naturally ventilated enclosure, the reliability and accuracy of such results must be thoroughly checked. In spite of these difficulties and even though people have been sceptical of CFD data in the past, its use in the consultancy industry has increased with time as better modelling techniques have been developed.

The Reynolds Averaged Navier-Stokes (RANS) approach is currently the most popular CFD formulation for fluid flow analysis. This technique uses turbulence models to solve for a steady state time-averaged prediction within the flow domain. The RANS technique has been used in the design stages of numerous buildings to predict the building’s ventilation flow patterns. However, since natural ventilation is typically an unsteady flow problem, the study of natural ventilation by RANS may need to be extended to include a transient approach (Jiang, 2004).
Over recent years, as high performance multi-processor parallel computers have become more readily available, interest in more complex approaches to turbulence simulation such as direct numerical simulation (DNS) and large eddy simulation (LES), which can be used for carrying out transient simulations, has grown. However, it is not yet understood how well such techniques perform when modelling natural ventilation. Two other alternatives with more reasonable computational costs worth mentioning here are Unsteady-RANS (URANS) and the Scale-Adaptive Simulation (SAS) approach. URANS, a variant of RANS, is a method in which the Reynolds averaged equations and models are solved including time dependence. SAS can be viewed as an improved URANS formulation which behaves in an LES-like manner in unsteady regions of the flow field and provides standard RANS capabilities in the stable flow regions.

CFD subdivides the geometrical domain under analysis into many small cells. Equations of mass, energy and momentum are discretised and solved in each cell. Clifford et al. (1997) suggest that CFD has many attractions when compared to the conventional method of building a scale model and testing in a wind tunnel. With CFD there is no need to build a physical model, it is easier to carry our parametric studies and detailed results at many points in space can be obtained, while it may be difficult to take such detailed and numerous measurements from a scale model. Advantages such as these led to the CFD simulation of buildings with various features such as inlet openings, stacks, plenums (Shao et al., 1993; Walker et al., 1993). CFD modelling has been used extensively in the analysis of airflow, temperature and contaminant distribution (Tsou, 2001). Flows within buildings have also been modelled with obstructions to the flow such as furniture and people (Gan et al., 1991). CIBSE (1997) describes CFD as “a very powerful technique” in predicting air movement and characteristics.

Another useful feature of CFD is the possibility for direct assessment of thermal comfort, air quality and effectiveness of a ventilation system. Gan and Awbi (1994) carried out CFD simulations using the VORTEX program on both mechanically and naturally ventilated rooms. Results were produced in the form of Predicted Mean Vote (PMV) and Predicted Percentage Dissatisfied (PPD) indices which are relevant to thermal comfort standards and for the spread of an indoor pollutant, such as CO₂ or other gases, give an assessment of the quality of indoor air. CFD solutions are
therefore capable of evaluating the performance of ventilation systems and are particularly useful for innovative designs involving passive or active systems. Conventional guidelines and rules of thumb are not applicable to such innovatively designed buildings.

CFD has the additional benefit of acting as a cross-check on newly developed configurations. Li et al. (2000) presented such a solution for natural ventilation of single and multi-zone buildings with multiple openings. An auxiliary concept of external pressure was introduced into the pressure-based multi-zone formulations. CFD was used to confirm the newly developed formulation implementation to a single-zone building with very large openings. Reasonable agreement was observed between the results.

Awbi (1989) was one of the early users of CFD to predict air flow and heat transfer in 2-D enclosures and the 3-D flow of a wall jet over surface-mounted obstacles. Good predictions of the temperature and air velocity distribution in a test room cooled by a ceiling jet were obtained by the CFD solution.

Ayad (1999) used CFD to study the ventilation properties of different opening configurations in a room. Six configurations of window openings were considered for the internal flows and results were compared with experimental values (Figure 3.12). CFD results showed that the placement of the openings in relation to each other was significant as it could enhance or reduce mean velocity at certain locations of the room. He reported that CFD results were helpful in assigning comfortable locations for humans inside the room. It was also found that the in-room mean velocity vectors were sensitive to upstream wind direction for a given wind speed while the effect of the upstream turbulence level on the in-room wind speed was negligible.
Gan (2006) used CFD to show that with increase in solar heat gains the ventilation rate generated by buoyancy sources in open cavities also increases. He explained that there is a point to which with increase in cavity width the buoyancy-induced ventilation also increases. After that point the ventilation rate either decreases (solar chimneys) or remains constant (multi-storey high double façades). This optimum width of an open cavity was found with the help of CFD to be between 0.55m and
0.6m for a solar chimney of 6m height. He went on further to explain that the integration of photovoltaics into a double façade could further enhance natural ventilation of the building and reduce the variation of the flow rate with storey height.

Méndez et al. (2008) analysed the ventilation flow pattern inside a two-bed hospital room; the room was divided by means of curtains and partition walls. The objective of the study was to optimise the room design from an indoor air quality point of view without affecting the patient’s privacy. The use of two air inlets or the removal of curtains separating the patients seemed the easiest solution but were expensive and not comfortable for the patients. CFD provided another simpler and cheaper solution i.e. the reduction of the height of the partition walls in the room which caused higher air-exchange efficiency than other alternatives (Figure 3.13). Mendez also suggested that air flow patterns were dependent on the geometry of the enclosure and hence no generalised standard could be established for air flow patterns. This means that for each specific case an individual CFD study was needed.

Figure 3.13: Ventilation profiles over a plane at a height of 2.3m (Méndez et al. (2008))
CFD predictions (RANS) together with wind tunnel tests were used to study the potential of using an active stack (a stack with built-in extract fan) to enhance night-time natural ventilation in a residential apartment (Wong and Heryanto, 2004). A total of 32 cases were investigated by varying the stack location, bedroom door operation (on/off), wind occurrence (on/off) and extract fan operation (on/off). CFD and wind tunnels tests were in good agreement with each other although it was observed that the CFD predictions predicted higher air velocities than obtained from wind tunnel experiments for cases where wind and active stack effects were considered. The study also revealed that in a naturally ventilated residential apartment, the external wind effect was still the most important factor to determine natural ventilation performance.

Kato et al. (1997) proposed a combined use of wind tunnel tests and CFD for cross ventilation of large indoor spaces. In this method, wind tunnel tests were first used to measure total pressure differences between windward and leeward openings and overall cross-ventilation air flow rates. Based on these measured values the air and contaminant distributions in the room were then predicted with CFD. The proposed method was implemented on a large-scale wholesale market building. It was concluded that the detailed analysis of indoor flow, temperature and contaminant fields, which could not be carried out in the wind tunnel tests, became possible using CFD. Another great merit of CFD analysis that was reported was the ease with which detailed analysis of ventilation efficiency could be carried out.

Jones and Whittle (1992) reviewed the application of CFD to building environmental design, examining major technical limitations in codes such as turbulence modelling, radiation models, lack of interaction with thermal models and the need for faster convergence for buoyant flows. They concluded that even though CFD codes could be successfully applied to building air flow prediction, they must be used with care and with the exercise of sound engineering judgement to get the best from them.

### 3.4. Steady State Analysis using CFD

#### 3.4.1. Reynolds-Averaged Navier Stokes (RANS) equations

In Reynolds-averaged approaches to turbulence, all of the unsteadiness is averaged out i.e. all unsteadiness is considered as part of the turbulence. The non-linearity of the Navier-Stokes equations on averaging gives rise to terms that must be modelled
(see Chapter 2). Any single Reynolds-averaged model will unlikely represent all turbulent flows equally well due to the inherent complexity of turbulence so turbulence models must be regarded as engineering approximations rather than scientific laws (Ferziger and Peric, 2002).

An evaluation of the performance of two RANS models for predicting natural ventilation flows driven by combined wind and buoyancy forces and where the wind flow assisted the buoyancy-driven flow was conducted by Cook et al. (2003b). The variation in the steady depth of the layer at ambient temperature with variation in areas of the openings of an enclosure was examined (Figure 3.14). The results from the CFD modelling were in good accordance with both analytical models and experimental data of Linden et al. (1990). A robust approach was also developed that demonstrated that pressure boundary conditions imposed directly at the openings can be used in conjunction with a reduced physical opening size to model the effects of wind pressure at inlets and outlets.

Asfour and Gadi (2007) compared the use of RANS and empirical coefficient based network models for predicting wind-induced ventilation in buildings (Figure 3.15). Comparison was conducted between the air flow rate calculated by a network model and the CFD software FLUENT 5.5 on buildings with various geometries and wind directions. The results obtained demonstrated that the standard k-ε model was accurate for predicting wind-induced natural ventilation in buildings. This method has been recommended as a CFD validation method for studies that do not have access to laboratory or full-scale testing facilities.

![Figure 3.14: CFD analysis by Cook et al. (2003) Velocity profile (left) and temperature profile (right) inside the enclosure](image)
From a computational point of view, indoor air flows have been investigated extensively during the past decades, particularly to assess turbulence modelling. Researchers have been very keen to identify which RANS-based turbulence model out-performed other models in terms of accuracy for specific applications. Through experiments, Fanger et al. (1988) demonstrated the significant impact of turbulence on human sensation of draughts in indoor environments. Chow and Li (2007) assessed four turbulence models by simulating fire-induced thermal plumes and compared the results with experimental data. The standard k-ε turbulence model (Lauder and Spalding, 1974) and three modified forms were tested. These were the low-Reynolds number (LRN) k-ε model (Chen, 1995b), a Chen-Kim modified k-ε
model (CK model) (Chen and Kim, 1987) and the Re-Normalization Group (RNG) (Yakhot et al., 1992) derived k-ε model. It was suggested that the use of the modified forms did not necessarily give better results and that it was perhaps better to tune the calibrated constants in the standard k-ε model. Furthermore, a more feasible approach proposed was the combination of different turbulence models (Chow and Mok, 1999).

Evola and Popov (2006) conducted an investigation for predicting wind driven natural ventilation in a cubic building. The idea was to compare the performance of two RANS based turbulence models, namely the standard k-ε model and the RNG model. Three different configurations were considered: single-sided ventilation with an opening on the windward wall, single-sided ventilation with an opening on the leeward wall and cross ventilation. The velocity distribution inside and around the building, as well as the ventilation rate and mean pressure coefficients on all of the building surfaces were determined and compared with both empirical expressions and experimental data. It was suggested that results obtained using the RNG model showed superior agreement with experimental data while the standard k-ε showed inaccuracy in the prediction of ventilation rates. This could be due to the fact that the k-ε model had difficulty representing flows near surfaces where turbulence damping effects were significant. It was also concluded that despite its greater accuracy, the RNG model required a slightly higher computational effort than the standard k-ε model. Another important result from this investigation was that positioning an opening on the leeward side rather than the windward side resulted in a larger ventilation rate within the building. However, this requires further investigation since different opinions have been expressed in the literature.

With the increased interest in natural ventilation, much research has been conducted looking at modelling of buoyancy-driven flows. The work by Ji et al. (2007) demonstrates the capability of RANS for predicting buoyancy-driven natural ventilation in connected spaces. They used the RNG k-ε turbulence model to study buoyancy-driven natural ventilation flow in a single-storey space connected to an atrium. A column of warm air was produced in the atrium by internal gains in the single-storey space which drove a ventilation flow. CFD predictions of airflow patterns, temperature distribution and ventilation flow rates agreed favourably with
both analytical and experimental data for two cases i.e. an atrium with and without ventilation openings at the bottom (Figure 3.16).

Another important finding of this study was that a tall atrium does not always enhance ventilation. The resistance caused by a small atrium outlet opening area may overcome the enhancement produced by the tall atrium. The study also looked at the influence of key CFD modelling issues such as boundary conditions, solution controls and mesh dependency.

Gan (2010) investigated the influence of the size of vertical external cavities used for buoyancy-driven air flow and heat transfer using the RNG k-ε CFD turbulence model (Figure 3.17). He considered two sizes of the computational domain – a small domain which had the same size as the physical cavity size and a larger extended domain. This extended cavity size was approximately 10 times the cavity width for asymmetric heating and 5 times for symmetric heating. He suggested that the extended domain size could be halved without significant loss of prediction accuracy.
but with substantial reduction in computational time. Gan concluded from his study that a difference was found in predicted air flow rate and heat transfer coefficient using the small and large extended domains. This difference was seen to be larger for wider cavities with asymmetric heating. He also suggested that a larger computational domain than the physical cavity size could provide more accurate simulation for buoyancy-driven natural ventilation. Presumably this was because a larger external cavity size created a more realistic reproduction of the external “open-boundary” conditions.

Figure 3.17: CFD predictions of buoyancy-driven natural ventilation in an atrium by GAN (2010)

Therefore, it was recommended that such large computational domains should be used for accurate prediction of heat transfer and flow rate in ventilation cavities with large openings for natural ventilation, particularly with multiple inlets and outlets,
asymmetric heat distribution on opposing walls, or asymmetric flow distribution at openings, unless a known (i.e. measured) flow profile could be prescribed at each opening. It was observed that in general, the more evenly the heat is distributed on the two walls of the vertical cavity with vertical inlet and outlet, the larger will be the flow rate but the heat transfer coefficient will be smaller.

Liu et al. (2009) looked at buoyancy-driven natural ventilation in buildings with an atrium using CFD and scale model tests (Figure 3.18). It was reported that the RNG $k$-$\varepsilon$ and zero-equation turbulence models showed better agreement between CFD results and measurements for a heated zone. In the atrium area zero-equation CFD models showed better results. A second important finding of the study was that temperature distribution in the atrium space was largely affected by the external ambient temperature rather than the thermal load inside the building.

![Figure 3.18: Temperature visualization under different ambient conditions Liu et al. (2009)](image)

The study also suggested that both the position and size of stack openings affected the overall temperature distribution within the atrium space. The study was carried out for a hot and humid climate after which it was concluded that buoyancy-only ventilation was not very effective due to insufficient pressure gradient caused by temperature difference. Additional efforts such as wind-driven ventilation, wind-
buoyancy ventilation or mechanically driven ventilation were necessary to achieve the required levels of thermal comfort.

Even though RANS modelling has remained a popular CFD approach for some time there are however limitations to its applications. Jiang et al. (2003) reported some of these limitations. Firstly, RANS modelling has been shown to be unable to correctly predict air flows around buildings as evident from the work of Lakehal and Rodi (1997). Secondly, natural wind varies in both speed and direction, so a transient prediction is required to fully describe the flow (Jiang and Chen, 2002).

Clifford et al. (1997) carried out an investigation on the case of single-sided ventilation to see how well CFD predicted the ventilation rate from velocity data. Results from testing a simple model in a wind tunnel were used to validate two RANS-based CFD turbulence models; the Reynolds-stress model and the k-ε model. It was noted that the k-ε model ignores secondary flows, whilst the Reynolds-stress model performed better. However, with the refining of the computational grid, neither model could predict the air flow at the opening. This, Clifford suggested, may be due to the time-dependent nature of the air exchange mechanism. For this reason, since flow through openings is such an important component of ventilation flows, unsteady flows are described next.

3.5. Time dependent flows

In practical engineering applications a wide variety of flows are inherently unsteady, due to turbulence. Turbulent flows in complex geometries are often observed to exhibit an oscillating behaviour of large coherent eddy structures, even in the case of steady state boundary conditions. A coherent structure is an eddy structure present in a flow for a relatively long time and is not only a short-term, high frequency transient phenomenon. For more information on coherent structures see Bonnet (1993).

Under certain conditions, multiple solutions for the flow rate exist in a natural ventilation system (Li et al., 2001). This may be due to the non-linear interaction between buoyancy and wind forces. Li et al. (2001) considered three examples: a single-zone building with two openings, a channel with two end openings and a two-zone building with two openings in each zone. Using analytical and numerical solutions it was demonstrated that all three cases exhibited hysteresis in flow rate.
These results are likely to have significant implications for multi-zone modelling of natural ventilation.

Yuan and Glicksman (2007) and (2008) have also reported that natural ventilation may have multiple steady states in combined wind and buoyancy driven mode. They investigated the quantitative relationship between the initial temperature and final steady state in a single space based on dynamic system analysis. In their study they considered a room with a buoyancy source on the floor and an opening at the top of the room to assist wind driven natural ventilation. According to their study, if the initial room temperature is low, the final steady state of the system will be dominated by the pressure difference between the indoor and ambient and will result in a downward flow. If the initial room temperature is relatively high, the final state of the system may be buoyancy dominated upward flow. They advise designers to avoid the complexities of multiple solutions as much as possible by avoiding the boundary conditions that can lead to multiple steady states presented in their paper. The extent to which this phenomena should be considered under practical conditions was analysed by Andersen (2007). His analysis showed that unambiguous solutions could be obtained if the difference between the indoor and outdoor temperature is known at the start, i.e. when the heat sources are turned on and the openings are opened.

Li et al. (2006) also report a bifurcation behaviour of flows driven by opposing buoyancy in two vertically connected open cavities. It was found that two stable fixed points exist for a certain range of strength ratios of the heat source/sink. The two stable steady flows showed hysteresis phenomenon. Both CFD and flow visualization confirmed the existence of two stable solutions.

In order to capture the dynamics of such complex flows, it is appropriate to use unsteady calculation methods. Some of these transient numerical techniques are now reviewed.

3.5.1. Unsteady RANS (URANS)

URANS is an attractive approach to resolve the unsteady behaviour mentioned above (Schwarze and Obermeier, 2006) because it is capable of providing values of variables as they change with time. URANS simulations are usually employed when long-term periodic oscillations in turbulent flows need to be captured. Turbulent
fluctuations of flow quantities are not resolved in the URANS approach but are still described by the turbulence model as in the RANS methodology. This helps in reducing the required memory and computing time especially in complex flow situations.

Sadiki et al. (2006) evaluated the performance of URANS to model combustion systems. They confirmed that the use of the URANS method employing a full Reynolds stress model was able to capture unsteady phenomena observed in swirling flows, such as precessing vortex core phenomenon. They also report that even though the use of Large Eddy Simulation (LES) is certainly increasing in engineering applications, the use of the URANS models will continue to be prevalent for some specific industry applications.

Schwarze and Obermeier (2006) considered two flow situations, the tundish flow (i.e. flow through a funnel) and a jet in a cross flow. The basic flow in a one-strand tundish is depicted in Figure 3.19. For these flows, relationships between the Strouhal number (St) (a non-dimensional frequency of the resolved unsteadiness) and the important flow parameters are known from experiments. In their investigation they used URANS models to resolve these relationships numerically. They reported that URANS predictions could indeed resolve frequencies and profiles of large-scale coherent structures in the flows they investigated. However, they also observed differences between the experimental findings and numerical data. They reported that URANS cannot resolve the precise trend with St. They assume that the details of flow that induce changes in St are smeared out in URANS simulations.
The accuracy of RANS turbulence models has been compared with URANS models in predicting complex flows with separation (Iaccarino et al., 2003). The unsteady flow around a square cylinder and a surface mounted cube have been predicted and compared with experimental data. It was shown that none of the numerical predictions using RANS produced good agreement with experimental data. It was observed that the flow never settled into a statistically stationary state but always displayed the existence of coherent vortex shedding in the flow. The study demonstrated that indeed URANS did predict periodic shedding and hence a better concurrence with experimental data.

Deevy et al. (2008) modelled a displacement ventilation room with an occupant with thermal radiation. To understand the influence of turbulent modelling a comparative study was made between URANS and the Detached Eddy Simulation (DES) approach described in Chapter 2 (Figure 3.20). The results showed that both URANS and DES gave good results though the DES results were in slightly better agreement with the experimental data.
Kaye et al. (2009) conducted numerical predictions to compare the transient flow development in a naturally ventilated space with a single localised heat source. The numerical predictions were compared with theoretical and experimental models. Eleven cases were studied overall covering a range of vent openings. It was observed that during the initial development of the room stratification, predictions agreed well with experimental results. CFD results were successful in predicting the depth of hot buoyant layer at the top of the room as well as the steady-state interface height separating the warm upper buoyant layer from the cooler air below in the room (Figure 3.21). Also RANS CFD predictions agreed well with the measured time it took for the buoyant upper layer to reach its maximum depth. However, for longer times, prediction was poor. They suggested this may be due to thermal diffusion and mixing at the interface between the upper and lower layers caused by the inflow via the floor level vents.
While URANS is successful in predicting turbulent flows, the results obtained from models such as DES and LES are believed to provide a more suitable approach to understanding complex turbulent flows since they take account of the turbulent unsteadiness differently, unlike URANS which still models this as in RANS. Gianluca and Durbin (2000), Shur et al. (1996), Travin et al. (2000), Spalart (2000) and Scotti and Piomelli (2002) all suggest that URANS modelling still lacks the accuracy for detailed flow prediction and analysis as required by natural ventilation studies.

3.5.2. Large Eddy Simulation (LES)

The most compelling case for the increase in the use of LES in the future can be made for engineering applications involving high Reynolds number (Re) flows (Pope, 2004a). For this regime, the transport processes of interest are affected by the large-scale energy containing motions and there is a cascade of energy, dominantly from the large scales numerically resolved by LES, to the statistically isotropic and universal small scales which are modelled in LES (Sub-Grid Scales). There are
therefore good reasons to expect LES to be successful, primarily because both the quantities of interest and the rate-controlling processes are determined by the resolved large scales.

LES has been used successfully for analysing airflows in and around buildings. Jiang et al. (2003) compared results from LES with wind tunnel tests for three test cases; single-sided ventilation with openings on the windward wall, single-sided ventilation with opening on the leeward wall and cross ventilation (Figure 3.22). The wind tunnel tests measured two-dimensional mean and fluctuating velocities inside and around building-like bluff bodies with openings and pressure distributions over them. They found good agreement between the wind tunnel tests and LES for the overall flow patterns, mean and fluctuating velocities around and within the model and in surface pressures. Some discrepancies were observed but these were found to be mainly due to the coarseness of the meshes used. As LES is capable of analysing the effects of fluctuating pressure on ventilation, Jiang et al. were able to find from their study that fluctuating pressures play an important role in determining flow rates in wind-driven, single sided ventilation. The Smagorinsky subgrid-scale model and a filtered dynamic SGS (FDS) model produced the same results, further confirming the fact that if the energy containing eddies are well resolved numerically, the SGS models should lose its overall influence on the results.
Figure 3.22: Measured and LES data comparison for (a) single-sided, windward ventilation, (b) single-sided, leeward ventilation and (c) cross ventilation (Jiang et al. (2003))

Worthy and Rubini (2003) on the other hand refute the argument that the choice of LES subgrid-scale model does not matter. In their study they investigated the behaviour of different LES subgrid-scale models in predicting flows of thermal
plumes. They suggested that the use of dynamic models was beneficial and should be used when dealing with temperature subgrid terms known as fluxes of the governing equations. It is perhaps possible that Worthy and Rubini used coarse meshes for the Reynolds numbers of their flow cases. This would imply that the SGS model had to characterise more energetic motions that is considered a risk in LES. In these circumstances a simple SGS model is not likely to be adequate. Therefore if relatively coarse grids are employed, the sub-grid scale model can play a more important role. With better and faster computer resources and the use of finer grids the differences between the subgrid-scale models becomes less apparent. This indicates the importance in LES CFD of careful mesh generation.

Jiang and Chen (2002) also looked at the benefits of using LES rather than wind tunnel tests to predict natural cross ventilation. They used LES with the Smagorinsky subgrid-scale model and compared the results with experimental data and on-site measurements. Steady wind tunnel tests were unable to reproduce the effects of wind as wind changes direction over time. They reported that wind tunnel tests showed the following discrepancies from experimental data: wind-pressure differences across the buildings; eddy size behind the buildings and wind speed distribution inside an apartment with cross ventilation. LES on the other hand showed good agreement with the experimental data.
Fluctuating inflows were also investigated by Hu et al. (2008) using LES for two separate cases. For case 1, in which the wind direction was normal to the building, the standard deviation of the fluctuating flow rate was smaller because the ventilation stream was mainly extracted from the mean flows. For case 2, in which wind direction was parallel to the building the approaching flows separate at the leading edges of the side walls, the energy conserved upstream has therefore been dissipated and the fluctuating energy transferred to small eddies. Consequently, the standard deviation of the fluctuating ventilation rate was much larger than the mean.

Figure 3.23: Velocity distribution around the buildings at 3m height from the ground with (a) wind from northwest direction and (b) a variable wind direction from north to west and a mean direction from northwest (Jiang and Chen (2002))
flow rate for case 2. Hu et al. suggest that traditional studies focus only on mean wind pressure distribution on the building envelope and that the fluctuating wind pressure for ventilation purposes is important but has not been studied in detail.

Figure 3.24: Turbulent kinetic energy distribution predicted by LES and experiment (Hu et al. (2008))

A comparison between RANS and LES models was carried out for single-sided natural ventilation driven by buoyancy forces for a room with large openings (Jiang and Chen, 2003). The experiment consisted of a full-scale test room placed in a larger test room to simulate an outdoor environment. Detailed measurements were taken inside and outside the test room of the air flow characteristics. These measurements were used to further validate the two CFD models. It was observed that the air temperature, air velocity and ventilation rates predicted by LES were in better agreement with the measured data than those computed by the RANS model.
This might be because the effect of the small scales on the large scales is predicted more accurately by the LES SGS model than the RANS turbulence model.

Another application of LES is in predicting the effects of wind flow around a group of buildings. Tutar and Oguz (2002) report that the correspondence between the results obtained from the LES approach and the experiments ‘seems to be good’. They suggest that an RNG sub-grid scale model seemed to be best suited for simulating atmospheric flow field around parallel buildings on the basis of flow parameter predictions and flow physics visualisation.

Figure 3.25: Time averaged velocity vectors (a) standard k-ε turbulence model (b) RNG k-ε turbulence model (c) realizable k-ε turbulence model (d) RNG based sub-grid scale turbulence model (e) Smagorinsky-Lilly sub-grid turbulence model and (f) experimental data (after Tutar and Oguz (2002))
Zhang and Chen (2000) also preferred to use a filtered dynamic subgrid scale model (FDSM) for LES of complex flows and results in better agreement with experimental data. Examples of such flows are: air flow with natural, forced and mixed convection in a room. They also used the Smagorinsky model but reported its performance for such flows was generally poor. It failed to predict even the mean flow parameters, such as the mean air velocity and temperature. Also the model was observed to over predict the turbulence intensity by one order. The study overall showed that LES with the FDSM has a good potential to simulate indoor air flow.

New subgrid scale models for LES are being developed. Guo et al. (2007) used a new SGS eddy diffusivity model in LES of scalar turbulence based on the modified Yaglom equation for scalar fluctuation at resolved scale. The evaluation was carried out by an LES analysis of scalar transport in decaying isotropic turbulence and fully turbulent channel flow. It was seen that the new model could achieve similar accuracy as that by the dynamic Smagorinsky model, with the computational time being reduced by 20%.

Tian et al. (2007) have also used the LES technique with an RNG SGS model to investigate the indoor air flow and contaminant particle concentration in two different rooms. The first room had no contaminants and LES predicted the velocity profiles in good agreement with the experimental data (Figure 3.26). The LES model also successfully captured the mean flow trends as well as instantaneous flow information, which can be very helpful for appropriate design and evaluation of a ventilation system.
Figure 3.26: Predicted instantaneous (a) velocity field and (b) total pressure profile mid-point in room 1 (after Tian et al. (2007))

Tian et al. (2006) compared the standard k-ε, RNG k-ε and RNG-based SGS model in simulating indoor air flow for which experimental data existed. It was observed that all three models provided good agreement with the measurements of air phase velocity (Figure 3.27). However, the RNG-based LES model provided the best agreement with the measurements. Also the RNG k-ε model gave better performance than the standard k-ε model. An added benefit of the RNG-based LES model was that it provided time-dependent low-Reynolds-number turbulence information to the particle phase, resulting in a more realistic particle dispersion and distribution than the conventional two-equation k-ε models. Thus Tian et al. suggest that the RNG-based model was better. However, in this study the same mesh was used for all three cases. The selection of the mesh was done by carrying out a grid independency check using the RNG k-ε model. This is in the author’s view is not what should be done in testing LES and a more robust method of mesh selection for LES needs to be adopted.
Jiang and Chen (2001) compared two subgrid-scale models of LES i.e. the Smagorinsky subgrid-scale model and the Filtered dynamic subgrid-scale model (FDS) for predicting the air flow in buildings with natural ventilation. It was reported that both Smagorinsky subgrid-scale model and FDS models were able to provide accurate flow results for most natural ventilation cases with fully or nearly fully developed turbulent flows. As the Smagorinsky subgrid-scale model is a much simpler model and requires less computing time than FDS hence the Smagorinsky subgrid-scale model would seem to be a more suitable model for such flow types. The Smagorinsky subgrid-scale model though performs poorly for predicting laminar flows and flows near walls as the model coefficient is a constant. For single-sided ventilation, the averaging procedure of calculating the air flow results in a lower ventilation rate and air change effectiveness and hence RANS might not be an appropriate choice. LES, which can provide instantaneous flow field can be more useful in this regard, however, this needs to be investigated further.
Finally, buoyant plumes rising from point heat sources in a naturally ventilated enclosure have been investigated using LES by Abdalla et al. (2007). The Smagorinsky sub-grid scale model was used for the unresolved small-scale turbulence. The Rayleigh number - a dimensionless number which gives a good indication as to whether the natural convection boundary layer is laminar or turbulent - was chosen such that the flow was in the range of transition from an original laminar point to a turbulent plume. Plume properties such as the source strength and rate of spread and also the ventilation properties such as the stratification height and temperature of stratified layer were calculated using LES (Figure 3.28, Figure 3.29). The predictions of the LES model showed good agreement with the theory of Linden et al. (Linden et al., 1990).

Figure 3.28: Isosurface of (a) low pressure and (b) temperature for the plume studied by Abdalla et al. (2007)
Although the use of LES has increased considerably over the last decade for a variety of applications, to the best of the author’s knowledge, no in-depth investigations have been performed on buoyancy-driven natural ventilation flows and in particular the prediction of multiple solution flows for buoyancy driven natural ventilation.

3.5.3. Detached Eddy Simulation (DES)

DES is a hybrid form of RANS and LES techniques whereby the model switches to an LES plus sub-grid scale formulation in regions where the mesh is fine enough for LES calculations. Regions where the turbulent length scale is less than the maximum grid dimension (usually near solid boundaries) are solved by RANS. Thus, the cost of computation is dramatically reduced with the use of DES as it does not demand as high a grid resolution as pure LES. Although DES was initially formulated
for the Spalart-Allmaras model (Spalart and Allmaras, 1992) and served as a wall model for LES, DES based on other models (such as the two equation models) behave as hybrid RANS-LES models. DES is a non-zonal approach and provides a single velocity field across the RANS and LES regions of solutions. However, the grid generation in DES is more complicated than for simple RANS or LES case due to the RANS-LES switch.

Hasama et al. (2008) employed both LES and DES to investigate the induced flow properties through a single opening. The first objective was to investigate the dependency of the induced room airflow on the opening shape and secondly the distribution of the mean and turbulent variables at the boundary plane of the opening. LES and DES were performed on the same grid. It was observed that DES over-estimated the sub-grid scale viscosity in the LES region. However, the difference between the two in regards to the mean properties of the room was negligible.

A modified version of DES known as Improved delayed DES (IDDES) (Shur et al., 2008) has been developed to cater for near-wall flows. Mockett et al. (2012) simulated flows over 2D hills and reported very good agreement with LES benchmark data. This was done with significantly reduced computational expense (an estimated factor of 34 reduction) than LES. However, the results were less satisfactory when the Reynolds numbers increased. Mylonas and Sayer (2012) also employed LES and DES to investigate forces acting on a yacht exposed to uniform incident flow at high Reynolds numbers. They report that both LES and DES gave accurate predictions of the forces on the yacht keel. They also suggest that LES exhibits higher sensitivity to the Smagorinsky constant and the sub-grid scale, whereas DES is more sensitive to the time step size.

3.6. Summary

It is concluded from the literature review that natural ventilation is an effective strategy to reduce carbon emissions from buildings. Natural ventilation has been investigated using experiments though they are often expensive to carry out. CFD on the other hand is being increasingly used to predict both buoyancy and wind driven natural ventilation. However it is the author’s opinion that the current research needs to focus on buoyancy-driven natural ventilation alone as to address windless days encountered during summer seasons.
Based on the previous work reviewed, some decisions have been made for the current work. Firstly, it is reported that the standard k-ε and RNG k-ε turbulence models are often seen to give the most accurate results for buoyancy-driven natural ventilation compared with the commonly used turbulence models. Both of these turbulence models need to be compared with each other in predicting a flow parameter e.g. volumetric flow against some experimental data. Secondly, the RANS approach has been frequently used to predict natural ventilation flows, however, with high computational power becoming readily available, more expensive approaches such as LES are worth investigation. For LES simulations it is observed that if the mesh is constructed carefully the effect of the SGS model is negligible. Thus an appropriate procedure needs to be followed in constructing the mesh for LES simulations. However, the Smagorinsky model has been reported to better in predicting natural ventilation flows (Jiang and Chen, 2001), thus it will be used as the SGS model for the simulations in the current work.

The review identified some gaps in knowledge relevant to the field of LES modelling of natural ventilation. The numerous ‘filling box’ experiments have not been repeated using CFD. This will be useful to do so that the CFD approach can be readily scrutinised for its performance. Additionally the interaction of turbulent plumes within buoyancy-driven natural ventilation plays an important role in the final ventilation pattern. The interaction of plumes has been investigated experimentally but there remains a gap of exploring this phenomenon using CFD. Multiple steady states in natural ventilation experiments have been reported in the literature. Little work has been done to investigate the occurrence of multiple steady state regimes in building ventilation using CFD. There is no work done that compares the two transient approaches i.e. URANS and LES in predicting multiple steady states identified in experiments. The current work addresses these issues in an attempt to fill the gaps in research reported in this chapter.
Chapter 4. Methodology

“Who knows the minds of men and how they reason and what their methodology is?”
– Walter Martin

4.1. Introduction
It was indicated in Chapter 1 that the primary objective of this work was to investigate the performance of LES in modelling buoyancy-driven natural ventilation. The purpose of this chapter is to introduce the available commercial software and then to choose CFD methods that were considered fit for the purpose of this study. An introduction to the benchmark test cases selected for use in the present research is also presented in this chapter. Theoretical models and experimental data from these benchmark test cases will be used to validate CFD predictions and assess their performance. Finally, the boundary conditions that were used to simulate the flows in the selected benchmark test cases are presented, together with the important topic of the methodology adopted for LES mesh design.

4.2. CFD codes
Ideal CFD software would be that which simulates flows accurately (i.e. results are in agreement with theoretical models and available experimental data), is simple to use, and has low computational cost. There are a variety of commercial CFD codes available in the market. The licence fees for these vary and hence selection is an important task. Some of the popular CFD codes used in the industrial/research environment are CFX (ANSYS, 2012), FLOW-3D (Flow Science, 2012), PHOENICS (CHAM, 2009), STAR-CD (CD-adapco, 2012), PowerFLOW (EXA, 2012) and the open source code OpenFOAM (OpenCFD Ltd, 2012). Selection of software was based on the following criteria:
• All-in-one package: All-in-one CFD codes help eliminate the problem of incompatibilities between different components such as mesh generator, flow solver and post-processor.

• The physics involved: It is important to make sure the software package includes what the flow problem of interest in the current work requires. E.g. is the code able to solve steady-state alone or can it also solve transient simulations?

• Has the CFD code been validated in the right application areas? The software package might have the capability to solve the desired problem but has the CFD code been used and validated by others with similar flow problems?

• User support: In the likely event of encountering problems, is there user support available to help rectify the problem?

• User friendliness: CFD codes are known to be overwhelming for new users. Thus it is important the user can quickly acquire competence and familiarity with the user interface and code complexity.

• Training: Many low cost CFD codes are in-house university based codes which may or may not have any training or tutorial manuals available to help the user.

Based on the above mentioned criteria it was decided for the present project to use PHOENICS initially (due to its ease of use) to help the author acquire familiarity with modelling fluid flow. With the complexity involved in LES simulations it was decided for the later applications in the present research to use the all-in-one ANSYS commercial package CFX. This includes a meshing module ICEM CFD which provides better meshing control to the user, which is a critical step in LES simulations. A brief overview of these two CFD software packages will now be given.

4.2.1. PHOENICS software
PHOENICS (CHAM, 2009), developed first in 1981, is a general purpose widely used CFD code. The PHOENICS code is a fully self-contained, structured grid code with grid generation, numerical solution, and post processing elements. It is written in Fortran and is relatively inexpensive to run. However, it uses first-order time discretisation and neglects terms of second order and higher in the algebraic formulations for time-dependent problems. PHOENICS is particularly useful for
newcomers to CFD, university teaching and research due to the user friendly interface, and was hence chosen for the first phase of this research.

4.2.2. ANSYS software

4.2.2.1. ICEM CFD
For the process of constructing a geometry and a mesh the ICEM CFD software (ANSYS, 2011c) was used. ICEM CFD is a general purpose grid generation program with output readable by over 100 fluid flow solvers. It can also be used to create, repair and simplify geometries intended to be imported into CFD solver programs. ICEM CFD with its advanced mesh editing capabilities and compatibility with CFX (ANSYS, 2012) was thus an ideal choice for this research project.

4.2.2.2. CFX
CFX (ANSYS, 2012), a commercially available CFD solver, was employed in this study to perform the main numerical calculations. Initiated in the UK, CFX software has its roots in the codes Flow3D and CFX-TASCflow and is one of the most popular CFD software codes used worldwide. The code has been successfully applied to various fluid dynamics related problems such as water flowing past ship hulls, gas turbine engines, aircraft aerodynamics, pumps, fans, HVAC systems, and more. It is also a useful research tool for ventilation studies to predict room air flow and heat transfer. CFX (ANSYS, 2012) has been used in a large number of research projects found in the literature reviewed in earlier chapters (e.g. Cook, 1998; Abdalla et al., 2007).

4.3. Investigative strategy
Benchmark solutions in CFD are indispensable for testing and validating new CFD algorithms and codes. Benchmarking is not only limited to testing new codes but also for examination of the performance of existing codes in their application to new physical problems. Benchmarking stems from the need to compare numerical values from CFD results with data which are accepted in the literature as a true test of code performance because of: (i) known analytical solutions, (ii) extensive prior calculations by a range of users, (iii) experimental test data. This is a more quantitative and conservative approach than merely looking at pictures or flow visualisations produced from CFD.
The major purpose of the benchmarks chosen in this study was to establish concrete evidence which estimated the capabilities of LES for predictions of buoyancy driven natural ventilation problems. It was particularly intended that a decisive answer should be sought to the question as to whether accurate predictions of the multiple steady states observed in experiments (as discussed in section 3.5) could be captured by LES.

4.3.1. A preliminary test case
Before the three main benchmark problems which form the primary focus of the current work are introduced, as explained above, a simple test case was used as a learning exercise and this is explained here. Since the test case involves salt bath modelling, a technique often used to investigate buoyancy-driven natural ventilation flows inside enclosures, a brief background description to this technique is provided.

4.3.1.1. Salt Bath Modelling
Buoyancy forces that exist in naturally ventilated buildings are represented in laboratory experimental studies by a density difference between two fluids. These fluids are often chosen to be fresh water and a salt-water solution (brine). By measuring local salt concentration (density) and velocity within the laboratory model the corresponding temperature and velocity of air flow in the target full-scale ventilation scenario being studied in the laboratory model can be estimated, as long as the laboratory model experiment is appropriately scaled to achieve geometric and dynamic similarity.

The lab set-up usually consists of submerging small models of the building made out of Perspex into a large tank of fresh water. Buoyancy flows are introduced in the model by introducing brine through nozzles or other forms of orifices. As brine is denser than fresh water the injected fluid in the laboratory model sinks, whereas in an airflow ventilation case with hot air plumes the buoyancy flows would be upwards. The laboratory models thus have to be inverted relative to the real problem. Dye is mixed with the brine solution in order to make the flow of brine visible. Holes drilled in the models can be opened or closed using plugs to represent vent openings. A typical salt bath modelling set-up is shown in Figure 4.1.
The preliminary test case chosen is based on the published work of Kaye and Linden (2004). Their paper reports on two axisymmetric plumes coalescing in a naturally ventilated enclosure. Two-plume coalescence results in a merged plume that rises to the ceiling from where the warm fluid can escape through openings. The fluid that is unable to escape travels sideways across the ceiling to the adjacent side walls and begins to descend. This eventually causes a temperature interface to form between the upper warm fluid layer and the lower ambient fluid layer (Figure 4.2).

Kaye and Linden developed an analytical model for the plume merge height and carried out experiments using salt bath modelling. This test case has been used in the present project to provide a learning curve for setting up correct CFD boundary conditions for buoyancy driven flow and investigating two RANS turbulence models, $k$-$\varepsilon$ (Launder and Spalding, 1974) and RNG $k$-$\varepsilon$ (Yakhot et al., 1992). It was decided to investigate this preliminary test case using the RANS approach only since this was viewed as stated above as merely a learning curve exercise.

Figure 4.1: Typical salt bath modelling setup (source: Linden and Kaye (2006))
The Benchmark 1 test case also used the same experimental work as noted above of Kaye and Linden (2004). The primary purpose of Benchmark 1 was to extend the study undertaken in the preliminary test case to include LES simulations of buoyancy-driven natural ventilation. For this reason it was decided to use a similar flow problem as the preliminary test case. The results analysis was extended to include not just the plume merge height, but also measured information on thermal interface height and plume volume flow rate. The performance of LES in modelling buoyancy-driven natural ventilation was evaluated on the basis of how accurately it predicted these various fundamental parameters compared to the Kaye and Linden (2004) analytical model and experimental data (Figure 4.3). This also brings novelty into the present research since plume-plume interaction has not previously been studied using LES.
Benchmark 2 test case

The Benchmark 2 test case focussed on the work of Chenvidyakarn and Woods (2005). Their paper reported the appearance of multiple steady states in the natural ventilation of an open plan office containing two stacks using laboratory experiments. They also used a small-scale cubic tank to represent the ventilated building (Figure 4.4). Two tubes attached to the ceiling were used as stacks whilst holes at the bottom of the tank acted as openings or vents. A uniform floor heat source was achieved using heating coils on the bottom of the tank whose heat input was altered by varying the voltage. By varying the history of how the flow was started up they observed three different steady state displacement ventilation regimes (Figure 4.5). Both URANS and LES approaches were used to study this test problem.
Figure 4.4: Small-scale model used in laboratory experiments by Chenvidyakarn and Woods (2005)

Figure 4.5: Three steady state ventilation regimes observed in laboratory experiments by Chenvidyakam and Woods (2005)
4.3.4. Benchmark 3 test case

After confirming the ability of LES to reproduce adequately the merging plume in Benchmark 1 and multiple steady state phases in Benchmark 2, a final Benchmark 3 problem was selected for the application of LES to a building geometry and flow. The aim of this benchmark was to test the application of LES to a realistic and representative building application typical of that considered by consulting engineers. Once again, a comparative study of URANS against LES method was carried out. The test case building selected was the naturally ventilated theatre Lichfield Garrick (Gorst, 2003), located in Lichfield, UK (Figure 4.6); this was chosen due to its typical high occupancy building form and a progressive complexity in building form and flow compared to Benchmarks 1 and 2.

Figure 4.6: Section of Lichfield Garrick auditorium (after Short and Cook (2005))

The criteria used in this research to assess and validate the predicted results against the benchmark test case data are as outlined by (Zhai et al., 2003):

- Qualitatively, the results from the CFD simulation should show the same trend as the experimental data or analytical models fitted to this data;
• Quantitatively, the discrepancies between the results of the CFD simulation and those of analytical or experimental data should be less than 30%.

4.4. Numerical method
The three basic numerical methods explored for the solution of partial differential equations are the Finite Difference Method (FDM), the Finite Element Method (FEM) and the Finite Volume Method (FVM). An integral technique applied to the conservation forms of the governing equations leads to the FVM method; in addition, FVM can be considered as a hybrid between classical FDM and FEM (With, 2001). Early work on LES has been carried out using Finite Difference schemes (Smagorinsky, 1963; Ferziger et al., 1977; Kim and Moin, 1985) but for the last two decades FVM have been used much more (Bastiaans et al., 2000; Abdalla et al., 2007). Thus the finite volume method is used as the default discretisation scheme for the LES simulations repeated here.

4.5. Time step selection

4.5.1. Time step selection for RANS/URANS
Although for steady state RANS predictions the time-dependent term is not strictly needed, it is often included so that the solution is progressed numerically through an artificial time to achieve steady state. The time-step in this case does not have to be chosen to resolve any real physical timescales, but rather an appropriate time step size is important in order to obtain a good convergence rate. CFX applies a false timestep as a means of under-relaxing the solution of the non-linear algebraic equations as they approach the final solution (ANSYS, 2011b). Since the solver is implicit (see below), a large time step size can be selected in order to achieve convergence quickly.

This so-called “Auto Timescale” option in CFX is robust but often conservative. For even faster convergence, selection of the “Physical Timescale” option allows for sufficient relaxation of the equation non-linearities but increased speed of approaching a converged steady-state solution.

A reasonable estimate of a physical global timescale of any flow problem can be made using the length of the fluid domain $L$, and the inlet condition specified mean velocity $U$:
This global residence time is only an overall estimate and is often required to be altered during the prediction of buoyancy driven flows in order to achieve smooth convergence. The time-step chosen for “numerical” time-stepping is often a small fraction of this, e.g. \( \Delta t = \frac{T}{100} \). Too large time steps result in divergence or “bouncy” convergence. On the other hand time steps that are too small result in very slow convergence (ANSYS, 2011a). However, for the first few time-steps it is often helpful to use a time step perhaps one or two orders of magnitude smaller than 4-1 to allow the (necessary) crude initial guesses to achieve reasonable values. Of course for URANS solutions, the time-step should be chosen to allow accurate resolution of the (usually periodic) real physical time-varying flows. This necessitates the estimate of the physical frequency likely to occur and then choosing a time step perhaps two orders of magnitude smaller as a cautious approach.

### 4.5.2. Time step selection for LES

Before the time step selection for LES predictions is discussed it is important to understand the terms explicit and implicit.

#### 4.5.2.1. Explicit time-marching methods

For this numerical approach, flow variables at a new time step at each cell are obtained from a discretised version of the transport equations approximated using only known values at the previous time level. Thus, each algebraic equation obtained from the discretised transport equation contains only a single unknown. Solution of these algebraic equations is therefore very fast. However the solution of the whole equation system is only conditionally stable. For large time steps the numerical method will display oscillations that grow as the solution proceeds eventually leading to solution divergence and failure.

Stability is described in terms of the Courant Friedrichs Levy (CFL) number or more simply the Courant number. The CFL number is a stability indicator deduced from the convective terms which are found to be the most serious cause of instability. In an explicit method, it is usually found that the maximum CFL number anywhere in the grid has to be less than unity to guarantee stability; this enables the time step to
be selected for the simulations. The Courant number essentially represents the ratio of the distance a fluid particle will convect in one time step to the local cell size, thus:

\[ CFL = \frac{u \times \Delta t}{\Delta x} \quad 4-2 \]

Where, \( u \) is the velocity in the \( x \)-direction, \( \Delta t \) is the time step and \( \Delta x \) is the cell size in the \( x \)-direction. Of course in general all 3 directions need to be considered to evaluate the cell CFL number, and in CFX this is allowed for by using the magnitude of the local velocity vector, and a characteristic cell size taken as 0.61xlargest edge length in finite volume. For explicit numerical methods \( \text{CFL}_{\text{max}} < 1 \) is thus a stability requirement. For accuracy, \( \Delta t \) must be small enough to provide accurate temporal discretisation of the fastest motions resolved (which are the smallest length scale resolved), and this (for second order accurate transient term discretisation) leads to a recommendation for \( \text{CFL}_{\text{max}} \) (i.e. considering CFL in all finite volumes) again to be between 0.1 and 0.5.

4.5.2.2. **Implicit time-marching methods**

In this numerical approach the flow variables at a new time step are calculated through algebraic equations which contain several values at the new time level as well as values at the previous level time. Thus a matrix inversion iterative process is needed to solve the algebraic equations. An implicit method is more stable than an explicit method and stability is not governed so strongly by the time step, i.e. \( \text{CFL}_{\text{max}} \) can be much larger (perhaps a factor of 10) and stable solutions observed when solving for RANS problems. However, for temporal accuracy when solving unsteady URANS or LES problems, \( \text{CFL}_{\text{max}} \) values between 0.5 and 1.0 are still recommended. CFX adopts an implicit solver due to the enhanced numerical stability which is of greater value in RANS CFD.
4.5.2.3. **Time step methodology for LES solution**

Initially the simulation is run with an adaptive time step; after the “startup” time (perhaps as much as 50,000 time steps) when the flow has “forgotten” the (guessed) initial conditions and the turbulence conditions have become established the time step is made constant at a value selected on the basis of CFL\( _{\text{max}} \). Although the solver is implicit, as noted above for accuracy it is recommended to keep the CFL\( _{\text{max}} \) in the range of 0.5 to 1.0 and the time step is calibrated to lie within this range. The simulation is then continued with constant \( \Delta t \) until a point is reached when monitor plots of flow field values at selected points in the flow domain are observed to display a statistically stationary state. From this point onwards the results are averaged to deduce time mean values for analysis and comparison purposes. A result file (with extension .res) is generated. The result file may be opened with the CFX post processor to analyse results.

**4.6. Boundary conditions**

Boundary conditions play a vital role in the accuracy of any CFD calculation. The following sub-sections outline the common boundary conditions applied to various parts of the computational domain.
### 4.6.1. Solid wall boundaries

Walls were assigned the ‘no-slip wall’ property which is the most common wall boundary condition implementation. This means the fluid immediately next to the wall assumes the same velocity as the wall, which is zero for stationary surfaces. The heat flux across the wall boundary is zero (i.e. an insulated adiabatic condition).

\[ q_w = 0 \]

This condition implies that the temperature gradient is zero at the wall (wall temperature and near wall node temperature are identical). However, for the velocity field, the no-slip condition implies a high velocity gradient exists near the walls. In turbulent flow this demands extremely fine grid near walls, which is computationally very expensive (and also then demands low Re versions of RANS turbulence models or SGS models). The classical approach to avoid the need for a very fine near wall grid is to adopt the ‘wall function’ approach as described next. The proper representation of these processes is critical to resolve the flow near a wall accurately.

Experiments show that the boundary layer flow near a wall can be sub-divided into a multi-layer form including a viscous sublayer and a logarithmic layer. The viscous sublayer is the closest to the wall, where the flow is almost laminar and the molecular viscosity plays an important role in momentum transfer. Further away from the wall is the logarithmic layer, where turbulence dominates the mixing process. In between these two layers is a transitional “buffer layer” where both viscous and turbulent mixing are of similar magnitude (see Figure 4.8)

![Figure 4.8: Multi-layer wall boundary description](source: ANSYS (2011a))
Theodore von Kármán (1930) proposed to describe this velocity distribution via a law known as the law of the wall. Figure 4.9 shows the various regions described above in the classical linear/logarithmic plot. Note that the velocity and wall distance are here expressed in non-dimensional ‘wall units’, thus:

$$ u^+ = \frac{\bar{u}}{u_*} \quad y^+ = \frac{\rho y u_*}{\mu}, \quad u_* = \sqrt{\frac{\bar{\tau}_\omega}{\rho}} $$

where $\bar{\tau}_\omega$ is the time-mean wall shear stress. The log-law portion of the profile may be expressed using the above variables as ($\kappa = 0.41$, $E = 9.0$)

$$ u^+ = \frac{1}{\kappa} \log(Ey^+) $$

This information can be used to allow a relatively coarse mesh, which cannot resolve the very steep near-wall gradient that defines the wall shear stress $\bar{\tau}_\omega$, to nevertheless calculate $\bar{\tau}_\omega$ accurately. This is done by ensuring the near wall grid node ($P_1$ in Figure 4.8) lies in the log-law region (i.e. $y^+_{P_1} > \approx 30$ and $< \approx 300$). Equation 4-5 is then used (knowing $u^+_{P_1}$ and $y^+_{P_1}$ from the current numerical solution) to calculate $\bar{\tau}_\omega$ which is used in the FV discretised momentum equations for cell $P_1$. This is done in slightly different ways, depending on RANS or LES mode of calculations.

![Figure 4.9: Logarithmic profile near a wall (source: Tominaga (2000))](image)
**RANS CFD**

CFX provides a near wall treatment known as the ‘Automatic near-wall treatment’ that corresponds to the above log-law concept. The Automatic near-wall treatment automatically switches from linear wall-functions ($u^+ = y^+$ for $y^+ < 11$) to a low Re buffer layer region profile $11 < y^+ < 30$ and a log-law profile for $y^+ > 30$ (see ANSYS (2011b) for details).

In addition to the use of a wall function to calculate the wall shear stress, further conditions have to be imposed to ensure accurate solution of the high Re k-ε equations at the near-wall nodes. CFX uses the classical approach to this, which is described in the CFX user manual (ANSYS, 2011b).

**LES CFD**

The wall function approach is basically the same for LES CFD and for RANS CFD. One implementation difference is that during the LES calculation, the time-mean values of $\langle \bar{u}_P \rangle^1$ and $\langle \bar{u}_i \rangle$ or $\langle \bar{r}_\omega \rangle$ are not available until a statistically stationary state is achieved. Until then, the normal practice is to use the latest available estimate for the time-mean quantities, and the instantaneous resolved wall shear stress is calculated from:

$$\bar{r}_\omega = \frac{\bar{u}_P}{\langle \bar{u}_P \rangle} \langle \bar{r}_\omega \rangle$$

4-6

4.6.2. Openings or Inflow/Outflow boundaries

Once again a similar approach is used in both RANS and LES predictions to calculate inflows and outflows through openings (connections between internal flow regions and external ambient) e.g. at the ends of stacks and at vents.

**RANS CFD**

CFX provides a specification of an ‘openings’ boundary condition which allows flow to enter or leave the domain depending on local conditions. In this study a loss coefficient was specified which is used to correct the Bernoulli (inviscid) approximation linking the pressure change across an opening to the flow through it. If $\Delta P$ represents the difference between the ambient static pressure (effectively the

1 $\langle \cdot \rangle$ indicates a time average of a filtered resolved quantity and an overbar indicates the instantaneous filtered quantity.
total pressure for a stagnant ambient) and the local static pressure inside the flow at the opening; then Bernoulli’s equation, corrected via a loss coefficient reads:

\[ \Delta P = \frac{1}{2} f \rho U_n^2 \]  

where, \( f \) is the loss coefficient and \( U_n \) is the normal component of time-mean velocity at the opening location. The relationship between loss coefficient and discharge coefficient is:

\[ f = \frac{1}{C_d^2} \]

The discharge coefficient, \( C_d \), can vary with Reynolds number. However, at high \( Re \) and for sharp edge openings a discharge coefficient \( C_d = 0.61 \) is usually taken as standard. The code is supplied with a value of the external ambient static pressure. If this is greater than the current calculated value of the internal opening static pressure, \( U_n \) is directed into the solution domain, if it is less \( U_n \) is outward. For \( \kappa, \varepsilon, T \) if the velocity is inward ambient values are used, if outward a zero gradient condition is applied and the internal value is set at the openings.

**LES CFD**

For LES the same dual-direction opening flow boundary condition was applied at domain openings as described for RANS. However, the internal pressure used in equation 4-7 now constantly fluctuates with time and hence the \( U_n \) velocity (used to specify the ‘filtered’ velocity on the boundary opening) will also fluctuate in time (as well as possibly direction), unlike the RANS steady state velocity.

**4.6.3. Solver Control and choice of convection discretisation scheme**

**RANS CFD**

For RANS simulations the ‘high resolution’ option in CFX was selected for convection discretisation rather than the ‘upwind’ setting. The upwind scheme is first-order accurate and robust but suffers from numerical diffusion and requires a finer mesh to produce numerically accurate solutions. The ‘high resolution’ blends pure 1\(^{st}\) order upwind (blending factor 0) with pure 2\(^{nd}\) order central differencing (blending factor 1). The blending factor is automatically varied between 0 and 1 in the high resolution option. The blend factor is varied on the basis of the local solution which
helps in achieving a bounded solution. In regions with low variable gradients the blending factor approaches 1 whilst in high gradient areas the value will be closer to 0 to help avoid over/under-shoots and for the purpose of improved robustness (ANSYS, 2011a).

To judge convergence of the steady state solution, the RMS of the residual values of all dependent variables were examined and convergence was achieved when all were less than $10^{-6}$.

**LES CFD**

A second order Backward Euler scheme was used for the transient term with the convection scheme set to ‘central difference’ rather than ‘high order’. Central difference scheme is non-dissipative on a uniform mesh which is important in LES CFD.

For LES, the question of solution convergence only applies to the in-time-step iterations used by the implicit method. The convergence criterion to decide on whether the present step was complete was that RMS residuals of velocity, temperature and pressure should again be less than $10^{-6}$. Since the time step is typically very small for LES, this was usually achieved with between 3 and 5 inner iterations.

**4.6.4. Domain initialisation**

To ensure that the plume would evolve in a stagnant flow and the stratified flow would develop quickly the following initial conditions were imposed; (i) all velocity components were set to zero and (ii) the temperature was set equal to the ambient temperature.

**4.6.5. Heat sources**

Boundary heat sources were also defined as no slip walls as described above, but a heat flux was specified on the wall boundary rather than an adiabatic condition. The precise value of the heat flux was different for each benchmark test case (units of W/m$^2$). Considering the domain as a control volume a positive value indicated heat flux into the domain as per convention.
4.6.6. Output control
For steady state RANS predictions output of variables was only triggered once when convergence was attained. On the other hand, for transient LES predictions the solution was saved every 1000 time steps in case the solver were to crash and then the solution could be recovered from one of the backups. Monitor points were placed in the domain to monitor temperature, velocity and pressure values in specified areas (i.e. areas of interest e.g. near heat sources, stacks, openings) during the simulation. This provided an insight into the flow development inside the computational domain and was also used as a basis to assess if the flow had reached a statistically stationary state. Additionally for LES, time series of temperature and velocity were also saved at selected points in order to evaluate spectral information.

4.7. Mesh selection methodology
There are three grid refinement strategies used in CFD. All three strategies are solution-based rather than pre-processing based. These are as follows:

- **R-refinement**: In this method the grid point number is fixed, however their position is changed based on selected areas of interest.
- **H-refinement**: In this method the grid is locally refined by increasing varying the number of grid points in a given region of space according to an assessment of local variable gradients.
- **P-refinement**: In this method the grid remains the same however the order of accuracy of the local spatial discretisation method is increased.

The problem with R-refinement is that it can lead to a depletion of grid points near features of interest. The P-refinement method is effectively being used in finite-element methods with very limited application to finite-volume methods (With, 2001). The most convenient method of grid refinement by far is thus H-refinement. Based on this information the H-refinement method was adopted in the current work.

**RANS CFD**
For RANS a suitable final mesh was selected by carrying out a grid sensitivity study. In this process various runs were performed using meshes of different resolution. Their results were then compared to analyse grid independence. Mesh resolution
was typically increased in areas of interest such as openings and heat sources and areas identified as possessing high variable gradients (such as the edges of jet plumes) from courser mesh solutions.

**LES CFD**

Adequate grid resolution to capture small scale flow features numerically accurately is an important requirement for all classes of CFD. Over several decades of user experience with RANS turbulence models, well established guidelines have become accepted, such as reported by Casey and Wintergerste (2000). This topic is not so well developed for LES CFD. LES is much more sensitive to grid design than RANS. For example, Vanella et al. (2008) have shown how LES predictions react more strongly to non-uniform grids. Since the grid size is LES also acts as the spatial filter size for removing sub-grid scale unsteady motions, then any sudden coarsening of the grid can lead to energy pile-up on the filter grid scale since this resolved energy has ‘nowhere to go’ as it moves into the coarser grid. This can even cause solution instability (note sudden refinement in the flow direction does not cause such large flow perturbations).

The most challenging area in the grid resolution context is the close to solid wall boundary region, where the energy containing eddies become very small and also scale on a viscous wall length scale ($\mu/\rho u_\tau$, where $u_\tau$ is the friction velocity = $\sqrt{\tau_\omega/\rho}$, $\tau_\omega$ being local wall shear stress). In these regions, Piomelli and Balaras (2002) have produced what have become accepted cell size criteria for well resolved LES of $\Delta x^+ < 100$, $\Delta y^+ < 2$, $\Delta z^+ < 10$ (x,y,z represent streamwise, wall normal and wall parallel co-ordinates and the $^+$ superscript indicates non dimensional wall units (e.g. $\Delta y^+ = \rho \Delta y u_\tau / \mu$)). These criteria would lead to exceedingly high cell numbers near walls in high Reynolds number flows. Fortunately, for the buoyant natural ventilation application of interest here, it is unlikely that the flow in the near wall boundary layers dominate the flow. Much more likely is that it is the turbulent eddy scales in the free shear regions on the edges of the buoyant jet plumes which control the turbulent entrainment. Grids to resolve such regions are neither so challenging as near wall boundary layers, and nor do they depend on Reynolds number since the eddy structures are only weakly dependent on Re. It is still necessary, however, to design the grid resolution carefully for accurate LES CFD.
Celik et al. (2005) have reviewed the several approaches proposed in the literature to guide LED grid design and assessment. Similarly, Gant (2010) has examined the performance of several assessment criteria suggested by Celik et al. (2006) for industrially relevant flows. Whilst various techniques have been suggested, the mesh density methodology chosen for the present work is based on the following steps, driven again by the belief that it is the free shear layer (plume boundary) turbulence that is important in the present application.

Mesh design and assessment uses the variables as defined below:

- $k_t$: total turbulence kinetic energy (time-mean)
- $k_{res}$: resolved turbulence kinetic energy
- $k_{SGS}$: SGS kinetic energy estimate
- $k_{RANS}$: RANS predicted turbulence energy
- $\mu$: fluid molecular viscosity
- $\mu_{SGS}$: SGS eddy viscosity
- $L$: integral turbulence length scale - RANS estimate ($k_{RANS}^{3/2}/\varepsilon_{RANS}$)
- $S$: Strain rate magnitude
- $Re_t$: turbulent Reynolds number ($\rho k_{RANS}^{1/2}L/\mu$)
- $\Delta$: filter width
- $\varepsilon_{RANS}$: RANS predicted dissipation rate
- $\varepsilon_{LES}$: LES estimated dissipation rate

**NB:** $k_t = k_{res} + k_{SGS}$

The mesh design procedure is as follows:

1) Using a RANS steady state solution obtained on the selected mesh, $Re_t$ and $L$ are calculated.

2) Analysis of $Re_t$ is used to confirm that the majority of the flow is determined by high Re free shear layers (i.e. $Re_t > 0(10^5)$) except for small regions near solid surfaces.

3) If it is assumed that an LES mesh provides good resolution when at least 80% of the total kinetic energy ($k_t$) is resolved (i.e. $k_{res} / k_t > 0.8$) (as suggested by Pope (2004b)), then, as shown in the analysis below, the mesh should be designed so that $L/\Delta > 12$. Using the RANS estimate for $L$ ($k_{RANS}^{3/2}/\varepsilon_{RANS}$) the mesh can be
checked to ensure that $\Delta$ satisfies this constraint, at least on the basis of an a-priori RANS solution.

The target condition that $L/\Delta$ should be greater than 12 for a suitable mesh for LES to satisfy the criterion $k_{res}/k_t > 0.8$ is deduced as follows. Two estimates can be made for the energy dissipation rate at any point in the flow, one based on the sub-grid scale model:

$$\varepsilon_{SGS} = C_\varepsilon \frac{k_{SGS}^{3/2}}{\Delta}$$  \hspace{1cm} (4-9)

where $C_\varepsilon$ is taken as 0.845 (Sagaut, 2005). The second assumes the usual high Re relationship between energy dissipation rate, turbulence energy and length scale based on an equilibrium cascade assumption:

$$\varepsilon = \frac{k_t^{3/2}}{L}$$  \hspace{1cm} (4-10)

Equating these two relationships and inserting $k_t = k_{res} + k_{SGS}$ gives:

$$C_\varepsilon \frac{k_{SGS}^{3/2}}{\Delta} = \frac{(k_{res} + k_{SGS})^{3/2}}{L}$$  \hspace{1cm} (4-11)

Thus

$$\frac{L}{\Delta} = \frac{1}{C_\varepsilon} \left(\frac{k_{res}}{k_{SGS}} + 1\right)^{3/2}$$  \hspace{1cm} (4-12)

For $\frac{k_{res}}{k_t} > 0.8$ this can be shown to lead to

$$\frac{L}{\Delta} > 12$$  \hspace{1cm} (4-13)

The ideas outlined above have been used to guide the mesh design for the LES simulations presented throughout this work.

4.8. Parallel processing computations

As explained in the introduction, LES is a very expensive CFD technique. The most powerful modern computers are parallel processor compute clusters i.e. a number of processors working at the same time. A domain decomposition approach was
adopted whereby the total solution was divided into sub-domains, with a sub-domain loaded onto each processor and each sub-domain exchanges information as the solution proceeds. Running LES CFD on a PC cluster greatly increases (depending on the number of parallel processors) the simulation speed compared to running it on a single processor. Parallel computation requires parallel coding. The Message Passing Interface (MPI) protocol, due to its portability across machines, has become one of the most widely used options. The simulations for this investigation were run on Loughborough University’s High Performance Computing (HPC) service (called “Hydra”) under an MPI protocol. However, BM1 using the RANS technique was simulated on a desktop PC with 8 processors in parallel. This was due to the fact at that stage of research the Hydra facility was not available.

Hydra used the Red Hat Linux operating system; it comprises a 1956-core 64-bit Intel Xeon cluster supplied by Bull. Hydra consists of 161 compute nodes, each having two six-core Intel Xeon X5650 CPUs and 24GB of memory with 40TB of user home storage. Communication between Hydra compute nodes is facilitated via an Infiniband network.

To provide an insight into the costs of running RANS/URANS and LES simulations, the typical mesh resolution, wall-clock runtime and computational power used for each of the benchmark problems to be reported below (BM1, BM2, BM3) are given in Figure 4.10, Figure 4.11 and Figure 4.12.

Figure 4.10: Computational and time costs for benchmark 1
From the above figures it is clear that both the mesh resolution and hence also run times were increased by around a factor of 10 when running LES instead of adopting a RANS/URANS approach. With higher mesh resolution the number of processors was also increased for LES, since for the same number of processors the run times
would obviously become even longer. The figures above for LES show the time to reach a statistically steady state once the ‘start-up’ period to forget initial conditions and establish turbulence throughout the solution domain has finished and not the complete simulation time for a specific benchmark. The start-up period from an initial zero velocity field can be considerable (50-100,000 time steps). However, this is considered a reasonable basis for estimation, since when one LES simulation has been obtained for a given problem, it can be used as an initial condition for the next set of flow conditions for example, and then the start-up time is not so significant.

Note also that the factor of 10 could be approximately halved if twice the number of processors had been used, so perhaps a useful guide line for LES calculations could be identified that access to a PC cluster of $\approx 100$ processors is needed before the cost relative to RANS CFD becomes acceptable – as long as the accuracy of prediction increases noticeably. This is the next task to examine and details of each benchmark flow are presented in the following chapters.

4.9. Summary

The PHOENICS and ANSYS CFX software are selected for the current study due to a number of reasons such as: ease of use, software validation, user support, training available etc. To validated CFD predictions they need to be compared with validated analytical solutions or experimental data known as benchmarks. Three benchmark test cases were chosen on the basis of their relevancy to the research problem. The first benchmark test case was based on the work of Kaye and Linden (2004). The second benchmark test case was grounded on the work of Chenvidyakarn and Woods (2005). The final test case investigated the naturally ventilated theatre Lichfield Garrick (Gorst, 2003), Lichfield, UK. The numerical method and boundary conditions that were used in this research have also been discussed in this chapter. Mesh generation process, which forms a significant stage of CFD, has been thoroughly explained for both conventional CFD and LES techniques. Finally, the cost in terms of time and computational power has been reported for all three benchmark test cases.
Chapter 5. Preliminary test case

“All achievements, all earned riches, have their beginning in an idea” – Napoleon Hill

5.1. Introduction
Chapter 4 has given an overview of the numerical methods that were adopted in this research project. However, as also mentioned in the previous chapter, experience in using the numerical procedure and associated settings (convection scheme, number of coefficient iteration loops turbulence model etc.) needed to be gained to ensure accurate modelling of natural ventilation problems. Preliminary RANS calculations of a model buoyancy-driven natural ventilation as a preliminary test case are reported here.

5.2. Background
Ventilated enclosures with multiple heat sources contain turbulent plumes that rise above the heat sources and interact with each other. Linden (1999) reports that this interaction influences the behaviour of the resulting ventilation flow and can affect ventilation flow rate. The behaviour of such plumes in a built environment context have been analysed by Kaye and Linden (2004). The experimental results obtained are used here to help assess RANS-based turbulence models for predicting the behaviour of such plumes. This will also provide supporting evidence and confirmation that the selection of an appropriate turbulence scheme is critical for modelling natural ventilation accurately.

5.3. The situation considered and associated theory
Buoyancy-driven natural ventilation was studied by Linden et al. (1990). The salt bath experimental work considered buoyancy-driven displacement ventilation in a small enclosure driven by a single continuous point source of buoyancy on the floor.
It was observed that steady stratification was produced consisting of two homogeneous layers of fluid separated by a horizontal interface at a height $h$ above the floor. The lower layer of fluid was at ambient density while the upper layer was at a density equal to the plume density at height $h$ (Figure 5.1 for two sources). They reported that the steady interface was formed where the volume and buoyancy fluxes through the upper (ceiling) openings equal that supplied to the upper layer by the plume.

Figure 5.1: Schematic representation of steady natural ventilation flow in an enclosure with notation; $(M)$ buoyancy flux, $(M_{\text{out}})$ buoyancy flux at outlets, $(q_1$ and $q_2$) heat sources of different strengths.

Pera & Gebhart (1975) have shown that the merging behaviour of two co-flowing fully turbulent plumes with sources at the same level is primarily dependent on their initial buoyancy fluxes $\hat{F}_1$ and $\hat{F}_2$, the ratio of these fluxes and the source separation $x_0$ (Figure 5.2). Plume merge height was found to be a function only of these parameters. If $z_m$ is the height at which the plumes merge then the analysis of Kaye and Linden (2004) predicted that:

$$\frac{z_m}{x_0} = \text{func} \left( \frac{\hat{F}_1}{\hat{F}_2} \right)$$

5-1
Here, $z_m$ is to be determined by plotting velocity profiles across the two plumes at various heights and noting where the separate plume maxima first disappeared (see Figure 5.2).

The scenario considered for this study is that shown in Figure 5.1 of a single space enclosure, with high and low-level openings for air flow and with two sources of buoyancy on the floor with a buoyancy flux ratio $\psi = F_2/F_1 = 0.45$. These values were chosen in order to compare the predicted flow rates from RANS CFD with the experimental data reported by Kaye and Linden (2004) for the same buoyancy flux ratio.

\[ \text{Figure 5.2: Schematic of two plumes showing merging height } z_m \text{ and the plume separation } x_0 \text{ (source: (Kaye and Linden, 2004))} \]

In order to estimate the merged plume flow rate and the steady state interface height it was important that the horizontal plane corresponding to the interface should be somewhere above the plume merge height $z_m$ but below the ceiling of the enclosure i.e. $z_m < h < H$. Initially the areas of openings in the floor and ceiling ($a_1$ and $a_2$) were chosen arbitrarily and the corresponding the “effective” opening area $A^*$, calculated using equation (5-2) (Hunt and Linden, 2001).
\[ A^* = \frac{C_D a_t a_b}{\left(\frac{1}{2}\left((C_D^2/C_e)a_t + a_b^2\right)\right)^{\frac{1}{2}}} \]  

5-2

The quantities \( C_e (=0.5) \) and \( C_D (=0.5) \) are the coefficients of expansion and discharge respectively.

This value of \( A^* \) was then used in equation (5-3) to establish the estimated normalised interface height \( \xi = h/H \), as defined by Linden et al. (1990).

\[ \frac{A^*}{H^2} = C^{3/2} \left[ \frac{\xi^2}{1 - \xi} \right] \]  

5-3

where,

\[ C = \frac{6\alpha}{10} \left[ \frac{9\alpha}{10} \right]^{1/3} \pi^{2/3} \]  

5-4

is a constant dependent upon the entrainment coefficient \( \alpha \) for the plume. Here 0.1 has been taken for the value of \( \alpha \) in accordance with the work of Linden et al. (1990).

5.4. CFD modelling assumptions

5.4.1. Computational domain

The computational domain considered was a cubic enclosure with a floor area of 25m\(^2\) and height of 5m. A view of the domain is shown in Figure 5.3. Two heat sources of strengths \( q_1 = 111.11 W \) and \( q_2 = 50 W \) were also placed on the floor. The two heat sources each had an area of 0.0081 m\(^2\) and were positioned symmetrically on the floor separated by a horizontal distance \( x_0 = 0.4 \) m. The opening area of upper and lower openings was 1.25m\(^2\) each. For convenience these openings were placed at the corners of the enclosure to ensure minimum interference with the plume mixing and merging process.
5.4.2. **Numerical solver**

The software package used for these CFD predictions was the PHOENICS (2009) code which uses the finite volume solution method on a staggered grid with a structured Cartesian coordinate system. The Boussinesq approximation (see chapter 2) was used to represent buoyancy effects and also a steady state RANS prediction was performed. The solution was considered converged when the global convergence criterion of 0.0001% was achieved.

5.4.3. **Grid refinement**

A preliminary study was carried out where the grid was systematically refined to examine grid sensitivity. The required grid density for grid independence depends mainly on the spatial discretisation technique selected for the non-linear convection terms. For the current work, convection terms were discretised using the HYBRID-differencing scheme (HDS) that is used in PHOENICS by default. HDS switches between the Upwind-Differencing Scheme (UDS) and the Central-Differencing Scheme (CDS) according to the relative size of the convective and diffusion fluxes across cell surfaces, characterised by a local cell Peclet number Pe. The CDS (second order accurate) is used for Pe < 2 while the UDS (first order accurate) is
used for $Pe > 2$. The cell Peclet number is the ratio of the convective to diffusive fluxes across a cell surface,

$$Pe = \frac{V \times L}{\alpha}$$  \hspace{1cm} 5-5

where $L$ is the local cell dimension, $V$ is the local cell velocity, and $\alpha$ is the relevant diffusion coefficient (total (i.e. molecular + turbulent) viscosity for momentum and thermal diffusivity for temperature).

A coarse grid was first selected to procure a solution quickly and establish confidence in the selected boundary conditions and solution domain size. This was then refined to improve resolution in high gradient regions such as openings, near heat sources and in the plume flow. The baseline (coarse) grid is referred to here as mesh A (Figure 5.4). In PHOENICS the baseline grid lines were distributed by the auto-mesher according to the following set of rules (PHOENICS User Documentation (CHAM, 2009)):

1. The maximum cell size was not allowed to exceed 5% of the domain size.
2. The ratio of the sizes of cells between one region and another was not allowed to exceed a set limit (1.5). (A region is a user-defined zone in space containing a flow-significant 'object' – e.g. the regions of heat source on the floor or the slot openings in the floor/ceiling).
3. If the maximum ratio is exceeded, the number of cells in a region was increased, and the spacing set according to a geometrical progression using a fixed expansion ratio (1.2), until either the ratio criterion was satisfied at both ends of the region, or the cells at both ends were less than a set minimum fraction (0.5%) of the domain size.

The resolution of the baseline grid was first doubled to produce a fine mesh density (mesh B Figure 5.4). Further refinement of the grid was then carried out specifically in areas where large gradients of solution variables (e.g. velocity or temperature) were identified in the mesh A solution. Failure to provide sufficient mesh density in these areas will result in the buoyant plume or the boundary layer flow being insufficiently resolved resulting in numerical smearing. Local grid refinement was
carried out in particular on the edges of the rising plumes. An example of baseline and refined grids is shown in Figure 5.4.

Figure 5.4: A comparative illustration showing mesh A (left) and mesh B (right)

The parameter used to judge solution sensitivity to mesh refinement was the total volume flow rate $Q$ in the merged plume at a height $z = 2.5$ m above the floor. $Q$ was estimated as described below. The results are shown in Table 5-1. Note that there is little variation (max 2.5%) in the estimated $Q$ between the baseline grid and the two refined grids, implying that the predicted solution is insensitive to grid changes and even the baseline grid resolves the flow adequately.

Table 5-1: Grid mesh settings and resulting volumetric flows

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Configuration</th>
<th>$Q$ (m$^3$/s)</th>
<th>total no. of cells</th>
<th>Grid size $(x,y,z)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>original</td>
<td>0.205</td>
<td>19980</td>
<td>(37,27,20)</td>
</tr>
<tr>
<td>B</td>
<td>2x overall</td>
<td>0.200</td>
<td>150960</td>
<td>(74,51,40)</td>
</tr>
<tr>
<td>C</td>
<td>2x source</td>
<td>0.203</td>
<td>25800</td>
<td>(43,30,20)</td>
</tr>
</tbody>
</table>

Based on work of others (Murakami et al. (1996), Chen (1995a), Murakami (Murakami, 1998) and Cook & Lomas (1997)) it was decided to study the performance of the $k$-$\varepsilon$ (Launder and Spalding, 1974) and RNG $k$-$\varepsilon$ (Yakhot et al., 1992) models in this problem.
5.4.4. Plume flow rate estimation

Kaye and Linden (2004) focused on the far-field behaviour of the plumes by making a series of flow measurements in the merged plume, using the technique described by Baines (1983). The results were plotted in the form of $z/x_0$ against a non-dimensional volume flow rate:

$$Q^* = \frac{Q^{3/5}F_1^{-1/5}}{x_0}$$  \hspace{1cm} 5-6

where, $F_1$ is the initial buoyancy flux in plume 1 and is given by (Batchelor, 1954) as:

$$F_1 = \frac{W_1 g}{C_p \rho_o T_o}$$  \hspace{1cm} 5-7

where, $W_1$ is the heat flux of the plume source, $g$ is gravitational acceleration, $C_p$ is specific heat, $\rho_o$ reference density and $T_o$ a reference temperature. Values of $Q^*$ were evaluated at different non-dimensional heights $z/x_0$.

The results were consistent with Baines (1983); the only difference was that all distances were scaled on the initial plume separation ($x_0$). The results were also scaled in terms of $F_1$ alone rather than the sum of the two buoyancy fluxes. Baines (1983), by measuring the distance from the source to the interface and the flow rate through the tank was able to measure the plume flow rate as a function of the distance from the source. The accuracy of the CFD simulations was assessed based on ability to predict this relationship accurately.

In order to calculate the predicted local volume flux $Q$ in the plume, velocity profiles obtained from the CFD solutions were plotted at different heights resulting in velocity profile curves as shown in Figure 5.5. The volume flux $Q$ is the area under the velocity profile curve. This can be calculated by integrating the area under the curve. Alternatively in this research the predicted profiles were first converted to equivalent “top-hat” profiles which can be used to represent their Gaussian counterparts. This was done as it was in accordance with the approach adopted by both Linden et al. (1990) and Cook (1998).
Here, $b_G$ is the radial distance from the plume axis to the point at which the velocity has fallen to 1/e of its peak value ($v_G$). The following two variables were then calculated using the numerical relationships between top-hat quantities and their Gaussian counterparts, as reported by Cook (1998):

$$b_T = \sqrt{2} b_G$$  \hspace{1cm} 5-8$$

$$v_T = \frac{v_G}{2}$$  \hspace{1cm} 5-9$$

Thus the volume flux in the plume could then be easily calculated using the following equation:

$$Q = \pi \times b_T^2 \times v_T$$  \hspace{1cm} 5-10$$

5.5. Results

5.5.1. Illustrative flow field results

The flow pattern within the enclosure predicted by the RANS CFD prediction ($k$-$\epsilon$) is shown in Figure 5.6. The velocity vector plot shows the direction of the expanding and rising plume above the heat sources which spreads laterally rapidly on reaching
the ceiling. Warm, buoyant air flows out through the upper openings and cool, ambient air is drawn in through the low-level openings. A contour plot of the velocity (Figure 5.7) further supports this flow pattern. The buoyancy ratio $\psi$ between the two plumes is clearly identified in the velocity contours in Figure 5.7 and the temperature contours in Figure 5.8 as $\psi = 0.45$ i.e. $F_2$ is lesser than $F_1$ for this solution. The region outside the plume is symmetrical in the velocity and temperature plots, showing that it is only the single merged plume that dominates the overall flow in the enclosure.

![Velocity vector plot representing the flow directions inside the enclosure](image)

From the thermal plot (Figure 5.8), the formation of the two layers of fluid separated by a horizontal interface is visible. It can also be observed that the upper layer is a uniform temperature (approx. $20.4^\circ$C) while the lower layer temperature is approx. $20^\circ$C (the ambient temperature). These results agree qualitatively well with the analysis of Linden et al. (1990) which confirms the suitability of the boundary conditions and the CFD setup.
Figure 5.7: Velocity contours on a plane perpendicular to the heat sources (x-y plane, z=2.5m), showing the coalescence of the two plumes using the RNG $k$-$\varepsilon$ turbulence model.

Figure 5.8: Temperature stratification inside the enclosure showing the two fluid layers separated by a horizontal interface (x-y plane, z=2.5m) using the RNG $k$-$\varepsilon$ turbulence model.
5.5.2. Comparisons with experiments

A plot of the measured non-dimensional flow rate against non-dimensional height from experimental data and the RANS solutions is shown in Figure 5.9 (k-ε model) and Figure 5.10 (RNG k-ε model) for the case of $\psi = 0.45$. The black dashed lines represent the experimental data (with the change in gradient indicating the merge height, represented by a red cross) while the green lines represent CFD predictions for each turbulence model. The original paper did not specify the level of uncertainty in experimental data.

The first thing to observe from the CFD predictions is that they confirm the behaviour noted in the experiments for a merged plume, i.e. there is a direct linear relationship between plume flow rate and distance away from the buoyancy source. However, the gradient of the predicted line (indicating the rate of entrainment of ambient fluid into the plume) is quite different for the two RANS turbulence models.

![Figure 5.9: Prediction of the plume flow rate using the k-ε turbulence model compared with the flow rate measurements for two merging plumes for buoyancy flux ratio $\psi=0.45$. The red cross indicates a change in gradient indicating the merge height.](image-url)
The graphs show that the RNG k-\(\varepsilon\) model predicts the entrainment relationship much more accurately than the standard k-\(\varepsilon\) model. An indication of the magnitude of the discrepancy between experimental and predicted values is given in Table 2.

**Table 5-2: Percentage discrepancies between CFD predictions and experimental data**

<table>
<thead>
<tr>
<th>RANS-based Turbulence Model</th>
<th>% discrepancy in slopes of experimental and CFD results</th>
</tr>
</thead>
<tbody>
<tr>
<td>k-(\varepsilon)</td>
<td>53.13</td>
</tr>
<tr>
<td>RNG k-(\varepsilon)</td>
<td>9.10</td>
</tr>
</tbody>
</table>

This result confirms the observations made by other authors and noted in the literature review of Chapter 3, that the RNG k-\(\varepsilon\) model is a superior model than the standard k-\(\varepsilon\) for buoyant plume applications.
5.6. Summary

Before a deeper study of natural ventilation using LES was undertaken, it was necessary to test the correct settings of boundary conditions and other code parameters such as mesh generation for a representative buoyant flow problem. In addition the opportunity to explore the sensitivity of the solution to the choice of RANS turbulence model was explored. The results presented in this chapter have confirmed the ability of the author to conduct CFD analysis of buoyancy driven natural ventilation type flow problems. It also demonstrated clearly how important the selection of an appropriate turbulence model is for RANS CFD analysis of buoyancy forces even in a very simple geometry. The results were compared both qualitatively and quantitatively with experimental data. The general flow patterns agreed well with the experimental work for both turbulence models. In terms of the volume flow rate prediction in the plume, it was observed that the RNG k-ε turbulence model showed much better agreement with the experimental data compared to the standard k-ε turbulence model.

Only a single value of $\psi$ was considered, so it was not established how well the RNG k-ε model would capture variations in this controlling parameter. This could have been done but it was considered that sufficient analysis had been completed to illustrate the sensitivity to RANS turbulence modelling, and to satisfy the ‘learning curve’ objective. The following chapters extend and complicate the natural ventilation scenarios studied and carry out and compare RANS, URANS and LES CFD analyses.
Chapter 6. Benchmark 1: LES of twin thermal plumes

“A man’s accomplishments in life are the cumulative effect of his attention to detail” – John Foster Dulles

6.1. Introduction

To ensure continuity from the preliminary test case, it was decided to adopt the same twin plume flow problem also as the Benchmark 1 test case. The first application of LES in this project to this natural ventilation problem is reported in this chapter.

The purpose of this benchmark was to assess the performance of LES in simulating the unsteady dynamics of two interacting, turbulent buoyant plumes in a naturally ventilated enclosure, and to provide information and experience for an LES study of more complex plume interactions and ventilation flows. The results are intended to provide a better understanding of the evolution of turbulent plumes and their unsteady turbulent structures. Comparisons of the results with the analytical model and experimental data by Linden and Kaye (2006) will also be used to evaluate the performance of LES in modelling buoyancy-driven natural ventilation.

6.2. The flow problem considered and associated theory

The flow problem considered for benchmark 1 is the same as in the preliminary test case. However in contrast to the preliminary test case, benchmark 1 used LES to model the buoyancy-driven natural ventilation within the enclosure.

The height of the steady interface formed between the upper warm layer and the lower ambient layer in a domain is an important parameter characterising this flow and will be used to validate the LES predictions. Linden and Kaye (2006) suggest that for two non-interacting unequal plumes a three layer stratification is possible. The stronger plume reaches the ceiling, spreads out and forms the first temperature
interface. The weaker plume reaches the upper layer stratification and spreads out, forming an intermediate layer (Figure 6.1). The effect of plume-plume interaction on this three layer stratification is dependent on the height at which the two plumes merge.

![Figure 6.1: Three layer stratification for non-interacting plumes](image)

If the two plumes merge below the predicted lower interface then a corrected interface height ($\xi'$) was evaluated by Linden and Kaye (2006) via:

$$\xi' = \xi + \varepsilon'$$  \hspace{1cm} 6-1

where $\xi$ is the uncorrected non-dimensional interface height (=h/H) and $\varepsilon'$ is a small perturbation to this interface height given by:

$$\varepsilon' \approx -\xi_v \left[ \frac{5\xi^4}{\left( \frac{A^*}{H^2C^{3/2}} \right)^2 + 5\xi^4} \right]$$  \hspace{1cm} 6-2

where,

$$\xi_v = \frac{y_v}{H}$$  \hspace{1cm} 6-3
and $y_v$ is the virtual original of the plume. For two unequal heat source plumes with a buoyancy flux ratio $\psi=0.5$, $y_v$ was given by Kaye and Linden (2004):

$$y_v = \frac{0.11 \times x_o}{\alpha}$$

where, $x_o$ is the heat source separation and $\alpha$ is the entrainment coefficient.

Linden et al. (1990) derived a relationship between the non-dimensional interface height $\xi$ and the effective opening area, $A^*$:

$$\frac{A^*}{H^2} = C^{3/2} \left[ \frac{\xi^5}{1 - \xi} \right]^{1/2}$$

where, the constant $C$ is given by:

$$C = \frac{6\alpha}{10} \frac{9\alpha^{1/3}}{\pi^{2/3}}$$

and $\alpha$ is the entrainment coefficient appropriate for top hat profiles ($C = 0.15$).

$A^*$ is the effective opening area formulated by Hunt and Linden (2001) to characterise geometric openings of areas $a_t$ and $a_b$ at the top and bottom of the space:

$$A^* = \frac{C_D a_t a_b}{\left[ \frac{1}{2} \left( \frac{C_D}{C_e} a_t^2 + a_b^2 \right) \right]^{1/2}}$$

where, $C_D$ and $C_e$ are the coefficients of discharge and expansion respectively; a value of 0.5 was used for both by Hunt and Linden (2001).

### 6.3. Computational methodology

#### 6.3.1. The computational domain and mesh generation

The computational domain used was a cubic enclosure as in the previous chapter but with a floor area of 1m x 1m and height 1m (Figure 6.2). This slight change in the geometry was made in order to reduce the size of the computational domain and to bring a similarity of the geometry with the geometry used by Abdalla et al. (2007).
This would help in the comparison of the iso-surfaces, plume structures, thermal interface structure etc.

The geometry and mesh for the computational domain were generated using ICEM (ANSYS, 2011c). Two heat sources, $q_1$ and $q_2$ were located close to the centre of the floor each with a geometric area of 0.0009m$^2$ and separated by a distance of 0.1m (centre to centre). Long rectangular openings were specified along the top and bottom side edges of the enclosure each with a geometric area of 0.05m$^2$. These values give a value of $A^*/H^2 = 0.0448$ and hence $\xi = 0.57$ from equation 6-5.

![Figure 6.2: Computational Domain](image)

The mesh design for LES was based on the guidelines presented in Chapter 4. To fulfil that criterion the mesh created had a resolution of 3million nodes (hexa elements) with ~150 in all co-ordinate directions. The mesh density however varied with finer mesh resolution near the heat sources and openings and coarser meshes away from the expected plumes axis. The $L/\Delta$ plot for the final designed mesh is shown in Figure 6.3. This shows that the $L/\Delta >12$ criterion was satisfied everywhere except (as expected) very close to the walls of the enclosure. The mesh resolution
for the free shear layer area of the enclosure is thus appropriate. Areas near the wall are not of prime concern and hence coarser mesh resolution is tolerated.

![Image](image_url)

**Figure 6.3**: L/Δ plot for designed mesh for BM1 LES simulations; (left) front view and (right) top view

### 6.3.2. LES software package and boundary conditions

Large Eddy Simulation (LES) was carried out using CFX (ANSYS, 2012). The Smagorinsky SGS model (Lilly, 1967) was used to model the effects of the sub-grid scale eddies.

All walls were assigned a no-slip boundary condition and the automatic wall function approach as described previously was adopted. Heat source strengths of $q_1=20\text{W}$ and $q_2=10\text{W}$ were used to drive the flow. Flow through the openings used the boundary condition approach explained in Chapter 4.

Initial conditions were set such that all velocity components within the computational domain were set to zero and the temperature inside the enclosure was set equal to the ambient temperature. This would ensure that the plumes would evolve initially in a stagnant flow and that stratified flow would develop quickly.

### 6.3.3. LES numerical details

The selection of the LES time step size was based on the criteria explained in chapter 4. The simulation was run with an adaptive time step until the start-up
transient had disappeared (after $\approx 8000$ time-steps). The start-up period was judged to be over when the change in the flow variables with time had flattened. After this a constant time step was maintained during statistical data gathering at a value of 0.02s, which, for the mesh and flow conditions which were established corresponded to a $\text{CFL}_{\text{max}}$ value of 0.7. The convergence criterion which determined the completion of each time step was that the root mean square (RMS) normalised values of equation residuals for velocity, temperature and pressure were less than $1 \times 10^{-6}$.

6.4. CFD results

6.4.1. Determining Statistical Stationarity

Statistically stationary flow (a steady time-mean state) is reached when the flow in the computational domain has fully evolved from its 'start-up' conditions and the transition to turbulent mixing is fully established. As per Linden et al. (1990) it was expected that approximately two homogeneous stratified layers would form within the enclosure. Thus, several temperature monitor points were placed in a vertical line (but away from the two plumes) distributed from the floor to the ceiling at a uniform 0.2m interval to track the development of the vertical temperature distribution over time and identify formation of such a regime.

A statistically steady state was considered to be achieved when the following criteria had been met:

i. time-mean ventilation flow rate was stable

ii. time-mean velocity, temperature and pressure values for the multiple monitor points inside the domain were all stable

These criteria were achieved after $\sim 90$ s of simulation time. This is faster than predicted by Kaye & Hunt (2004) whose model predicted a steady state interface to be reached after 230s for the flow conditions studied here. However, as discussed below, significant overturning and mixing at the side walls was observed in the CFD simulations that increased the rate of deepening of the warm upper layer and hence reduced the time taken to reach a steady state. It is not believed that the estimate of Kaye and Hunt (2004) allowed the effect of this to be taken into account.

A buffer of a further 30s was allowed for before statistical data gathering of time averaged flow variables was begun; the statistics were taken over a time period of
30s (Figure 6.4). This time period was thought to be sufficient as the fluid had travelled \(~6\) times through the enclosure during this time and any unsteady phenomena should have become established at a stationary state.

![Figure 6.4: Snapshot of the transient values of flow through the enclosure at each opening to illustrate period of start-up, buffer and transient statistics](image)

6.4.2. Mean flow field and interface height

Once the flow had reached steady state, the performance of LES was tested by examining the behaviour of the predicted interface height ($\xi$) and comparing it with the analytical model of Kaye and Linden (2004). Following the formulation presented by Linden and Kaye (2006) for unequal plumes which merge below the interface height (which is the case for $\psi = 0.5$), the corrected non-dimensional interface height was observed to be $\xi' = 0.65$ in the experiments. It is worth noting that in the geometry of Figure 6.2, the enclosure is relatively narrow (half width to height ratio = 0.5). Therefore, the outflow from the plume after impingement on the ceiling will be turned down at the side walls and cause some mixing of the warm stratified fluid with
the cooler ambient fluid below. For this aspect ratio (0.5) the penetration depth of the downwards deflected fluid is expected to be about 0.43m (Kaye and Hunt 2007). This means that the vertical penetration of these downwards deflected wall jets will almost reach to the steady state interface height and therefore the turbulence induced by these flows will almost certainly cause interfacial mixing and a diffuse interface, which will introduce some uncertainty in the measured value for h.

The LES predicted time-mean temperature distribution (Figure 6.5) clearly displays the location of plume coalescence as well below the interface and the formation of a two layer strongly stratified flow as indicated by theory. The merged plume mixing is observed to be fairly rapid as the peak temperature in the centre of the merged plume almost disappears before ceiling impingement. The plume is not quite symmetrical with respect to the enclosure global flow; this may be because of small non-convergence of the time-mean values or perhaps some slight lateral "flapping" of the plume. The lateral wall jets caused by impingement transforming into downwards wall jets on the side walls are also clearly visible; the slight asymmetry shows the left hand downward flow to be stronger than the right hand, penetrating to perhaps ¼ of the enclosure height before being dissipated.

Figure 6.5: Mean temperature contours predicted by LES (x-y plane, z=0.5m) for ψ = 0.5
Figure 6.6: Mean temperature contours predicted by RANS (RNG k-ε) (x-y plane, z=0.5m) for $\psi = 0.5$.

Figure 6.7 shows a time-mean vertical temperature profile plotted (x=0.1, z=0.1) well away from the enclosure centre line.

As can be seen in Figure 6.7 the temperature remains the same below a height of 0.45m and above 0.8m with the interface located within this range. This is in stark contrast to the step change in temperature at the interface height assumed by the analytical model of Linden and Kaye (2006). The transition layer between the lower ambient temperature fluid and the upper warm fluid extends over approximately 0.3m in the LES predictions. This is considerably larger than the value predicted using the model of Kaye et al. (2010) of 0.07m but this was based on the molecular diffusivity of heat in air and, by ignoring any turbulent effects is bound to be a large underestimate. This discrepancy is certainly due also in part to the turbulent mixing driven by the overturning flow discussed above.

A RANS RNG k-ε (selected on the basis of the results obtained in Chapter 5) prediction using the same mesh as that used for LES is shown in Figure 6.6. It is clear that the RANS temperature solution varies greatly from the LES. The RANS
predicted plume merge point is much higher, the plume cross-section is more slender, and the merged plume mixing much weaker so that peak temperatures are observed to persist throughout the lateral ceiling wall jets after impingement right into the enclosure corners. The mixed fluid indicated by green/yellow colours is much stronger, and finally the interface is not horizontal but tilted upwards towards the side walls. The interface height for the RANS solution is determined in the same way and implies an interface height of 0.77m as also shown in Figure 6.7.

![Graph showing temperature profile](image)

**Figure 6.7:** Vertical temperature profile comparing theoretical and predicted temperature interface heights in the domain. The vertical profile is plotted on a vertical line located at $(x=0.1, z=0.1)$

The LES predicted interface height has been determined by identifying the minimum value of the gradient of the temperature distribution curve. The temperature distribution curve shown in blue (Figure 6.7) is obtained from LES CFD data. Slope of this curve is illustrated in Figure 6.8. The minimum value of the slope lies at $26^\circ C$ which corresponds to an LES predicted interface height of 0.57m in Figure 6.7.
Cook (1998) and Abdalla et al (2007) also predicted a similar diffused behaviour of the interface using RANS and LES respectively. Abdalla et al (2007) have also suggested that the nature of the stratification may be attributed to the turbulent diffusion of heat induced by the unsteady motion of the plume and mixing due to overturning of the plume outflow at the side walls (Kaye and Hunt, 2007), and this is certainly confirmed by the current calculations. The discrepancy between analytical and computation for the interface height is +18.5% for RANS and -12% for LES: This is the first indication from the current work that LES can provide increased accuracy compared to RANS for turbulent buoyant flows relevant to natural ventilation applications.

6.4.3. Instantaneous flow field

Instantaneous temperature plots on a plane passing through the heat sources provide a good indication of the flow dynamical behaviour during the flow start-up period (Figure 6.9 (a)-(d)). Figure 6.9(a) at t=0.5s after the simulation was first started suggests that both plumes are initially laminar between the source and a certain height above the floor (approximately 50% of the enclosure height).
Figure 6.9: Instantaneous temperature contours on an x-y plane for $\psi = 0.5$, $(z=0.5)$ and at times (a) $t_1=0.5$sec,(b) $t_2=2$sec, (c) $t_3=3$sec,(d) $t_4=10$sec

Figure 6.9(b) illustrates that after just 2s the plumes start to show evidence of instabilities leading to the foundation of eddy structures in the shear layer and plume-plume interaction has begun just as the flow has first reached the ceiling. Figure 6.9(c) and (d) show that both plumes have become very turbulent after just 3s elapsed time after flow initiation. Figure 6.9(c) shows significant interaction between the plumes with breakdown of individual plume identities, even more vigorous turbulence and a corresponding increase in the entrainment of cooler surrounding fluid. Figure 6.9(d) shows that after 10s of flow development the plumes have merged approximately 0.4m above the heat sources. The cooler surrounding air is
entrained strongly into the plume and driven upwards towards the ceiling where it spreads towards the side walls and at this time has begun to descend to form the upper mixed warm layer. This warm air subsequently forms the interface that separates the warm upper layer from the ambient lower layer.

Figure 6.10 depicts the instantaneous temperature field on an x-y plane at z=0.5m (left) and a y-z plane at x=0.5m (right) at the much later time of t=150s after the solution has achieved a statistically stationary state. The 3D nature of the initial region of the plume is visualised by comparing the temperature contours in the lower half of the enclosure between left and right planes in Figure 6.10.

![Figure 6.10: Instantaneous temperature contours over vertical planes. x-y plane, z=0.5 (left) y-z plane x=0.5, (right)](image)

It is noticeable that although there is a continuous breakdown of eddies from the plume shear layer throughout its travel from the floor to the ceiling, the breakdown is significantly accelerated during travel through the temperature interface and in the upper warm layer. This may be due to the interaction of plume eddies and smaller turbulent eddies present in the warm upper layer generated by plume impingement and the turbulence in the wall jets on the ceiling and the side walls. Note also that these images in Figure 6.10 show clear evidence of plume flapping in the upper layer both laterally towards the right (in Figure 6.10 left) and towards the front (in Figure 6.10 right)
Qualitatively the instantaneous temperature contours demonstrate that the plume remains highly turbulent throughout its motion from the heat source to the ceiling. This can be confirmed quantitatively by examining the variation in the instantaneous z-direction (w) velocity along the vertical y-axis (normalised by the maximum vertical velocity $V_m$) (Figure 6.11). The plot shows that for both plumes, significant front/back motions develop immediately in close proximity to the heat sources. The mean z-direction velocity is close to zero but large perturbations exist, both positive and negative, over the whole enclosure height. Comparing the plots for both plumes for the entire passage from heat source to ceiling, it is observed that plume 1 is more turbulent than plume 2.

6.4.4. Plume merge height

In order to determine the merge height ($y_m$) of the two plumes, LES predicted time-mean temperature or velocity profiles can be plotted. These profiles can then be used to determine the merge height (Kaye and Linden, 2004). When the velocity profiles of the two plumes can no longer be distinguished from each other it is reasonable to consider the plumes to have merged. Figure 6.12 illustrates the merging of the velocity profiles of two unequal strength plumes (for $\psi = 0.5$).

It can be observed that above a height of 0.45m the profiles coalesce, two distinct maxima can no longer be identified and hence the plumes are considered to have merged. This is slightly higher than the height of 0.35m predicted by Kaye & Linden (2004) for this value of $\psi$.

The discrepancy is possibly due to the finite extent of the enclosure inhibiting the drawing together of the plumes and a small but finite virtual origin offset at the base of each plume.
Figure 6.11: Instantaneous w velocity normalised by max value of velocity $V_m$ plotted along y-axis

Figure 6.12: Merging Gaussian profiles of the two plumes for $\psi = 0.5$
6.4.5. Ventilation flow rate

In order to test the performance of LES further, a series of flow rate estimates were made in the merged plume following the technique proposed by Baines (1983) and also used by Kaye and Linden (2004). The volume flux in a self-similar buoyant plume is given theoretically by (Kaye and Linden, 2004):

\[ Q = \left( \frac{5F}{4\alpha} \right)^{1/3} \left( \frac{6\alpha y}{5} \right)^{5/3} \]  

Assuming a value of \( \alpha = 0.09 \), Kaye and Linden (2004) indicated that the flow rates above and below the point of coalescence can be written as a fraction of non-dimensional distance as:

\[ \left( \frac{y}{x_o} \right)_{\text{below}} = 2.28 \left( 1 + \psi^{1/3} \right)^{-1/3} Q^{3/5} F_1^{-1/5} \]  
\[ \left( \frac{y}{x_o} \right)_{\text{above}} = 3.013 \left( 1 + \psi \right)^{-1/5} Q^{3/5} F_1^{-1/5} + y_v \]

where \( y_v = 0.11 \) (from equation 6-4) was suggested, based on the predictions of Kaye & Linden (2004). The theoretical predictions as described by equations 6-9 and 6-10 were offset in order to make sure that the volume flux \( Q \) had a zero value at \( y/x_o = 1.1 \) (with \( x_o = 0.1 \)). This is because the theoretical values consider a zero volume flux at the physical origin of heat sources (i.e. \( y/x_o = 0 \)) whilst in reality the volume flux extrapolate to zero at the virtual origin i.e. \( y/x_o = -1.1 \) (Figure 6.13).

LES values were calculated using parameters deduced from Gaussian fits to the predicted plumes using the same relationships as outlined in chapter 5. The results from LES could not be compared directly with the RANS predictions presented in Chapter 5 (Figure 5.10) since the geometries were different. Therefore, RANS (RNG k-\( \varepsilon \)) predictions were repeated for the geometry used in benchmark 1 and plotted next to the predictions of LES. The LES predictions in Figure 6.13 clearly provide a better fit to the theoretical predictions than RANS (RNG k-\( \varepsilon \)).
6.4.6. Vortex structures

Coherent structures - large-scale energetic organised turbulent eddies - within a flow, are a well-known feature of high Re turbulent flows. The understanding of the dynamics of such structures can help understanding of turbulence phenomena (in particular mixing) and also guide turbulence modelling methods (Hussain and Melander, 1991).

An instantaneous pressure isosurface is shown in Figure 6.14 and illustrates both vortex ring and spiral structures which form early in the plumes close to each heat source and grow as the plume width increases downstream. Structures similar to these were also present in the LES simulations of single plumes by Abdalla et al. (2007) and Zhou et al. (2001) although those applications were dominated by pure momentum sources. The plumes simulated herein are not forced but are passively generated by buoyancy sources. Further investigation is needed to understand the source of the spiral pressure structures. These large scale energetic structures contribute significantly to the increase of plume width via their dominance of the
The structures from both plumes grow separately with height until the plume edges collide and the structured nature of the coherent motions is lost. As the plume enters the interface its width stops increasing and the coherent structures break down into smaller scale structures, accelerating in the upper warm layer.

The plot of a temperature isosurface (Figure 6.15) confirms the presence of small scale eddy structures in the upper part of the plume and, in the upper warm layer. It is also worth noting that in an instantaneous snapshot the interface surface is not a pure horizontal plane but undulating over a height of approximately 0.2m these distinctions being caused by the eddy structures unsteady with the interface. This supports the findings in section 5.2 of the temperature across the interface being a diffuse layer rather than a step change. This smeared temperature interface is thus directly attributed to turbulent mixing (Kaye et al., 2010) driven in part (i.e. at the lateral edges of the interface) by overturning of the plume outflow at the enclosure edges (Kaye & Hunt 2007).

![Instantaneous pressure isosurface (P= -0.028Pa) at time =150s and coloured by velocity](image)

Figure 6.14: Instantaneous pressure isosurface (P= -0.028Pa) at time =150s and coloured by velocity
When the Reynolds number is large, a cascade of fluctuating energy from large to small scales precedes fluctuating kinetic energy dissipation into internal energy by fluid viscosity at the smallest scales of motion (the Kolmogorov scale ($\eta$)). Fourier analysis helps to identify the distribution of turbulent energies among different eddy wavelengths or frequencies, representing different scales of turbulence and their temporal characteristics (Mathieu and Scott, 2000). The velocity spectra can be readily interpreted physically in terms of the transfer of energy between different scales of turbulence and dissipation of turbulent energy by viscosity. The relationship between the frequency and the spatial scales is reciprocal i.e. low frequencies correspond to large spatial scales and vice versa.

Figure 6.16 shows an LES predicted frequency spectrum for the vertical velocity at a point in the centre of the domain and between the two plumes as they merge (location ($0.5, 0.3, 0.0$)). A generic feature of all high Re turbulent jet flows is the $-5/3$ law (List, 1982; Kostovinos, 1991). This slope can be observed in Figure 6.16 which confirms that the present flow exhibits fully turbulent characteristics. A faster roll-off of energy is expected to occur at higher frequencies due to numerical effects. As
long as this happens only when the energy level has dropped significantly compared to the level of energy containing frequencies, this is considered to be an adequately resolved LES.

The fact that there exists a local peak in the low frequency, energy containing part of the spectrum (labelled A at a frequency of ~0.08Hz), suggests a low frequency oscillation is present in the flow, probably a slow meandering of the plumes laterally back and forth as noted earlier.

![Power spectral density of the vertical velocity at x, y, z = 0.5, 0.3, 0.0](image)

Figure 6.16: Power spectral density of the vertical velocity at x, y, z = 0.5, 0.3, 0.0

6.5. Summary

LES CFD has been used to investigate the interaction of two turbulent buoyant plumes in a buoyancy-driven naturally ventilated enclosure. Theory suggested a normalised interface height of 65% whereas LES predicted 57%. This 12% under prediction is thought to be due to the omission in the theory of a diffuse flow at the interface caused by mixing. For the same test case, RANS CFD (RNG k-ε) predicted a normalised interface height of 77% resulting in a larger discrepancy of 18.5%.

Vertical velocity profiles plotted across the two plumes suggested that the plumes were predicted to merge at a height of 0.45m above the heat sources. Theory
suggested a merge height of 0.35m. This discrepancy was thought to be due to the small but finite virtual origin offset of 0.11m neglected in the theory as the heat sources in the CFD model has a finite area.

The LES predictions of volume flux in the merged plume overpredicted slightly the trend in increase in plume flow rate with height along the plume trajectory. However, when the offset due to the virtual origin was applied to the theoretical relation, the agreement improved considerably.

Instantaneous temperature plots and pressure and temperature isosurfaces revealed vortical and spiralling coherent structures present in both plumes near the heat sources. These structures grew laterally, increasing the plume widths until they interacted with one another, causing a rapid breakdown of the eddy structures and merging of the two plumes. The interface surface is unsteady and non-planar and acts as a resistance to the turbulent structures moving within the warm upper layer. The non-planar nature is thus caused by the interactions of vortices of different scales in the upper warm layer.

Spectral analysis of the vertical velocity in the region between the two plumes suggested the existence of a low-frequency motion, possibly a slow (≈ 0.1Hz) meandering motion of the plumes laterally back and forth. The spectrum of the velocity field at high frequencies obeyed the -5/3 power law which is a characteristic of fully developed turbulent flows which gave confidence that the turbulence was accurately resolved by LES.

In conclusion application of an LES CFD approach was found to be successful in elucidating the fluid dynamics of two interacting buoyant plumes in a naturally ventilated enclosure. LES was also able to predict mean values of the flow which agreed favourably with the theory of Kaye and Linden (2004) and represented approximately a halving of error in some important flow parameters relative to RANS (RNG k-ε) CFD. The characteristic frequency spectrum of this type of flow was also reproduced.
### Table 6-1: Summary table of comparisons with comments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>LES</th>
<th>RANS</th>
<th>Analytical</th>
<th>Experimental</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature Interface thickness</td>
<td>0.3m</td>
<td>0.15m</td>
<td>Step change</td>
<td>-</td>
<td>Both LES and RANS predicted a diffused interface due to turbulent diffusion of heat induced by unsteady motion of plume and mixing due to overturning phenomena at side walls</td>
</tr>
<tr>
<td>Interface height</td>
<td>0.57m</td>
<td>0.77m</td>
<td>0.65m</td>
<td>-</td>
<td>LES exhibits 12% whilst RANS exhibits 18.5% discrepancy compared to theory. This discrepancy is thought to be due to omission of a diffuse flow at the interface caused by mixing.</td>
</tr>
<tr>
<td>Plume merge height</td>
<td>0.45</td>
<td>-</td>
<td>-</td>
<td>0.35</td>
<td>Discrepancy possibly due to virtual origin problem</td>
</tr>
<tr>
<td>Fast Fourier Analysis</td>
<td>Follows the -5/3 law</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>High Re turbulent jet flows exhibit -5/3 slope on the energy cascade. This generic feature was observed for the LES predictions</td>
</tr>
</tbody>
</table>
Chapter 7. Benchmark 2: Buoyant flow in an enclosure with ceiling vent stacks and lower openings – multiple solutions

“Take advantage of the ambiguity in the world. Look at something and think what else it might be” – Roger von Oech

7.1. Introduction
This chapter reports on a study that investigated the use of both RANS and LES CFD in predicting the multiple steady states that have been observed in experiments of a particular buoyancy-driven natural ventilation scenario. Multiple steady states in a naturally ventilated space have been reported in the experimental work of Chenvidyakarn and Woods (2005). The results obtained from their paper are therefore used here to assess the performance of the computational results of this study.

7.2. Background
Chenvidyakarn and Woods (2005) investigated natural ventilation in a laboratory experiment scaled to represent an open-plan office using water model experiments (Figure 7.1). The space was ventilated through two ceiling stacks open to the ambient (of different heights) and lower openings to the external ambient located near the base of the enclosure mimicking a doorway (see Figure 7.1). A uniform distribution of heat was assumed on the floor to represent occupancy and to produce this an electrically heated unit was distributed over the enclosure floor. It was reported that for the various conditions of geometry of stack heights and openings
and heating rates up to three different steady state ventilation regimes were observed.

In the first regime, warm air exits through the taller stack while ambient air is drawn in through the shorter stack and through the lower openings (Figure 7.2a). In the second regime, warm air exits through both stacks whilst drawing air in through the lower openings (Figure 7.2b). Finally in the third regime, ambient air is drawn in through the taller stack and lower openings whilst the warm air exits through the shorter stack (Figure 7.2c). The factors affecting which final steady state is attained are the geometry of the enclosure and the flow history (i.e. prevailing flow conditions in the enclosure before a change is made in the geometry of the enclosure).

To the best of the author’s knowledge, no attempt has yet been made to examine whether any CFD approach (either RANS or LES) is capable of capturing completely which steady state is achieved under which flow circumstances.
In their paper Chenvidyakarn and Woods present a formulation for the temperature inside the room at steady state, $T_{in,ss}$ ($^\circ$C) as follows:

$$T_{in,ss} = T_E + \left( \frac{H_h}{\rho C_p A^* \sqrt{g/\alpha H}} \right)^{2/3}$$  \hspace{1cm} 7-1

where, $T_E$ (°C) is the exterior temperature, $H_h (W)$ is the heat gain from occupants and equipment, $C_p$ (J/kg K) is the heat capacity of air, $\rho$ (kg/m$^3$) is the density of air and $A^*$ is the effective area of the openings. $A^*$ was again formulated as in Hunt and Linden (2001) to represent openings of area $a_t$ and $a_b$ at the top and bottom of the space respectively:
\[ A' = \frac{C_D a_t a_b}{\left[ \frac{1}{2} \left( \frac{C_p^2}{C_e} \right) a_t^2 + a_b^2 \right]^{1/2}} \]  

Also, Chenvidyakarn and Woods (2005) define a dimensionless room temperature, \( \theta \):

\[ \theta = \left( \frac{T_{in} - T_E}{T_{in,ss} - T_E} \right) \]  

and dimensionless time, \( \tau \):

\[ \tau = \frac{t}{t_s} \]

where \( t_s \) (s) is a dimensional timescale to converge to equilibrium given by

\[ t_s = \frac{V}{A' (g \alpha^* H)^{1/2} (T_{in,ss} - T_E)^{1/2}} \]

where, \( V \) is the volume of the room (m\(^3\)), \( g \) is the gravitational constant (m/s\(^2\)) and \( \alpha^* \) is the volume expansion constant (1/K).

They presented a relationship between the dimensionless room temperature and the dimensionless time to converge to equilibrium as shown in Figure 2. It is observed from this figure that for \( \tau > 3.5 \), \( \theta > 0.99 \) and so the room has essentially reached steady state.
7.3. Numerical details

7.3.1. Computational geometry and mesh

The geometry generated for the CFD analysis was identical to the small scale model reported by Chenvidyakarn and Woods (2005) (Figure 7.4).

In the case of RANS predictions, it was decided to investigate whether using a URANS approach would capture any slow plume oscillations or unsteadiness of such flow. For URANS predictions mesh independency was achieved with a mesh resolution of 1.6million. The mesh was particularly fine in the stack regions. The RNG k-ε turbulence model (Chapter 2) was again used for the URANS simulations.
For LES the best practice guidelines described in Chapter 4 was again used to design an acceptable mesh. This resulted in a mesh resolution of 27 million nodes. The L/Δ plot is shown in Figure 7.5. As expected the L/Δ ratio is above 12 in most regions of the computational domain (i.e. the main enclosure and the stacks) except for the regions near the walls.
7.3.2. Boundary conditions

Water at 23°C was used as the working fluid in the simulation (as water at room temperature was used in the original experiment). The floor was set a boundary condition corresponding to a uniformly distributed heat source with a total heat input of 90W which was in accordance with the experimental study. The stack openings as well as the bottom opening were assigned the ‘opening’ boundary condition described earlier. Amongst other lower openings, a single opening was set as an opening whilst the others were assigned an adiabatic wall boundary condition. The selection of the opening area for the lower opening was based on the data provided in the paper for a specific flow regime.
Initially the flow solution was assigned an ambient temperature of 23°C with all three components of velocity equal to zero. The walls were assumed to be adiabatic and assigned the ‘no-slip’ (wall function) boundary condition.

7.3.3. The URANS and LES approach
For the case of URANS, maximum Courant number ($CFL_{\text{max}}$) was maintained in the slightly larger range of 1.0 to 5.0. This was deemed acceptable since URANS does not have to resolve temporal frequencies associated with the smallest resolved eddies such as LES; the likely resolved frequencies will be probably two orders of magnitude larger (if any unsteadiness is predicted). Initially the time step of 0.02s was used for LES during the start-up period. A physical time step of 0.06s was chosen on the basis that the $CFL_{\text{max}}$ for LES should be between 0.5 and 1.0. Figure 7.6 shows the temperature transient over time steps for a few points in the flow indicating the typical trend.

![Snapshot of the evolution of dynamical values of instantaneous temperature within the domain using LES](image)

7.4. Methodology
The main purpose of the current study was to study the capability of CFD to predict the multiple steady states observed originally by Chenvidyakarn and Woods (2005). However for the presence of a certain regime the boundary conditions used were
critical. A diameter of 7mm was used for the lower opening as it was observed in the experimental study that all three steady states were possible in this case.

7.4.1. Regime B
Chenvidyakarn and Woods describe that the flow naturally evolves into regime B (Figure 7.2b). They reported that “depending on the history of the flow, the heights of the room and stacks, the area of the bottom hole and the cross-sectional areas of the stacks, the system is capable of producing up to three steady state displacement ventilation regimes”. It was decided to keep all these factors constant except for the history of the flow. In real buildings, history of the flow often changes due to changes in occupancy.

7.4.2. Regime A and C
For regime A and C, ambient air was introduced into the building via the short and tall stacks respectively (representing cold draughts that can occur in reality). This was done by temporarily changing the boundary condition at the opening from ‘opening’ to ‘inlet’ with a normal velocity component of 0.015m/s for regime A and 0.02m/s for regime C. These values were based on the outflow velocities from the same openings during regime B. Using these flow conditions as the starting point/history of the flow and keeping all other boundary conditions the same, the simulations were started. After a time period of 30s the ‘inlet’ boundary condition was changed back to an ‘opening’ boundary, thus allowing the flow to decide for itself at what condition it would stabilise. It was observed that flow in each case continued to entrain ambient air from either stack and would continue to do so until reaching a statistically steady state. This triggered the development of both regimes A and C.

7.5. Results

7.6. Steady state solution
Steady state was considered to be reached when the flow in the computational domain had evolved from the initial stagnant conditions to a steady flow pattern and that the transport of mass, momentum and energy within the flow had reached statistically steady rates. In order to determine if a steady state had been reached within the domain, monitor points were placed in the centre of the domain (Figure 7.4). The lowest monitor was 5cm from the floor with 5 more monitors above
it at intervals of 2cm. These monitor points would update information on the temperature and velocity conditions in the domain. These monitor points will also be used to extract the average room temperatures. Four other monitor points, placed at either end of both the stacks were used to provide information about the flow direction in the domain. Steady state was considered to be achieved when the following criteria had been met:

- ventilation flow rate was unchanging;
- velocity, temperature and pressure values at all monitor points were stable

Figure 7.7 shows the evolution of the average room temperature over time for both URANS and LES against theoretical predictions. It can be seen from the figure that both URANS and LES predict the room temperature accurately although once again LES shows improved level of prediction (0.15% error for LES, 1.42% error for URANS). Both show the room to reach steady state in about 1.6 hours.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig7_7.png}
\caption{Comparison of the time to adjust to steady state as predicted by URANS, LES and the theory}
\end{figure}

It is worth investigating how the relationship between the dimensionless room temperature $\theta$, and the dimensionless time to converge to equilibrium, $\tau$, holds for
both URANS and LES. According to the work of Chenvidyakarn and Woods (2005) when \( \tau > 3.5 \) then \( \theta \sim 1 \). It can be seen from Figure 7.8 that LES performs more accurately in this regard than URANS which over-predicts \( \theta \) and has not reached steady state at \( \tau \sim 3.5 \). (Note that in Figure 7.7 the room temperature at steady state is being compared while in Figure 7.8 it is the time to reach steady state that is being compared based on the dimensionless time \( \tau \) used by Chenvidyakarn and Woods (2005)).

![Figure 7.8: Relationship between the dimensionless room temperature, \( \theta \), and the dimensionless time to converge to equilibrium, \( \tau \)](image)

### 7.7. Multiple steady states

Snapshots for both URANS and LES simulations can be seen in Figure 7.9 and Figure 7.10 respectively. These illustrate temperature plots over a plane passing midway through the domain. Cold ambient air can be seen to be drawn into the domain down through the stacks to produce regimes A and C.

LES, on the other hand, is able to elucidate this behaviour e.g. in regime A the plume takes on a more meandering behaviour whereupon reaching the floor it breaks down whilst in regime C the plumes are more turbulent and break down before they reach
the mid height of the domain. Additionally it can be seen that for regime B, LES predicts the presence of cold draughts at the right-hand end of the floor. URANS however, fails to capture such behaviour. This is expected due to the averaging techniques inherent in the URANS method. The URANS solutions were observed to not maintain any unsteadiness in its steady state predictions. This means that plotting Figure 7.9 at a later time looked the same. This however was not the case with LES which maintained unsteadiness in its statistically steady state.

Additionally, the room should be well mixed and thermally uniform. The URANS temperature plots however suggest a temperature interface (vertical temperature gradient) albeit small in all three regimes (Figure 7.9) at a height of approximately 14cm from the floor. LES results, however, suggest that this difference in temperature is due to large recirculating eddies caused by warm convection currents adjacent to the left wall.

Using instantaneous temperature profiles through the stacks, the process of some regimes switching from one to another can be witnessed. For example, Figure 7.11 shows the taller stack of the enclosure during the switch from regime C to regime B. Initially ambient air currents flow down through the taller stack making their way into the room (Figure 7.11a). During the switch warm air from the enclosure begins to make its way up the centre of the taller stack (Figure 7.11b). As this warm air builds up in the stack being supplemented by more warm air from the enclosure cold ambient currents are restricted to the side walls of the stack (Figure 7.11c). Gradually the warm air expands radially taking up the entire stack and restricting any further ingress of ambient air. As the buoyancy forces increase in the stack warm air exits out through the stack (Figure 7.11d).
Figure 7.9: Temperature plot at $t = 320s$ on a plane midway through the domain using URANS illustrating (a) Regime A, (b) Regime B and (c) Regime C (dotted black lines representing an interface)

Figure 7.10: Temperature plot at $t = 320s$ on a plane midway through the domain using LES illustrating (a) Regime A, (b) Regime B and (c) Regime C
Figure 7.11: Instantaneous temperature plots of the taller stack of the building during the switch from regime C to regime: (a) $t = t_{ss,C}$, (b) $t = t_{ss,B} + 190.05s$, (c) $t = t_{ss,B} + 198.05s$ and (d) $t = t_{ss,B}$

### 7.8. Comparison with analytical model

Figure 7.12 and Figure 7.13 show the variation of the inside room temperature, $T_{in}$, for the three regimes with changes in the bottom opening ratio, $A^*/A^*$, for the analytical and both CFD models. The figures plot dimensional temperature, $T^{*}_{in,ss}$.

\[
T^{*}_{in,ss} = \frac{(T_{in,ss} - T_E)}{(T_H - T_E)}
\]

where $T_H$ is the temperature of the heat source. Again, the original paper did not specify the level of uncertainty in experimental data.
Good agreement is observed between theory and CFD for regime B at larger doorway areas using URANS. However, as the doorway area reduces i.e. $A_{3}^{*}/A_{1}^{*} < 1.0$ the dimensional room temperature is under-predicted for regime B and over-predicted for regimes A and C. On the other hand LES appears to be more accurate throughout the opening area change explored, showing very close agreement with experimental data fit.

![Figure 7.12: Comparison between theory (dotted lines) and URANS predictions (marker points) of dimensionless room temperature, $T_{inss}^{*}$, with changes in area of bottom opening, $A_{3}^{*}/A_{1}^{*}$ (dotted lines show theory)](image-url)
7.9. Summary

Multiple steady states in buoyancy-driven natural ventilation have been investigated using LES and URANS. The theoretical model shows that the average room temperature of the enclosure should be 31.60°C. LES predicted an average temperature of 31.65°C (0.15% discrepancy) and URANS predicted 32.05°C (1.42% discrepancy).

The relationship between the dimensionless room temperature $\theta$, and the dimensionless time to converge to equilibrium, $\tau$, was also predicted. According to theory, when $\tau > 3.5$ then $\theta \sim 1$. This was predicted well by both modelling techniques although LES proved to be more accurate than URANS.
Using the 7mm bottom opening, three steady state regimes were predicted by both LES and URANS in line with theoretical expectations. The URANS method however was unable to either capture the detail of the flow structures or maintain the unsteadiness in steady state which was predicted by LES. This is expected due to the averaging techniques inherent in the URANS method. URANS also predicted a weak vertical temperature gradient in the domain which was not observed in the experimental work which suggests a well-mixed enclosure. This phenomenon was correctly predicted by LES which predicted the flow to comprise recirculating convection currents in the region where URANS had predicted a vertical temperature gradient. This has practical implications of URANS falsely suggesting presence of a temperature interface which might finally result in designers altering the opening areas.

The differences between LES and URANS performance in predicting the different regimes for all values of the bottom opening area ratio and the respective room temperatures were investigated. It was observed that URANS did not perform well in predicting the room temperatures for opening size ratios with diameters less than 6mm. URANS over-predicted the temperatures, especially for regime A. LES on the other hand performed well for all area ratios. By its nature, LES requires far more computing power than URANS. In this work, the LES cases required approximately five times more time than URANS (using the same hardware platform).

In conclusion it can be stated that LES was more successful than URANS in revealing the multiple steady states and predicting values of flow reported by Chenvidyakarn and Woods (2005).
<table>
<thead>
<tr>
<th>Parameter</th>
<th>LES</th>
<th>URANS</th>
<th>Analytical</th>
<th>Experimental</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steady state room temperature</td>
<td>31.65°C</td>
<td>32.05°C</td>
<td>31.6°C</td>
<td>-</td>
<td>Both URANS and LES predict average room temperature accurately however LES shows improved level of prediction</td>
</tr>
<tr>
<td>Time to reach steady state</td>
<td>at τ&gt;3.5, θ=1</td>
<td>at τ&gt;3.5, θ=1</td>
<td>at τ&gt;3.5, θ=1</td>
<td>-</td>
<td>In predicting the time to reach steady state temperatures, LES followed theory more accurately than URANS</td>
</tr>
<tr>
<td>3 steady states</td>
<td>predicted</td>
<td>predicted</td>
<td>-</td>
<td>Reported</td>
<td>Both URANS and LES predicted the three steady states reported in experiments</td>
</tr>
<tr>
<td>Unsteadiness in the flow</td>
<td>Captured</td>
<td>Did not capture</td>
<td>-</td>
<td>Reported</td>
<td>The URANS solution eventually converged into a RANS solution whilst LES continued to predict unsteadiness in the statistically steady state</td>
</tr>
<tr>
<td>Dimensionless room temperatures</td>
<td>Accurate for lower opening area less than 6mm</td>
<td>Inaccurate for lower opening area less than 6mm</td>
<td>-</td>
<td>-</td>
<td>URANS over predicted temperatures, especially for Regime A</td>
</tr>
</tbody>
</table>
Chapter 8. Benchmark 3: URANS and LES practicality assessed on an auditorium test case

“Today’s practicality is often no more than the accepted form of yesterday’s theory” – Kenneth L. Pike

8.1. Introduction

The previous chapters have reported on the performance of LES in comparison with popular CFD techniques such as RANS and URANS. It was observed that LES performs better in predicting measured values and provides many more details about the fluid flow. However, these CFD tools have been investigated in this research in order to help practitioners use them for ventilation system creation during the design stage of a building. Important factors of natural ventilation that have been ignored in the previous test cases are design considerations and the occupant thermal comfort which is important to the practitioner. No matter how much data a CFD technique may provide, if it does not contribute significantly to this type of information then its preference over conventional CFD techniques already in use in the industry is questionable. This chapter hence investigates the advantage of using LES over URANS in terms of the information it provides to the practitioner and at what cost. Another aim of the current chapter is to use a benchmark problem which is not simplified to a small box (for the purpose of research) but to investigate a full-scale, real building geometry. For this purpose an auditorium is investigated with a large open space where buoyancy effects are prominent.
8.2. Background

The Lichfield Garrick is a remodelled civic hall located at Lichfield, UK. The building has two main performance spaces: the studio space and the main auditorium (Figure 8.1). For the purpose of this research the studio space is neglected as it is mechanically ventilated. The main auditorium has two sets of raked seating (one at ground level and another on a balcony) and high heat gains. Fresh air is provided from hidden plena through openings below the raked seating. Fresh air is also supplied on both sides of the stage into the auditorium via a plenum underneath the stage. Stale air exits the auditorium space via eight stacks; six above the auditorium space and two above the stage area. This kind of scenario is ideal for investigating buoyancy-driven natural ventilation flows. Technical data that will be used in this research has been obtained from Short and Cook (2005).

![Figure 8.1: The Lichfield Garrick auditorium with the studio space and stairwells blurred out.](image)

8.3. Numerical procedure

8.3.1. Computational mesh and domain

In this benchmark test case the building was built to scale in the CFD meshing software. The purpose was to make sure practitioners could import already built Computer Aided Design (CAD) models into CFD software without scaling them down for subsequent LES analysis. As mentioned earlier the studio space and the stairwell
were ignored as they did not influence the natural ventilation flow in the main auditorium directly.

The main auditorium space hosted 17 rows of raked seating (5 on the balcony and 12 on the ground floor). Every row of seating was separated by an ambient air inlet. The orchestra pit and the two openings under the stage area were placed right at the foot of the stage as in the original design. Four rows of high power spot lights (two on top of the seating area and two over the stage area) were introduced to serve as artificial lighting in the auditorium. Six stacks over the seating area and two over the stage area were also included as in the original design. The proscenium arch was also kept in the CFD model as it was likely to play a critical part in the prevailing ventilation flow patterns in the space. The 3D model of the auditorium built in ICEM CFX is shown in Figure 8.2. The dimensions of each of these features are given in Table 8-1.

![Figure 8.2: Auditorium model built in ICEM CFX](image-url)
Table 8-1: Dimensions of important features of the auditorium model for benchmark 3

<table>
<thead>
<tr>
<th>Section</th>
<th>Dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Seating row area</td>
<td>17 rows @ 1m x 15m</td>
</tr>
<tr>
<td>Opening area between seating</td>
<td>15 rows @ 0.25m x 15m</td>
</tr>
<tr>
<td>Stack opening area (over seating)</td>
<td>6 @ 1.5m x 3m</td>
</tr>
<tr>
<td>Stack opening area (over stage)</td>
<td>2 @ 1.5m x 2m</td>
</tr>
<tr>
<td>Stage area</td>
<td>10m x 15m</td>
</tr>
<tr>
<td>Stage opening area</td>
<td>2 @ 1m x 4.5m</td>
</tr>
<tr>
<td>Proscenium arch</td>
<td>5m x 15m</td>
</tr>
<tr>
<td>Lighting row</td>
<td>4 rows @ 0.5m x 15m</td>
</tr>
</tbody>
</table>

For URANS predictions a mesh independency check was carried out to select an optimum mesh. This optimum mesh was selected on the basis of volumetric flow through the enclosure and had a resolution of 3million nodes. The turbulence model selected for the URANS technique was again the RNG k-ε turbulence model.

Building on the experience acquired in the previous benchmarks, the L/Δ ratio again served as the basis for mesh design (Figure 8.3). The final mesh density chosen was 50million nodes. Due to limitations of computational power and CFD software licences available the mesh resolution could not be increased further. Thus, maintaining the mesh size at 50million, the mesh distribution was varied to increase resolution close to the stack, stage, lighting and occupancy areas since the gradients in both temperature and velocity were expected to be higher in these areas. It can be seen from Figure 8.3 that in the middle of the auditorium the L/Δ ratio dropped below 12 and so the mesh does not exactly fit the best practice guideline. In ideal circumstances further mesh refinement should be carried out, but this was not possible given the available time and resources. It was decided to proceed with the mesh shown since most of the regions where turbulence would be created were adequately resolved, but the above limitation has to be noted.
8.3.2. Boundary conditions

Boundary condition data for the flow condition under study have been acquired from a confidential consultancy report by Cook and Lomas (2002). An ambient temperature of 24°C was assumed for this benchmark. This was done to represent an early evening performance time period during hot summer days in Litchfield. No external wind was imposed on the model in order to assess the buoyancy-driven ventilation strategy without the presence of wind.

A discharge coefficient of 0.6 was assumed for all openings in the auditorium. The heating load in the auditorium is presented in Table 8-2. The radiative component of a section’s heat gain was imposed on its neighbouring walls from where it was convected into the adjacent air.

Table 8-2: Heat loads used in CFD simulations

<table>
<thead>
<tr>
<th>Area</th>
<th>Heat output (kW)</th>
<th>Convective: Radiative %ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Auditorium</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Occupants (500)</td>
<td>50</td>
<td>50:50</td>
</tr>
<tr>
<td>Lighting</td>
<td>20</td>
<td>90:10</td>
</tr>
<tr>
<td>Stage</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Occupants (100)</td>
<td>10</td>
<td>50:50</td>
</tr>
<tr>
<td>Lighting</td>
<td>30</td>
<td>90:10</td>
</tr>
</tbody>
</table>
8.3.3. URANS and LES numerical details

For the URANS predictions, instead of an adaptive time step, a physical time step of 0.1s was used at the beginning of the simulation run (up to ~100 time steps). As the iterative processes ‘marched in time’ the physical time step was tuned to make sure the CFL number was in the 1.0 to 10 range (timestep ~ 1s). Monitor plots were placed in the domain to observe the dynamic change in values of temperature and velocity as the simulation progressed (Figure 8.4). A snapshot of the instantaneous temperatures for points 1 and 2 using URANS is presented in Figure 8.5. It is observed that for about the first 50 time steps no rise in temperature occurs for points 1 and 2. However after this time period the temperatures gradually rise until ~150 time steps. From here on the temperatures seems to reach a statistically stationary state. Even though the temperature might seem to dampen out for point 1 after t=250s, it was observed at later times that the amplitude of fluctuations does not dampen.

Figure 8.4: Monitor points. Location of point 1 (x,y,z = 5,12,7.5) and 2 (x,y,z = 23,11,7.5) shown in red whilst others in green
For LES simulations a time step of 0.01s was used in the start-up period where variations in variable values are expected to be high and thus in order to avoid the simulation from crashing. Once the start-up period was over (~30s) the timestep was increased to a value of 0.05s with CFL$_{\text{max}}$ value of ~0.6. Monitoring values of temperatures and velocities throughout the domain indicated when the flow reached statistically steady state. The vertical momentum component was also monitored to assess if a statistically steady state had been reached. It was observed that at 200s the flow had attained a statistically steady state though a buffer was allowed for a further 40s i.e until 240s. From 240s to 320s statistical data collection was carried out for FFT analysis (to be discussed in a later section). In Figure 8.6 the instantaneous temperatures using LES for point 1 and 2 are presented in order to illustrate the different periods of the simulation. It can however be observed that occasional high amplitude fluctuations occurs and thus the sample time may not be enough. Note also that significantly more high frequency information is present in the LES time series captured to URANS, as expected.
8.4. CFD results

8.4.1. Instantaneous temperature field

For the purpose of comparing the temperature contours obtained from the URANS and LES predictions an x-y plane is passed through the domain at z=4.5m. Temperature contours on this plane are shown in Figure 8.7 (a)-(e). Figure 8.7(a) shows the temperatures at t=15s after start-up conditions. The URANS method predicted kidney-like structures rising from the light sources and semi-laminar plumes rising from the occupant seating area. LES on the other hand for the same instant predicted the plumes rising from both the occupant seating and lighting area to be highly turbulent. Both URANS and LES however show no visible signs of plume rise from the stage area.

Figure 8.7(b) shows snapshots at t=35s for URANS and LES. Even though the overall temperature distribution throughout the auditorium seems to be similar for both the approaches, much more fine scale detail in the LES is clearly observed. Additionally LES predicts small structures in the middle of the domain that URANS fails to predict. A visible steady rise of heat from the stage area is predicted by both approaches at this time interval.
At \( t=55\)s (Figure 8.7(c)) differences in the overall temperature distribution between the URANS and LES in predictions begin to emerge. This is particularly observed in the steady heat rise from the stage area. URANS predicts steady plumes rising above the stage area whilst in the LES predictions, plume rise is observed only in the very rear of the stage area. Further along the simulation at \( t=100\)s shown in Figure 8.7(d) URANS continues to predict rising plumes from the stage area however these rising plumes are still not visible in the LES predictions. The question occurs whether LES is actually unable to predict a phenomenon whilst URANS can or whether LES predicts it in a different location, or moving from one location to another? This is worth investigating and will be dealt with in one of the following sections.

Lastly in Figure 8.7(e) at \( t=200\)s the temperature distribution for both URANS and LES is similar in the near stack regions and the interface structure that is developed at the lighting level. However LES predicts cooler temperatures near the stage area and in the middle open space area of the auditorium as compared to URANS. Additionally in the LES predictions one can establish local flow patterns within the enclosure. For example the lighting above the seating area continues to entrain ambient air from openings under the seating area which causes two local ambient air currents in the enclosure.
Figure 8.7: Instantaneous temperature plots using URANS and LES predictions at time $t =$ (a) 15s (b) 35s (c) 55s (d) 100s and (e) 200s.
8.4.2. Statistically steady state

The temperature contours at the end of the run i.e. t=320s are shown in Figure 8.8 for URANS and LES. It is observed that overall temperature distribution using both the approaches is dissimilar with the temperature values predicted by URANS being slightly higher compared to LES. It is also revealed that the interface height over the stage area is lower than the lighting level using URANS and higher using LES. Also it is noticed that the URANS approach predicts a much more uniform temperature in the auditorium. LES on the other hand divides the auditorium into two regions i.e. a cooler stage area and a comparatively hotter seating area with about 1°C difference. This is thought to be due to formation of a local flow pattern over the stage which LES predicted. This will be investigated later using streamline plots.

Both URANS and LES predict the orchestra pit in front of the stage being the coolest region of the auditorium with LES predicting the stage area to be of similar temperatures. URANS also predicts a current of hot air rising in front of the top seating area which LES predicts to break into smaller structures. CIBSE (2006) recommends a comfortable temperature range of 24-25°C for auditoria. Both URANS and LES predict all the occupancy to be within this temperature range.

Figure 8.9 illustrates the velocity contours on the same x-y plane at z=4.5m for both URANS and LES. Again local velocity patterns differ between both approaches. In the LES plot, high velocity (~0.45m/s) currents are observed both on the stage and above the stage area. These are completely missing in the URANS predictions. Fanger et al. (1988) from experiments advised that at a velocity of 0.45m/s up to 60% of occupants sense draughts and will feel dissatisfied. It is hence seen that 60% of the people on stage and in the last 5 seating rows from the rear (ground floor) will feel dissatisfied according to LES. This can be a major finding in the design stages as something can be done to inhibit these draughts and maintain satisfaction of the occupants. URANS was deficient in predicting such a phenomenon and its associated design considerations.

Figure 8.10 illustrates time averaged temperature plot over the statistically steady state period. It can be observed that LES predicts a more planar temperature interface which is expected however URANS predicts a very non planar interface.
The presence of a cooler back stage and vortex over the stage is still captured in the time mean temperature plots of LES unlike in URANS predictions.

Figure 8.8: Instantaneous temperature contours at statistically steady state for URANS and LES at t=320s
Figure 8.9: Velocity plots for BM3 test case using URANS and LES at t=320s
Figure 8.10: Time averaged temperature plots over the statistically steady state for BM3 test case using URANS and LES
8.4.3. Velocity streamlines

Streamlines are curves that are plotted by tangents to the velocity vector of the flow. Effectively a streamline is a path a fluid particle would take through the fluid domain. 3D Streamlines (coloured by velocity) for 50 seed points are plotted using both URANS and LES. The assumption of a steady state flow is assumed when the streamlines were created. The streamline plots (Figure 8.11) make some very important clarifications. Firstly it is observed that LES predicts a fluid particle to travel many times in the stage area of the enclosure before leaving the enclosure through the stack as compared to URANS. This is confirmed by the fact that even though both URAN and LES streamlines have 50 seed points, the streamline in the LES plot are much denser as compared to URANS.

Additionally it is seen that a large vortex forms over the stage area which gives rise to the draughts discussed earlier. Due to these draughts the rising plumes from the stage were not visible in the LES prediction as they were entrained quickly into the vortex before they could form plume like structures above the stage area. Also worth noting is the fact that in LES, ambient air drawn in from the openings in front of the stage area, is then entrained into the vortex over the stage and escapes later via the stacks. Hence the residence time of a fluid particle is mostly spent over the stage. On the other hand URANS predicts fluid to enter through the openings under the stage, travel to the stage area where it is immediately pushed to the rear wall of the stage and escapes later through the stack. During design stages these results can be of great importance in deciding if in the event of a fire, smoke will reside over the stage area (as predicted by LES) or will escape quickly via the stack (as predicted by URANS). Contrarily the designers might want stage smoke during a performance to stay longer on the stage rather than being pushed to the back of the stage. With the increased accuracy of LES issues such as these can be addressed.
Figure 8.11: Streamline plots (colored by velocity) using URANS and LES
8.4.4. Flow rate through the enclosure

To compare URANS and LES quantitatively the volumetric flow rate through the enclosure was monitored (Figure 8.12). This volumetric flow rate plot also confirms that by $t=200$s the flow had developed into a statistically steady state. Volumetric flow rates are expressed in terms of air changes per hour (ACH) in the enclosure. The ACH predicted by both the approaches remains quite similar in the start-up period of the simulation (i.e. $30<t<100$) however as the time passes a deviation between the values of ACH predicted by the two approaches becomes apparent. At $t=320$s URANS predicted an ACH of 15.34 whilst LES predicted a lower ACH of 14.8. This 3.6% discrepancy might be of significance when the prevailing ACH just meets the minimum ACH levels. The ACH predicted by both the approaches is well above the minimum required (for this case ~5 ACH). However URANS predicts a 3.52% higher ACH compared to LES. This difference is attributed to higher temperature difference across the stack openings which cause higher flow rates through the stacks.

![Figure 8.12: Air change per hour plotted against time for URANS and LES](image-url)
8.4.5. Fourier analysis

As explained in Chapter 6 Fourier analysis helps identify the distribution of the different scales of turbulence intensity (represented by frequencies). A Fast Fourier analysis is something that is not usually carried out in consultancies, however it is worth finding out how well resolved are the LES results for this benchmark. Again the velocity spectra are plotted against frequency. Figure 8.13 shows the location of the three points where the statistical data was analysed. These were chosen at points of interest i.e the upper seating area, the lower seating area and the stage area.

Figure 8.13: Location of the three points where FFT statistics analysed. (x,y,z) of (a) Point 1 (5,10,7.5) (b) Point 2 (12,6,7.5) and (c) Point 3 (22,4,7.5)

Figure 8.14 shows the power spectral density of the vertical velocity v (chosen in line with the work of (Abdalla et al., 2007)) for the three points. The characteristic -5/3 slope is clearly observed in the figure which confirms that the present flow exhibits fully turbulent characteristics. A significant drop in levels of energy at higher frequencies compared to the energy containing frequencies is observed.
(approximately of the order $10^3$). Thus this is considered to be an adequately resolved LES.

Typically the time-sequence data passed to FFT corresponds to a single period of periodically repeating signal. Because in most cases including this case, the first and the last data do not coincide, the repeated signal will thus have large discontinuities. This produces high-frequency components in the resulting Fourier modes which is termed an aliasing error. This problem can be avoided by conditioning the input signal before the transform by “windowing” it with an appropriate windowing method. In the current work the Hanning windowing method was used (Blackman and Tukey, 1958). However, this still resulted in an aliasing error which can be observed at higher frequencies in Figure 8.14. Additionally it can be observed that there exists a dip in the FFT of point 3 (at ~0.01Hz). This may be because the time data series for point 3 was not long enough to capture any physical phenomenon. This can be confirmed by observing the instantaneous fluctuating velocity $v$. Figure 8.15 illustrates the instantaneous vertical velocity $v$ plotted against time at the three points mentioned above. The plot demonstrates the periods of statistically steady states for each of the points. It can be seen that the point from where statistical data collection begins; for point 3 the flow has not reached a statistically steady state early on. This means not enough time may have elapsed for a phenomenon to be repeated at point 3 and thus to be captured in the FFT plot. A longer time length is required for a better FFT analysis.
Figure 8.14: Power spectral density of the vertical velocity at point 1, 2 and 3

Figure 8.15: Instantaneous velocity $v$ plotted against time for point 1, 2 and 3 with the horizontal dashed lines showing statistically steady state periods
8.5. Summary

Both URANS and LES have been used to predict buoyancy driven natural ventilation flow in a real auditorium building. The aim was to assess the performance of the two CFD techniques and compare their costs.

The flow inside the auditorium took 200s to reach statistically steady state but simulations were carried out until 320s for both URANS and LES. Using 8 processors for URANS it took approximately 2.5 days to carry out the simulation for a mesh of 3 million nodes. On the other hand LES resulted in a mesh of 50 million nodes and took 28 days to reach statistically steady state for the flows in the enclosure using 60 processors. It was concluded that using up to 100 processors the simulation time could be halved. Still, LES would be costly in terms of simulation time compared to URANS.

Comparing the temperature plots from both URANS and LES it is concluded that URANS tends to smear out small details of the flow which LES captures. These small scale details become important when the driving forces in the naturally ventilation system are weak. Additionally URANS tends to predict a more uniform temperature distribution in the auditorium whilst LES distinguishes the stage area to be cooler than the seating area due to a local vortex present over the stage that entrained cool ambient air from the openings underneath the stage. Generally URANS was seen to predict higher temperatures inside the auditorium as compared to LES.

Velocity plots from URANS and LES elucidate the presence of a vortex over the stage area in the LES predictions which URANS does not reveal. This vortex causes draughts at the front of the stage area which can have major design implications depending on the requirement of the desired flow pattern. This also has an effect on the occupant comfort and the sensation of draught in the auditorium which LES takes into account more readily.

Streamline plots for both URANS and LES reconfirms the hypothesis made above by showing that URANS shows air to move to the rear of the stage area and quickly escape the building whilst LES predicts ambient air to recirculate many times over the stage area before making its way out via the stacks.
No major difference was observed in predicting the flow rate through the building using the two CFD approaches. The increase in flow rate through the enclosure seems to be similar with URANS over predicting the flow rate (a deviation of 3.52% from LES). This is thought to be due to the over prediction of temperature across the openings by URANS. This over prediction of temperatures is thought to be caused by under prediction of mixing which means the eddy viscosity being calculated by URANS is of lower value.

Table 8-3: Summary table of comparisons with comments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>LES</th>
<th>URANS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Indoor temperature</td>
<td>Divides the auditorium in two regions with a 1°C temperature difference</td>
<td>Predicts a more uniform temperature in the auditorium due to under prediction of mixing</td>
</tr>
<tr>
<td>Draughts</td>
<td>Predicts draughts at ~0.45m/s both on and above the stage</td>
<td>Presence of draughts are completely missing in URANS predictions</td>
</tr>
<tr>
<td>Streamlines</td>
<td>Longer travel time of fluid and formation of a vortex over the stage</td>
<td>Shorter travel time of fluid and its immediate travel to the rear of the stage area</td>
</tr>
<tr>
<td>ACH</td>
<td>14.8</td>
<td>15.34</td>
</tr>
<tr>
<td>FFT</td>
<td>Exhibits the -5/3 gradient in the energy cascade</td>
<td>-</td>
</tr>
<tr>
<td>Cost</td>
<td>Needed 50 processors and 28 days run time</td>
<td>Needed 8 processors and 2.5 days run time</td>
</tr>
</tbody>
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Chapter 9. Summary, conclusions and future work

“If you follow reason far enough it always leads to conclusions that are contrary to reason” – Samuel Butler

9.1. Research strategy

As part of the present research the performance of the LES CFD approach has been assessed for modelling buoyancy-driven natural ventilation and its performance compared to the more conventional RANS-based CFD approach. The methodology involved the application of the LES method, first to simple geometries and then to more realistic benchmark problems of buoyancy-driven natural ventilation flows. Test cases were chosen based on their relevance to the application of interest and the availability of extensive experimental data. The CFD codes were selected for their validated use in the area of interest, ease of use, as well as available training and user support.

The performance of LES in predicting buoyancy-driven natural ventilation flows was assessed in Benchmark 1 using both LES and RANS techniques. This flow problem consisted of plume-plume interaction in an enclosure with openings on the floor and the ceiling level as reported by Kaye and Linden (2004). The ability of both LES and URANS techniques was further evaluated for predicting multiple steady states as reported in the experimental work of Chenvidyakarn and Woods (2005) in Benchmark 2. In Benchmark 3, the aim was to test the application of URANS against LES in a realistic and representative building application typical of that considered by consulting engineers.

To the knowledge of the author the application and thorough validation of the LES technique to the range of buoyancy affected flow problems in the present work is the
first of its kind. Experimental techniques such as salt bath modelling and conventional RANS CFD have been extensively used to investigate buoyancy-driven natural ventilation, however this work provides an alternative approach. A review of the research ‘map’ of this field shows that there are typically two trends of research method investigating buoyancy-driven natural ventilation. A trend to adopt conventional CFD and RANS turbulence modelling is observed when the overall flow description in an enclosure is of interest whilst minimising cost; experimental studies are carried out when the particular focus of the study is turbulence or multiple steady states in fluid flow. This study thus lies on the research ‘map’ of this field in such a way that it tries to combine both these trends into a single research methodology i.e. LES. This work has attempted to elucidate both the accuracy and cost of running LES by comparing results with conventional RANS CFD as well as experimental data. Using LES CFD, detailed and accurate fluid flow predictions could become faster and cheaper than experimental techniques and more accurate than RANS CFD. The current results are generally in good agreement with previous work and expand this by providing deeper insight into flows dominated by buoyancy and natural convection. This work also provides “user guidelines” from CFD model geometry creation, through to setting up the flow problem (in particular mesh generation), control of the solver during the simulation and the type of results to be expected from a well-designed application of LES.

The LES technique is not new, however, due to its reliance on extensive computational resources; its application has been limited. With the recent upsurge in large computational resources becoming readily available (e.g. PC clusters) the work reported in this thesis provides clear indications of the benefits of using LES and sheds light on its feasibility as a tool for consulting engineers. The work also provides a framework for future studies to assess the performance of LES in its application to more complex problems.

9.2. Conclusions from benchmark test cases

9.2.1. Benchmark 1
Following a preliminary test case, Benchmark 1 investigated the plume-plume interaction, evolution and associated unsteady turbulent structures in detail using LES. It was found that the temperature interface height, which is an important
parameter characterising this flow, was predicted accurately by LES but with a discrepancy of 14% compared to theoretical data. RANS (RNG k-ε) predicted the same interface height with a discrepancy of 18.4%. The plume merge height was predicted with a discrepancy of 28.5%. This discrepancy was thought to be due to the virtual origin problem due to the finite area of heat sources in the CFD model. The volume flux predicted by LES agreed well with theory of Kaye and Linden (2004), however RANS predictions deviated from theory, especially at larger distances from the heat sources. Instantaneous temperature plots, pressure and temperature isosurfaces revealed vortex and spiralling coherent structures in the plumes. The non-planar structure of the temperature interface was attributable to the interactions of different turbulent eddy scales in the upper warm layer. Spectral analysis of the LES results confirmed a well resolved LES and the adherence of the velocity field at higher frequencies to the -5/3 power law, characteristic of fully turbulent flows.

9.2.2. Benchmark 2
For Benchmark 2, URANS was able to predict the average room temperatures within 1.42% of theory whilst LES predicted temperatures within 0.15% compared to the theoretical model of Chenvidyakarn and Woods (2005). The time to reach steady state temperatures was predicted more accurately by LES than URANS. All three steady states reported in the experimental work were captured using both LES and URANS, however URANS reported some flow features (such as the presence of a temperature interface and inaccurate temperatures) in the enclosure which were misleading. On the other hand LES was able to give an insight into the true nature of these flow features. LES also revealed the presence of cold draughts at the floor level which URANS was not able to capture. This can have significant implications on the thermal comfort of the occupancy present on the floor level. Additionally it was observed that with varying the lower opening area, the temperatures predicted by URANS were over-predicted relative to the experimental data for openings with small diameters. Of significant importance is the finding that URANS was unable to predict the unsteadiness of the flow (so in fact the URANS solution converged to a RANS solution) which LES was naturally able to capture.

9.2.3. Benchmark 3
In the Benchmark 3 test case, once again URANS over-predicted the temperatures in an auditorium compared to LES. From velocity plots it was observed that LES
predicted flow features (such as small scale vortices) that would cause the sensation of draughts in the auditorium. URANS smeared out the presence of these along with other smaller flow structures and URANS is thus not as capable as LES in predicting comfort related features of the flow. Additionally 3D streamlines predicted by LES provided a better insight (such as residence time, flow separations, vortex formation etc.) into the travel pattern of fluid in the domain compared to URANS. Quantitative comparison of volumetric flow rates predicted by LES and URANS showed that URANS over predicted the rates with a deviation of 3.52% compared with the LES values. These findings confirm the superiority of LES over conventional RANS and URANS approaches to modelling buoyancy-driven natural ventilation. Throughout this work it was observed that RANS/URANS over predicted the temperatures compared to LES and theory.

9.3. Contribution to knowledge

The value of this work lies in the evaluation of LES for modelling buoyancy-driven natural ventilation. The implications of this are that both researchers and consulting engineers are now better equipped to decide if the complexity of their problem would benefit from the application of LES and how much computational resources they must have available in order to run LES accurately.

Most notably, this is the first study (to the author’s knowledge) to investigate the holistic effectiveness of LES in buoyancy-driven natural ventilation flow problems. Holistic effectiveness, refers to the use of LES to investigate fine details of flow (such as plume-plume interactions) or if needed the overall flow evolution, development and multiple steady states (if they exist) for a real auditorium building. Furthermore, the study has enabled the useful identification of the minimum computational power (i.e. ~100 processors) and resulting time requirement (i.e. ~2 weeks) for practitioners who wish to adopt LES into their modelling of natural ventilation systems design.

The results provide compelling evidence for consulting engineers that LES has reached a stage where it has a viable role to play in the design of buildings. This study also suggests that this approach appears to be effective in countering challenging natural ventilation problems which can help in gaining a deeper understanding of natural ventilation. Based on the results presented here, it is reasonable to suggest that LES could be taken further to include applications to
smoke dispersion, occupant comfort, pollutant/particle transport associated with breathing, sneezing, coughing etc. With increased use of LES as a design tool it is hoped that better buildings with improved occupant comfort and reduced carbon footprint could be designed resulting in a healthier environment for future generations.

The following points, based on this work, provide valuable guidance for CFD practitioners who wish to use LES for modelling internal space buoyancy-driven natural ventilation.

- Since internal space buoyancy-driven flow is likely to be at high Re number and the turbulence will be dominated by free shear edges, mesh generation should be guided by two aspects (helped by an a-priori RANS calculation):
  - check that Re_l is high, except in small near-wall layers
  - use an estimate of the integral length scale (L) to generate mesh dimensions such that L/Δ>12, where Δ is the filter width
- If the evolution of the flow is not important, RANS should be used to predict the steady state flow. LES can then be used to look at critical flow features such as plume-plume interaction, formation of vortices, multiple steady states etc. in minimum computational “start-up time.”
- As long as Re_l is high over most of the solution domain the Smagorinsky SGS model should prove adequate
- Use the low dissipation central difference convection scheme
- Use the Second Order Backward Euler scheme for the transient term
- For convergence the residual RMS target should be 10^{-6}
- Use 1-5 coefficient loops for convergence control within each iteration
- Maintain the time steps such that CFL_{max} is in the range of 0-0.5.
- If FFT analysis is planned ensure the time step size is kept constant throughout the statistical data collection period
- Save backups every 500 time steps. In case of power cut or a simulation crash this can save many days of simulation time.
- Approximately 100 processors in parallel are recommended to run viable LES simulations in a reasonable run time
9.4. Limitations of the research

Although this work has looked holistically at the effectiveness of LES in modelling buoyancy-driven natural ventilation, additional work is needed to give LES predictions further confidence. Guidelines have been presented, however there are further guidelines for effective use of LES that remain to be explored. Due to time limitations DES was not investigated in this study but should be explored as another alternative. This technique is potentially useful because of its ability to save computational time compared to LES, particularly if near-wall resolution of the flow is thought to be necessary. The current predictions of LES using the Smagorinsky SGS model were satisfactory, but future studies should also explore other SGS models. Future studies should apply LES to other plume configurations such as colliding plumes, arrays of plumes, dual flow within the same opening etc. For benchmark 1 test case, it needs to be investigated what causes higher flow rates using URANS compared to LES. In regards to Benchmark 2, it needs to be investigated why URANS is unable to predict temperatures accurately for smaller lower opening areas. At present the Benchmark 3 test case was only explored using CFD techniques. There is a need to verifying the CFD results with experimental or field data. Finally, the effects of wind on the air flow within the enclosure for all three benchmark test cases have been ignored in this study. It would be interesting to investigate how wind affects the ventilation pattern in the enclosures. Rigorous validation of LES for other benchmarks will make it possible to have more confidence and accurately use the LES tool in engineering practice.
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**List of contributions**