

# IMPROVED DUST DISPERSION MODELLING FOR SURFACE QUARRIES

AN OPTIMIZED RANS  $k - \varepsilon$  APPROACH

Author: Genora M. D. Joseph, BSc.(Hons), MSc.



UNITED KINGDOM • CHINA • MALAYSIA

A thesis submitted to the University of Nottingham for the degree of  
Doctor of Philosophy

Department of Chemical and Environmental Engineering, The  
University of Nottingham

October 2015

## Abstract

Conventional dust dispersion models which employ Gaussian concentration distributions are routinely applied to predict the dispersion and deposition of fugitive dust arising from quarrying activity. However, these models are known to over-predict the long range transport of particulates beyond the confines of the quarry pit, because their complex terrain algorithms are unable to accommodate the steep gradients which are typically encountered in quarry excavations. They therefore cannot account for the internal flow regimes which contribute to the removal of suspended particulates from the air stream.

Consequently, a need arises within the extractive industries, for improved dust dispersion models that are not constrained by quarry topography. This research project attempts to address this deficiency in the modelling of dust emissions from quarry blast events, by presenting an optimized RANS  $k - \varepsilon$  approach which can adequately simulate the flow-field in which particulates are entrained under a range of meteorological conditions.

The stages involved in the incremental development of the numerical model are documented in the thesis, and commence with characterization of the atmospheric boundary layer. In particular, the Monin-Obukhov Similarity Theory is applied to parametrize the atmospheric surface layer, which exerts the most influence on the dispersion and deposition of near-ground particulate emissions.

Modifications to the standard  $k - \varepsilon$  model coefficients and the inclusion of buoyancy source terms have been adopted in this work, in accordance with previous studies by Alinot and Masson (2005). These modifications ensure that the turbulence closure equations are compatible with Monin-Obukhov Similarity scaling of the atmospheric surface layer. The Businger-Dyer flux profile functions have been employed to introduce stability modifications to the logarithmic velocity, temperature and turbulence profiles which have been defined at the inlet boundaries of the computational domain to enable numerical representation of both adiabatic and diabatic atmospheric conditions. Furthermore, the Lagrangian Discrete Phase Model has been coupled with Eulerian solution of the flow field to provide a robust means of replicating fugitive dust dispersion through the stochastic tracking of injected particulates. The project also presents a consolidated post-processing methodology to incorporate wind direction variability due to mesoscale atmospheric effects into the CFD model. This methodology use the Moore (1976) equation to parametrize the standard deviation of wind direction variability and proposes a novel, Gaussian probability weighted averaging procedure to arrive at a resultant plume which accounts for the influence of mesoscale wind variability on particulate trajectory and improves the  $k - \varepsilon$  predictions of lateral spreading of the dust plume.

Simulations of flow and dispersion over a series of idealized cosine depressions of varying aspect ratio have been used to assess model predictions of the flow regime and the corresponding plume attenuation within artificial valleys. To allow the model to accommodate negative terrain elevations and to produce profiles of the flow variables which conform to

wall topography, a wall-distance scalar has been introduced to ensure consistency of the inlet profile with the flow solution within the domain. These simulations have demonstrated that the proposed model surpasses UK-ADMS in terms of its ability to resolve strong recirculation regimes in deep depressions.

The project culminates in a case study of the Old Moor Quarry in Buxton, Derbyshire. This case study tests the viability of the proposed  $k - \varepsilon$  model and validates the model predictions of dust dispersion with field measurements obtained over the course of a monitoring campaign of approximately one month duration. Meteorological pre-processing steps in accordance with the findings of Holtslag and Van Ulden (1983) have been employed to derive atmospheric surface layer input parameters from routine meteorological data measured at the quarry site, eliminating the need for sophisticated meteorological measurements. Dust dispersion predictions obtained using the conventional dust dispersion model UK-ADMS, have been compared to the CFD model results to demonstrate the improved prediction accuracy of the proposed  $k - \varepsilon$  approach. Notably, the CFD model is shown to account for the various flow regimes which arise due to the combined effects of the site meteorology and the complex terrain of the quarry excavation.

Importantly, the statistical Performance metrics, FAC2, MG, FB and NMSE recommended by Hanna et al. (2004) for the evaluation of dispersion model performance, have been used to assess the accuracy of fugitive dust deposition predictions obtained from the proposed model. The performance evaluation exercise indicates that the buoyancy modified  $k - \varepsilon$  model outperforms UK-ADMS for all of the metric tests. The incorporation of the wind variability weighted averaging procedure in the case study simulations is seen to reduce uncertainty due to random error, quantified by NMSE. This due to the fact that the wind variability averaging procedure evens out outlying predictions which may be due to the inherent stochasticity of the DPM model.

## Acknowledgements

I feel an enduring sense of gratitude for the support that I received from my supervisors, Dr Ian S. Lowndes and Dr David M. Hargreaves. Throughout the duration of my research project, I have been able to confidently rely on Dr Lowndes' extensive knowledge of air pollution modelling and the extractive industries. Dr Hargreaves has been a bastion of knowledge on atmospheric physics and Computational Fluid Dynamics and his academic guidance and steadfast support through the successes and hurdles have kept me committed to the task. I am grateful to my supervisors for their patience, their dedication to teaching and their unwavering belief in my ability to complete this thesis. I feel honoured to have had the opportunity to carry out my research under their esteemed direction.

I am grateful to the University of Nottingham, International office and the Faculty of Engineering for making this research project possible through the Dean of Engineering Research Scholarship for International Excellence. I wish to thank the University of Nottingham HPC Services for meeting my computing needs during the final phase of my research. I also wish to thank Dr Stephen Ambrose for being a source of moral and technical support over the past four years.

I feel truly blessed for the outpouring of love and support that I received from my family and friends throughout this journey. I cannot thank my mother Shirley enough, for my life, for her love, her hard work and sacrifice in raising me and for being a shining example of perseverance and strength. I am grateful to my dear 10 year-old daughter Njemile, who has been patient, helpful and understanding beyond her years.

I also wish to thank my dear friend Shelly who has been a motivating force throughout this endeavour - tolerating my frequent and gratuitous wailing and always calmly reminding me that the PhD was entirely within my reach! My uncles, Dr Jeffrey Blaize and Ralph Blaize have been such wonderful paternal influences in my life and I remain eternally grateful. I have felt the abiding love and faith of my friends, Barbara, Abeo, Nelly, Amy, Verna Sharika even across the oceans. I am also grateful to my friends Lydia, Ed, Dr. Olajumoke Ajao-Adelakun and Leandra, in Nottingham and Leeds who have all generously helped with childcare.

I am thankful to my Grandfather who sadly passed away during my studies, for his prayers, his words of wisdom and his faith in me. Finally, I thank God for the determination and health to see this project through to completion.

## Contents

|                                                                             |             |
|-----------------------------------------------------------------------------|-------------|
| <b>Contents</b>                                                             | <b>iv</b>   |
| <b>List of Figures</b>                                                      | <b>viii</b> |
| <b>List of Tables</b>                                                       | <b>xv</b>   |
| <b>Nomenclature</b>                                                         | <b>xvii</b> |
| <b>1 Introduction</b>                                                       | <b>1</b>    |
| 1.1 A Brief History of Quarrying, from Ancient to Modern Times . . . . .    | 1           |
| 1.2 The Need for Improved Quarry Dust Dispersion Models . . . . .           | 2           |
| 1.3 Aims and Objectives . . . . .                                           | 4           |
| 1.4 Overview of Thesis Content . . . . .                                    | 5           |
| <b>2 Literature Review</b>                                                  | <b>7</b>    |
| 2.1 Surface Quarries . . . . .                                              | 7           |
| 2.1.1 Definition of Fugitive Dust . . . . .                                 | 7           |
| 2.1.2 Dust Generation from Quarry Processes . . . . .                       | 9           |
| 2.1.3 Monitoring and Measurement of Fugitive Dust . . . . .                 | 17          |
| 2.2 The Use of Numerical Models to Predict Quarry Dust Dispersion . . . . . | 20          |
| 2.2.1 Limitations of Conventional Dust Dispersion Models . . . . .          | 22          |
| 2.2.2 CFD application to Atmospheric Dispersion Modelling . . . . .         | 23          |
| 2.2.3 Dispersion Model Inter-comparison Studies . . . . .                   | 25          |
| 2.2.4 CFD Dispersion Modelling of Flow over Quarry Topography . . . . .     | 30          |
| 2.3 Characterization of The Atmospheric Boundary Layer . . . . .            | 33          |
| 2.3.1 Surface Layer Structure and Meteorology . . . . .                     | 37          |
| 2.3.2 ABL Profiles and Thermal Stability Classes . . . . .                  | 42          |

|          |                                                                                                      |           |
|----------|------------------------------------------------------------------------------------------------------|-----------|
| 2.3.3    | The Significance of the Froude Number in Stratified Flows . . . . .                                  | 44        |
| 2.3.4    | Profiles of Velocity, Temperature and Turbulence . . . . .                                           | 46        |
| 2.3.5    | Energy and Turbulence Scales in the ABL . . . . .                                                    | 47        |
| 2.3.6    | The Special Case of the Convective Mixed Layer . . . . .                                             | 49        |
| 2.3.7    | Measuring ABL Meteorological Parameters . . . . .                                                    | 52        |
| 2.3.8    | Wind Direction Variability . . . . .                                                                 | 54        |
| 2.4      | Summary . . . . .                                                                                    | 57        |
| <b>3</b> | <b>Optimization of the Numerical model</b>                                                           | <b>58</b> |
| 3.1      | The Navier-Stokes Equations . . . . .                                                                | 58        |
| 3.2      | The FLOWSTAR Complex Terrain Module . . . . .                                                        | 60        |
| 3.3      | Numerical Modelling Using CFD . . . . .                                                              | 62        |
| 3.3.1    | Selection of a RANS Turbulence Closure Model . . . . .                                               | 64        |
| 3.3.2    | Finite Volume Discretization of the Calculation Domain . . . . .                                     | 66        |
| 3.3.3    | Numerical Errors and RANS Limitations . . . . .                                                      | 68        |
| 3.4      | Obtaining Homogeneous ABL Profiles using the ANSYS FLUENT $k - \varepsilon$ model                    | 69        |
| 3.4.1    | $k - \varepsilon$ Model Solver Settings . . . . .                                                    | 70        |
| 3.4.2    | Appropriate Boundary Conditions . . . . .                                                            | 73        |
| 3.4.3    | Stream-wise Gradients in the Undisturbed ABL and the Role of Wall<br>Functions . . . . .             | 75        |
| 3.4.4    | Model Coefficients and the Inclusion of Buoyancy Effects . . . . .                                   | 78        |
| 3.4.5    | The Boussinesq Approximation . . . . .                                                               | 79        |
| 3.5      | Replicating the Alinot and Masson (2005) ABL Profiles . . . . .                                      | 79        |
| 3.5.1    | Formulation of $k$ , $\varepsilon$ and Energy Source Terms . . . . .                                 | 84        |
| 3.5.2    | Testing the homogeneity of the ABL Profiles . . . . .                                                | 85        |
| 3.5.3    | Comparison with Alinot and Masson (2005) Results and Monin-Obukhov<br>Similarity profiles . . . . .  | 89        |
| 3.6      | Summary . . . . .                                                                                    | 93        |
| <b>4</b> | <b>Accounting for Wind Direction Variability in Lagrangian Particle Disper-<br/>sion Simulations</b> | <b>94</b> |
| 4.1      | Past Studies of Wind Direction Variability . . . . .                                                 | 94        |
| 4.2      | Parametrizing Wind Direction Variability . . . . .                                                   | 95        |
| 4.3      | Methodology . . . . .                                                                                | 99        |
| 4.3.1    | The Computational Domain . . . . .                                                                   | 100       |
| 4.3.2    | DPM Boundary Conditions and Injection Parameters . . . . .                                           | 100       |
| 4.3.3    | Meteorological Conditions . . . . .                                                                  | 102       |
| 4.3.4    | Wind Variability Simulations . . . . .                                                               | 103       |
| 4.3.5    | The Influence of the Lagrangian Integral Time Scale Constant . . .                                   | 105       |
| 4.4      | Results and Discussion . . . . .                                                                     | 108       |
| 4.4.1    | Homogenous ABL Profiles . . . . .                                                                    | 108       |
| 4.4.2    | DPM Accretion Results . . . . .                                                                      | 109       |
| 4.5      | Summary . . . . .                                                                                    | 121       |

|          |                                                                                                           |            |
|----------|-----------------------------------------------------------------------------------------------------------|------------|
| <b>5</b> | <b>Flow and Dispersion over Idealised Depressions</b>                                                     | <b>122</b> |
| 5.1      | Flow within Valleys . . . . .                                                                             | 122        |
| 5.1.1    | Numerical Simulation of Valley Flows . . . . .                                                            | 126        |
| 5.2      | Methodology . . . . .                                                                                     | 126        |
| 5.2.1    | Introduction of a Wall Distance Scalar in the Numerical Model . . .                                       | 126        |
| 5.2.2    | Validation of the $k-\varepsilon$ Model with Wind Tunnel Results from Ishihara<br>et al. (1999) . . . . . | 128        |
| 5.2.3    | The Computational Domain for Flow over Cosine Depressions . . .                                           | 134        |
| 5.2.4    | Mesh Independence Study . . . . .                                                                         | 135        |
| 5.3      | Results and Discussion . . . . .                                                                          | 140        |
| 5.3.1    | The Influence of Idealized Terrain on the Flow-field . . . . .                                            | 140        |
| 5.3.2    | Correlation of the Froude Number to Flow Separation . . . . .                                             | 149        |
| 5.3.3    | The Influence of the Depressions on Particle Dispersion . . . . .                                         | 151        |
| 5.3.4    | Comparison of $k-\varepsilon$ and UK-ADMS Turbulence Profiles . . . . .                                   | 156        |
| 5.3.5    | Comparison of $k-\varepsilon$ and UK-ADMS Dry Deposition Predictions . .                                  | 163        |
| 5.4      | Summary . . . . .                                                                                         | 166        |
| <b>6</b> | <b>A Case Study of Old Moor Quarry</b>                                                                    | <b>168</b> |
| 6.1      | Overview of the Case Study . . . . .                                                                      | 168        |
| 6.2      | Old Moor Quarry Location . . . . .                                                                        | 169        |
| 6.3      | Meteorological Pre-processing Routine . . . . .                                                           | 172        |
| 6.3.1    | Site Meteorological Measurements . . . . .                                                                | 172        |
| 6.3.2    | Surface Radiation Balance . . . . .                                                                       | 172        |
| 6.3.3    | Fractional Cloud Cover . . . . .                                                                          | 174        |
| 6.3.4    | Surface Sensible Heat Flux Computations . . . . .                                                         | 174        |
| 6.3.5    | Calculating the Monin-Obukhov Length . . . . .                                                            | 176        |
| 6.3.6    | Treatment of the Convective Mixed Layer . . . . .                                                         | 178        |
| 6.4      | Characterization of Blast Emissions . . . . .                                                             | 178        |
| 6.5      | Artificial Terrain Simulations . . . . .                                                                  | 182        |
| 6.5.1    | Discretizing the Computational Domain . . . . .                                                           | 182        |
| 6.5.2    | Specification of the Initial Blast Velocity . . . . .                                                     | 187        |
| 6.5.3    | Examination of the Wind-field and Dust Dispersion within the Quarry                                       | 187        |
| 6.6      | Actual Terrain Simulations . . . . .                                                                      | 203        |
| 6.6.1    | The Influence of upwind topography . . . . .                                                              | 205        |
| 6.6.2    | Evaluating the $k-\varepsilon$ Model Uncertainty . . . . .                                                | 211        |
| 6.6.3    | Performance Metrics for Dispersion Model Evaluation . . . . .                                             | 211        |
| 6.6.4    | Using Frisbee Gauge Measurements to Validate the Model . . . . .                                          | 213        |
| 6.6.5    | Discussion of the $k-\varepsilon$ Model Performance . . . . .                                             | 217        |
| 6.6.6    | $k-\varepsilon$ Model Predictions of In-pit Dust Retention . . . . .                                      | 223        |
| 6.7      | Summary . . . . .                                                                                         | 228        |

|          |                                                                                  |            |
|----------|----------------------------------------------------------------------------------|------------|
| <b>7</b> | <b>Conclusions and Further Work</b>                                              | <b>229</b> |
| 7.1      | Conclusions . . . . .                                                            | 229        |
| 7.1.1    | Numerical Model Optimization . . . . .                                           | 231        |
| 7.1.2    | Validation of the buoyancy modified $k - \varepsilon$ dispersion model . . . . . | 233        |
| 7.1.3    | Limitations of the Model . . . . .                                               | 234        |
| 7.2      | Further Work . . . . .                                                           | 235        |
| 7.2.1    | Application to other source types . . . . .                                      | 235        |
| 7.2.2    | Improving boundary layer characterization . . . . .                              | 235        |
| 7.2.3    | Emission factors . . . . .                                                       | 236        |
| 7.2.4    | Improved validation techniques . . . . .                                         | 236        |
| 7.2.5    | Automating the simulations . . . . .                                             | 236        |
| <b>A</b> | <b>UDF to Introduce Inlet Profiles and Buoyancy Modifications to FLUENT</b>      |            |
|          | $k - \varepsilon$ Model                                                          | <b>238</b> |
| <b>B</b> | <b>Cuboid Source Particle Injection File Code</b>                                | <b>251</b> |
| <b>C</b> | <b>MATLAB Wind Variability Averaging Script</b>                                  | <b>253</b> |

## List of Figures

|     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |    |
|-----|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| 2.1 | Airborne dust particle aerodynamic diameter classified according to fractional penetration into the human respiratory tract (Jimenez et al., 2011). . .                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | 8  |
| 2.2 | Extraction and processing sequence at rock quarry from DEFRA (2004). . .                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 10 |
| 2.3 | Typical configuration of blast drill holes and explosive charge for a bench blast at a rock quarry, from Kulatilake et al. (2010). . . . .                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 11 |
| 2.4 | Horizontal velocity profile of advancing blast cloud with time, estimated from video footage (Silvester et al., 2006). . . . .                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 12 |
| 2.5 | Crushing and screening sequence at a rock quarry from DEFRA (2004). . .                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | 14 |
| 2.6 | Quarry benches and face excavation profile of a typical rock quarry, showing the arrangement of haul roads and extraction faces and the various slope angles for slope stability considerations (Hem, 2012). . . . .                                                                                                                                                                                                                                                                                                                                                                                                            | 16 |
| 2.7 | Non-directional Frisbee gauge in-situ (AEA Technology plc, 2011). . . . .                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 18 |
| 2.8 | A comparison of the solutions produced by the (a) FLUENT AD (b) FLUENT DPM models to the UK-ADMS model predictions of ground level and plume centreline concentrations for a gaseous plume emitted from a 50 m stack located at 100 m in a domain of size 1000 m $\times$ 500 m $\times$ 150 m, from Riddle et al. (2004). The solid line and $x$ markers represents FLUENT and UK-ADMS concentration predictions at the plume centreline respectively. The dashed lines and $+$ markers denote FLUENT and UK-ADMS concentrations at ground level respectively. The distance on the x-axis is measured from the source. . . . . | 26 |
| 2.9 | A plot of UK-ADMS plume dispersion models (a) horizontal plume dispersion at stack height, (b) vertical section along plume centreline (c) ground level concentration. Concentration in $\mu\text{gm}^{-3}$ , from Riddle et al. (2004). . . . .                                                                                                                                                                                                                                                                                                                                                                                | 28 |

|      |                                                                                                                                                                                                                                                                      |    |
|------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| 2.10 | A plot of the solution of FLUENT DPM plume dispersion models (a) horizontal plume dispersion at stack height, (b) vertical section along plume centreline (c), ground level concentration. Concentration in $\mu\text{gm}^{-3}$ , from Riddle et al. (2004). . . . . | 29 |
| 2.11 | A comparison of the particulate deposition predictions obtained using FLUENT $k - \varepsilon$ (top) and UK-ADMS (bottom) to model dispersion at a UK quarry under neutral atmospheric conditions from Silvester et al. (2009). . .                                  | 31 |
| 2.12 | Structure and approximate heights of the layers which comprise the Atmospheric Boundary Layer, adapted from Kaimal and Finnigan (1994). . . . .                                                                                                                      | 34 |
| 2.13 | The effects of the roughness canopy on the ABL, the aerodynamic roughness height and the zero-plane displacement. . . . .                                                                                                                                            | 36 |
| 2.14 | Diurnal cycle of atmospheric boundary layer evolution from Kaimal and Finnigan (1994). . . . .                                                                                                                                                                       | 38 |
| 2.15 | Turbulent eddy structure in the daytime convective ABL from Kaimal and Finnigan (1994). . . . .                                                                                                                                                                      | 39 |
| 2.16 | Turbulent eddy structure in the night-time stable ABL from Kaimal and Finnigan (1994). . . . .                                                                                                                                                                       | 40 |
| 2.17 | Displacement of adiabatically lifted air parcel (Jacobson, 1999). . . . .                                                                                                                                                                                            | 42 |
| 2.18 | Illustration of the dividing streamline concept showing the dividing streamline height and separation of the streamlines above and below a hill (Leo et al., 2015). . . . .                                                                                          | 45 |
| 2.19 | Profiles of velocity, wind direction and potential temperature in the convective ABL (Kaimal and Finnigan, 1994). . . . .                                                                                                                                            | 50 |
| 2.20 | Profiles of normalised velocity, potential temperature and buoyancy variances and turbulent dissipation rate in the convective ABL (Caughey and Palmer, 1979) . . . . .                                                                                              | 51 |
| 2.21 | Spatial and temporal scales of atmospheric turbulence, adapted from Isaksen et al. (2009) . . . . .                                                                                                                                                                  | 56 |
| 3.1  | FLOWSTAR regularly spaced grid over an isolated hill with domain boundaries defined by wind-aligned rectangle (CERC Ltd, 2011). . . . .                                                                                                                              | 62 |
| 3.2  | Illustration of finite volume discretization for a 2-dimensional structured grid. . . . .                                                                                                                                                                            | 67 |
| 3.3  | SIMPLEC pressure-velocity coupling algorithm iterative steps to solve the discretized equations using initial guessed field for pressure, velocity and transported variables from Versteeg and Malalasekera (1995). . . . .                                          | 72 |
| 3.4  | Illustration of staggered grid system to allow evaluation of velocity components on alternate grid for pressure interpolation. . . . .                                                                                                                               | 73 |
| 3.5  | Diagram of flat terrain modelling domain. . . . .                                                                                                                                                                                                                    | 75 |
| 3.6  | Law of the wall for smooth and sand-grained roughened surfaces showing law of the wall for the viscous sublayer, buffer layer and log region (Blocken et al., 2007b). . . . .                                                                                        | 76 |

|      |                                                                                                                                                                                                                                                                                                                          |     |
|------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|
| 3.7  | Wall function fitting of logarithmic inlet velocity profile at centre of wall adjacent cell Blocken et al. (2007b). . . . .                                                                                                                                                                                              | 78  |
| 3.8  | Image of the hexahedral mesh used to discretize the empty computational domain. Flow variable were plotted on vertical rakes at positions indicated on the $y=0$ plane, highlighted in blue. The region encircled in the dashed red circle is magnified to show geometric cell growth in the vertical direction. . . . . | 81  |
| 3.9  | Magnified region of the empty computational domain, showing cells of uniform width and length, with geometric growth of cell heights in $z$ -direction to capture large variations of flow variables in near-wall region. . . . .                                                                                        | 82  |
| 3.10 | Non-dimensional temperature profiles for the neutral, stable and unstable test cases (Alinot and Masson, 2005). . . . .                                                                                                                                                                                                  | 83  |
| 3.11 | Stable ABL profiles of non-dimensionalized a) $u$ , b) $T$ , c) $\varepsilon$ and d) $k$ , from vertical rakes located at $x=0$ m (dashed line), $x=212.5$ m (crosses) and $x=400$ m (circles). . . . .                                                                                                                  | 86  |
| 3.12 | Neutral ABL profiles of non-dimensionalized a) $u$ , b) $T$ c) $\varepsilon$ and d) $k$ , from vertical rakes located at $x=0$ m (dashed line), $x=212.5$ m (crosses) and $x=400$ m (circles). . . . .                                                                                                                   | 87  |
| 3.13 | Unstable ABL profiles of non-dimensionalized a) $u$ , b) $T$ , c) $\varepsilon$ and d) $k$ , from vertical rakes located at $x=0$ m (dashed line), $x=212.5$ m (crosses) and $x=400$ m (circles). . . . .                                                                                                                | 88  |
| 3.14 | Comparison of Fluent test, Alinot and Masson (2005) and M-O normalized flow and turbulence profiles for the stable ABL, $u(h)=10 \text{ ms}^{-1}$ , $I(h) = 8\%$ , $h_{ref}=35$ m. . . . .                                                                                                                               | 90  |
| 3.15 | Comparison of Fluent test, Alinot and Masson (2005) and M-O normalized flow and turbulence profiles for the neutral ABL, $u(h)=10 \text{ ms}^{-1}$ , $I(h) = 8\%$ , $h_{ref}=35$ m. . . . .                                                                                                                              | 91  |
| 3.16 | Comparison of Fluent test, Alinot and Masson (2005) and M-O normalized flow and turbulence profiles for the unstable ABL, $u(h)=10 \text{ ms}^{-1}$ , $I(h) = 8\%$ , $h_{ref}=35$ m. . . . .                                                                                                                             | 92  |
| 4.1  | Frequency distribution of wind direction variability angles measured at a height of 2 m at 1 minute intervals in the nocturnal ABL, for a 4 month observation a period, from Mahrt (2010). . . . .                                                                                                                       | 96  |
| 4.2  | Wind direction variability angular changes as a function of wind speed, measured at a height of 2 m at 1 minute intervals in the nocturnal ABL, for a 4 month observation a period, from Mahrt (2010). . . . .                                                                                                           | 97  |
| 4.3  | Variation of $\sigma_\theta$ with wind speed, for Cardington field observations reproduced from Davies and Thomson (1999). . . . .                                                                                                                                                                                       | 98  |
| 4.4  | The computational domain, showing position of cuboid volume source. . . .                                                                                                                                                                                                                                                | 101 |
| 4.5  | Wind variability method at different $\sigma_\theta$ increments, neutral ABL $c_L = 0.15$ , $\sigma_\theta = 5^\circ$ at a) $x = 140$ m, b) $x = 170$ m, c) $y = 100$ m. . . . .                                                                                                                                         | 104 |

|      |                                                                                                                                                                                                                                                       |     |
|------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|
| 4.6  | Homogenous turbulence profiles, a) Unstable ABL, b) Neutral ABL, c) Stable ABL, d) Normalized Temperature for the stability classes used in the wind variability simulations . . . . .                                                                | 108 |
| 4.7  | Stable DPM accretion plots with different $c_L$ values, $\sigma_\theta = 5.7^\circ$ , a) $x=135$ m, b) $y=100$ m . . . . .                                                                                                                            | 112 |
| 4.8  | Unstable DPM accretion and UK-ADMS 5.0 plots, $\sigma_\theta = 5.0^\circ$ , a) $x=135$ m, b) $y=100$ m . . . . .                                                                                                                                      | 114 |
| 4.9  | Neutral DPM accretion and UK-ADMS 5.0 plots, $\sigma_\theta = 5^\circ$ , a) $x=135$ m, b) $y=100$ m . . . . .                                                                                                                                         | 115 |
| 4.10 | Stable DPM accretion and UK-ADMS 5.0 plots, $\sigma_\theta = 5.7^\circ$ , a) $x=135$ m, b) $y=100$ m . . . . .                                                                                                                                        | 116 |
| 4.11 | Dry deposition contours ( $\text{kgm}^{-2}\text{s}^{-1}$ ) for an unstable ABL, a) UK-ADMS, b) base FLUENT, and c) FLUENT WMV $c_L = 0.05$ . . . . .                                                                                                  | 118 |
| 4.12 | Dry deposition contours ( $\text{kgm}^{-2}\text{s}^{-1}$ ) for a neutral ABL, a) UK-ADMS, b) base FLUENT and c) FLUENT WMV $c_L = 0.05$ . . . . .                                                                                                     | 119 |
| 4.13 | Dry deposition contours ( $\text{kgm}^{-2}\text{s}^{-1}$ ) for a stable ABL, a) UK-ADMS, b) base FLUENT and c) FLUENT WMV $c_L = 0.05$ . . . . .                                                                                                      | 120 |
| 5.1  | 2D valley profiles for 3, 5 and 8 aspect ratio valleys used in wind tunnel study by Snyder et al. (1991). Solid lines correspond to ideal shapes, whilst markers represent measured shapes. . . . .                                                   | 123 |
| 5.2  | Profiles of $u/U_\infty$ for (a) 3, (b) 5 and (c) 8 aspect ratio valleys from Snyder et al. (1991), the solid lines indicate results from numerical simulations, whilst the triangular markers represent wind tunnel measurements. . . . .            | 124 |
| 5.3  | Profiles of $I = \sigma_u/U_\infty$ for (a) 3, (b) 5 and (c) 8 aspect ratio valleys from Snyder et al. (1991), the solid lines indicate results from numerical simulations, whilst the triangular markers represent wind tunnel measurements. . . . . | 125 |
| 5.4  | Plane at $y = 0$ through $\alpha = 4$ depression illustrating $z'$ field and values for points P1 and P2. . . . .                                                                                                                                     | 128 |
| 5.5  | Experimental section of wind tunnel and cross-section of scale model of 3D cosine squared hill employed by Ishihara et al. (1999). . . . .                                                                                                            | 129 |
| 5.6  | Computational domain and boundary conditions used to perform full scale simulations of the 3D hill in Ishihara et al. (1999) . . . . .                                                                                                                | 130 |
| 5.7  | Enlargement of mesh region enclosed in red rectangle showing grid refinement near hill on ground surface Ishihara et al. (1999). . . . .                                                                                                              | 131 |
| 5.8  | Cross-section of mesh showing vertical cell distribution above and around cosine squared hill. . . . .                                                                                                                                                | 131 |
| 5.9  | Comparison of a) normalized $u$ component of velocity and b) normalized $\sigma_u$ profiles over cosine squared hill computed by the modified $k - \varepsilon$ to those obtained in wind tunnel experiments by Ishihara et al. (1999). . . . .       | 133 |
| 5.10 | The computational domain, showing dimensions of the fetch and depression and imposed boundary conditions. . . . .                                                                                                                                     | 134 |

|      |                                                                                                                                                                                        |     |
|------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|
| 5.11 | The unstructured face mesh on the ground surface showing the effects of the size function around the depression. . . . .                                                               | 136 |
| 5.12 | The mesh on a vertical slice through the centre of the depression, showing clearly the growth of cell size with height. . . . .                                                        | 137 |
| 5.13 | Comparison of unstable turbulent kinetic energy profiles over $\alpha=4$ depression for coarse, medium and fine grids. . . . .                                                         | 139 |
| 5.14 | Flow profiles across $\alpha=8$ depression at $y = 0$ of a) $\hat{u}$ and b) $I$ . . . . .                                                                                             | 141 |
| 5.15 | Flow profiles across $\alpha=4$ depression at $y = 0$ of a) $\hat{u}$ and b) $I$ . . . . .                                                                                             | 142 |
| 5.16 | Flow profiles across $\alpha=2.67$ depression at $y = 0$ of a) $\hat{u}$ and b) $I$ . . . . .                                                                                          | 143 |
| 5.17 | Flow profiles across $\alpha=2$ depression at $y = 0$ of a) $\hat{u}$ and b) $I$ . . . . .                                                                                             | 144 |
| 5.18 | Velocity vector plots for the stable ABL on a central plane $xz$ plane through the depression for aspect ratios (a) 8, (b) 4, (c) 2.67 and (d) 2. . . . .                              | 146 |
| 5.19 | Velocity vector plots for the neutral ABL on a central plane $xz$ plane through the depression for aspect ratios (a) 8, (b) 4, (c) 2.67 and (d) 2. . . . .                             | 147 |
| 5.20 | Velocity vector plots for the unstable ABL on a central plane $xz$ plane through the depression for aspect ratios (a) 8, (b) 4, (c) 2.67 and (d) 2. . . .                              | 148 |
| 5.21 | Stable temperature profiles at the depression centre $(x_0, y_0)$ compared to the adiabatic temperature profile for depression aspect ratios of (a) 8, (b) 4, (c) 2.67, (d) 2. . . . . | 149 |
| 5.22 | Non-dimensionalised concentration contour plots, $\hat{C}$ , for the stable ABL, for depression of aspect ratio (a) 8 ,(b) 4 ,(c) 2.67 ,(d) 2. . . . .                                 | 153 |
| 5.23 | Non-dimensionalised concentration contour plots, $\hat{C}$ , for the neutral ABL, for depression of aspect ratio (a) 8 ,(b) 4 ,(c) 2.67 ,(d) 2. . . . .                                | 154 |
| 5.24 | Non-dimensionalised concentration contour plots, $\hat{C}$ , for the unstable ABL, for depression of aspect ratio (a) 8 ,(b) 4 ,(c) 2.67 ,(d) 2. . . . .                               | 155 |
| 5.25 | Comparison of UK-ADMS and FLUENT a) $\hat{u}$ and b) $I$ profiles for the stable ABL over the $\alpha = 8$ depression. . . . .                                                         | 157 |
| 5.26 | Comparison of UK-ADMS and FLUENT a) $\hat{u}$ and b) $I$ profiles for the neutral ABL over the $\alpha = 8$ depression. . . . .                                                        | 158 |
| 5.27 | Comparison of UK-ADMS and FLUENT a) $\hat{u}$ and b) $I$ profiles for the unstable ABL over the $\alpha = 8$ depression. . . . .                                                       | 159 |
| 5.28 | Comparison of UK-ADMS and FLUENT a) $\hat{u}$ and b) $I$ profiles for the stable ABL over the $\alpha = 2$ depression. . . . .                                                         | 160 |
| 5.29 | Comparison of UK-ADMS and FLUENT a) $\hat{u}$ and b) $I$ profiles for the neutral ABL over the $\alpha = 2$ depression. . . . .                                                        | 161 |
| 5.30 | Comparison of UK-ADMS and FLUENT a) $\hat{u}$ and b) $I$ profiles for the unstable ABL over the $\alpha = 2$ depression. . . . .                                                       | 162 |
| 5.31 | Comparison of UK-ADMS and FLUENT dry deposition contour plots for the $\alpha = 8$ depression for a) stable, b) neutral and c) unstable atmospheric conditions. . . . .                | 164 |

|      |                                                                                                                                                                                                                                                             |     |
|------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|
| 5.32 | Comparison of UK-ADMS and FLUENT dry deposition contour plots for the $\alpha = 2$ depression for a) stable, b) neutral and c) unstable atmospheric conditions. . . . .                                                                                     | 165 |
| 6.1  | Contour map of Old Moor Quarry showing site elevations and surrounding areas. . . . .                                                                                                                                                                       | 170 |
| 6.2  | Aerial view of Old Moor Quarry on 12 <sup>th</sup> September 2005. . . . .                                                                                                                                                                                  | 171 |
| 6.3  | Aerial view of Old Moor Quarry on 31 <sup>st</sup> December 2006. . . . .                                                                                                                                                                                   | 171 |
| 6.4  | Old Moor wind speed and wind direction wind rose during measuring period                                                                                                                                                                                    | 173 |
| 6.5  | Psychrometric curve according to Holtslag and Van Ulden (1983) . . . . .                                                                                                                                                                                    | 176 |
| 6.6  | Frequency distribution of PGT stability classes at Old Moor quarry at the time of blasting for the measurement period from June 9 <sup>th</sup> to July 19 <sup>th</sup> . . .                                                                              | 177 |
| 6.7  | All initial blast cloud locations for bench blasting conducted during the measurement period. . . . .                                                                                                                                                       | 181 |
| 6.8  | Representative blast locations, from averaging groups of blasts in close proximity of each other. . . . .                                                                                                                                                   | 181 |
| 6.9  | Specification of domain boundaries for prevailing wind direction, $\theta = 90^\circ$ . .                                                                                                                                                                   | 183 |
| 6.10 | Plan view of surface mesh on the quarry bench floors and bench faces. . . .                                                                                                                                                                                 | 185 |
| 6.11 | Prismatic layer near the wall in region 1 and cell refinement imposed on benches. . . . .                                                                                                                                                                   | 186 |
| 6.12 | Dust accretion for static injection with initial particle injection velocity of $0 \text{ ms}^{-1}$ . . . . .                                                                                                                                               | 188 |
| 6.13 | Dust accretion for initial particle injection velocity of $25 \text{ ms}^{-1}$ . . . . .                                                                                                                                                                    | 189 |
| 6.14 | The difference between the $0 \text{ ms}^{-1}$ and $25 \text{ ms}^{-1}$ Accretion profiles. . . . .                                                                                                                                                         | 190 |
| 6.15 | Comparison of normalized profiles of the $u$ -velocity component for stability classes A, B, C and D for a) $90^\circ$ prevailing wind direction and b) $270^\circ$ counter-wind direction. . . . .                                                         | 192 |
| 6.16 | Normalized contour plots of $u$ velocity component at $y = -90 \text{ m}$ for $270^\circ$ wind under a) stability class A and b) stability class D. . . . .                                                                                                 | 194 |
| 6.17 | Comparison of turbulence intensity profiles for stability classes A, B, C and D for a) $90^\circ$ prevailing wind direction and b) $270^\circ$ counter-wind direction. .                                                                                    | 196 |
| 6.18 | Contour plots of $I = \sqrt{2/3k}/ u_h $ at $y = -90 \text{ m}$ for $270^\circ$ wind under a) stability class A and b) stability class D. . . . .                                                                                                           | 197 |
| 6.19 | Comparison of normalized profiles of the $v$ -velocity component for stability classes A, B, C and D for a) $90^\circ$ prevailing wind direction and b) $270^\circ$ . . . . .                                                                               | 199 |
| 6.20 | Comparison of normalized profiles of the $w$ -velocity component for stability classes A, B, C and D for a) $90^\circ$ prevailing wind direction and b) $270^\circ$ counter-wind direction. . . . .                                                         | 200 |
| 6.21 | Hourly averaged particle mass concentration iso-volume for non-dimensionalized concentration greater than $5 \times 10^{-4}$ , $90^\circ$ wind direction a) Stability class A, b) Stability class B, c) Stability class C and d) Stability class D. . . . . | 201 |

|      |                                                                                                                                                                                                                                                                                                      |     |
|------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|
| 6.22 | Hourly averaged particle mass concentration isovolume for non-dimensionalized concentration greater than $5 \times 10^{-4}$ , $270^\circ$ wind direction a) Stability class A, b) Stability class B, c) Stability class C and d) Stability class D. . . . .                                          | 202 |
| 6.23 | The boundaries of the computational domain used for the actual terrain simulations. . . . .                                                                                                                                                                                                          | 204 |
| 6.24 | Non-dimensionalized $u_\theta$ contour plots for $\theta = 310.1^\circ$ , on $16^{th}$ June. . . . .                                                                                                                                                                                                 | 206 |
| 6.25 | Non-dimensionalized $u_\theta$ contour plots for $\theta = 306.2^\circ$ on $6^{th}$ July. . . . .                                                                                                                                                                                                    | 207 |
| 6.26 | Non-dimensionalized $u_\theta$ contour plots for $\theta = 258.2^\circ$ , on $22^{nd}$ June. . . . .                                                                                                                                                                                                 | 208 |
| 6.27 | non-dimensionalized $u_\theta$ contour plots for $\theta = 240.5^\circ$ on $21^{st}$ June. . . . .                                                                                                                                                                                                   | 209 |
| 6.28 | non-dimensionalized $u_\theta$ contour plots for $\theta = 230.6^\circ$ , on $19^{th}$ June. . . . .                                                                                                                                                                                                 | 210 |
| 6.29 | Layout of Frisbee dust gauge positions relative to quarry pit. The gauges are indicated by solid black circles labelled DG1 to DG10. . . . .                                                                                                                                                         | 214 |
| 6.30 | Dust deposition observations compared to CFD and ADMS predictions, with and without wind variability correction and emission factor reduction for a) raw data and b) data on a logarithmic scale. The dotted line represents 2:1, solid line represents 1:1 and dashed line represents 1:2 . . . . . | 218 |
| 6.31 | Dust deposition observations compared to CFD and ADMS predictions for a) data normalized by the mean observed deposition and b) data normalized by the mean predicted deposition. The dotted line represents 2:1, solid line represents 1:1 and dashed line represents 1:2 . . . . .                 | 219 |
| 6.32 | Comparison of datasets falling within a factor of 2 of the observed deposition for ADMS and CFD predictions. . . . .                                                                                                                                                                                 | 220 |
| 6.33 | Comparison of datasets falling within a factor of 2 of the observed deposition for ADMS and CFD predictions after quantile-quantile data conditioning. . . . .                                                                                                                                       | 221 |
| 6.34 | a) UK-ADMS contour plot of dry deposition compared to the b) CFD Accretion rate contour for blast event on the $9^{th}$ of June. . . . .                                                                                                                                                             | 224 |
| 6.35 | a) UK-ADMS contour plot of dry deposition compared to the b) CFD Accretion rate contour for blast event on the $16^{th}$ of June. . . . .                                                                                                                                                            | 225 |
| 6.36 | a) UK-ADMS contour plot of dry deposition compared to the b) CFD Accretion rate contour for blast event on the $22^{nd}$ of June. . . . .                                                                                                                                                            | 226 |
| 6.37 | Comparison of the $k - \varepsilon$ model estimates of in-pit retention, to empirical estimates derived from Cole and Fabrick (1984) formula . . . . .                                                                                                                                               | 227 |

## List of Tables

|     |                                                                                                                                                                                  |     |
|-----|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|
| 2.1 | Maximum Particulate aerodynamic diameter of particle size range and the corresponding size fractions which comprise total fugitive dust according to BS6069 part 2:1994. . . . . | 8   |
| 2.2 | The types and crushing mechanisms of crushing plant at a typical stone quarry (DEFRA, 2004). . . . .                                                                             | 13  |
| 2.3 | Sources of dust at typical surface quarries and relevant dust abatement measures (Ghose and Majee, 2001; Kissell, 2003). . . . .                                                 | 15  |
| 2.4 | Aerodynamic roughness height for different types of surface cover Jacobson (1999) and USEPA (2008a). . . . .                                                                     | 37  |
| 2.5 | PGT Stability classes correlated to $L_{M0}$ and $R_i$ (Barthelmie, 1999; Woodward, 1999; Ashrafi and Hoshyaripour, 2008). . . . .                                               | 44  |
| 2.6 | Meteorological measurement quality objectives for multi-pollutant monitoring from USEPA (2008b) . . . . .                                                                        | 52  |
| 3.1 | Comparison of grid size and CPU resource demands for URANS and LES treatment of wall-bounded flow problem (Eggenspieler, 2011). . . . .                                          | 63  |
| 3.2 | Alinot and Masson (2005) $C_{\varepsilon 3}$ curve fitting expression coefficients . . . . .                                                                                     | 79  |
| 3.3 | $k - \varepsilon$ turbulence closure model constants . . . . .                                                                                                                   | 79  |
| 3.4 | Under-relaxation factors and convergence criteria for the computation of flow variables. . . . .                                                                                 | 80  |
| 3.5 | Alinot and Masson (2005) flow properties for the stable, neutral and unstable ABL. . . . .                                                                                       | 84  |
| 4.1 | Meteorological parameters used to define the three stability classes in the wind variability simulations. . . . .                                                                | 102 |
| 4.2 | Values of the Kolmogorov constant proposed by Degrazia and Anfossi (1998) for different atmospheric stability conditions. . . . .                                                | 107 |

|      |                                                                                                                                                                                                                                                                |     |
|------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|
| 4.3  | Values of the time scale constant derived from values of the Kolmogorov constant proposed in the literature . . . . .                                                                                                                                          | 107 |
| 4.4  | Lateral Plume Spread Predictions . . . . .                                                                                                                                                                                                                     | 117 |
| 5.1  | Meteorological Parameters . . . . .                                                                                                                                                                                                                            | 135 |
| 5.2  | Mesh refinement parameters for fine, medium and coarse meshes. . . . .                                                                                                                                                                                         | 135 |
| 5.3  | Coarse-grid Richardson error estimates . . . . .                                                                                                                                                                                                               | 138 |
| 5.4  | Buoyancy frequency and Froude number values for the stable ABL over the depressions. . . . .                                                                                                                                                                   | 150 |
| 6.1  | Values of $T$ and $\gamma/s$ at $P=1000$ mb, Holtslag and Van Ulden (1983) . . . .                                                                                                                                                                             | 175 |
| 6.2  | Average values of $L_{MO}$ corresponding to each PGT stability class for all meteorological data . . . . .                                                                                                                                                     | 177 |
| 6.3  | Coordinates of the centre point of the bench faces. . . . .                                                                                                                                                                                                    | 180 |
| 6.4  | Coordinates of blast bounding vertices and the average emission rate for each blast. . . . .                                                                                                                                                                   | 180 |
| 6.5  | Bounding vertices and average emission rate of representative blast calculated from averaging groups of overlapping blast. . . . .                                                                                                                             | 182 |
| 6.6  | Computational domain boundary conditions applied for different ranges of wind direction for the domain illustrated in Figure 6.23. . . . .                                                                                                                     | 204 |
| 6.7  | Coordinates of Frisbee Gauges in the domain. . . . .                                                                                                                                                                                                           | 215 |
| 6.8  | Values of $u_h$ , $\theta$ and $\sigma_\theta$ for blast events contributing the most to accumulated mass of dust at the gauges. . . . .                                                                                                                       | 215 |
| 6.9  | Predicted dust deposition from CFD and UK-ADMS numerical models compared to site observations of accumulated dust on Frisbee Gauge . . . . .                                                                                                                   | 216 |
| 6.10 | Statistical Performance metrics computed for CFD, with and without wind variability at 100% and 50% of emission factor, and UK-ADMS. Subscript “ <i>cond</i> ” denotes performance metrics computed after quantile-quantile conditioning of datasets . . . . . | 222 |

## Nomenclature

|                 |                                                              |
|-----------------|--------------------------------------------------------------|
| $\alpha$        | Aspect ratio                                                 |
| $\alpha_{PT}$   | Priestley-Taylor evaporation parameter                       |
| $\alpha_P$      | Pressure under relaxation factor                             |
| $\beta$         | Thermal volumetric expansion coefficient of air ( $K^{-1}$ ) |
| $\beta_r$       | Surface moisture constant                                    |
| $\beta_g$       | Buoyancy parameter ( $Kms^{-2}$ )                            |
| $\delta_{ij}$   | Kronecker-delta operator                                     |
| $\dot{m}_{avg}$ | Average fugitive dust emission rate ( $kgs^{-1}$ )           |
| $\ell$          | Characteristic Eddy length scale (m)                         |
| $\Gamma$        | Surface layer height (m)                                     |
| $\gamma$        | Psychrometric constant ( $PaK^{-1}$ )                        |
| $\Gamma_c$      | Full vegetation cover coefficient                            |
| $\Gamma_s$      | Bare soil cover coefficient                                  |
| $\kappa$        | von-Karman constant                                          |
| $\lambda$       | Thermal conductivity ( $Wm^{-1}K^{-1}$ )                     |
| $E$             | Latent heat flux ( $Wm^{-2}$ )                               |
| Fr              | Froude number                                                |

|                          |                                                                                      |
|--------------------------|--------------------------------------------------------------------------------------|
| NMSE <sub>r</sub>        | Random component of normalized mean square error                                     |
| NMSE <sub>s</sub>        | Systematic component of normalized mean square error                                 |
| NMSE                     | Normalized mean square error                                                         |
| R <sup>2</sup>           | Correlation coefficient                                                              |
| Re <sub>p</sub>          | Relative Reynolds number                                                             |
| $\mu$                    | Dynamic viscosity (kgm <sup>-1</sup> s <sup>-1</sup> )                               |
| $\mu_t$                  | Turbulent viscosity (kgm <sup>-1</sup> s <sup>-1</sup> )                             |
| $\overline{\phi}$        | Mean of scalar quantity                                                              |
| $\overline{A}$           | Weighted average accretion rate (kgm <sup>-2</sup> s <sup>-1</sup> )                 |
| $\overline{u_i}$         | Mean component of wind velocity (ms <sup>-1</sup> )                                  |
| $\phi_i$                 | Fluctuating component of scalar quantity                                             |
| $\phi_\varepsilon$       | $\varepsilon$ similarity flux function                                               |
| $\phi_{m,h}$             | Non-dimensional flux function for momentum/heat                                      |
| $\Pi_{m,h}$              | Buckingham-Pi Theory non-dimensional $\Pi$ groups for momentum/heat                  |
| $\Psi_h$                 | Monin-Obukhov Similarity function for heat                                           |
| $\psi_{m,h}$             | Diabatic non-dimensional flux integral term for momentum/heat                        |
| $\Psi_m$                 | Monin-Obukhov Similarity function for momentum                                       |
| $\rho$                   | Density of air (kgm <sup>-3</sup> )                                                  |
| $\rho_p$                 | Particle density (kgm <sup>-3</sup> )                                                |
| $\sigma$                 | Stefan-Boltzmann constant ( $5.67 \times 10^{-8}$ Wm <sup>-2</sup> K <sup>-4</sup> ) |
| $\sigma_\alpha$          | Total wind direction variability (deg)                                               |
| $\sigma_{\theta t}$      | ABL wind direction variability (deg)                                                 |
| $\sigma_\theta$          | External wind direction variability (deg)                                            |
| $\sigma_\theta$          | Standard deviation of wind variability (deg)                                         |
| $\sigma_\Theta^2$        | Temperature variance (K <sup>2</sup> )                                               |
| $\sigma_{k,\varepsilon}$ | Prandtl numbers for $k$ and $\varepsilon$                                            |

|                   |                                                                                                          |
|-------------------|----------------------------------------------------------------------------------------------------------|
| $\sigma_T$        | Turbulent Prandtl number                                                                                 |
| $\sigma_{u,v}^2$  | $u, v$ velocity variance components ( $\text{m}^2\text{s}^{-2}$ )                                        |
| $\sigma_y$        | Horizontal plume dispersion parameter (m)                                                                |
| $\sigma_z$        | Vertical plume dispersion parameter (m)                                                                  |
| $\tau$            | Surface shear stress ( $\text{Nm}^{-2}$ )                                                                |
| FAC2              | Proportion of data within factor of 2 of observations                                                    |
| FB                | Fractional Bias                                                                                          |
| MG                | Geometric mean bias                                                                                      |
| Pr                | Prandtl number                                                                                           |
| $\Theta$          | Potential Temperature (K)                                                                                |
| $\Theta_*$        | Convective layer scaling temperature (K)                                                                 |
| $\tilde{f}$       | Fourier transform function                                                                               |
| $\tilde{u}_{i,d}$ | Perturbation velocity ( $\text{ms}^{-1}$ )                                                               |
| $\varepsilon$     | Turbulent kinetic energy dissipation rate ( $\text{m}^2\text{s}^{-3}$ )                                  |
| $\varepsilon_p$   | Turbulent dissipation rate in wall adjacent cell ( $\text{m}^2\text{s}^{-3}$ )                           |
| $\varphi$         | Wall distance scalar (m)                                                                                 |
| $\zeta$           | Stability parameter                                                                                      |
| $a$               | Surface albedo                                                                                           |
| $A_i$             | Accretion rate for individual direction variation ( $\text{kgm}^{-2}\text{s}^{-1}$ )                     |
| $a_n$             | Alinot and Masson (2005) $C_{\varepsilon 3}$ curve fit coefficient                                       |
| $a1, a2, a3$      | Morsi and Alexander (1972) drag law constants for smooth spherical particles                             |
| $C$               | Mean concentration of a pollutant ( $\text{kgm}^{-3}$ )                                                  |
| $C(x, y, 0)$      | Near-ground concentration ( $\text{kgm}^{-3}$ )                                                          |
| $c_1$             | Empirical Swinbank (1963) heat transfer constant ( $5.31 \times 10^{-13} \text{ Wm}^{-2}\text{K}^{-6}$ ) |
| $c_2$             | Constant radiation flux ( $\text{Wm}^2$ )                                                                |
| $c_3$             | Surface heating coefficient                                                                              |

|                                                                  |                                                                                        |
|------------------------------------------------------------------|----------------------------------------------------------------------------------------|
| $C_\mu, C_{\varepsilon 1}, C_{\varepsilon 2}, C_{\varepsilon 3}$ | $k - \varepsilon$ model coefficients                                                   |
| $C_A$                                                            | Frisbee gauge collection area ( $\text{m}^2$ )                                         |
| $C_D$                                                            | Dimensionless drag coefficient                                                         |
| $c_G$                                                            | Ground cover coefficient                                                               |
| $C_{ks}$                                                         | Roughness constant                                                                     |
| $c_L$                                                            | Lagrangian integral time scale constant                                                |
| $C_o$                                                            | Kolmogorov constant                                                                    |
| $c_p$                                                            | Specific heat capacity of air at constant pressure ( $\text{kJkg}^{-1}\text{K}^{-1}$ ) |
| $C_{x,y,z}$                                                      | Pollutant concentration ( $\text{kgm}^{-3}$ )                                          |
| $D$                                                              | Depression/pit depth (m)                                                               |
| $d$                                                              | Zero plane displacement height (m)                                                     |
| $D_j$                                                            | Diffusion coefficient ( $\text{m}^2\text{s}^{-1}$ )                                    |
| $d_p$                                                            | Particle equivalent spherical diameter (m)                                             |
| $E$                                                              | Total Energy (J)                                                                       |
| $E_{coarse}$                                                     | Coarse grid error                                                                      |
| $E_{fine}$                                                       | Fine grid error                                                                        |
| $E_{ks}$                                                         | Empirical rough wall constant                                                          |
| $f\%$                                                            | Percentage cloud cover                                                                 |
| $f_{1,2}$                                                        | Fine/coarse grid solutions                                                             |
| $f_{100\%}$                                                      | Percentage cloud cover at 100% relative humidity                                       |
| $f_c$                                                            | Fractional canopy cover                                                                |
| $F_{dry}$                                                        | Dry deposition flux ( $\text{kgm}^{-2}\text{s}^{-1}$ )                                 |
| $F_D$                                                            | Specific drag force per unit velocity ( $\text{s}^{-1}$ )                              |
| $F_s$                                                            | Grid convergence safety factor                                                         |
| $G$                                                              | Ground heat flux ( $\text{Wm}^{-2}$ )                                                  |
| $g$                                                              | Acceleration due to gravity ( $\text{ms}^{-2}$ )                                       |

|           |                                                                              |
|-----------|------------------------------------------------------------------------------|
| $G_b$     | Buoyancy production term ( $\text{m}^2\text{s}^{-3}$ )                       |
| $G_k$     | Shear production term ( $\text{m}^2\text{s}^{-3}$ )                          |
| $GCI$     | Grid Convergence Index                                                       |
| $H$       | Boundary layer depth (m)                                                     |
| $h_{1,2}$ | Fine/coarse grid spacing                                                     |
| $h_c$     | Critical Froude number height (m)                                            |
| $h_{ref}$ | Reference height (m)                                                         |
| $I$       | Turbulent intensity                                                          |
| $k$       | Turbulent kinetic energy ( $\text{m}^2\text{s}^{-2}$ )                       |
| $K^+$     | Incoming solar radiation ( $\text{Wm}^{-2}$ )                                |
| $k_{1,2}$ | Fourier wave numbers in $x, y$ direction                                     |
| $K_h$     | Turbulent exchange coefficient for heat ( $\text{m}^2\text{s}^{-1}$ )        |
| $K_m$     | Turbulent exchange coefficient for momentum ( $\text{m}^2\text{s}^{-1}$ )    |
| $k_p$     | Turbulent Kinetic energy in wall adjacent cell ( $\text{m}^2\text{s}^{-2}$ ) |
| $k_s$     | Equivalent sand-grain roughness height (m)                                   |
| $k_s^+$   | Dimensionless equivalent wall roughness                                      |
| $L$       | Width of depression/pit (m)                                                  |
| $l$       | Inertial sub-range length scale (m)                                          |
| $L^+$     | Incoming long-wave radiation ( $\text{Wm}^{-2}$ )                            |
| $L^-$     | Outgoing long-wave radiation ( $\text{Wm}^{-2}$ )                            |
| $L_e$     | Eddy length scale (m)                                                        |
| $L_{MO}$  | Monin-Obukhov length (m)                                                     |
| $l_m$     | Characteristic mixing length (m)                                             |
| $M_T$     | Total collection mass of dust (kg)                                           |
| $N$       | Brunt-Väisälä buoyancy frequency ( $\text{s}^{-1}$ )                         |
| $\nu$     | Kinematic viscosity ( $\text{m}^2\text{s}^{-1}$ )                            |

|              |                                                                               |
|--------------|-------------------------------------------------------------------------------|
| $P$          | Absolute pressure (Pa)                                                        |
| $p$          | Formal order of accuracy of solution                                          |
| $P^*$        | Initial SIMPLEC pressure estimate (Pa)                                        |
| $P'$         | SIMPLEC Pressure correction term (Pa)                                         |
| $P_0$        | Atmospheric pressure (Pa)                                                     |
| $p_i$        | Probability of occurrence of wind direction variation                         |
| $Q$          | Heat flux ( $\text{Wm}^{-2}$ )                                                |
| $Q^*$        | Net surface radiation ( $\text{Wm}^{-2}$ )                                    |
| $Q_s$        | Pollutant emission rate ( $\text{kgs}^{-1}$ )                                 |
| $Q_w$        | Surface sensible heat flux ( $\text{Wm}^{-2}$ )                               |
| $R$          | Gas constant of air ( $\text{Jkg}^{-1}\text{K}^{-1}$ )                        |
| $r$          | Grid refinement ratio                                                         |
| $r_d$        | Radial distance from depression centre (m)                                    |
| $R_f$        | Flux Richardson number                                                        |
| $R_i$        | Non-dimensional Richardson number                                             |
| $Re_\Gamma$  | Global Reynolds number                                                        |
| $Re_z$       | Local Reynolds number                                                         |
| $RH$         | Relative humidity                                                             |
| $RH_{crit}$  | Threshold relative humidity for cloud formation                               |
| $RH_e$       | Critical relative humidity                                                    |
| $s$          | Slope of saturation specific humidity-temperature curve ( $\text{PaK}^{-1}$ ) |
| $S_\epsilon$ | Turbulence dissipation rate source term ( $\text{m}^2\text{s}^{-3}$ )         |
| $S_C$        | pollutant source term ( $\text{kgm}^{-3}$ )                                   |
| $S_E$        | Energy source term (J)                                                        |
| $S_k$        | Turbulent kinetic energy source term ( $\text{m}^2\text{s}^{-2}$ )            |
| $S_{u_i}$    | Momentum source term ( $\text{Nm}^{-3}$ )                                     |

|                       |                                                                    |
|-----------------------|--------------------------------------------------------------------|
| $T$                   | Absolute temperature (K)                                           |
| $T_0$                 | Reference Temperature (K)                                          |
| $T_*$                 | Surface layer scaling temperature (K)                              |
| $T_{\text{exposure}}$ | Exposure duration (s)                                              |
| $T_A$                 | Meteorological averaging time (hr)                                 |
| $T_a$                 | Near-surface air temperature (K)                                   |
| $T_D$                 | Temperature at valley edge (K)                                     |
| $T_L$                 | Lagrangian integral time (s)                                       |
| $T_s$                 | Ground surface temperature (K)                                     |
| $T_w$                 | Wall temperature (K)                                               |
| $T_z$                 | Temperature profile (K)                                            |
| $U_0$                 | Unperturbed wind speed ( $\text{ms}^{-1}$ )                        |
| $U_{10}$              | Reference wind speed at 10 m ( $\text{ms}^{-1}$ )                  |
| $u_*$                 | Friction velocity ( $\text{ms}^{-1}$ )                             |
| $u_h$                 | Wind velocity at reference height $h$ ( $\text{ms}^{-1}$ )         |
| $u_i$                 | Velocity component in $i$ direction ( $\text{ms}^{-1}$ )           |
| $u'_i$                | Fluctuating component of wind velocity ( $\text{ms}^{-1}$ )        |
| $U_m$                 | Unperturbed wind speed at top of middle layer ( $\text{ms}^{-1}$ ) |
| $u_p$                 | Particle velocity ( $\text{ms}^{-1}$ )                             |
| $u_z$                 | $u$ velocity component profile ( $\text{ms}^{-1}$ )                |
| $v_d$                 | Deposition velocity ( $\text{ms}^{-1}$ )                           |
| $v'_d$                | Turbulent component of deposition velocity ( $\text{ms}^{-1}$ )    |
| $v_t$                 | Gravitational setting velocity ( $\text{ms}^{-1}$ )                |
| $w_*$                 | Convective layer scaling velocity ( $\text{ms}^{-1}$ )             |
| $X_o$                 | Observed value of deposited mass (kg)                              |
| $x_o$                 | $x$ coordinate at pit/depression centre (m)                        |

|             |                                                  |
|-------------|--------------------------------------------------|
| $X_p$       | Predicted value of deposited mass (kg)           |
| $y^+$       | Dimensionless wall distance                      |
| $y_p$       | Distance to centroid of wall adjacent cell (m)   |
| $z'$        | Wall distance (m)                                |
| $z_0$       | Aerodynamic roughness height (m)                 |
| $z_i$       | Mixing layer depth (m)                           |
| $z_r$       | Terrain profile (m)                              |
| $z_s$       | Height of the source (m)                         |
| $z_s(x, y)$ | Shape profile of Ishihara et al. (1999) hill (m) |
| $Re_*$      | Friction Reynolds number                         |

## 1.1 A Brief History of Quarrying, from Ancient to Modern Times

Quarries have been central to the advancement of human civilization ever since early humans devised rudimentary tools and infrastructure to improve the habitability of their natural environments. Mineral extraction was one of the earliest forms of human industry, supplying ancient civilizations with stone for building, religious symbolism and the creation of tools, weapons and household implements (Tripcevich and Vaughn, 2013). The earliest history of large-scale quarrying activity recorded in Aswan, Egypt pre-dates 3500 BC. The ancient Egyptians constructed their Great Pyramids and obelisks from stone extracted from quarries in the Nile River basin (Kelany et al., 2009; Coulson, 2012). Using the stone products of quarries, other civilisations such as the Ancient Peruvians, Greeks and Chinese also built monumental structures- Machu Picchu, the Parthenon and the Great Wall respectively - which even today invoke wonder and awe in observers. In modern times, quarrying has advanced considerably, becoming a highly mechanised industry, however, the products of quarries are still inextricably linked to nearly every aspect of human industry and commerce.

Presently, surface quarries and their associated industries are nationally important to the UK, both in terms of the employment generated by the quarry sector and the significant economic contribution of mineral-based commodities to Gross Domestic Product (GDP) BGS (2014). Within the European Union, the UK is considered an important producer of quarry minerals, 80% of which are consumed by the construction sector (Highley et al., 2004; BGS, 2014). The Office for National Statistics estimates that the trade value of mineral based products was £2.4 billion in 2012. In particular, limestone and dolomite were the highest grossing mineral ores, contributing £543 million to the UK economy in 2012 (Bide et al., 2013; Office for National Statistics, 2014).

## 1.2 The Need for Improved Quarry Dust Dispersion Models

The main environmental emission associated with this extractive industry is fugitive dust, primarily generated from the attrition of granular rock and the subsequent entrainment of particulates into the ambient air. To give an idea of the polluting potential of UK quarries, the National Atmospheric Emissions Inventory (NAEI) has estimated a gross  $\text{PM}_{10}$  emission factor for all types of mineral extraction of 0.03 tonnes per kilo-tonne of extracted mineral. Consequently, surface quarries have been identified as significant primary contributors of  $\text{PM}_{10}$  and  $\text{PM}_{2.5}$  to the UK National Atmospheric Pollution Inventory (MacCarthy et al., 2011). Thus, they are regulated and permitted under the Integrated Pollution Prevention and Control (IPPC) regime of the Pollution Prevention Control Regulations 2003, and quarry operators are required to implement dust abatement strategies which minimize fugitive dust emissions and enable their installations to meet National Air Quality Objectives (NAQOs) for particulate matter. The UK Minerals Policy contained in the Technical Guidance to the National Planning and Policy Framework (DCLG, 2012) advises quarry operators to conduct a dust assessment study to identify site parameters which are likely to increase the potential for adverse impacts from dust emission. The Framework further recommends examination of the interaction between dust generating activities, site meteorology, topography and receptor locations and endorses the use of computer modelling techniques to fulfil this objective.

According to the Secretary of State's Guidance for Quarry Processes, quarry operators are required to adopt Best Available Techniques (BAT) for preventing and reducing dust emissions (DEFRA, 2004). It is recommended that this be achieved through the implementation of an Environmental Management System (EMS) which can assist in ensuring that quarry operations do not breach air quality objectives. During the planning and permitting stage of any quarry installation, operators are required to submit an audit and assessment of dust emissions likely to originate from both mobile and static sources during the projected lifetime of the quarry (AEA Technology plc, 2011). To this end, USEPA AP-42 emission factors are used in conjunction with calibrated plume dispersion models to facilitate successful positioning of monitoring networks and allow operators to evaluate the efficiency of abatement techniques.

Conventionally, numerical dispersion modelling methods have involved the application of Gaussian-based models such as the UK Atmospheric Dispersion Modelling System (UK-ADMS) and the US Environmental Protection Agency equivalent, AERMOD, to predict the dispersion of fugitive dust plumes from quarry emission sources and ensure regulatory compliance. However, whilst these models have relatively fast solution times and are able to predict dust dispersion under a range of meteorological conditions, Gaussian model algorithms offer an over-simplified resolution of the atmospheric flow-field and are therefore more suited to the modelling dispersion of gaseous plumes emitted from elevated sources over flat terrain. In this regard, Lowndes et al. (2008) concluded that the reliability of conventional Gaussian model predictions is reduced where the entrainment and dispersion of fugitive dust is complicated by in-pit and surrounding topography as well as the dynamic

nature of dust emissions.

Furthermore, within a typical quarry, the terrain gradient is likely to exceed the 1:3 tolerance imposed for reliable application of the Gaussian model complex terrain algorithm. Indeed, work by Silvester et al. (2009) has demonstrated that conventional Gaussian models are severely challenged by complex terrain and are unable to account for in-pit fugitive dust retention due to terrain effects. As a result, they significantly over-predict the long-range transport of particulates by as much as 60%. Consequently, the use of Gaussian model predictions to inform the selection and implementation of fugitive dust abatement strategies for compliance with environmental regulations is likely to result in over-design of these abatement systems. As far as the Environmental Agency is concerned, conventional dispersion models are fit for purpose, their over-predictions inadvertently ensure that quarries consistently operate within a large factor of safety with regard to dust abatement. However, whilst the conservativeness of conventional model predictions may be favourable for environmental protection, it is uneconomical for quarry operators. A need therefore arises to develop new dispersion models which can handle complex terrain and by extension, resolve the internal flow regimes which occur as a result of significant perturbation of the Atmospheric Boundary Layer by pit topography. Ultimately, these models will safeguard against considerable over-design of dust abatement systems, thus proving beneficial for quarry productivity and unit operating costs.

To this end, Silvester et al. (2009) have demonstrated that Computational Fluid Dynamics (CFD) models such as the standard  $k - \varepsilon$  turbulence model, may be used under neutral stability conditions to satisfactorily replicate the complex internal flow regimes observed within surface quarries. Silvester et al. (2009) also recommended consideration of atmospheric stability conditions to obtain more realistic predictions of the atmospheric dispersion of fugitive dust that may arise under actual meteorological conditions. Therefore, this project seeks to develop CFD models which can replicate the dust dispersion and deposition patterns observed from surface quarry blasts under the range of meteorological conditions measured on site. The computational demand of two equation RANS models such as the standard  $k - \varepsilon$  turbulence model is relatively low compared to other CFD methods. Consequently, this model may be applied to investigate the effects that different meteorological conditions can have on the dispersion of fugitive dust emitted from multiple bench blasting events.

In recent years, the results of studies which have applied the standard  $k - \varepsilon$  model as an atmospheric boundary layer modelling tool have been communicated in peer reviewed literature. In particular, Alinot and Masson (2005) demonstrated that the  $k - \varepsilon$  model coefficients and closure equations may be modified to make them compatible with the Monin-Obukhov Similarity scaling laws which characterise the atmospheric surface layer. The adoption of this transformation, permits the use of the standard  $k - \varepsilon$  model to investigate the dispersion of fugitive dust emissions from surface quarries under actual meteorological conditions.

### 1.3 Aims and Objectives

#### Research Aim

The major driver of this research project is the identified need to address the shortfalls of current quarry dust dispersion modelling practice. Therefore, the principal aim of the project is to propose a Computational Fluid Dynamics model which can satisfactorily predict the near source dispersion and deposition of fugitive dust from quarry blast emissions under a range of meteorological conditions representative of diurnal variations in atmospheric stability. The project will also seek to perform a critical evaluation of the dust deposition predictions of the proposed  $k - \varepsilon$  turbulence model and compare its performance to that of UK-ADMS.

#### Research Objectives

The modelling methodology will be carried out in a series of discrete stages, in order to extend the functionality of the standard  $k - \varepsilon$  model and adapt it for use as a coupled quarry dust dispersion model. Throughout this process of model development, the research project will seek to meet the following main objectives,

1. to explore the characterization of the atmospheric surface layer and the selection of a set of mathematical equations to parametrize the surface layer flow-field under stable, neutral and unstable atmospheric stability conditions.
2. to implement an approach for maintaining horizontal homogeneity of the undisturbed atmospheric profiles in the  $k - \varepsilon$  model, which is universally applicable to the stable, neutral and unstable atmosphere.
3. to develop a method of accounting for mesoscale wind direction variability in the CFD model which delivers lateral plume spread predictions on par with those of UK-ADMS.
4. to use the proposed  $k - \varepsilon$  model to investigate the influence of idealized valley topography on the structure of the turbulent flow-field and the subsequent dispersion of particulates entrained in this flow-field. Additionally, the study of flow over idealized topography will be used to precisely ascertain the terrain aspect ratios which challenge the reliability of UK-ADMS predictions.
5. to implement a strategy for deriving the requisite atmospheric parameters from routinely measured meteorological variables in order to adequately describe the turbulent state of the atmosphere in the proposed  $k - \varepsilon$  model.
6. To use field measurements of dust deposition to validate the proposed  $k - \varepsilon$  CFD model and evaluate the degree of uncertainty in model predictions through the use of various statistical performance metrics. In this way, it will be possible to verify whether quantifiable gains in prediction accuracy may be realised through the use of CFD modelling methods.

## 1.4 Overview of Thesis Content

### Chapter 2: Literature Review

Chapter 2 will give context to the problem being studied, by presenting a description of surface quarry operations, the associated mechanisms of dust liberation and the classification and monitoring of fugitive dust. An overview of various dispersion modelling approaches is presented including a number of CFD approaches that have been employed by other researchers to predict dispersion over complex terrain. The second section of this chapter presents a critical review of the literature used to establish the appropriate mathematical characterization of the atmospheric boundary layer.

### Chapter 3: Optimization of the Numerical Model

This chapter presents an evidenced argument to support the application of a buoyancy modified  $k - \varepsilon$  model for dispersion modelling from near-surface fugitive dust emissions. In particular, the chapter examines how the challenge of maintaining horizontal homogeneity of atmospheric profiles can be overcome. The chapter will describe the implementation of stability modifications to the turbulence closure equations as well as appropriate boundary conditions and solver settings which can enable replication of stable, neutral and unstable atmospheric flow-fields.

### Chapter 4: Accounting for Wind Direction Variability

The under-prediction of lateral plume spread observed in CFD models by Riddle et al. (2004) is discussed in this chapter. A methodology is presented to incorporate wind direction variability in the model to account for the contribution of mesoscale atmospheric phenomena to lateral dispersion of a pollutant plume. The Discrete Phase Model (DPM) will be coupled to the turbulence model for the stochastic tracking of particles and calibration of the DPM model constant  $c_L$  will be examined.

### Chapter 5: Flow and Dispersion over Idealized Depressions

This chapter presents an analysis and discussion of the results of the CFD model simulation of the atmospheric flow-field predicted over a series of idealized, circular depressions of cosine profile and with aspect ratios of 8, 4, 2.67 and 2, respectively. The combined effects of varying aspect ratio and atmospheric stability on the predicted flow-field will be examined. Moreover, the effects of terrain-induced flow-field perturbations on the dispersion of particulates will be studied.

### Chapter 6: A Case Study of Old Moor Quarry

This thesis will culminate in a case study of dust dispersion and deposition from the Old Moor limestone quarry situated in Buxton, Derbyshire. In the first instance, the effects of the internal pit terrain on the flow-field will be investigated without the influence of external orography. Following on from this, the computational domain will be extended to include external orography, thereby permitting an examination of the influence of external

landforms on the flow-field. The chapter will describe the model validation exercise in which dust deposition field measurements will be used to validate the model in accordance with model performance criteria recommended by Hanna et al. (2004).

### **Chapter 7: Conclusions and Further Work**

This thesis concludes with a summary of the major findings of each component of the research project and how these have strengthened the case for the adoption of CFD methods in surface quarry fugitive dust dispersion studies. Recommendations for further work will be made to outline a course for future improvements to the numerical model which were outside the scope of this project.

## 2.1 Surface Quarries

Every aspect of surface mining operations can generate significant fugitive dust emissions which have the potential to produce adverse effects on the environment, human health, occupational safety and quarry productivity (Appleton et al., 2006; Kingman et al., 2009). Therefore, for any surface quarry installation, mineral throughput demands are tempered by increasingly stringent environmental standards to mitigate the harmful effects of fugitive dust and maintain acceptable ambient air quality. These have contributed to an increase in the planning and operational constraints faced by quarry operators.

### 2.1.1 Definition of Fugitive Dust

Fugitive dust consists of particulate emissions to the ambient air from diffuse sources, where the resultant flow stream is unconfined. These emissions arise from the abrasion or attrition of rock and soil material through mechanical means or wind action and are difficult to quantify (USEPA, 1998). The studies of Appleton et al. (2006) and Silvester et al. (2009) have adopted the definition of quarry fugitive dust as consisting of particulates with aerodynamic diameters ranging between 1 to 75  $\mu\text{m}$ , according to British Standard BS6069 part 2:1994. Mass fractions for particle size ranges which constitute fugitive dust are given in Table 2.1, from which it may be observed that particles of maximum aerodynamic diameter  $\leq 10 \mu\text{m}$  form 50% of the sampled mass fraction, in accordance with recommendations in the Michigan Department of Environmental Quality air emissions calculation technical report (MDEQ, 2014).

The UK National Atmospheric Emissions Inventory is primarily concerned with the finer particulates of aerodynamic diameter  $\leq 10 \mu\text{m}$ , as this size fraction has a longer suspension time due to its low deposition velocity and is transported further than coarser fractions. Particles in this size range are classified as either thoracic or respirable particles because they are small enough to be aspirated beyond the human larynx (BSI, 1993), whereby they may contribute to the onset of various pulmonary disorders and pneumoconioses in quarry

Table 2.1: Maximum Particulate aerodynamic diameter of particle size range and the corresponding size fractions which comprise total fugitive dust according to BS6069 part 2:1994.

| Dust size range ( $\mu\text{m}$ ) | Maximum particle aerodynamic diameter of size range ( $\mu\text{m}$ ) | Size fraction |
|-----------------------------------|-----------------------------------------------------------------------|---------------|
| 30 - 75                           | 75                                                                    | 0.30          |
| 10 - 30                           | 30                                                                    | 0.20          |
| 2.5 - 10                          | 10                                                                    | 0.45          |
| 1.0 - 2.5                         | 2.5                                                                   | 0.05          |

workers and nearby receptor populations (NIOSH, 1974; WHO, 2000). Figure 2.1 illustrates the various classifications of fugitive dust applied by BSI (1993) according to the degree of penetration into the human respiratory tract. Coarser particulates of aerodynamic diameter  $30\text{ }\mu\text{m}$  to  $100\text{ }\mu\text{m}$  are termed inhalable dust and do not penetrate beyond the upper airways, they do however contribute to soiling, atmospheric turbidity and may increase the wear of mechanical equipment (Cleaner Quarries, 2004). Thoracic dust particulates of aerodynamic diameter between  $10\text{ }\mu\text{m}$  and  $30\text{ }\mu\text{m}$  are generally deposited in the trachea or bronchial tubes. However, the respirable particulates of diameter less than  $10\text{ }\mu\text{m}$  are the most hazardous to human health as these can penetrate to the alveoli and those with a diameter of about  $2\text{ }\mu\text{m}$  are likely to experience maximum deposition in the alveolar region (WHO, 2000).

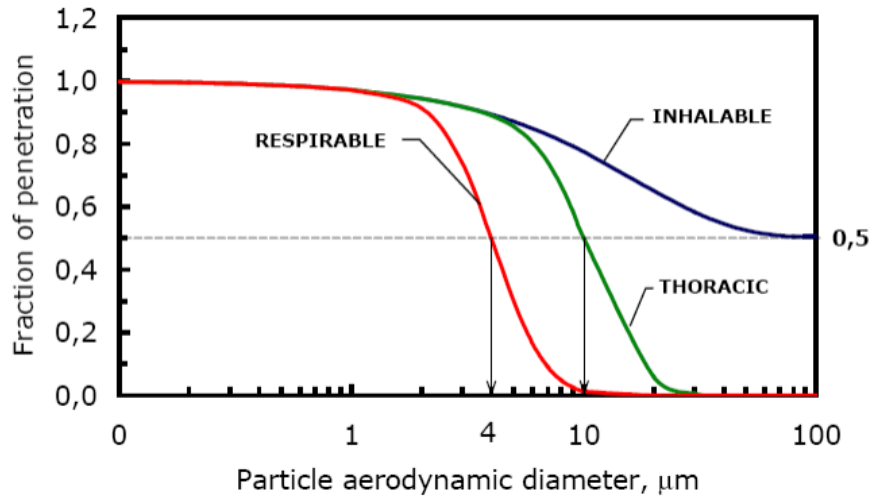


Figure 2.1: Airborne dust particle aerodynamic diameter classified according to fractional penetration into the human respiratory tract (Jimenez et al., 2011).

### 2.1.2 Dust Generation from Quarry Processes

Figure 2.2 illustrates the sequence of extraction and processing activities at a typical limestone quarry. The extracted mineral rocks are transported between each stage of processing via unpaved haul roads which are constructed from graded and compacted parent rock material. Due to the frequency of mechanical disturbance to the unpaved road surface, haul roads are the principal generator of fugitive dust in surface quarries, accounting for over 50% of total fugitive dust emission (Ghose and Majee, 2001). However, Watson and Chow (2000) and Kissell (2003) note that dust abatement strategies such as road wetting and the application of dust suppressant chemicals can achieve haul road dust control efficiencies of between 70 to 90%. Thompson and Visser (2007) advise that reduction of vehicle speeds can also alleviate haul road dust emissions. Furthermore, Countess (2001) and Veranth et al. (2003) observed that a significant proportion - as much as 75%, of haul road dust entrained in the flow-field at heights of 1 to 2 m above the road surface by vehicle attrition or wind action, settles out within 6 m of the road edge in the absence of strong vertical wind components.

The drill and blast mining method is commonly employed at limestone quarries as an economical and reliable means of displacing and fragmenting the rock face to extract the minerals (Simangunsong et al., 2004). Kose et al. (2005) estimated that 20-25% of unit production costs of quarry operations goes towards achieving optimal fragmentation. The initial rock fragmentation and the resultant blast pile size distribution achieved through blasting must conform to quarry plant capabilities. In particular, the type and capacity of the loading, transport and comminution machinery will have been selected and sized to operate efficiently within specific rock fragmentation size ranges. A secondary blast objective is to produce a looser packed muck pile profile, thereby improving mineral reclaim, handling and processing efficiency. The bench blasting method involves a sequential number of operations including,

- (i) drilling of a number of holes to a given depth and pattern along a length of rock bench as illustrated in Figure 2.3,
- (ii) charging these holes with explosives and detonators,
- (iii) packing of charged holes with inert materials to facilitate optimum rock fragmentation and blast pile profile.

Post blast, the material is loaded by hydraulic or electric mobile shovels onto flat-bed dump trucks for transport to the quarry primary crushing circuit.

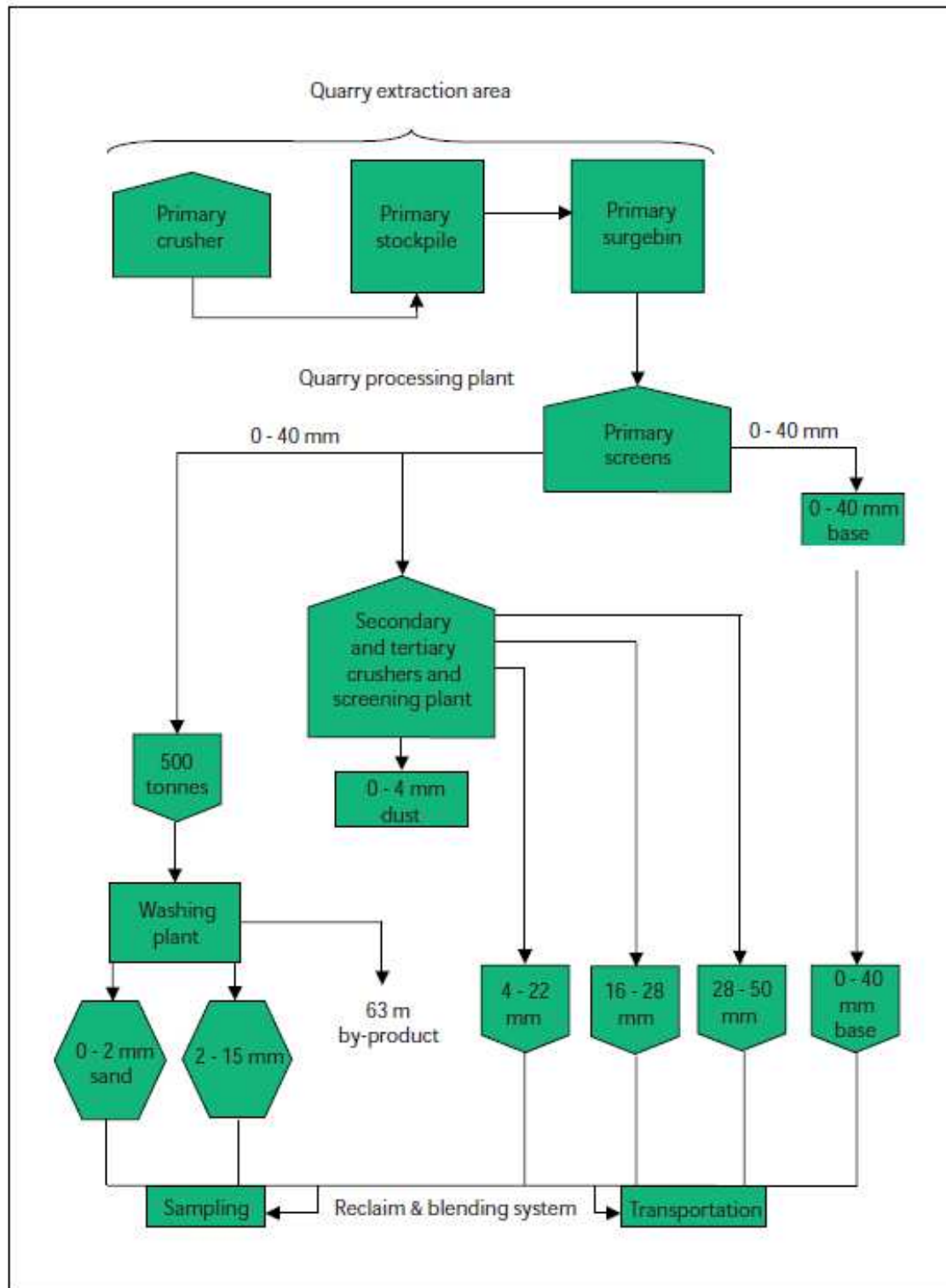


Figure 2.2: Extraction and processing sequence at rock quarry from DEFRA (2004).

The most commonly used explosive charge consists of a combination of Ammonium Nitrate and 5.8-8% fuel oil (ANFO) (USEPA, 1980). Cevizci and Ozkahraman (2012) recently described the different blast design practices that may be employed to optimize the fragmentation. In particular, stemming has been used to pack the top of drill holes with inert materials atop the explosive charges, to direct energy from expanding blast gases laterally into the fragmentation of the surrounding rock mass, rather than out the top of the drill hole. Mitchell (2009) observed that improved rock fragmentation is associated with increased generation of fines, which are a potential source of fugitive dust emissions. Currently, the optimization of blast design is principally driven by a desire to improve the processing efficiency of the product as opposed to minimization of fines. However, research studies carried out by Djordjevic (2002) and Onederra (2004) have examined the use of finite element numerical methods to model blast-induced rock fragmentation and demonstrated that numerical models of blast fragmentation could be used to optimise blast design and ultimately reduce the generation of fines. The dispersion of the fugitive dust emissions

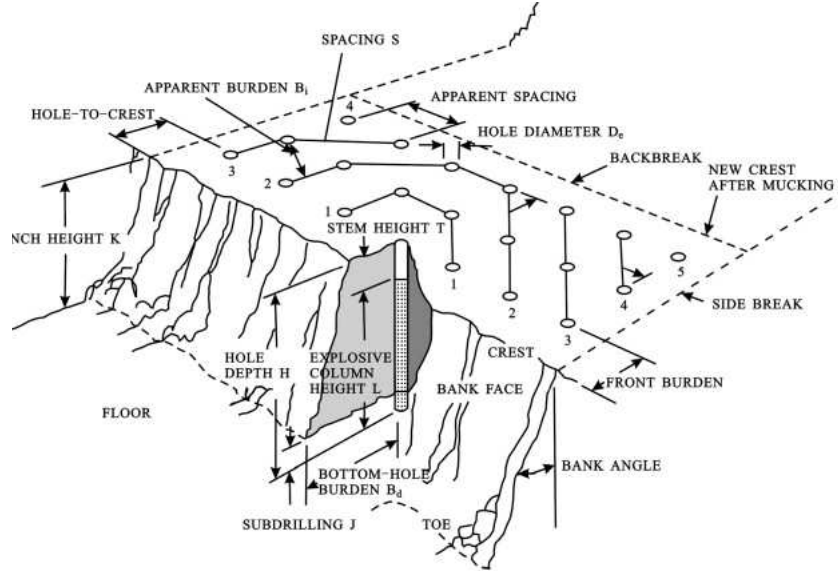


Figure 2.3: Typical configuration of blast drill holes and explosive charge for a bench blast at a rock quarry, from Kulatilake et al. (2010).

produced on a bench blast are heavily influenced by the prevailing atmospheric conditions. Initially, the momentum of the blast dust cloud is quickly dampened by the surrounding atmosphere and particles are subsequently transported by the wind field (Silvester et al., 2009). Silvester et al. (2006) used frames captured at intervals of 0.4 s from video footage of a representative blast to estimate the initial momentum of the blast cloud. The horizontal extent of the blast front in each of the frames was used to deduce the horizontal velocity profile of the cloud. Figure 2.4 shows that the initial velocity of the blast cloud rapidly decays from a peak of  $25 \text{ ms}^{-1}$  to that of the background flow regime within about 3 s of the explosion.

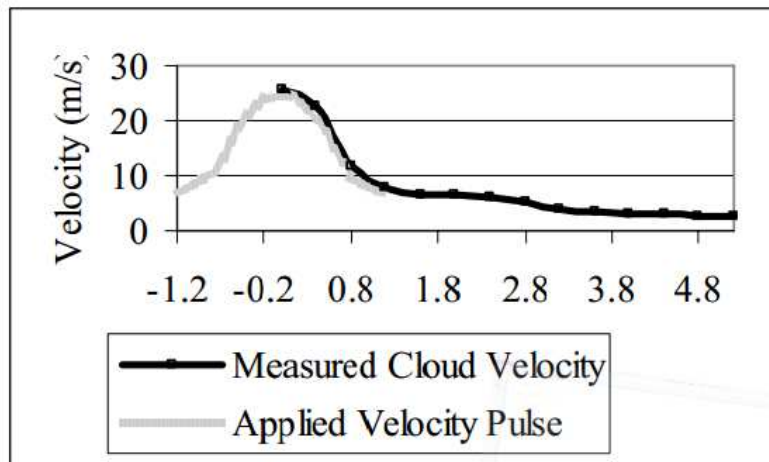


Figure 2.4: Horizontal velocity profile of advancing blast cloud with time, estimated from video footage (Silvester et al., 2006).

Blast emissions are essentially instantaneous particulate injections which entrain a relatively high mass loading of dust particles into the ambient air and whilst fugitive dust from other sources can be effectively mitigated through the use of emissions control devices and dust suppression measures, active control strategies for fugitive dust from bench blasting can prove costly and difficult to implement. For example, the use of wet suppression measures, involving wetting of the bench and the surrounding rock surfaces prior to a blast can interfere with the performance of explosives and detonators. Consequently, at many surface quarries, blast emissions are generally not subject to active control strategies and instead passive dust mitigation is relied upon, hence Ghose and Majee (2001) and the Department for Communities and Local Government in DCLG (2005) have advised quarry operators to utilise knowledge of site meteorology, surrounding topography and vegetative cover to minimise fugitive dust emission and dispersion from a blast.

In addition to haul road and blast sources, fugitive dust emissions are also generated when rock from the muck pile is loaded into trucks and transported to the processing plant, where extracted material is transferred via conveyors to crushing and screening equipment. The quantity of dust generated at each stage of production depends on the volume of aggregates extracted and the physical properties of the mineral, namely moisture content, brittleness and percentage fines (Countess Environmental, 2006). At intermediate stages of the processing cycle, aggregates are often stored in uncovered stockpiles which are susceptible to wind erosion. Dust emission from stockpiles peaks during the loading and reclaim of material, fortunately, the erodibility of a stockpile is reduced over time by consolidation of the material (Countess Environmental, 2006).

Size reduction of extracted mineral rocks is carried out in comminution circuits as illustrated by Figure 2.5. The types of primary and secondary crushing plant installed at a quarry

depend on the desired mineral quality and the intended use of the finished rock (DEFRA, 2004). The main types of crushing plant that may be employed at a quarry processing circuit are listed in Table 2.2, Within the processing circuit, the intermediate mineral product may

Table 2.2: The types and crushing mechanisms of crushing plant at a typical stone quarry (DEFRA, 2004).

| Crusher type          | Crushing mechanism                                            | Processing stage                                |
|-----------------------|---------------------------------------------------------------|-------------------------------------------------|
| Jaw crusher           | Use mechanical jaws to apply pressure to break rock           | primary crushing                                |
| Impact crusher        | Use force of impact against rotating or stationary components | tertiary crushing                               |
| Gyratory/cone crusher | Crushing head rotating against rocks in cone chamber          | primary (gyratory), secondary & tertiary (cone) |
| Attrition crusher     | Use abrasion to produce fine aggregates                       |                                                 |

be separated into specific size fractions by the use of appropriately sized mesh screens. Rocks may also be washed to remove excess fines and deleterious material which may adversely affect the finished aggregate quality (DEFRA, 2004).

From the aforementioned description of quarry processes, it is clear that the extraction and processing of mineral ores at surface quarries involve considerable attrition of the parent rock, which in the absence of satisfactory abatement measures may result in the liberation of significant quantities of fugitive dust. Therefore quarry operators have come to rely on the dust abatement measures listed in Table 2.3, for the mitigation of excessive dust generation from the main sources of fugitive dust identified within the quarry.

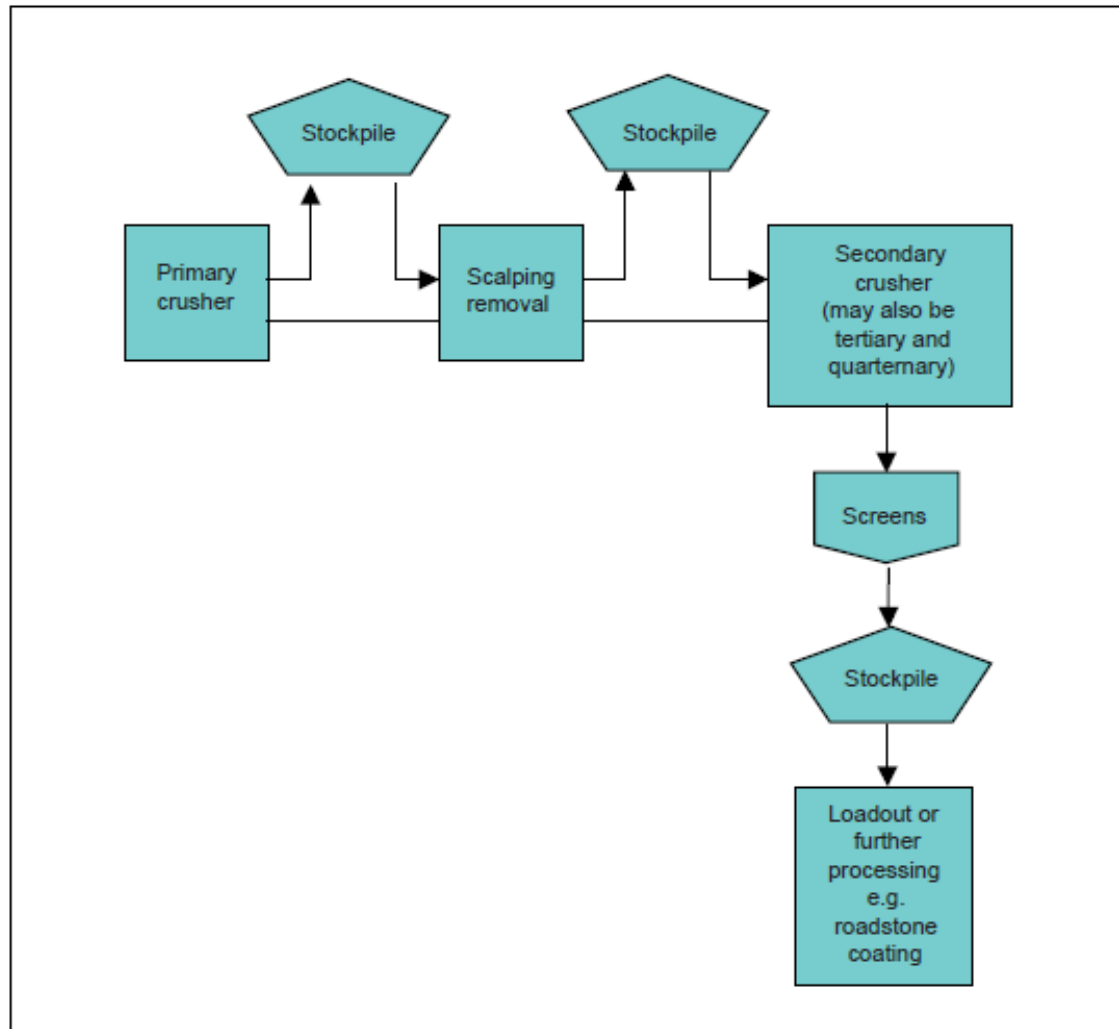


Figure 2.5: Crushing and screening sequence at a rock quarry from DEFRA (2004).

Table 2.3: Sources of dust at typical surface quarries and relevant dust abatement measures (Ghose and Majee, 2001; Kissell, 2003).

| Fugitive Dust Source        | Control Measures                                                                                                                                                                  |
|-----------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Drilling                    | Cyclone and bag filters, water and detergent suppression of dust                                                                                                                  |
| Blasting                    | water sprays, using knowledge of atmospheric conditions                                                                                                                           |
| Unpaved haul roads          | haul road wetting, application of surfactants, soil stabilizers, use of geo-textiles and polymer membranes, hygroscopic compounds such as calcium chloride, lime, sodium silicate |
| Loading and unloading       | manual water sprays with detergent, enclosures around loading and unloading areas                                                                                                 |
| Mobile processing equipment | Water sprays, cyclones, filters                                                                                                                                                   |
| Stockpiles                  | water sprays, vegetation barriers                                                                                                                                                 |
| Windblown dust              | water sprays, stockpile enclosures, vegetation barriers                                                                                                                           |

The complex topography of a surface quarry, illustrated in Figure 2.6, arises from the construction of slopes and benches which allow safe access to, and maximize the recovery of the target minerals. In hard-rock quarries, multi-bench slopes are designed to provide access to mineral workings at different elevations and also as a safety feature to catch falling debris (Allington et al., 2007). Due to slope stability considerations, the dimensions and slope angles of quarry benches are dependent on the geological properties of the rock-face. Additionally, the bench configuration will be guided by excavation capabilities of on-site equipment and the orientation and grade restrictions imposed on ramps and haul roads. Typically, the heights and face angles of the benches may be selected to maximize the quantity of minerals that may be safely exploited at minimal unit production cost (Kose et al., 2005; Matheson and Duthie, 2010), however, in many UK quarries, after-use and restoration plans may also inform the design of haul road slopes and benches (Allington et al., 2007).

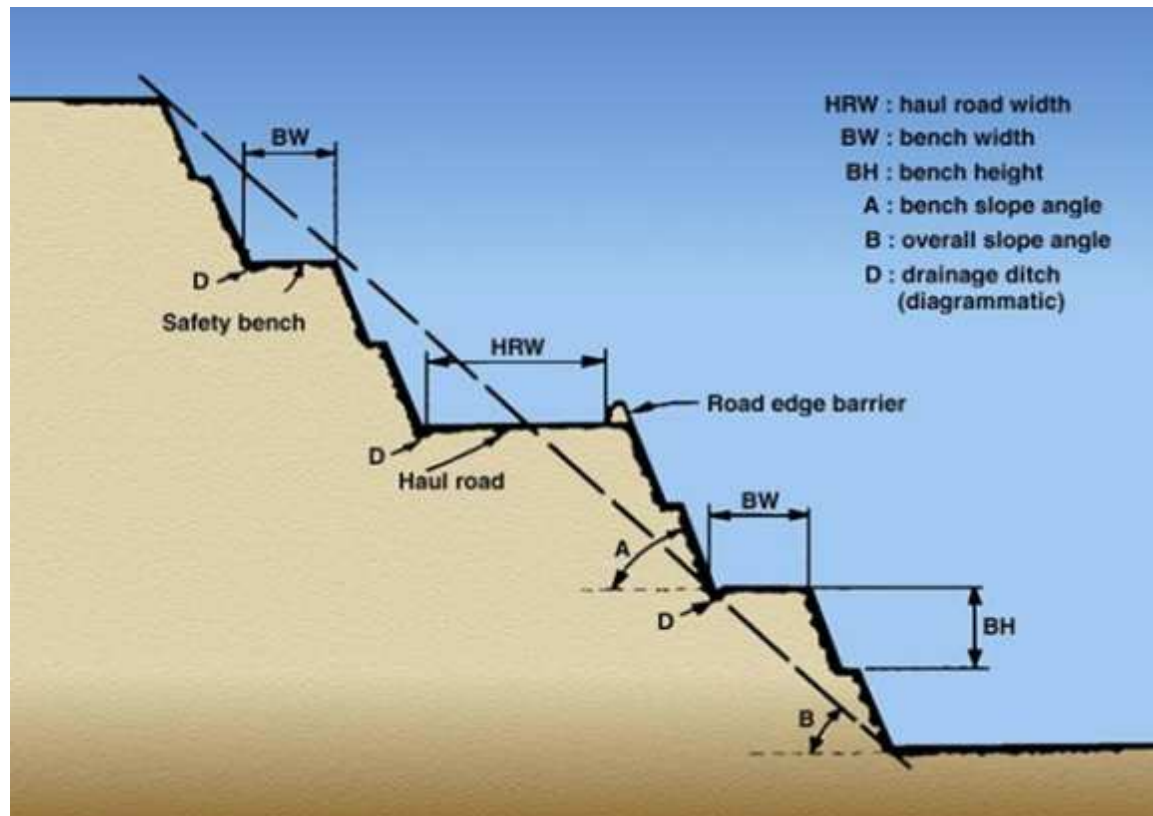


Figure 2.6: Quarry benches and face excavation profile of a typical rock quarry, showing the arrangement of haul roads and extraction faces and the various slope angles for slope stability considerations (Hem, 2012).

### 2.1.3 Monitoring and Measurement of Fugitive Dust

In 2008, rock quarrying contributed 11.9 kilotonnes of  $PM_{10}$  to the total UK National  $PM_{10}$  inventory of 132.9 kilotonnes, accounting for half the  $PM_{10}$  contribution from the extractive industries and ranking as the third largest  $PM_{10}$  emission source after combustion and agriculture (AEA Technology plc, 2011). Consequently, the monitoring of particulate emissions from surface quarries is required by the Environmental Permitting Regulations (EPR) 2010 and the EU Integrated Pollution Prevention and Control (IPPC) Directive (2008/1/EC). Dust monitoring campaigns are expected to establish baseline particulate levels, assess the environmental impact of quarry operations and quantify the effectiveness of dust abatement measures (Agency, 2013). Quarry operators have recourse to various dust measurement techniques which may involve active or passive sampling of the dust-laden air. As an example of active sampling methods, high volume air samplers may be employed to capture particulates from a sampled air stream isokinetically removed from the ambient air flow by a constant flow exhaust pump. The quantity and size distribution of the dust carried by the sampled air stream may be measured using a combination of gravimetric and optical analysis methods.

The Tapered Element Oscillating Microbalance (TEOM) is another example of an active monitoring system which may be used to sample particulates of a specific size range from the air stream. Dust-laden air is drawn into the TEOM, where dust particles collect on replaceable filter cartridges mounted on the narrow end of a hollow tapered tube. The base of the tube is fixed, the narrow tip which supports the filter medium is free to oscillate (Patashnick and Rupprecht, 1991). Particles accumulating on the filter cartridges increase the mass of the free end of the tapered element and alter the frequency of oscillations of the tube. An electronic feedback system which uses a combination of a Light Emitting Diode (LED) and photo transistor relays a signal to a counter allowing the frequency of oscillation to be stored in the memory of a data processing unit. The particle mass is subsequently determined, using the equations of motion for simple harmonic oscillations (Cantrell et al., 1996). By combining the particle mass loading with the flow rate of air through the system, the TEOM is able to offer continuous, real-time measurements of airborne dust concentration (Patashnick and Rupprecht, 1991). Active sampling methods such as the TEOM, have the ability to offer both directional sensitivity and short-term measurements, but they are costly to operate and are typically used to address acute occupational health and safety concerns (AEA Technology plc, 2011).

Alternatively, passive dust monitoring systems involve the use of stationary deposition gauges which rely on the collection of impacted dust and are suitable for the long-term (one week to one month) monitoring of nuisance dust. Passive gauges are typically mounted at heights of between 1 m to 2 m above the ground surface, free of flow obstructions such as vegetation and buildings which may bias the sample collected.

Non-directional sampling systems consist of gauges which collect dust falling out of the air stream from any direction, followed by gravimetric analysis of the deposited dust. The most popular passive gauge is the omni-directional Frisbee gauge, which consists of a pole mounted Frisbee-shaped collector with a collection bottle for rainwater as shown in Fig-

ure 2.7. Frisbee gauges have an optimal aerodynamic shape and therefore offer higher collection efficiencies than other non-directional deposition gauges such as the BS 1747: Part 1 deposit gauge and ISO deposit gauge (Vallack, 1995; Agency, 2013). Hall et al. (1994) note that Frisbee gauges are susceptible to dust blow-out in high winds, and their average collection efficiency is only about 50% in typical wind conditions. Vallack (1995) recommend that poor collection efficiency and susceptibility to wind blow-out may be easily remedied by the use of either a polyester foam insert or a liquid paraffin coating which allows the Frisbee to retain the collected dust. Frisbee gauges are best suited for measuring dust deposition in  $\text{mgm}^{-2}\text{day}^{-1}$  over a range of exposure time periods, typically lasting from one week up to one month.



Figure 2.7: Non-directional Frisbee gauge in-situ (AEA Technology plc, 2011).

Directional sampling and measurement methods are preferred where it is necessary to establish the directionality of the dust emission such as to differentiate the contributions of multiple sources. Directional monitoring of dust can be achieved using the DustScan<sup>TM</sup> technique which involves the use of a network of vertically mounted cylindrical sticky pads to intercept and collect a representative sample of the dust fraction being transported in the air stream (Datson and Fowler, 2007). Unlike the gravimetric, passive Frisbee sampling methods described previously, an optical image analysis of the dust size fractions collected on the network of the Dustscan<sup>TM</sup> cylindrical collection tapes, allows for an estimation of dust flux from a specific direction. The airborne dust concentration is determined by an evaluation of the loss of light reflectance transmitted by the sticky pads due to dust soiling, expressed as Effective Area Coverage (EAC%) (Datson and Fowler, 2007; Agency, 2013). The DustScan<sup>TM</sup> system and other directional methods such as dust slides which assess dust

soiling rate on the basis of loss of reflectance, are preferred for short term measurements ranging from one to two weeks.

In order that quarry operations remain compliant with Environmental Regulations, dust emission measurements must not exceed statutory limits stipulated in the ambient air quality standards. In the UK, the National Air Quality Objectives (NAQOs) set the maximum airborne concentrations limits for  $\text{PM}_{10}$ , such that the 24 hour mean is  $50 \mu\text{gm}^{-3}$ , not to be exceeded more than 35 times per year and the annual mean is  $40 \mu\text{gm}^{-3}$  (DEFRA, 2009). Statutory limits for dust deposition are not officially established, however UK custom and practice thresholds dictate that dust deposition levels exceeding the annual mean of  $200 \text{mgm}^{-2}\text{day}^{-1}$  constitute a serious nuisance (AEA Technology plc, 2011).

## 2.2 The Use of Numerical Models to Predict Quarry Dust Dispersion

Zanetti (1990) described dispersion modelling as an important intermediate step in the design and implementation of emission reduction and control measures. To this end, new generation Gaussian models with improved algorithms such as UK-ADMS, AERMOD and CALPUFF are approved for use by the UK Environmental Agency to support Environmental Impact Assessments submitted as part of current or future planning and permitting applications for quarry installations (Appleton et al., 2006; Carruthers et al., 2009).

Di Sabatino et al. (2007) noted that due to their widespread use, Gaussian dispersion models have benefited from extensive model validation and standardization of modelling protocols, and offer the advantage of permitting the user to model the contribution of a large number of emission sources simultaneously for many hours of meteorological data within a short processing time. Riddle et al. (2004) proposed that the UK-ADMS Gaussian model was well suited for modelling the dispersion of pollutants from elevated sources in simple terrain scenarios, since it placed a relatively low demand on computational resources and offered a simple numerical set-up. Gaussian-based modelling packages, such as UK-ADMS, include a utility to extract terrain data from digital formats available on National databases (Ordnance Survey National Transfer format), removing the need for extensive surveys of landforms surrounding a surface quarry (CERC Ltd, 2011). Moreover, both UK-ADMS and AERMOD are equipped with meteorological pre-processors which are able to compute atmospheric parameters to characterize the atmospheric boundary layer from routine meteorological data, thereby eliminating the need for sophisticated meteorological instruments to directly measure these variables (Carruthers et al., 2009).

However, it is well known that Gaussian model algorithms suffer from several inherent limitations related to over-simplification of the flow-field. In the case of UK-ADMS, the FLOWSTAR algorithm is used to model the flow over complex terrain. This algorithm uses a linearized analytical solution of the momentum and continuity equations and offers a simplified treatment of topography in which the Froude number is used as a critical model parameter in separated flows (CERC Ltd, 2011). The linearization of the flow equations employed in the UK-ADMS complex terrain model algorithm is based on small perturbation theory by Jackson and Hunt (1975) which is restricted to terrain gradients below 1:3. The theory assumes that terrain in-homogeneities produce small perturbations in the flow-field relative to mean flow quantities. However, this assumption is not valid in cases where separation of the flow occurs (Finardi et al., 1997). In the case of surface quarries, the linearized flow model and by extension the complex terrain algorithm are incompatible with the quarry topography, which produces large perturbations in the atmospheric flow-field. Consequently, the small perturbation treatment applied to complex terrain compromises the ability of Gaussian model to satisfactorily replicate the actual dust dispersion in the near-field of the quarry pit.

Additionally, Gaussian model predictions may suffer from inconsistencies among similar model types or different versions of the same model even with the same data set due to intrinsic differences in model algorithms (Hall et al., 2000). For instance, later version of

UK-ADMS offer substantially greater terrain resolution capabilities than earlier versions and the UK-ADMS treatment of complex terrain is vastly different to that of AERMOD (Carruthers et al., 2011). Also, the formulation of the Gaussian equation implies that model accuracy is severely challenged by low wind speeds (Holmes and Morawska, 2006). The reliability of Gaussian model approximations is further reduced for near-ground releases because the vertical dispersion of near-ground releases may depart considerably from the Gaussian probability density function (Smith, 1995). Complex terrain field studies have revealed that Gaussian models can over-predict pollutant fluxes by as much as 60% and they are inapplicable to dispersion problems involving spatial variations in surface heat flux (Lowndes et al., 2008). Therefore, El-Fadel et al. (2009) recommended that UK-ADMS should only be relied upon as a qualitative prediction tool for dispersion over complex terrain.

Regulatory Gaussian models are commonly used in conjunction with emission factors equations; most of which have been developed empirically by the US-EPA through the use of regression analysis to estimate emissions from fugitive dust sources in surface coal mines (USEPA, 1980, 1998). US-EPA emission factors equations have correlated the emission rate from various dust generating activities with parameters which affect the potential for dust liberation, such as frequency of activity, soil moisture and fines content (Watson et al., 2000). One such example is the US-EPA AP-42 emission factor equation for estimating the mass of Total Suspended Particulates (TSP) released from blasting a bench of height not exceeding 21 m and plan area,  $A$ ,

$$EF_{TSP} = 0.00022A^{1.5}. \quad (2.1)$$

The accuracy and universal applicability of US-EPA emission factor equations to dynamic or intermittent dust sources such as haul roads have been disputed in work by Claiborn et al. (1995) and Venkatram (2000) mainly because they are based on the assumption that fugitive dust sources are fixed continuous emitters of particulates, and they rely on obscure input variables, resulting in notable variances between predicted and observed emission factors. US-EPA AP-42 Emission factor estimates are often based on limiting assumptions which may be site and source specific (Countess Environmental, 2006), as these models were developed for surface coal mines in the western United States and may not necessarily be suitable for generalizing the emission rate of an entire source category (Countess Environmental, 2006). Venkatram (2000) proffered that US-EPA emission factor equations potentially overestimate mean  $PM_{10}$  emission by as much as 60-100% for paved roads. Recognizing the limitations of their emission factor equations, the US-EPA recommends supplementing the equations with state or local information which may improve the AP-42 methodology. The Michigan Department of Environmental Quality (MDEQ) specifically address dust emissions from limestone quarry bench blast events, thus presenting an emission factor equation relating filterable  $PM_{10}$  emissions to blast tonnage,

$$EF_{PM_{10}} = 0.038 \text{ kg/tonne}. \quad (2.2)$$

Even so, there is a high degree of uncertainty associated with using the MDEQ emission factor equation to estimate dust emissions from bench blasting in UK limestone quarries.

Not least because of differences in geomorphology, mineral composition and site meteorology. Generally, the choice is stark for quarry operators who wish to quantify dust emissions and emission factor equations are preferred over the laborious and costly task of directly quantifying dust emissions from each source type (Venkatram, 2000; Countess Environmental, 2006). Thus US-EPA AP-42 and MDEQ emission factor equations have become the de facto means of computing emission rates from fugitive dust sources at coal and limestone surface quarries respectively.

### **2.2.1 Limitations of Conventional Dust Dispersion Models**

The limitations in modelling flow over complex terrain faced by conventional Gaussian models have led researchers to seek alternative methods to simulate the dispersion of pollutants over such terrain. Studies by Apsley and Castro (1997), Castro and Apsley (1997) and Duranti et al. (1998) have explored numerical modelling of flow over complex topography, building upon the findings of the Russian Hill (RUSHIL) experiments conducted by Khurshudyan et al. (1981). The Khurshudyan et al. (1981) experiments have been cited as one of the earliest wind tunnel investigations into atmospheric flow and dispersion over 2D hills of varying aspect ratios. The study examined the modifications to the turbulence structure of the flow-field induced by the presence of hills and the effects on the dispersion of a pollutant emitted from an elevated source at different positions relative to the hills. Khurshudyan et al. (1981) found that the dispersive characteristics of the pollutant plume were extensively modified by the presence of a steep hill and the resultant recirculation region in the lee of the hill. In a later study, Chatzipanagiotidis and Olivari (1996) concluded that although terrain induced modifications to the flow-field are pronounced in the near-field, the effects of complex topography are less significant in the far-field. Field studies by Wiggs et al. (2002) into aeolian sediment transport over valleys, indicated that valley topography can alter the local wind regime to a sufficient extent to produce even up to synoptic scale meteorological variations with significant implication for the dispersion of pollutants. In light of the preceding, it is apparent that small perturbation theory by Jackson and Hunt (1975) cannot be extrapolated to complex terrain scenarios where flow separation is present and instead, non-linear numerical methods, namely CFD, are required for modelling the flow-field over complex terrain (Palma et al., 2008).

CFD models enable the simulation of the turbulent transport of momentum, heat and mass by solving the non-linear Navier-Stokes equations of fluid flow and are applicable to a large range of meteorological and topographic conditions (Scargiali et al., 2005). Furthermore, CFD methods can offer superior replication of dispersion scenarios over complex terrain as evidenced by the results of the study by Silvester et al. (2009). CFD models have been more conventionally applied to wind engineering problems and near-field dispersion modelling in the urban environment, where the presence of buildings induce large perturbations in the atmospheric flow-field (Tominaga and Stathopoulos, 2009; Gousseau et al., 2011; Tominaga and Stathopoulos, 2012). However, studies by researchers such as Gorlé et al. (2009), Pontiggia et al. (2009), Pontiggia et al. (2011), Sabatino et al. (2008), Di Sabatino et al. (2007) and Blocken et al. (2008) demonstrate that CFD can also be successfully applied to

model pollutant dispersion, where there is a degree of geometric complexity and localised grid refinement may be required to fully resolve the flow around obstacles (Riddle et al., 2004; Pontiggia et al., 2009).

### 2.2.2 CFD application to Atmospheric Dispersion Modelling

Direct Numerical simulation (DNS) methods can provide transient solutions of the full Navier-Stokes equations of fluid flow, thereby enabling the resolution of turbulence at all length scales. Thus, three dimensional turbulence structures in the flow, which greatly affect the transport of momentum, heat and mass can be explicitly resolved. However, the application of DNS to the prediction of dispersion phenomena is confined to flows with low to moderate Reynolds numbers and simple geometries (Squires and Eaton, 1991; Poinso et al., 1995; Ling et al., 1998; Saeedi et al., 2014 (In Press, Corrected Proof)). In order to fully resolve flow turbulence using DNS, Anderson Jr (1995) and Coleman and Sandberg (2010) note that the computational domain is required to be large enough to capture large scale turbulence structures while simultaneously possessing a grid resolution fine enough to solve for the smallest scales of turbulence in the energy dissipating range of the turbulence spectrum. Accordingly, Sagaut (1998) and Pope (2000) estimate that the number of computational grid points,  $N_g$ , required to fully resolve a turbulent flow problem is a function of the Reynolds number,  $Re$ , resulting in  $N_g = Re^{9/4}$ . This constraint implies that the application of DNS to resolve large Reynolds number flows which possess a wide range of length scales is impractical because of the high demand in computational resource that such an endeavour would incur.

CFD numerical models which apply finite-volume discretization of the fluid domain and solve the Navier-Stokes equations of fluid flow in each control volume have gained much traction in the area of dispersion modelling. Large Eddy Simulation (LES) models present a coarse grid approach to resolving large scale three-dimensional turbulence and are therefore able to predict the effects of recirculation regimes on pollutant dispersion at significantly lower computational expense than DNS (Sagaut, 1998). LES applies a filtering approach to differentiate large scale motions from the small scale eddies which are subject to sub-grid scale modelling (Pope, 2000). With the application of LES methods, the objective is to resolve the anisotropic, energy-containing eddies and as such, sub-grid filtering decomposes the velocity into a resolved component which represents the large energy containing eddies and a residual component which can be modelled by an eddy-viscosity approach such as the Smagorinsky-Lilly model (Pope, 2000). Studies by Cai et al. (1995), Baggett (1998) and Diebold et al. (2013) have demonstrated that LES can encounter difficulties when solving atmospheric flow problems in which small scale turbulent motions in the near ground region of complex geometries have a significant bearing on transport of flow properties. In fact, Pope (2004) cautions that LES cannot be employed to resolve these near wall motions without incurring significant computational expense which is comparable to that of DNS methods.

Reynolds-Averaged Navier-Stokes (RANS) models are the most commonly applied CFD model in dispersion modelling studies and are particularly attractive for industrial appli-

cations due to their comparatively low computational demand. These models apply a Reynolds decomposition to separate flow variables into mean and fluctuating components, with the fluctuating components being attributed to flow turbulence. The Reynolds stresses which arise from this treatment are solved through application of the Boussinesq Hypothesis where the stresses are related to the mean rate of strain and by extension the mean velocity gradients by a constant of proportionality  $\mu_t$ , which represents the turbulent eddy viscosity. The turbulent eddy viscosity is subsequently solved by means of turbulence closure equations. In the case of the standard  $k - \varepsilon$  turbulence model, closure of the RANS equations is achieved through the solution of transport equations for turbulent kinetic energy,  $k$ , and its dissipation rate,  $\varepsilon$ . The assumption of turbulence isotropy which underpins modelling of the Reynolds stresses in eddy viscosity models is only truly valid for small-scale turbulence (Tennekes and Lumley, 1972), hence the modelling of recirculation regimes dominated by anisotropic, larger scale motions presents a challenge to RANS models (Maurizi, 2000; Santos et al., 2009). Reynolds Stress Models (RSM) use different transport equations to calculate individual Reynolds stresses and account for anisotropy in horizontal and vertical turbulent fluctuations, they therefore offer better resolution of pollutant dispersion than isotropic RANS models, albeit at greater computational resource costs than isotropic two-equation models (Gromke et al., 2008).

Apart from the limitations of the assumption of turbulence isotropy, maintaining homogeneous atmospheric profiles throughout the length of the computational domain remains a challenge in the implementation of RANS models. The correct reproduction of the ABL in RANS models depends on the imposition of fully developed velocity and turbulence profiles at the domain inlet to implicitly represent the influence of an upstream fetch not modelled in the computational domain (Gorlé et al., 2009). To this end, the popular Richards and Hoxey (1993) profiles are imposed at the domain velocity inlets to model neutral atmospheric boundary layer flows. However, studies by Hargreaves and Wright (2007), Blocken et al. (2007b) and Blocken et al. (2007a), which have utilised the standard  $k - \varepsilon$  model, noted that atmospheric boundary layer profiles do not remain horizontally homogeneous throughout the computational domain due to incompatibility of the inlet profile with wall functions imposed by the model to resolve the near-wall viscous sub-layer. Hence, the profiles are observed to decay along the domain, leading to discrepancies between the simulated and measured values. Blocken et al. (2007b) and Hargreaves and Wright (2007) recommended that the problem of horizontal inhomogeneity could be alleviated by harmonizing the profile and model values of roughness through the use of an equivalent sand-grain roughness. Moreover Alinot and Masson (2005) was able to obtain homogeneous profiles for stable, neutral and unstable atmospheric conditions by making the model coefficients congruous with Monin-Obhukov similarity scaling of the atmospheric surface layer.

Hybrid models such as Detached Eddy Simulation (DES) which combine a near-ground RANS approach with an LES approach for the outer flow regions have steadily gained popularity because they combine the advantages of both CFD methods. However, the DES models suffer from disparities in velocity profile predictions when the flow transitions from RANS to LES regions (Baggett, 1998; Piomelli et al., 2003). Chen et al. (2012)

propose the use of a novel Constrained Large Eddy Simulation (CLES) approach to eliminate the logarithmic layer mis-match between the RANS and LES zones of conventional DES simulations. Their methodology involves a typical LES solution of the flow field with the implementation of a dual approach sub-grid scale model which applies a Reynolds-stress constraints near the wall but defaults to a traditional LES sub-grid model in the remaining sub-grid region. Since both DES and CLES approaches involves a full LES solution of parts of the flow-field, their computational resource requirements are not expected to differ vastly from that of traditional LES.

### **2.2.3 Dispersion Model Inter-comparison Studies**

The performance of UK-ADMS has been extensively evaluated for a range of emission stack heights and meteorological conditions using both wind tunnel and field datasets. In particular, validation of the model with field measurements of tracer gas concentration from the Kinkaid, Indianapolis and Prairie Grass experimental campaigns have demonstrated that the model performs well for predicting the dispersion of emissions from elevated stacks situated on flat terrain (Carruthers et al., 1994, 1995, 1998). Therefore a good starting point for the evaluation of a new dispersion model is a comparison of its performance to that of UK-ADMS under dispersion site conditions for which UK-ADMS is known to perform reliably.

In this vein, Riddle et al. (2004) performed a model inter-comparison study between FLUENT and UK-ADMS, illustrated in Figure 2.8,

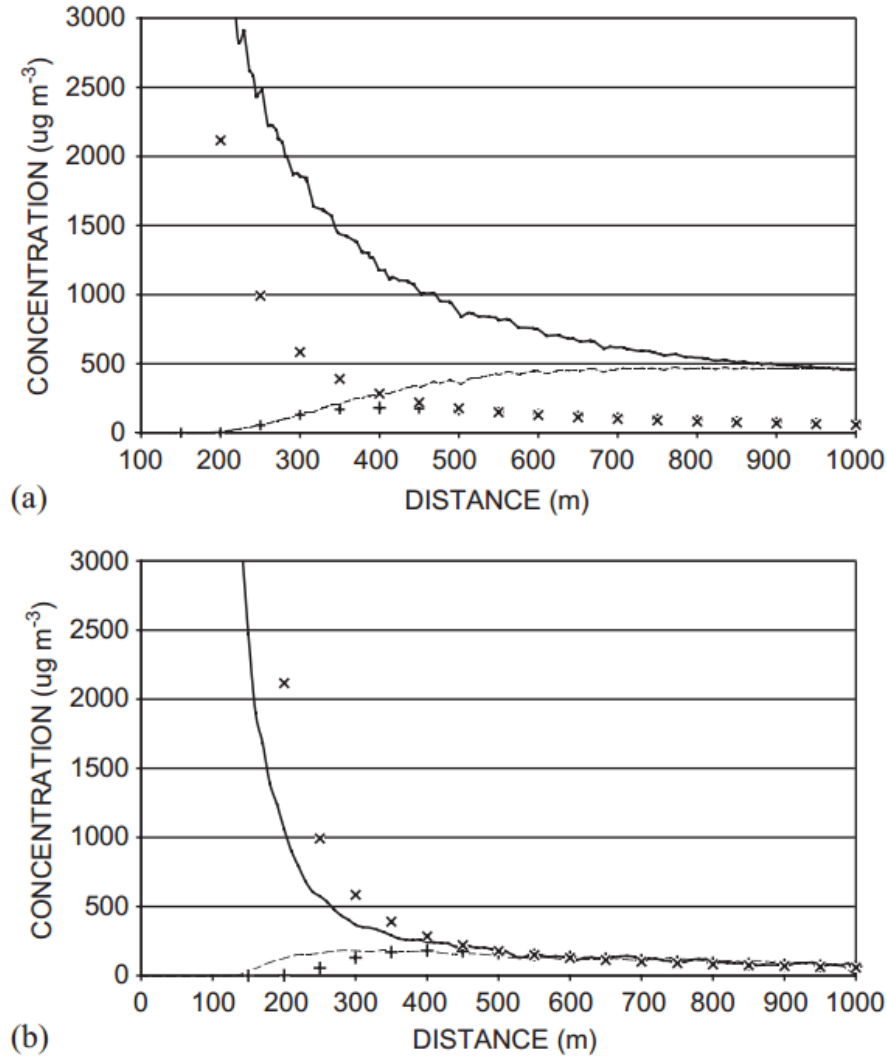


Figure 2.8: A comparison of the solutions produced by the (a) FLUENT AD (b) FLUENT DPM models to the UK-ADMS model predictions of ground level and plume centreline concentrations for a gaseous plume emitted from a 50 m stack located at 100 m in a domain of size  $1000\text{ m} \times 500\text{ m} \times 150\text{ m}$ , from Riddle et al. (2004). The solid line and  $x$  markers represents FLUENT and UK-ADMS concentration predictions at the plume centreline respectively. The dashed lines and  $+$  markers denote FLUENT and UK-ADMS concentrations at ground level respectively. The distance on the x-axis is measured from the source.

They found that the dispersion of gas emitted from a single 30 m stack in their computational domain was best predicted by coupling the Eulerian solution of the flow field obtained from the FLUENT Reynolds Stress Model (RSM) with a Lagrangian Particle tracking model. In FLUENT's Lagrangian Discrete Phase Model (DPM), which provides stochastic tracking of individual particles, Riddle et al. (2004) represented the gaseous plume using massless particles. The results obtained by Riddle et al. (2004) in Figure 2.8, show that when compared to the DPM model, the less computationally intensive Advection-Diffusion (AD) method vastly over-predicts both the ground level and plume centreline predictions. Indeed, Squires and Eaton (1991) advised that particulate dispersion is best assessed using a Lagrangian method where the frame of reference is attached to the individual particles. Dispersion models based on a coupled Euler-Lagrange approach permit the modeller to harness the benefits of both types of model. They exploit the computational efficiency of the Eulerian approach to produce a preliminary solution of the flow-field and combine it with the higher accuracy Lagrangian method to deal with sub-grid scale, particle-oriented aspects of pollutant dispersion (Burger et al., 2002; Li et al., 2006).

In analysing the results of their dispersion study conducted using the DPM tracking model, Gorlé et al. (2009) noted that the Lagrangian Integral time-scale constant,  $c_L$ , defined as the ratio of the Lagrangian integral time to the Eulerian integral time, was analogous to the turbulent Schmidt number,  $Sc_t$  used in the AD method and defined as the ratio of momentum diffusivity  $\nu_t$  to mass diffusivity  $D_t$  due to atmospheric turbulence. The value of  $c_L$  is used to modify the Lagrangian Integral time  $T_L$  which theoretically represents the lifetime of turbulent eddies in the flow. An increase in the time scale constant corresponds to an increase in  $T_L$ , the time over which the fluctuating velocity component is held constant. This in turn translates to a decrease in the frequency of velocity fluctuations which are used to characterize the instantaneous flow velocity in particle trajectory computations (Tian et al., 2006).

In the dispersion studies conducted by Apsley and Castro (1997) and Gousseau et al. (2011), the limitations of isotropic models are result in under-prediction of the lateral plume spread due to underestimation of the turbulent kinetic energy resulting from the use of Reynolds averaging and the eddy-viscosity assumption. Riddle et al. (2004) demonstrated that the under-prediction of lateral plume spread present in CFD models, as shown in Figure 2.9 and Figure 2.10, was avoided in UK-ADMS, through the inclusion of a model to replicate the characteristic meandering of the prevailing wind direction observed in atmospheric flows.

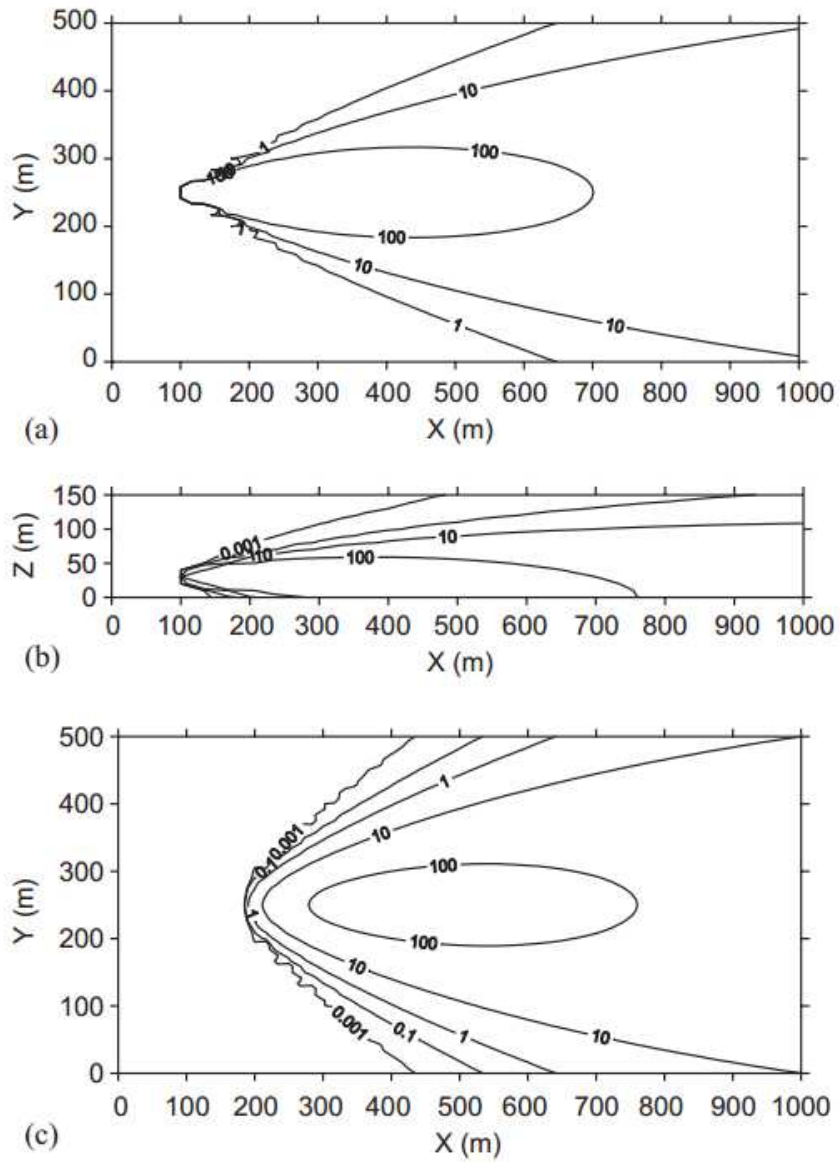


Figure 2.9: A plot of UK-ADMS plume dispersion models (a) horizontal plume dispersion at stack height, (b) vertical section along plume centreline (c) ground level concentration. Concentration in  $\mu\text{gm}^{-3}$ , from Riddle et al. (2004).

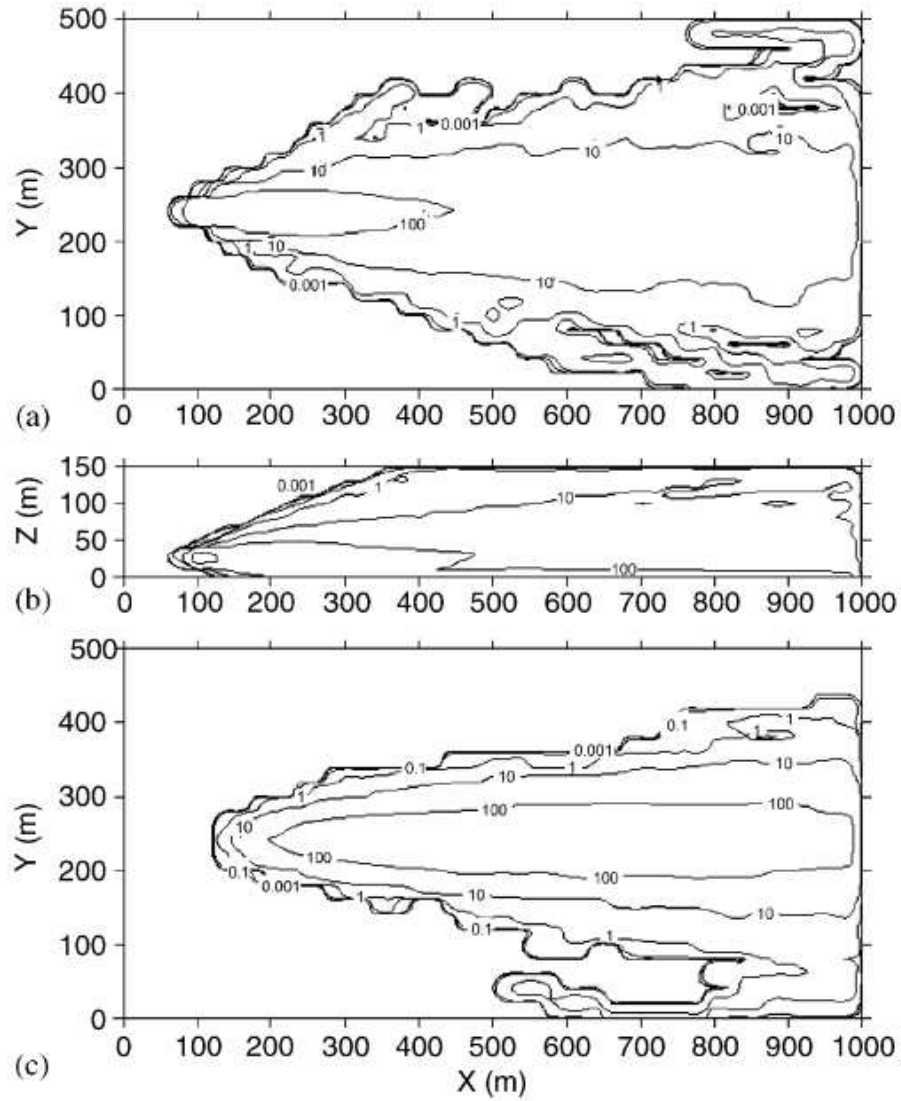


Figure 2.10: A plot of the solution of FLUENT DPM plume dispersion models (a) horizontal plume dispersion at stack height, (b) vertical section along plume centreline (c), ground level concentration. Concentration in  $\mu\text{gm}^{-3}$ , from Riddle et al. (2004).

Blocken et al. (2008) advised that the adoption of an unsteady RANS (uRANS) simulation model to account for this transient meandering of the flow might assuage the problem of underestimation of lateral plume spread in non-buoyant plume dispersion. Arguably, while transient simulations may minimise the extent of under-prediction of lateral plume spread, the incorporation of temporal discretisation in RANS CFD models is still somewhat removed from actual atmospheric phenomena, and it may seem counter-intuitive to conduct transient simulations in a time-averaged model. In a recent study, de Mello and Yanagihara (2010) propose the inclusion of an additional equation to account for the variance of pollutant concentration fluctuations in the steady state turbulence model, which may provide a reasonable alternative solution method to current computationally expensive transient simulations. In the same vein, Quinn et al. (2001) and Vervecken et al. (2013) proposed the use of probability weighted summation of solutions produced from a number of simulations performed to represent the full range of direction variability of the mean wind. Even after the phenomenon of wind direction variability has been duly accounted for, the challenges of modelling complex topography using an isotropic turbulence model must be surmounted. Therefore, Maurizi (2000) recommended calibration of the model constants for atmospheric flows to counter the complex terrain limitations of the standard  $k - \varepsilon$  model and improve its turbulent kinetic energy predictions.

#### **2.2.4 CFD Dispersion Modelling of Flow over Quarry Topography**

There are compelling arguments to perform CFD model dispersion studies to produce more realistic models of particulate plume dispersion over complex topography. However, there are few studies in the literature that document the results of CFD investigation of the dispersion and deposition of fugitive dust. Furthermore, the pollutant dispersion studies which incorporate complex terrain effects, such as those by Chatzipanagiotidis and Olivari (1996), Blocken et al. (2008) and Chavez et al. (2011), only considered the neutral stability atmosphere wherein the effects of thermal buoyancy are absent. In these studies, the model predictions were typically validated against scaled wind tunnel measurements and there is a scarcity of studies that have attempted to compare numerical model predictions of dispersion with field measurements of pollutant fluxes under a range of meteorological conditions. In one of the few instances involving field validation, Hong et al. (2011) employed an LES model to simulate the wind field over a test region in South Korea and subsequently used this validated model to predict the dispersion of livestock odour over this area. Their model predictions were found to correlate well with field measurements. In another example, Scargiali et al. (2005) considered the dispersion of chlorine gas over a 30 km<sup>2</sup> mountainous region in Eastern Sicily using a CFX  $k - \varepsilon$  code. To include the effects of thermal buoyancy, they introduced modifications to the RANS equations for turbulent kinetic energy and its dissipation rate. They concluded that predicted ground level concentrations were attenuated by the presence of downwind complex terrain. The findings of these studies are encouraging, and support the selective use of CFD models to predict fugitive dust dispersion over complex topography for a range of meteorological conditions beyond the idealised neutral atmospheric condition.

In contrast to naturally occurring land topography, quarry excavations are often characterized by sharp changes in elevation due to the steep gradients of the extraction benches. To date, only a handful of researchers have addressed the specific challenges to dispersion modelling presented by quarry topography. Under neutral stability conditions, Silvester et al. (2009) demonstrated that more accurate flow-field resolutions and deposition predictions can be achieved for the near source dispersion of particulates from an open pit quarry by employing a suitably calibrated CFD model compared to UK-ADMS. A comparison of the predicted particulate deposition patterns generated by the UK-ADMS and CFD models are shown on Figure 2.11,

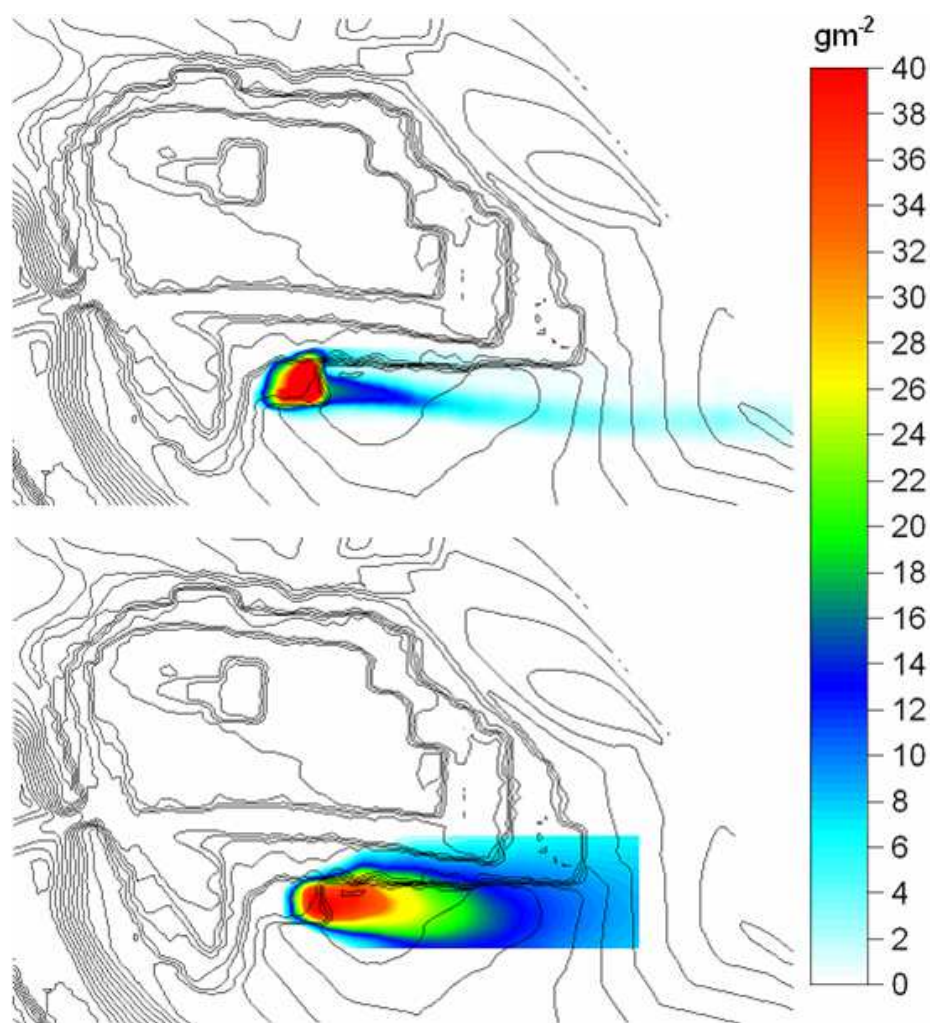


Figure 2.11: A comparison of the particulate deposition predictions obtained using FLUENT  $k - \varepsilon$  (top) and UK-ADMS (bottom) to model dispersion at a UK quarry under neutral atmospheric conditions from Silvester et al. (2009).

Their study concluded that on average, approximately 50% of emitted particulates were deposited and retained within the pit boundaries. These model predictions correlated well with pit retention values prescribed by UK Environmental regulations. Furthermore, the degree of pit retention was found to depend on the location of the emission source, the direction of the prevailing wind and the nature of the local flow regime generated within the pit cavity. Importantly, Silvester et al. (2009) acknowledged the need to incorporate atmospheric stability effects into such model investigations to develop a more comprehensive picture of the dust dispersion and deposition.

Chinthala and Khare (2011) have recently used CFD models to investigate the nature of the flow structures which develop in open pit coal mines of varying depth. Their study concluded that as the depth of the pit increased, there was an associated strengthening of the recirculation flows in the pit cavity. The deepest cavities experienced almost complete decoupling of the in-pit flow regime from the atmospheric boundary layer over the open pit and the internal flow was dominated by large vortex structures. Conversely, for shallower depth pits the penetration of the external atmospheric boundary layer into the pit cavity was more likely to give rise to an internal flow regime dominated by smaller vortex structures with associated secondary vortices.

Flores et al. (2014) applied DES to resolve turbulence and predict the dispersion of particles injected inside a large open pit copper mine in northern Chile. The depth of the pit was of the same order of magnitude as the height of the daytime atmospheric boundary layer. In addition, the pit was situated in a desert region and subject to intense insolation, thus Flores et al. (2014) anticipated that the recirculation flow regime observed by Silvester et al. (2009) would be greatly exacerbated under these conditions, leading to the formation of large scale rotations well outside the remit of a RANS-based modelling approach. Notwithstanding its limitations, Blocken et al. (2008), Tominaga and Stathopoulos (2009) and Chavez et al. (2011) conclude that the standard  $k-\varepsilon$  model presents a good compromise between computational demand, results accuracy and model stability. Moreover, research by Alinot and Masson (2005), which substantially informs the modelling methodology of the original research work presented in this thesis, has selected the two equation standard  $k-\varepsilon$  model for closure of the RANS equation because of the relative ease of deriving the  $k$  and  $\varepsilon$  turbulence transport properties from routine meteorological data. Furthermore the model equations and coefficients can be readily adapted to make them compatible with Monin-Obukhov similarity theory, which has been found to adequately characterize the near surface atmosphere.

### 2.3 Characterization of The Atmospheric Boundary Layer

The dispersion of pollutants emitted into the troposphere is strongly dependent on the background wind systems which characterize the Atmospheric Boundary Layer (ABL) (Silvester et al., 2009), and in order to obtain a reasonably accurate numerical simulation of atmospheric flow, the turbulence parameters and boundary conditions which characterize the ABL must be appropriately defined. The ABL occupies the lowest 1 to 2 km of the troposphere, where the flow structure is influenced by turbulent exchanges of momentum and heat with the Earth's surface (Sutton, 1953; Kaimal and Finnigan, 1994). In the free atmosphere above the ABL height  $H$ , (Figure 2.12), the wind structure is independent of shear at the surface and the airflow approximates to that of an inviscid fluid, where the Coriolis force balances the pressure gradient force and near-geostrophic flow is attained (Kaimal and Finnigan, 1994).

Atmospheric flows are random and chaotic due to thermal and mechanically generated turbulence (Garratt, 1994) and their large range of characteristic length scales and high Reynolds numbers are not amenable to exact wind tunnel or numerical simulation (Folz and Wallace, 2010). Additionally, an accurate replication of the ABL is difficult to achieve in laboratory or numerical wind tunnels due to the non-stationary nature of atmospheric turbulence, by which atmospheric motions occur at temporal scales ranging from a few seconds to several days. Fortunately, turbulent motions which affect the dispersion of atmospheric pollutants occur at temporal scales of less than a day (Garratt, 1994), therefore air pollution modelling can be accommodated by resolving microscale and mesoscale motions as opposed to the larger synoptic scale motions. Moreover, the length scales of turbulent eddies are constrained by the depth of the atmospheric boundary layer, whereby for dispersion modelling over homogeneous terrain, atmospheric turbulence is frequently simplified to a two dimensional problem, primarily concerned with dispersion in the vertical and stream-wise directions.

Figure 2.12 indicates the typical structure of the ABL. In the roughness sub-layer, turbulence is strongly affected by the individual roughness elements and the turbulent kinetic energy is dissipated by fluid viscosity (Garratt, 1994). The inertial sub-layer is dominated by microscale turbulence and the velocity profile is logarithmic in the absence of thermal buoyancy effects. The roughness sub-layer and inertial sub-layer together comprise the surface layer which is of particular importance to micro-meteorological studies, since the largest height dependent variations in meteorological parameters occur in this layer. Near ground pollutant releases, such as fugitive dust emissions from surface quarries occur entirely within the surface layer therefore accurate predictions of quarry dust dispersion are contingent upon the resolution of the turbulent flow field in the surface layer.

Unlike the surface layer, the outer layer is affected by the Coriolis forces arising from the Earth's rotation, and under daytime convective conditions, turbulent mixing due to free convection ensures an almost uniform distribution of the flow variables such as velocity and temperature. Tennekes and Lumley (1972), Kaimal and Finnigan (1994) and Garratt (1994), discuss the existence of a transitional buffer region between the surface layer and

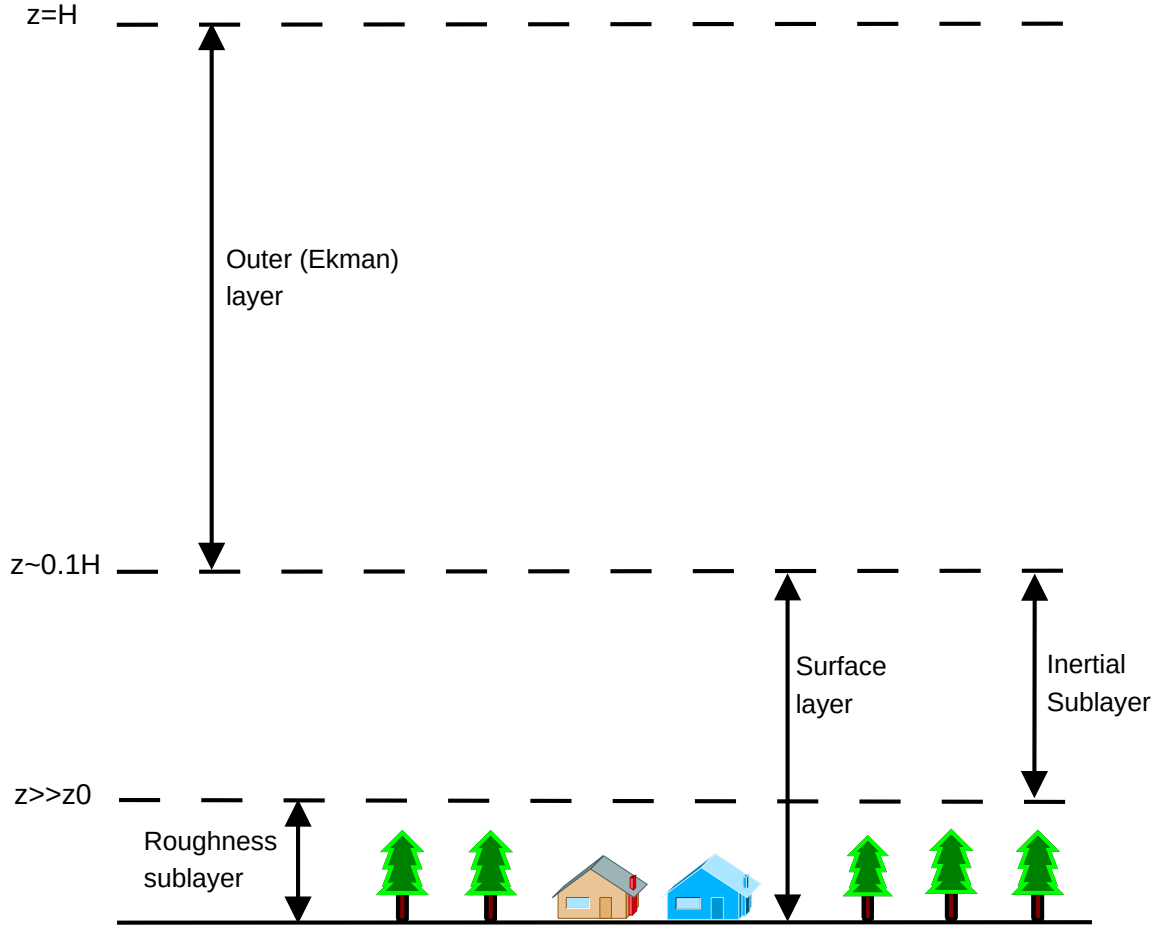


Figure 2.12: Structure and approximate heights of the layers which comprise the Atmospheric Boundary Layer, adapted from Kaimal and Finnigan (1994).

mixed outer layer, where both surface layer and outer layer scaling laws are applicable. The gradient-diffusion hypothesis known as K-theory is applied to describe the turbulent transport processes of heat and momentum in the atmosphere (Berkowicz and Prahm, 1979). K-theory states that turbulent diffusion is analogous to molecular diffusion of gases, where fluxes of gaseous properties occur along their gradients. Thus, K-theory relates the turbulent flux of a flow variable to the vertical gradient of its mean, resulting in momentum and heat fluxes in the atmosphere which are proportional to the vertical gradients of mean velocity and mean temperature respectively (Kaimal and Finnigan, 1994),

$$\tau = K_m \rho \frac{\partial \bar{u}}{\partial z}, \quad (2.3)$$

$$Q = K_h \rho c_p \frac{\partial \bar{\Theta}}{\partial z}. \quad (2.4)$$

In Equations 2.3 and 2.4, the subscripts  $m$  and  $h$  denote momentum and heat respectively.  $c_p$  and  $\rho$  represent the specific heat capacity at constant pressure and the density of the air respectively.  $K_m$  and  $K_h$  are the turbulent exchange coefficients for momentum and heat. The turbulent exchange coefficient for momentum has the units of length  $\times$  velocity (Kaimal and Finnigan, 1994), such that

$$K_m \propto u_* z = \kappa u_* z \quad (2.5)$$

and the constant of proportionality is the von-Karman constant,  $\kappa$  (Garratt, 1994).  $\Theta$  is the potential temperature, which is the temperature of an air parcel originally at pressure  $P$  and absolute temperature  $T$  after it is brought adiabatically to the reference pressure,  $P_0=10^5\text{Pa}$ ,

$$\Theta = T \left( \frac{P_0}{P} \right)^{R/c_p}, \quad (2.6)$$

where  $R$  is the gas constant of the air.

A shear stress  $\tau$ , arises at the ground surface as a consequence of the no-slip boundary condition, whereby tangential forces develop between the moving viscous fluid and the stationary surface to balance frictional drag and maintain the state of motion (Schlichting and Gersten, 2000). Shear stress at the surface can therefore be expressed in terms of a reference friction velocity at the surface  $u_*$ ,

$$\tau = \rho u_*^2. \quad (2.7)$$

Manipulation of Equations 2.3, 2.5 and 2.7 leads to,

$$\frac{\partial \bar{u}}{\partial z} = \frac{u_*}{\kappa z} \quad (2.8)$$

which upon integration yields the logarithmic mean wind profile equation for the neutral ABL, which implies the absence of thermal buoyancy effects,

$$\bar{u} = \frac{u_*}{\kappa} \ln \left( \frac{z}{z_0} \right). \quad (2.9)$$

In Equation 2.9, the constant of integration,  $z_0$ , is defined as the aerodynamic roughness height. This height provides a correction to the velocity profile by accounting for the removal of momentum from the flow field by aerodynamic drag arising due to presence of roughness elements immersed in the flow (Shaw and Pereira, 1982). Kaimal and Finnigan (1994) estimated that this length is typically 1/30 of the height of the average roughness element. Over a dense roughness canopy, the wind-field may be sufficiently obstructed by roughness elements such that it is necessary to introduce a zero-plane displacement height

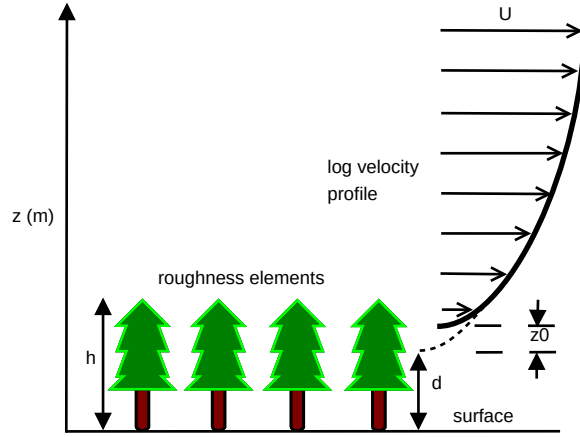


Figure 2.13: The effects of the roughness canopy on the ABL, the aerodynamic roughness height and the zero-plane displacement.

$d$ , to compensate for the displacement of the momentum sink from the ground surface as shown in Figure 2.13 (Shaw and Pereira, 1982).

The zero-plane displacement height defines the height above the surface that the logarithmic velocity profile extrapolated downwards would decay to zero in the absence of the roughness elements. Accounting for both these length scales in the log velocity profile equation leads to the expression,

$$\bar{u} = \frac{u_*}{\kappa} \ln \left( \frac{z - d}{z_0} \right). \quad (2.10)$$

The presence of roughness elements disturbs the mean flow and increases turbulent eddy formation by increasing the shear stresses in the flow (Santos et al., 2009). Studies by Bottema (1997), Chan (2001), Cao and Tamura (2007) and Cao et al. (2012) proposed that establishing the roughness configuration of a given site is particularly important for dispersion modelling, not least because surface roughness determines the surface friction characteristics. Moreover, any transitions in roughness profile may provoke local momentum advection phenomenon that may impact on plume dispersion (Chan, 2001). Cao et al. (2012) recognised that surface roughness compounds the effect of complex topography on flow phenomenon such as boundary layer separation and reattachment. Table 2.4 provides a list of representative values of surface roughness and zero-plane displacement height for different categories of surface cover. The value prescribed by USEPA (2008a) for surface quarries accounts for the presence of artificial landforms such as benches and slopes, thus when the quarry terrain is explicitly modelled, a smaller value of surface roughness would be required. This is likely to be an intermediate value between that of the surrounding surface cover and bare rocks.

Table 2.4: Aerodynamic roughness height for different types of surface cover Jacobson (1999) and USEPA (2008a).

| Surface type                    | $z_0$ (m)       | Reference     |
|---------------------------------|-----------------|---------------|
| Smooth sea                      | 0.00001         | Garratt(1992) |
| Rough sea                       | 0.000015-0.0015 | Garratt(1992) |
| Ice                             | 0.00001         | Oke(1978)     |
| Snow                            | 0.00005-0.0001  | Oke(1978)     |
| Level desert                    | 0.0003          | Sehmel(1980)  |
| Short grass                     | 0.003-0.01      | Oke(1978)     |
| Long grass                      | 0.04-0.1        | Oke(1978)     |
| Agricultural crops              | 0.04-0.2        | Oke(1978)     |
| Bare rocks                      | 0.05            | USEPA (2008a) |
| Quarries/Strip mines/<br>Gravel | 0.3             | USEPA (2008a) |

### 2.3.1 Surface Layer Structure and Meteorology

The structure of the ABL evolves continuously during the day due to diurnal heating and cooling cycles at the surface (Figure 2.14). Indeed, atmospheric boundary layer processes are essentially driven by friction and short-wave solar radiation absorbed at the ground surface during the day. Consequently, two distinct states of the ABL emerge; namely the day-time unstable boundary layer illustrated in Figure 2.15, where the net positive heat flux from the surface gives rise to thermal convection, and the night-time stable ABL illustrated in Figure 2.16, where long-wave radiative cooling of the surface creates a ground based temperature inversion which suppresses mixing and damps out turbulent exchanges throughout the depth of the stable nocturnal ABL (Jacobson, 1999). Over the course of the day, as the ground surface is heated by solar radiation, the nocturnal inversion rises as the layer of thermally enhanced turbulent mixing above the ground deepens forming the convective daytime ABL (Figure 2.14). The inversion layer at the top of the convective ABL is distorted by turbulent eddies which frequently penetrate the inversion (Jacobson, 1999). The production of turbulence in the ABL is dependent on the fluxes of heat at the surface and the law of conservation of energy implies that an energy balance exists between incoming and out-going radiation. The characteristics of the ground surface such as surface albedo which describes the reflectivity and the Priestley-Taylor parameter, which is related to evapotranspiration potential at the surface also determine the availability of energy for the generation of atmospheric turbulence.

In both the day-time and night-time ABL, the prevalence of wind shear near the surface implies that the flow in the surface layer is dominated by forced convection due to mechanical turbulence, ergo the sharpest vertical gradients of flow properties are observed in this region. Garratt (1994), Kaimal and Finnigan (1994) and Jacobson (1999) define the surface layer

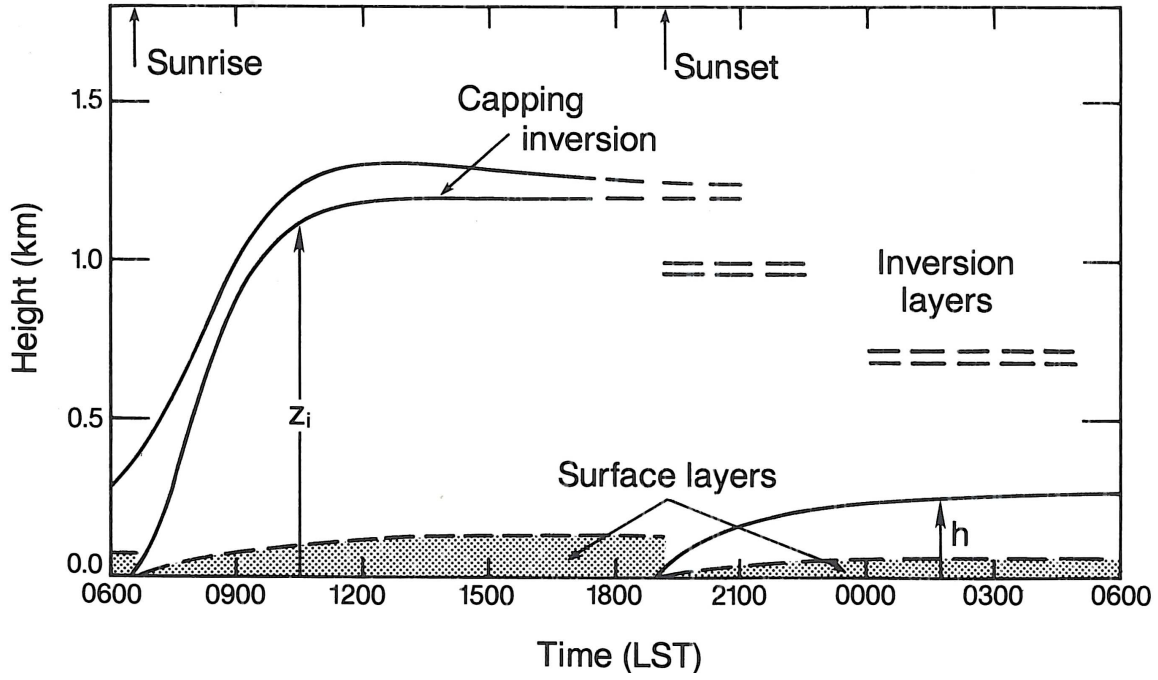


Figure 2.14: Diurnal cycle of atmospheric boundary layer evolution from Kaimal and Finnigan (1994).

as consisting of the bottom 10% of the ABL where shear stress is approximately constant. Monin-Obukhov Similarity theory proposes scaling laws to describe the turbulent state of the constant shear, atmospheric surface layer in terms of characteristic parameters which govern the flow, namely the surface fluxes of momentum, buoyancy and temperature and the height above the surface. Therefore the Monin-Obukhov similarity relationships relate the vertical profiles of the non-dimensionalized flow variables to the friction velocity,  $u_*$ , the buoyancy parameter  $\beta_g$ , the scaling temperature at the surface  $T_*$ , and the vertical coordinate  $z$ . These scaling parameters are themselves functions of the surface layer height  $\Gamma$  and physical properties of the fluid (density  $\rho$ , dynamic viscosity,  $\mu$ , thermal conductivity  $\lambda$  and specific heat capacity at constant pressure,  $c_p$ ) (Barenblatt, 1979). From Equation 2.7,  $u_*$  is given by,

$$u_* = \sqrt{\frac{\tau}{\rho}}. \quad (2.11)$$

The surface layer scaling temperature and the buoyancy parameter are defined as follows,

$$T_* = -\frac{(\overline{w'\Theta'})}{u_*} \quad (2.12)$$

$$\beta_g = \frac{g}{T_0}, \quad (2.13)$$

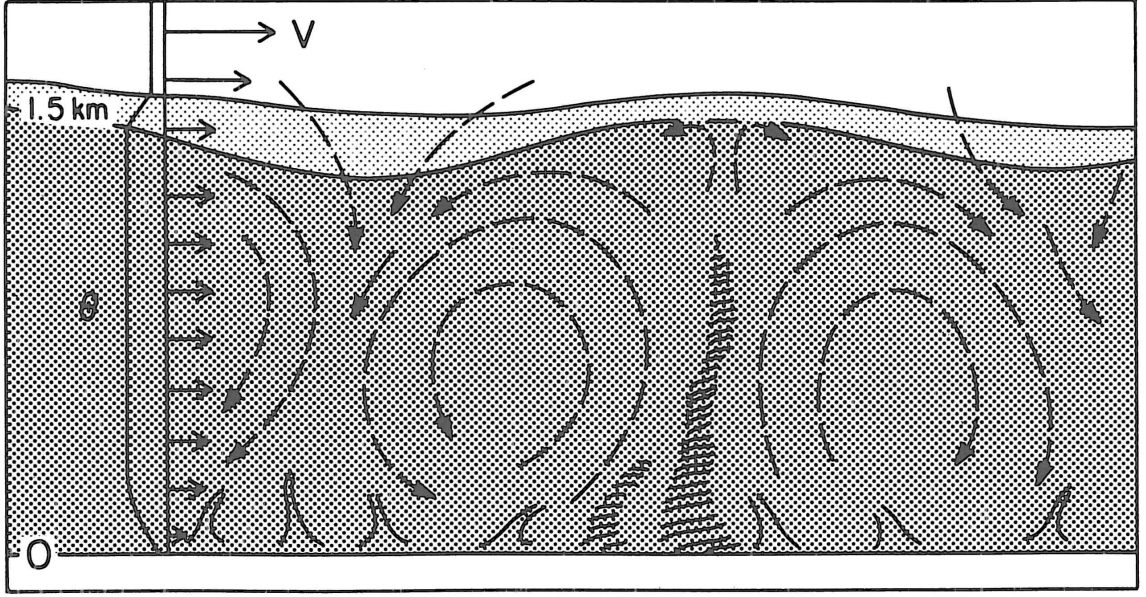


Figure 2.15: Turbulent eddy structure in the daytime convective ABL from Kaimal and Finnigan (1994).

where shear stress  $\tau$  and  $\overline{w'\Theta'}$  represent the momentum and potential temperature fluxes at the surface respectively. The sensible heat flux from the surface drives the exchange of temperature so that  $T_*$  can be expressed in terms of the surface sensible heat flux,

$$T_* = -\frac{Q_w}{\rho c_p u_*}. \quad (2.14)$$

By applying Buckingham II-Theorem, Monin and Obukhov (1954) derived the following functional relationships for momentum and potential temperature in the stationary, horizontally homogeneous surface layer,

$$\Pi_m = \frac{z}{u_*} \frac{\partial u}{\partial z} = \Phi_m \left( \frac{z}{L_{MO}}, Re_z, Re_\Gamma, Pr \right), \quad (2.15)$$

$$\Pi_h = \frac{z}{T_*} \frac{\partial \Theta}{\partial z} = \Phi_h \left( \frac{z}{L_{MO}}, Re_z, Re_\Gamma, Pr \right), \quad (2.16)$$

Buckingham II-Theorem presents a procedure to arrive at the dimensionless groups which govern a flow by first identifying and grouping the independent flow variables into functions. The number of functions depends on the number of non-repeating variables identified for the system. The functional forms of the dimensionless groups denoted by  $\Pi$  are determined through dimensional analysis of the variables in each function.

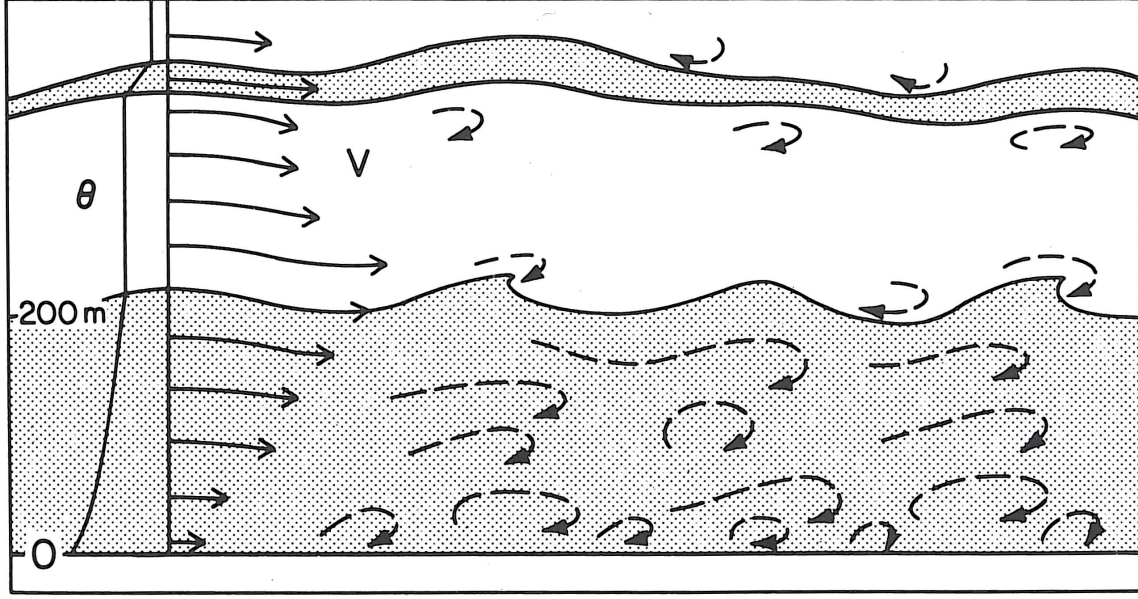


Figure 2.16: Turbulent eddy structure in the night-time stable ABL from Kaimal and Finnigan (1994).

In the preceding functions,  $Pr$  is the dimensionless Prandtl number, a ratio of momentum diffusivity to thermal diffusivity expressed by,

$$\frac{K_m}{K_h} = \frac{\mu c_p}{\lambda}. \quad (2.17)$$

Based on work by Prandtl 1932, Obukhov 1946 and Monin 1950, the assumption of similarity in the surface layer between the characteristically large local and global Reynolds numbers of the flow,  $Re_z = u_* z / \nu$  and  $Re_\Gamma = u_* \Gamma / \nu$ , permits the derivation of Monin-Obukhov similarity law which is independent of the flow Reynolds numbers,

$$\frac{z}{u_*} \frac{\partial u}{\partial z} = \Psi_m \left( \frac{z}{L_{MO}}, Pr \right) \quad (2.18)$$

$$\frac{z}{T_*} \frac{\partial \Theta}{\partial z} = \Psi_h \left( \frac{z}{L_{MO}}, Pr \right). \quad (2.19)$$

In the local and global Reynolds number equations,  $\nu$  is the kinematic or specific viscosity, a ratio of the dynamic viscosity to the density of the flow.

From the Monin-Obukhov Similarity theory, the Monin-Obukhov length,  $L_{MO}$  emerges as a representative thermal length scale for the surface layer under different stability conditions, such that, atmospheric parameters normalised by appropriate powers of the scaling parameters in Equations 2.11 2.12 and 2.13 become universal functions of the stability parameter,

$\zeta = z/L_{MO}$  (Barenblatt, 1979; Kaimal and Finnigan, 1994). The Monin-Obukhov length corresponds to the height at which thermal forcing exceeds mechanical shear (Foken, 2006; Folz and Wallace, 2010) and is used to categorise the steady state, horizontally homogeneous atmospheric surface layer (Businger et al., 1971).  $L_{MO}$  is computed from,

$$L_{MO} = -\frac{u_*^3}{\kappa(g/\overline{\Theta})(\overline{w'\Theta'})}, \quad (2.20)$$

relating the potential temperature flux and the surface sensible heat flux in the two expressions for  $T_*$ , and giving  $L_{MO}$  in terms of absolute temperature,

$$L_{MO} = -\frac{\rho c_p u_*^3}{\kappa(g/T_0)Q_w}. \quad (2.21)$$

In Equation 2.21,  $T_0$  is a reference temperature, generally taken as the near surface air temperature  $T_a$  (Holtzlag and Nieuwstadt, 1986). Negative values of the Monin-Obukhov length indicate convective conditions with a corresponding net positive heat flux, where dispersion and dilution of pollutants are rapid due to thermally enhanced turbulent mixing. On the other hand, positive values of  $L_{MO}$  are indicative of a stable stratification of the ABL where the heat flux is negative, consequently the generation of turbulence is suppressed as heat is lost to the surface and the potential for dilution and dispersion of pollutants is reduced. The value of the Monin-Obukhov length approaches infinity for the neutral, adiabatic atmosphere.

The non-dimensionalized forms of the neutral wind and potential temperature profile equations agree well with Monin-Obukhov similarity theory (Kaimal and Finnigan, 1994),

$$\phi_m = (\kappa z/u_*)(\partial \overline{u}/\partial z) \quad (2.22)$$

$$\phi_h = (\kappa z/T_*)(\partial \overline{\Theta}/\partial z), \quad (2.23)$$

such that  $\phi_m$  and  $\phi_h$  are functions of  $\zeta = z/L_{MO}$  in the surface layer. For values of  $|\zeta| < 1$ , Monin and Obukhov (1954) deduced that  $\phi_m$  and  $\phi_h$  could be taken as the first term of a Maclaurin power series (Garratt, 1994), such that  $\phi_{m,h}$  possesses the form,

$$\phi_{m,h} = 1 + \beta \zeta. \quad (2.24)$$

The forms of the similarity functions applied in work by Alinot and Masson (2005) to define the stability modification to the inlet profiles of velocity and temperature are those derived from experiments conducted by Businger et al. (1971) to determine the flux-profile relationships in the surface layer,

$$\phi_m = \begin{cases} \left(1 - 16\frac{z}{L_{MO}}\right)^{-\frac{1}{4}} & -2 \leq L_{MO} \leq 0, \\ 1 + \frac{5z}{L_{MO}} & 0 \leq z/L_{MO} \leq 1. \end{cases} \quad (2.25)$$

$$\phi_h = \begin{cases} \left(1 - 16 \frac{z}{L_{MO}}\right)^{-\frac{1}{2}} & -2 \leq L_{MO} \leq 0, \\ 1 + \frac{5z}{L_{MO}} & 0 \leq z/L_{MO} \leq 1. \end{cases} \quad (2.26)$$

### 2.3.2 ABL Profiles and Thermal Stability Classes

The derivation of the logarithmic wind profile equation is based on the neutral atmospheric condition, which occurs when the sensible heat flux from the surface is zero and the stability parameter therefore tends to zero with  $\phi_m = \phi_h \approx 1$ . However, the neutral stability condition is an idealised atmospheric condition which typically marks the transition between the nocturnal stable ABL and the daytime unstable ABL; although neutral conditions may also arise on windy days with near complete cloud cover of the sky where mechanical turbulence far surpasses thermally generated turbulence. Under neutral conditions, buoyancy effects are absent and an adiabatically lifted parcel of air as shown in Figure 2.17 will have the same temperature as the ambient air, and will thus remain at equilibrium with its surroundings. In contrast, the stable and unstable conditions are more persistent states of the atmosphere and will give rise to displacement of an adiabatically lifted parcel. In the stable case, a temperature inversion occurs at the surface due to net long-wave radiative cooling (Segal, 1989), thus an air parcel which is cooler and denser than the ambient air will be forced back to its initial position. Conversely in an unstable atmosphere, the parcel will be warmer and less dense than its surroundings and will rise under the influence of thermal buoyancy forces.

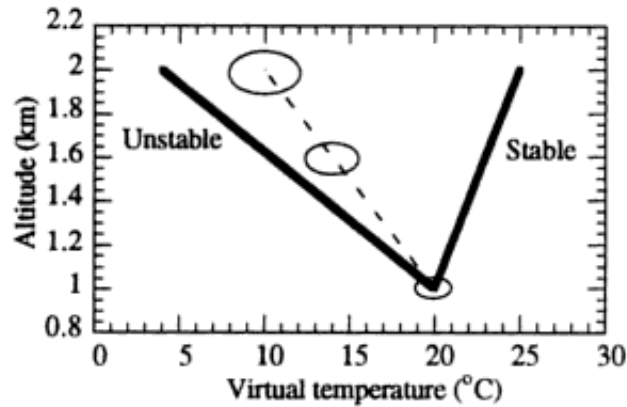


Figure 2.17: Displacement of adiabatically lifted air parcel (Jacobson, 1999).

Accordingly, atmospheric stability can be said to describe the resistance of the atmosphere to vertical motions. It can be quantified in terms of the frequency of oscillation of the air parcel about the position at which it is in thermal equilibrium with its surroundings, known

as the Brunt-Väisälä buoyancy frequency,

$$N = \sqrt{\frac{g}{\Theta} \frac{\partial \Theta}{\partial z}} \approx \sqrt{\frac{g}{\rho} \left( -\frac{\partial \rho}{\partial z} \right)}, \quad (2.27)$$

where  $\Theta$  is a reference potential temperature, and under the assumption that the air behaves as an ideal gas, the buoyancy frequency can be given in terms of density.  $N^2 = 0$  implies that no oscillations occur, as is the case for neutral atmospheric conditions, whilst  $N^2 > 0$  corresponds to the stable atmosphere where the parcel oscillates about its initial position.  $N^2 < 0$  is associated with unstable atmospheric conditions which enhance vertical motions, thus allowing the buoyant parcel to continue to rise.

Atmospheric stability is also an indicator of the relative contribution of thermal buoyancy to ABL turbulence and increasing atmospheric stability will suppress the formation of turbulent eddies which vertically transfer momentum and heat. According to Santos et al. (2009) and Gualtieri and Secci (2011), the production of turbulent kinetic energy and the velocity and temperature profiles which develop throughout the depth of the ABL are dependent on atmospheric stability conditions. Nieuwstadt and Duynkerke (1996) described the various stability classifications of the atmosphere as prototypes of the ABL, which are determined by prevailing meteorological conditions. The Pasquill-Gifford-Turner scheme was developed to classify atmospheric stability and has been frequently employed in pollutant dispersion studies as a means of qualitatively assessing turbulence and the dispersive potential of the atmosphere (Mohan and Siddiqui, 1998). However numerical models rely on quantitative indicators of atmospheric stability such as the Monin-Obukhov length as these can be readily incorporated into flow-field computations.

Apart from the Monin-Obukhov length scale, other quantitative indicators have been used to describe the stability of the atmosphere in terms of the relative contribution of mechanical shear and thermal buoyancy to the generation of turbulent kinetic energy. One such index is the non-dimensional Richardson Number,  $R_i$ ,

$$R_i = \frac{(g/\bar{\Theta})(\partial \bar{\Theta}/\partial z)}{(\partial \bar{u}/\partial z)^2}. \quad (2.28)$$

The contributions of buoyancy and shear to turbulence can be formulated in terms of the eddy covariances leading to the flux Richardson number  $R_f$ ,

$$R_f = \frac{(g/\bar{\Theta})\overline{w'\Theta'}}{\overline{u'w'}(\partial \bar{u}/\partial z)} \simeq \frac{K_h}{K_m} \quad (2.29)$$

Mohan and Siddiqui (1998) indicate that both Richardson numbers and the Monin-Obukhov Length provide reasonable coverage of all the stability classes defined in the Pasquill-Gifford-Turner (PGT) scheme and Table 2.5 gives practical correlations between PGT stability classes and these stability parameters.

Table 2.5: PGT Stability classes correlated to  $L_{MO}$  and  $R_i$  (Barthelmie, 1999; Woodward, 1999; Ashrafi and Hoshyaripour, 2008).

| Stability Class   | PGT Class | $L_{MO}$                 | $R_i$                    |
|-------------------|-----------|--------------------------|--------------------------|
| Strongly Unstable | A         | $-100 < L_{MO} < 0$      | $R_i < -0.86$            |
| Unstable          | B         | $-1000 < L_{MO} < -100$  | $-0.86 \leq R_i < -0.37$ |
| Weakly Unstable   | C         | $-10^5 < L_{MO} < -1000$ | $-0.37 \leq R_i < -0.10$ |
| Neutral           | D         | $L_{MO} >  10^5 $        | $-0.10 \leq R_i < 0.053$ |
| Stable            | E         | $10 < L_{MO} < 100$      | $0.053 \leq R_i < 0.134$ |
| Strongly Stable   | F         | $0 < L_{MO} < 10$        | $0.134 \leq R_i$         |

### 2.3.3 The Significance of the Froude Number in Stratified Flows

Atmospheric stability has been defined in terms of the buoyancy frequency  $N$ , which represents the interaction of gravitational and buoyancy forces on an air parcel. It is now necessary to consider the Froude number which can be used to classify stratified flows over complex terrain in terms of the ratio of inertial to gravitational forces (Ryan and Lamb, 1984). Under stable ABL conditions, the shallow ABL is likely to be greatly disturbed by complex terrain obstacles, and the Froude number  $Fr$  is an important parameter in assessing how the flow behaves in the vicinity of these obstacles (Ryan and Lamb, 1984; Kaimal and Finnigan, 1994).

$$Fr = \frac{\bar{u}}{Nh}, \quad (2.30)$$

where  $\bar{u}$  is the mean wind velocity in the stream-wise direction at the upwind edge of the obstacle,  $N$  has been already defined as the Brunt-Väisälä buoyancy frequency. The height of the terrain obstacle is represented by  $h$ .

The dividing streamline concept, illustrated in Figure 2.18, was formulated by Sheppard (1956) to approximate the behaviour of stably stratified flows over three dimensional hills. The dividing streamline concept defines a dividing streamline height,  $h_c$ , above which fluid parcels upstream of a 3D obstacle, possess sufficient kinetic energy to surmount the obstacle (Snyder et al., 1985; Leo et al., 2015). Below  $h_c$ , the fluid parcels pass around the sides of the obstacle. A linearised form of the concept is incorporated in the flow solvers of analytical dispersion models such as UK-ADMS and AERMOD to determine whether a pollutant plume entrained in the flow approaching a complex terrain obstacle impinges on the obstacle surface or is transported over it, with important implications for the computation of pollutant concentrations on the windward and leeward faces of the obstacle (Kaimal and Finnigan, 1994). The Sheppard (1956) integral formulation for determining the dividing streamline height is derived from an energy balance between the flow kinetic energy at a height  $h_c$  upwind of an obstacle and the potential energy over the obstacle,

$$\frac{1}{2}\bar{u}^2 = \int_{h_c}^h (h-z)N^2(z)dz. \quad (2.31)$$

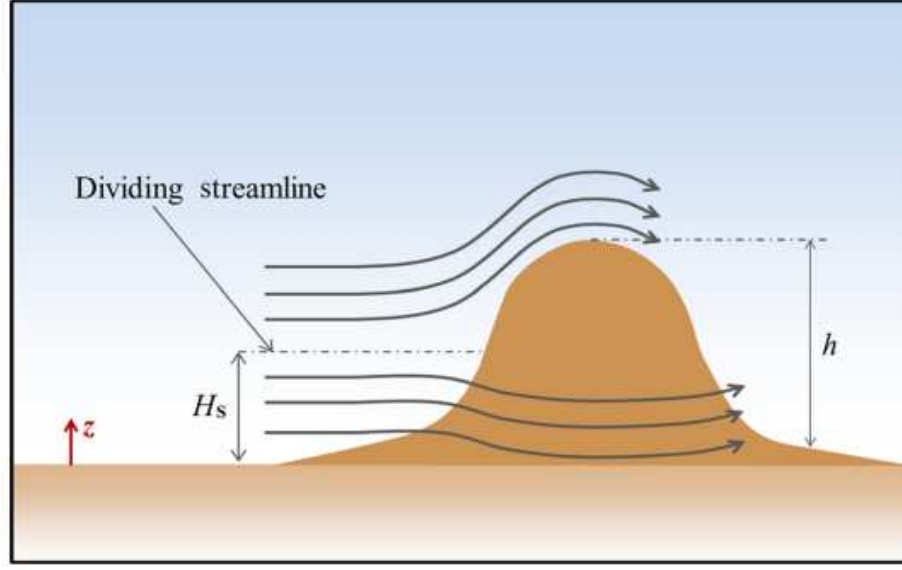


Figure 2.18: Illustration of the dividing streamline concept showing the dividing streamline height and separation of the streamlines above and below a hill (Leo et al., 2015).

Linearisation of the Sheppard (1956) formula is achieved by assuming a constant density gradient which corresponds to a constant buoyancy frequency as per Equation 2.27, and uniform velocity of the approach flow. Consequently, the Sheppard (1956) formula reduces to a simple linear equation, which relates the dividing streamline height to the Froude number of the flow and the height of the terrain obstacle,

$$h_c = h(1 - Fr). \quad (2.32)$$

Laboratory studies by Snyder et al. (1985); Hunt and Snyder (1980) have demonstrated that the concept is broadly applicable to flow separation phenomena over and around small symmetrical and axisymmetrical hills. However, the dividing streamline concept is less reliable for more complex topography where the assumption of a uniform mean flow velocity and density gradient are less plausible, and the turbulent perturbations in the flow are significant (Ryan and Lamb, 1984).

Much of the theory relating to the use of the dividing streamline height has been developed and applied to the flow-fields experienced over isolated hills. However, for obvious reasons, this current study is interested in how the concept relates to the flow-field within valleys. Under the assumption that a valley is in essence, an inverted hill, it likely that an analogous flow scenario develops in the vicinity of a valley, where the dividing streamline height can be used to approximate the critical height at which the flow at the base of a valley has sufficient kinetic energy to surmount the wall of the valley cavity and exit over the trailing edge. Below this height the flow is blocked within the valley cavity. Thus the critical Froude number for

valley flows is equivalent to the critical Froude number  $Fr = 1$  for isolated hills specified in work by Jackson and Hunt (1975), which indicates whether the flow will go over the hill or be blocked upstream and separate around the hill. The Froude number formulation implies that a combination of weak wind, stable atmospheric conditions and deep valleys are likely to give rise to low values of  $Fr$  which indicate the formation of separated flows. In instances where the approach flow is characterized by strong winds upward of  $5 \text{ ms}^{-1}$ , such as those seen in the neutral and near-neutral ABL, ventilating flows are more likely because the buoyancy frequency approaches zero and the Froude number tends to infinity. Work by Grainger and Meroney (1993) examined the influence of Froude number on the persistence of stable inversions within depressions. This work found that inversions that occur within a depression are likely to be flushed out at Froude numbers in excess of 1.6. Such flows are classified as ventilating flows and are responsible for sweeping pollutant emissions out of the valley. Grainger and Meroney (1993) indicated that for the range  $1.3 < Fr < 1.6$ , although localised recirculation may occur, the air in the valley remains coupled to the free atmosphere above. At Froude numbers below 1.3, a separate internal flow regime develops within the valley and any temperature inversion within the valley is exacerbated.

#### 2.3.4 Profiles of Velocity, Temperature and Turbulence

In CFD models, the accuracy of numerical simulations of the ABL are strongly dependent on the manner in which the boundary and initial conditions which characterize a particular atmospheric flow regime are described in the model. The log velocity law is typically used to characterize the constant shear stress surface layer, and is frequently imposed as the inlet velocity profile in CFD simulations (Richards and Hoxey, 1993). Integration of Equations 2.23 yields modified velocity and temperature profiles for the non-neutral ABL (Kaimal and Finnigan, 1994; Gualtieri and Secci, 2011),

$$u(z) = \frac{u^*}{K} \left[ \ln \left( \frac{z}{z_0} \right) - \psi_m \right], \quad (2.33)$$

$$\Theta(z) - \Theta_w = \frac{T^*}{K} \left[ \ln \left( \frac{z}{z_0} \right) - \psi_h \right], \quad (2.34)$$

where  $\psi_m$  and  $\psi_h$  are diabatic terms which are integrals of the non-dimensional wind shear  $\phi_m$ , and temperature flux  $\phi_h$

$$\psi_m = \int_{z_0}^z [1 - \phi_m] \frac{dz}{z}, \quad (2.35)$$

$$\psi_h = \int_{z_0}^z [1 - \phi_h] \frac{dz}{z}. \quad (2.36)$$

Due to the relation,

$$\frac{\partial \Theta}{\partial z} = \frac{\partial T}{\partial z} + \frac{g}{c_p}, \quad (2.37)$$

the temperature profile equation can be expressed in terms of the absolute temperature,  $T_z$ .

$$T(z) = \frac{T^*}{\kappa} \left[ \ln \left( \frac{z}{z_0} \right) - \psi_h \right] - \frac{g}{c_p} (z - z_0) + T_w. \quad (2.38)$$

Based on the Businger-Dyer flux profile functions, where  $\phi_h = \phi_m^2$  Alinot (2003) applied the stability modified profile equations for velocity and temperature to characterize the flow at the inlets of their computational domain. For  $L_{MO} < 0$ ,

$$u(z) = \frac{u^*}{\kappa} \left[ \ln \left( \frac{z}{z_0} \right) + \ln \left( \frac{8\phi_m^4}{(\phi_m + 1)^2(\phi_m^2 + 1)} \right) - \frac{\pi}{2} + 2 \tan^{-1} \left( \frac{1}{\phi_m} \right) \right] \quad (2.39)$$

$$T(z) = \frac{T^*}{\kappa} \left[ \ln \left( \frac{z}{z_0} \right) - 2 \ln \left[ \frac{1}{2} (1 + \phi_m^{-2}) \right] \right] - \frac{g}{c_p} (z - z_0) + T_w \quad (2.40)$$

and for  $L_{MO} > 0$ ,

$$u(z) = \frac{u^*}{\kappa} \left[ \ln \left( \frac{z}{z_0} \right) + \phi_m - 1 \right] \quad (2.41)$$

$$T(z) = \frac{T^*}{\kappa} \left[ \ln \left( \frac{z}{z_0} \right) + \phi_m - 1 \right] - \frac{g}{c_p} (z - z_0) + T_w. \quad (2.42)$$

### 2.3.5 Energy and Turbulence Scales in the ABL

Turbulent kinetic energy quantifies the intensity of turbulent fluctuations in the atmosphere which are directly responsible for the transport of momentum, heat and mass (Srivastava and Sarthi, 2002). Therefore it is important to select appropriate numerical methods that can capture the spatial and temporal characteristics of the turbulent motions which most greatly influence dust dispersion from the depressions that form surface quarries. In the energy-containing range, large eddies with length scales of the same order of magnitude as the depth of the atmospheric boundary layer, derive their energy directly from buoyancy and shear and contain most of the energy of the flow (Kaimal and Finnigan, 1994). These larger eddies in turn supply energy to progressively smaller eddies in the inertial sub-range in an energy cascade process. The smallest eddies at the end of the energy cascade are affected by molecular viscosity and their kinetic energy is dissipated as heat (Libby, 1996). The rate of transfer of energy delivered from the large eddies to smaller eddies in the inertial sub-range is in equilibrium with the energy dissipated by viscosity at the smallest length scales (Tennekes and Lumley, 1972; Arya, 1988), such that the turbulent kinetic energy dissipation rate  $\varepsilon$  is represented by,

$$\varepsilon \sim u^2 \cdot \frac{u}{l} \quad (2.43)$$

where  $u$  is a turbulence velocity scale such that  $k = 1/2u^2$  and  $l$  is the characteristic length scale of turbulence in the inertial sub range. The Kolmogorov Similarity Hypothesis supposes that the energy cascade process dispenses away with the anisotropy of the large eddies, because the decay of large eddies into smaller ones retains none of the directionality of

the larger eddies, giving rise to an inertial sub-range in which turbulence is locally isotropic and its statistical properties are governed by the dissipation rate (MacCready, 1962),

$$\varepsilon = \left( \frac{\tau}{\rho} \right) \frac{\partial u}{\partial z}, \quad (2.44)$$

substituting in  $u_*$  based on the relation in Equation 2.11 and applying K-theory, the profile equation for the turbulent dissipation rate in the neutral ABL is obtained,

$$\varepsilon = \frac{u_*^3}{\kappa z}. \quad (2.45)$$

For the non-neutral atmosphere, Alinot (2003) applied the stability modified profiles for the turbulent dissipation rate given by,

$$\varepsilon = \frac{u_*^3}{\kappa z} \phi_\varepsilon, \quad (2.46)$$

where,

$$\phi_\varepsilon = \begin{cases} \left( 1 - \frac{z}{L_{MO}} \right) & -2 \leq z/L_{MO} \leq 0, \\ \phi_m - \frac{z}{L_{MO}} & 0 \leq z/L_{MO} \leq 1. \end{cases} \quad (2.47)$$

Based on the estimation of eddy wavelengths at the dissipation range and large eddy limit of the inertial sub-range, MacCready (1962) concluded that formulae based on the turbulence isotropy assumption of the inertial sub-range can be applied at heights of up to 200 m in the ABL. However, MacCready (1962) also noted that this was contingent on the stability conditions of the atmosphere. Thus, although RANS models are unable to resolve the larger, anisotropic, energy-containing eddies, their assumption of turbulence isotropy is compatible with the spectral characteristics of turbulence in the inertial sub-range and they can be applied to model near-surface regions of the flow which are dominated by smaller turbulent motions.

### 2.3.6 The Special Case of the Convective Mixed Layer

At surface quarries, the majority of fugitive dust generating activities, including bench blasting, occur during the day when atmospheric conditions are predominantly unstable. The Monin-Obukhov Similarity theory has been applied to characterize the surface layer under both stable and convective conditions, however, above the surface layer turbulence parameters become insensitive to surface shear stress and no longer scale with the friction velocity  $u_*$  and height  $z$  (Garratt, 1994). A new scaling velocity  $w_*$  and temperature  $\Theta_*$  are defined for the convective mixed layer to reflect the dependence of mixed layer turbulence on the surface heat flux and the mixing height,  $z_i$  (Kaimal and Finnigan, 1994),

$$w_* = \left[ \frac{g}{\Theta} (\overline{w'\Theta'}) z_i \right]^{1/3} \quad (2.48)$$

$$\Theta_* = \frac{(\overline{w'\Theta'})}{w_*}. \quad (2.49)$$

Using Equation 2.20,  $w_*$  can be written in terms of  $L_{MO}$

$$w_* = \left( \frac{z_i}{\kappa |L_{MO}|} \right)^{1/3}. \quad (2.50)$$

In Figure 2.19, it can be seen that the mean profiles of velocity and temperature are approximately constant in the mixed layer as thermally enhanced turbulence succeeds in ensuring that the properties of the fluid are well mixed. In particular, the horizontal turbulent fluctuations, represented by the velocity variances  $\sigma_u^2$  and  $\sigma_v^2$  as well as the turbulent dissipation rate are approximately constant as seen in Figure 2.20 according to Caughey and Palmer (1979),

$$\frac{\sigma_{u,v}^2}{w_*^2} \simeq 0.35, \quad (2.51)$$

$$\frac{\varepsilon z_i}{w_*^3} \simeq 0.6. \quad (2.52)$$

In contrast to the horizontal variances, the vertical velocity variance  $\sigma_w^2$  and temperature variance  $\sigma_\Theta^2$  experience some variability in the mixed layer, and aircraft observations by Lenschow et al. (1980) have led to the following variance profiles,

$$\frac{\sigma_w^2}{w_*^2} = 1.8 \left( \frac{z}{z_i} \right)^{2/3} \left( 1 - 0.8 \frac{z}{z_i} \right)^2, \quad (2.53)$$

$$\frac{\sigma_\Theta^2}{\Theta_*^2} \approx 1.8 \left( \frac{z}{z_i} \right)^{-2/3}. \quad (2.54)$$

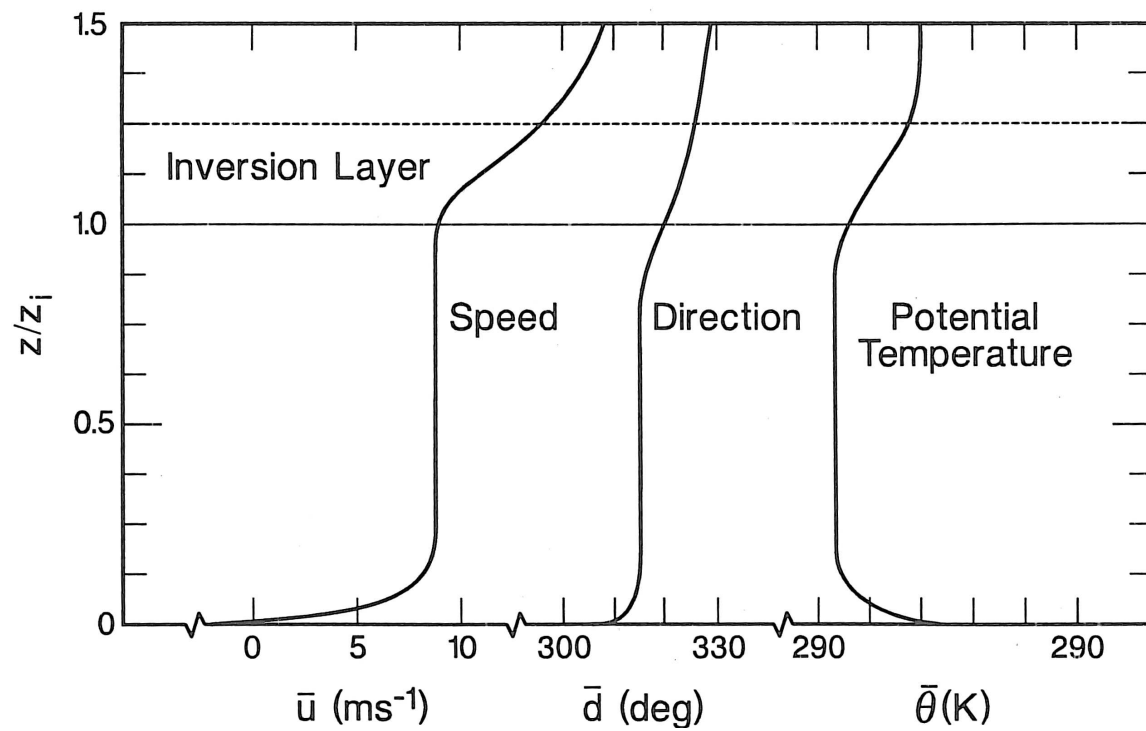


Figure 2.19: Profiles of velocity, wind direction and potential temperature in the convective ABL (Kaimal and Finnigan, 1994).

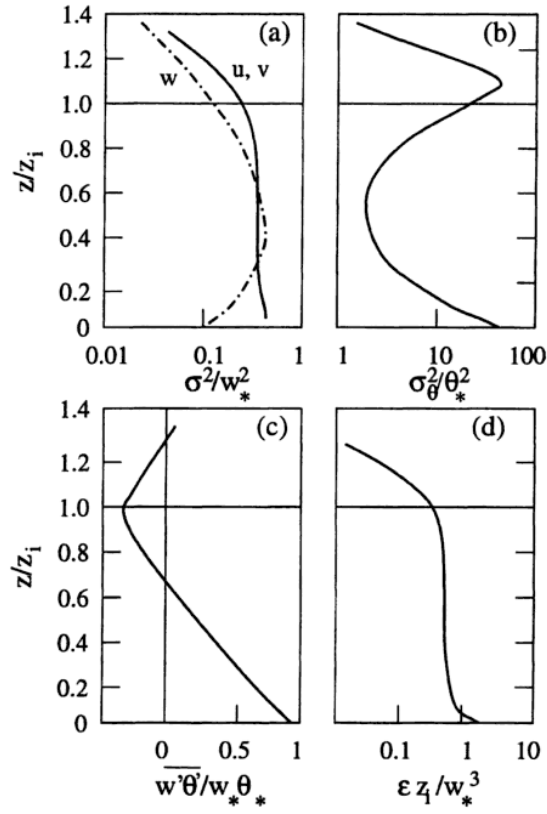


Figure 2.20: Profiles of normalised velocity, potential temperature and buoyancy variances and turbulent dissipation rate in the convective ABL (Caughey and Palmer, 1979)

### 2.3.7 Measuring ABL Meteorological Parameters

The various parameters which define the structure of the ABL have been discussed, and profile equations, including those proposed by Alinot and Masson (2005) to describe the vertical transfer of momentum and heat in the ABL, have been examined. It is now necessary to consider how the scaling parameters representative of the turbulent state of the atmosphere can be derived from routine meteorological data.

The Quality Assurance Handbook for Air pollution Measurement Systems: Volume IV (USEPA, 2008b), provides guidance to the air pollution monitoring community on the collection of meteorological input data for multi-pollutant monitoring networks. Table 2.6 includes both the required and optional meteorological measurement parameters (indicated by an asterisk) as well as the measurement quality objectives which must be met. The minimum recommended sampling frequency for meteorological measurements is one hour.

Table 2.6: Meteorological measurement quality objectives for multi-pollutant monitoring from USEPA (2008b)

| Parameter                             | Method                        | Range            | Resolution |
|---------------------------------------|-------------------------------|------------------|------------|
| Ambient temperature (K)               | Thermistor                    | 243.16 to 320.16 | 0.1        |
| Relative humidity (%)                 | Psychrometer/hygrometer       | 0 to 100         | 0.5        |
| Wind speed ( $\text{ms}^{-1}$ )       | cup/probe sonic anemometer    | 0.5 to 50        | 0.1        |
| Wind direction ( $^{\circ}$ )         | wind vane or sonic anemometer | 0 to 360         | 1.0        |
| Solar radiation* ( $\text{Wm}^{-2}$ ) | Pyranometer                   | 0 to 1100        | 10         |
| Precipitation* ( $\text{mmhr}^{-1}$ ) | Tipping bucket                | 0 to 25          | 0.2        |
| Barometric pressure* (Pa)             | Aneroid barometer             | 600 to 1100      | 0.5        |

Once routine meteorological variables have been measured on site, an appropriate methodology must be adopted to derive the surface layer scaling parameters that are required by the numerical model. Under daytime insolation, Holtslag and Van Ulden (1983) devised a scheme to determine the fluxes of heat and momentum from the surface radiation budget; this scheme forms the basis for the UK-ADMS meteorological pre-processor. During the day, most of the radiation incident on the ground surface is in the form of short wave solar radiation, although some of the longer wavelengths of the electromagnetic spectrum are also present. Depending on the reflectivity of the surface, quantified by the surface albedo, a fraction of the incoming short-wave radiation is reflected back into the atmosphere. The surface also emits low energy radiation with wavelengths in the longer range of the electromagnetic spectrum, a percentage of this longer wavelength radiation is returned to the

ground through back-scattering due to the cloud cover and atmospheric turbidity. Thus, the net radiation at the surface  $Q^*$  is determined from the balance between incoming and outgoing radiation,

$$Q^* = (1 - a)K^+ + L^+ - L^-, \quad (2.55)$$

where  $a$  is the surface albedo,  $K^+$  is the incoming solar radiation (insolation) and  $L^+$  and  $L^-$  are the incoming and outgoing long-wave radiation respectively. Swinbank (1963) postulated that the incoming clear-sky long-wave radiation is a function of emissivity and radiation temperature of the atmosphere and Holtslag and Van Ulden (1983) proposed the use of a cloud cover correction factor to allow for the reflection of long-wave radiation back to the surface by clouds. Therefore the incoming long-wave radiation is expressed as,

$$L^+ = c_1 T_a^6 + c_2 N, \quad (2.56)$$

where  $c_1$  is an empirical constant determined by Swinbank (1963), equivalent to  $5.31 \times 10^{-13} \text{ Wm}^{-2}\text{K}^{-6}$ ,  $T_a$  is the near surface ambient air temperature in Kelvin, and  $c_2$  is a constant radiation flux of  $60 \text{ Wm}^{-2}$  which represents the contribution of cloud cover to incoming long-wave radiation in the mid-latitudes and  $N$  was defined earlier in this chapter, Equation 2.27, as the Brunt-Väisälä buoyancy frequency.

The outgoing long-wave radiation on the other hand, is a function of the ground surface emissivity and surface radiation temperature,  $T_s$ . Thus from the Stefan-Boltzmann law, assuming that the ground surface behaves as a black-body with respect to out-going long-wave radiation, Holtslag and Van Ulden (1983) found that,

$$L^- = \sigma T_s^4, \quad (2.57)$$

here  $\sigma = 5.67 \times 10^{-8} \text{ Wm}^{-2}\text{K}^{-4}$  and is the Stefan-Boltzmann constant; a constant of proportionality relating the outgoing long-wave radiation to the fourth power of the surface radiation temperature.

Since surface temperature is not routinely measured at meteorological stations, Holtslag and Van Ulden (1983) recommended that the outgoing long-wave radiation equation be expressed in terms of the more commonly measured near surface air temperature  $T_a$ ,

$$L^- = \sigma T_a^4 + 4\sigma T_a^3(T_s - T_a), \quad (2.58)$$

where the second term on the right-hand side is a temperature correction term which accounts for the temperature difference between the surface and lower atmosphere under daytime convective conditions. The temperature correction term was deduced by Holtslag and Van Ulden (1983) through field measurements of  $Q^*$ ,  $K^+$  and surface sensible heat flux  $Q_w$ . The field investigations by Holtslag and Van Ulden (1983) also provide a convenient parameter substitution for the temperature correction term in Equation 2.58, as they indicate that the temperature correction term can be approximated by a fraction of the net radiation  $Q^*$ ,

$$4\sigma T_a^3(T_s - T_a) = c_3 Q^*. \quad (2.59)$$

In Equation 2.59,  $c_3$  is a surface heating coefficient which Holtslag and Van Ulden (1983) estimated as 0.12. Thus, by substituting the expressions for  $L^+$  and  $L^-$  into the equation for  $Q^*$ , they derived an expression for net radiation at the surface which uses routine meteorological variables,

$$Q^* = \frac{(1 - a)K^+ + c_1 T_a^6 - \sigma T_a^4 + c_2 N}{1 + c_3}. \quad (2.60)$$

In keeping with the Law of Conservation of Energy, the net solar radiation at the surface is balanced by the ground heat flux, latent heat flux and surface sensible heat flux (Arya, 1988), giving an energy balance equation of the form,

$$Q^* = Q_w + \lambda E + G. \quad (2.61)$$

where  $G$  is the ground heat flux and represents energy absorbed by the surface medium through conduction. The latent heat flux,  $\lambda E$ , denotes the energy required to drive the process of evaporation at the surface and is dependent on both the availability of water at the surface and surface wind speed (Flint and Childs, 1991). Once the sensible heat flux, is determined from Equation 6.2, Holtslag and Van Ulden (1983) recommend an iterative process to determine  $L_{MO}$ , where initial computations of the friction velocity are obtained using the neutral log-law velocity equation.

### 2.3.8 Wind Direction Variability

Dispersion models rely on the input of meteorological data, which are typically averaged over time scales ranging from several minutes to one hour. At these time scales, it becomes necessary to consider the implications of atmospheric motions which exceed the turbulence scale. Figure 2.21 illustrates the full range of spatial and temporal scales at which atmospheric motions occur, however local atmospheric dispersion phenomena are primarily influenced by microscale and mesoscale motions.

Recalling the notion that in contrast to vertical dispersion which is constrained to the depth of the ABL, the horizontal dispersion of a pollutant plume is virtually unconfined and consequently the horizontal spread of the plume is influenced by mesoscale and in some cases synoptic scale atmospheric phenomena, which produce low frequency oscillations of the wind (Vickers et al., 2008; Davies and Thomson, 1999).

Any atmospheric phenomenon which influences wind structure can give rise to wind direction variability, thus gravity waves, drainage flows, topographic effects and cloud cover variations are among the likely causes suggested by Davies and Thomson (1999) and Mahrt (2010). Wind direction variations occur for all classes of atmospheric stability and terrain complexity, but it is noted in work by Anfossi et al. (2005) that oscillations of the wind direction dominate the flow and are therefore the primary drivers of plume dispersion in stable, low wind conditions, where turbulent mixing is suppressed. To dispel any ambiguity which may arise over what is meant by low wind conditions, the definition provided by Deaves and Lines (1998) is invoked here, where low wind conditions are defined as instances

where the mean wind speed,  $\bar{u}$ , is less than or equal to the root mean square horizontal turbulent velocity,  $\sigma_u$ . This equates to wind speeds below  $1 \text{ ms}^{-1}$  in convective conditions and  $0.5 \text{ ms}^{-1}$  in neutral and stable conditions.

A study by Mahrt (2010) examined surface wind variability for the stable boundary layer and found that the standard deviation of wind direction was inversely proportional to the wind speed. Field measurements by Davies and Thomson (1999) indicated that at wind speeds above  $5 \text{ ms}^{-1}$ , the wind direction variability remains approximately constant, suggesting that a minimum, constant value of the standard deviation should be used to account for wind direction variability above a threshold wind speed of  $5 \text{ ms}^{-1}$ .

The UK-ADMS models (CERC Ltd, 2011) adopt the formulation proposed by Moore (1976) to account for wind direction variability and imposes a limit of  $\pm\pi/6$  to the standard deviation of wind direction to restrict wind direction variability to realistic values in low wind conditions, thus according to Moore (1976), the component of wind variability due to motions which exceed the turbulence scale is given by:

$$\sigma_\theta = 0.065 \sqrt{\frac{7T_A}{U_{10}}}, \quad (2.62)$$

for  $-\pi/6 \leq \sigma_\theta \leq \pi/6$ , where  $\sigma_\theta$  represents the wind direction variability in radians,  $T_A$  is the averaging time in hours and  $U_{10}$  is the mean wind speed in  $\text{ms}^{-1}$  at a reference height of 10 m above the ground.

The observation that the wind direction variability increases with averaging time is represented in Moore (1976) empirical formulae and also emerges in work by Davies and Thomson (1999) and Mahrt (2010). Since air quality standards can require assessment of pollutant concentrations at various averaging times, it is therefore useful to adopt a formulation for wind variability which captures the dependence on averaging time, thus the Moore (1976) equation has been used to parametrize wind direction variability in this research project.

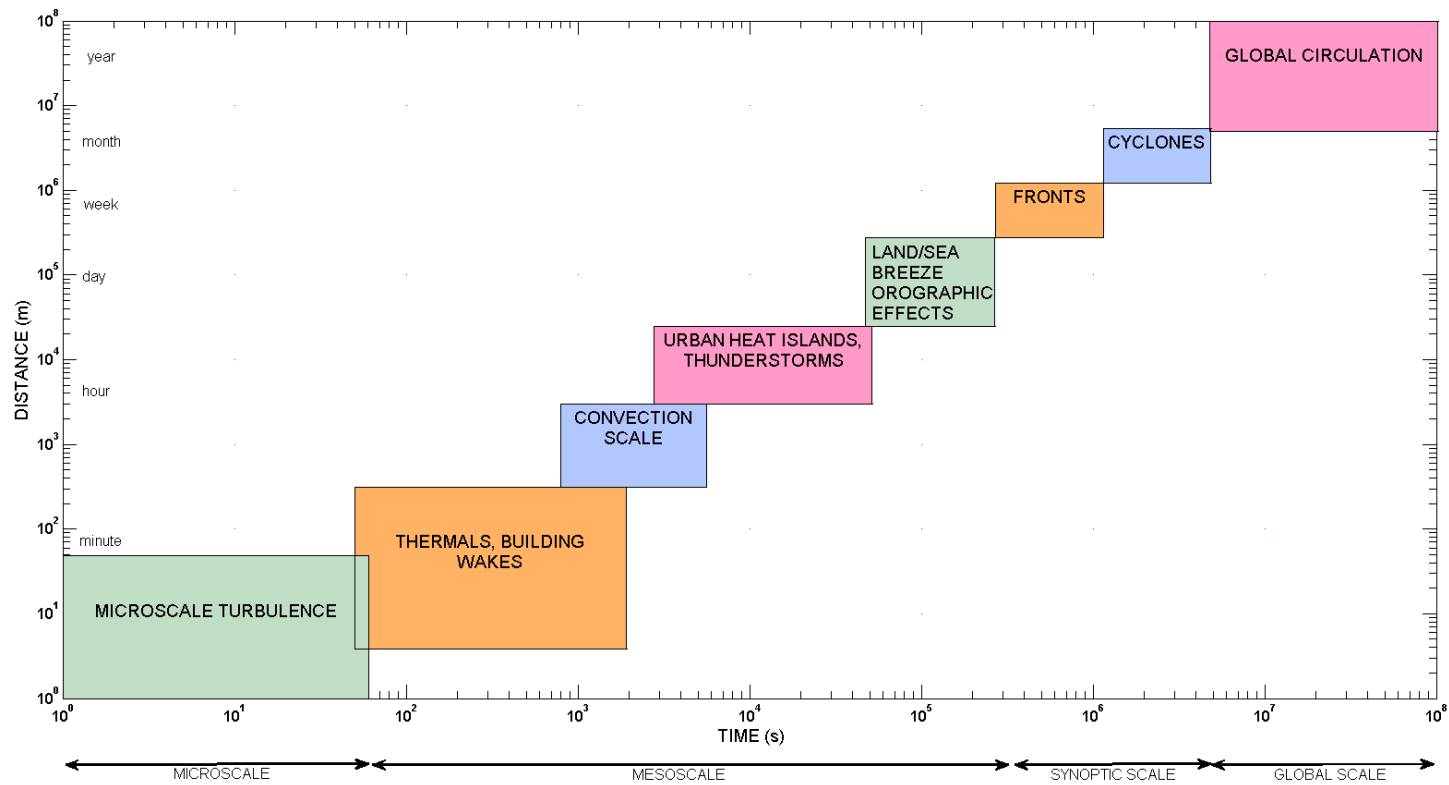


Figure 2.21: Spatial and temporal scales of atmospheric turbulence, adapted from Isaksen et al. (2009)

## 2.4 Summary

The Literature Review has presented extensive discourse on how aspects of quarry dust dispersion modelling might be handled. The dust liberation mechanisms which exist at surface quarry installations have been explored and a scope of operation has been put forward for the proposed numerical model. Discussion of the structure of the atmospheric surface layer has led to the identification of a set of mathematical equations based on Monin-Obukhov Similarity Theory, that can be used to represent the turbulent state of the atmosphere and enable replication of the turbulent flow-field in which dust particles are entrained. This chapter has examined the Froude number and its use as an indicator of flow separation over complex terrain. A means to parametrize the standard deviation of wind direction arising from mesoscale atmospheric motions has been considered. It has emerged, from a survey of the available Literature, that researchers such as Alinot and Masson (2005) have successfully used the  $k - \varepsilon$  turbulence model in conjunction with buoyancy-modified inlet profile equations to simulate the atmospheric surface layer under variable stability conditions. Therefore, these findings will be used in formulating the mathematical basis for the numerical model developed in this research project.

## Optimization of the Numerical model

### 3.1 The Navier-Stokes Equations

Numerical models can offer the opportunity to study atmospheric flows which would otherwise be difficult to replicate in a wind tunnel. They can accommodate complex geometries, variable topography and a broad range of meteorological and physical conditions at relatively low costs compared to wind tunnel scale model experiments (McAlpine and Ruby, 2004). Furthermore, numerical models can be constructed and solved in a relatively short time for prognostic and diagnostic air pollution applications.

Numerical models produce specific solutions of the Navier-Stokes equations which govern the motion of a fluid in three dimensional space. The Navier-Stokes equations are derived by relating the dynamics of the flow to the Conservation Laws of Physics. Firstly, from the Law of Conservation of Mass, the continuity equation can be obtained for a fixed control volume, where the rate of change of mass is equal to the net flux of mass into the control volume,

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

In Equation 3.1, tensor notation has been adopted to denote flow in three dimensions. In accordance with Newton's Second Law of Motion, the rate of change of momentum of a fluid parcel in each of the three directions of a Cartesian coordinate system is expressed in terms of the balance of pressure, surface stresses and external forces acting on the parcel,

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial P}{\partial x_j} + \mu \left( \frac{\partial^2 u_i}{\partial x_j \partial x_j} \right) + \rho g_i + S_{u_i}, \quad (3.2)$$

where  $p$  is the pressure,  $g_i = (0, 0, -g)$  is the gravity vector and  $S_{u_i}$  represents an external momentum source term.

For a moving fluid, the Law of Conservation of Energy is manifested through the First Law of Thermodynamics, where the rate of change of energy of a parcel of fluid is the sum of the net heat flux across the boundaries of the parcel and the rate of work done on the parcel by

surface and body forces acting on the fluid. Therefore, the total energy of the fluid parcel is comprised of mechanical and thermal components,

$$\frac{(\partial \rho E)}{\partial t} + \frac{\partial(\rho u_j E)}{\partial x_j} = -\frac{\partial p u_j}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ \lambda \frac{\partial T}{\partial x_j} \right] + \mu \left[ \frac{\partial}{\partial x_j} u_j \frac{\partial^2 u_i}{\partial x_j \partial x_j} \right] + S_E, \quad (3.3)$$

where  $\lambda$  is the thermal conductivity of the fluid and  $S_E$  is an energy source term which represents the contribution of external sources to the total energy of the fluid.

Following from the general form of the Navier-Stokes and Energy equations, the transport equation for a scalar variable, such as the concentration of pollutant, consists of transient, advective, diffusive and source terms. Therefore, the concentration field of a pollutant entrained in a fluid medium may be determined from the Advection-Diffusion equation,

$$\frac{\partial C}{\partial t} + \frac{\partial(u_j C)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ D_j \frac{\partial C}{\partial x_j} \right] + S_C, \quad (3.4)$$

where  $D_j$  is the mass diffusion coefficient of the pollutant species and  $C = \rho Y$  is the mean concentration of the pollutant, with  $Y$  being the mass fraction of pollutant.  $S_C$  is a pollutant source term.

The randomness of turbulent flows is best considered using a stochastic modelling approach (Tennekes and Lumley, 1972; Libby, 1996), thus Reynolds decomposition is an important treatment of the statistics of turbulence which has been embedded in the physics of eddy viscosity models and has been implemented to disaggregate the flow into mean and fluctuating components. Employing vector notation to represent the directionality of the flow, the Reynolds decomposition of the instantaneous velocity vector is given as,

$$u_i = \overline{u_i} + u'_i, \quad (3.5)$$

and the instantaneous value of a scalar quantity  $\phi$  is expressed as,

$$\phi = \overline{\phi} + \phi'. \quad (3.6)$$

The time-averaged mean component represented by an over-bar, is obtained from an ensemble average over an averaging time which is greater than the lifetime of turbulent eddies in the flow, such that the mean of a field variable can be established in addition to general trends in its fluctuating components (Libby, 1996). In this way, solution of the Navier-Stokes equations is constrained to mean properties of the flow. From Reynolds averaging over the time interval  $t_0$  to  $t_0 + \Delta t$ , the mean  $u$  velocity is obtained,

$$\overline{u_i} = \frac{1}{\Delta t} \int_{t_0}^{t_0 + \Delta t} u_i \, dt, \quad (3.7)$$

The fluctuating component denoted by a prime, represents the contribution of turbulence to variation from the mean value of the flow variable. By definition, the mean of the fluctuating components is zero,

$$\overline{u'_i} = \frac{1}{\Delta t} \int_{t_0}^{t_0 + \Delta t} u'_i \, dt \equiv 0. \quad (3.8)$$

However, the fluctuating components are correlated such that the mean of their covariance terms have non-zero values (Tennekes and Lumley, 1972),

$$\overline{u'_i u'_j} \neq 0, \quad (3.9)$$

Reynolds decomposition of the variables in the Navier-Stokes equations and Reynolds averaging leads to the appearance of these covariance terms in the momentum and energy equations. In particular, the fluctuating velocity covariance terms appear, so that after Reynolds averaging, the stress tensor becomes,

$$\frac{\partial}{\partial x_j} \left( \mu \frac{\partial \overline{u_i}}{\partial x_j} - \overline{\rho u'_i u'_j} \right), \quad (3.10)$$

where the term  $\overline{\rho u'_i u'_j}$  is known as the Reynolds stresses and represents the effects of turbulent stresses which act to deform the fluid (Versteeg and Malalasekera, 1995).

### 3.2 The FLOWSTAR Complex Terrain Module

Under steady-state conditions, the transient term in the Advection-Diffusion equation (Equation 3.4) disappears. Furthermore, by assuming a constant wind speed, with the x-axis oriented in the direction of the mean wind, diffusive transport can be considered negligible relative to advective transport in the along-wind direction, leading to,

$$u \frac{\partial C}{\partial x} = D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} + Q_s \delta(x) \delta(y) \delta(z - z_s). \quad (3.11)$$

where  $Q_s \delta(x) \delta(y) \delta(z - z_s)$  is the pollution emission rate from a point source located at  $(0, 0, z_s)$  specified in mass per unit time,  $u$  is the along-wind velocity,  $D_y$  and  $D_z$  are the mass diffusion coefficients in the  $x$  and  $y$  directions respectively. Applying the boundary conditions:  $C = 0$  as  $|y|$  and  $z$  tend to infinity,  $C(0, y, z) = 0$  and

$$-D_z \frac{\partial C}{\partial z} = 0, \quad z = 0, \quad (3.12)$$

the Gaussian plume model is obtained as a solution to Equation 3.11 in the limits  $0 < x < \infty$ ,  $-\infty < y < +\infty$  and  $0 < z < \infty$ ,

$$C(x, y, z) = \frac{Q_s}{2\pi\sigma_y\sigma_z u} \exp\left(\frac{-y^2}{2\sigma_y^2}\right) \left\{ \exp\left(\frac{-(z - z_s)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z + z_s)^2}{2\sigma_z^2}\right) \right\} \quad (3.13)$$

where  $C(x, y, z)$  is the pollutant concentration at co-ordinates  $(x, y, z)$ , whilst  $\sigma_y$  and  $\sigma_z$  are the standard deviations of the concentration distribution in the crosswind and vertical directions respectively. The second exponential terms accounts for reflection of the plume at the ground. The Gaussian plume equation is applied in analytical dispersion models such as UK-ADMS to calculate the concentration field of a pollutant plume, wherein complex topography and variable meteorological conditions are accommodated through modifications

to plume spread parameters  $\sigma_y$  and  $\sigma_z$  based on flow-field computations of the complex terrain model.

The inability of UK-ADMS to accurately predict fugitive dust dispersion from surface quarries arises due to the simplified treatment of terrain-induced perturbations in the ABL and has been discussed extensively in Chapter 2. In UK-ADMS, the FLOWSTAR algorithm is used to model the atmospheric flow-field over complex terrain. FLOWSTAR is a simple numerical model which provides analytical solutions to linearised flow equations of continuity and momentum (CERC Ltd, 2011). These solutions to the Navier-Stokes equations are based on small perturbation theory devised by Jackson and Hunt (1975). Perturbation velocities and pressures are substituted into the equations of fluid motion to modify the flat-terrain flow-field to account for the presence of complex terrain. Furthermore, the non-linear terms in the flow equations are represented as functions of the mean flow.

FLOWSTAR divides the flow-field into three layers, the first of these is a near-ground *inner layer* where perturbation shear stresses are important, but not thermal stratification. Above the inner layer is a *middle layer*, in which the effects of perturbation shear stresses are felt, however the effects of thermal stratification can again be ignored. The *outer layer* is not influenced by shear stress, but its turbulent structure is dominated by the effects of thermal stratification.

In order to model the flow-field over complex terrain, FLOWSTAR first constructs a regularly spaced 2D grid to describe the extents of the topographic area entered by the user via a terrain file or Ordnance Survey digital terrain NTF (National Transfer Format) file, as shown in Figure 3.1. The boundaries of this domain are defined in the model by a rectangle aligned with the wind direction. This approach is repeated for each wind direction entered in the meteorological module. The spacing of the grid points is specified by the user and the allowable grid density ranges from 32 x 32 to 256 x 256. The FLOWSTAR algorithm produces a Fourier transform which only captures the main spatial structure of the terrain, and the less significant terrain features are filtered out. The Fourier transforms are inverted to determine the flow perturbation velocities, which are subsequently used to adjust the flow velocity and ultimately modify the plume spread parameters and height of the plume centreline (Hill et al., 2005; CERC, 2013). The Fourier transform of the terrain is given by,

$$\tilde{f} = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) e^{-i(k_1 x + k_2 y)} dx dy, \quad (3.14)$$

where  $k_1$  and  $k_2$  are the wave numbers in the  $x$  and  $y$  directions respectively, only the first 32 are considered and higher frequency sinusoids are eliminated. The transform takes the following general form for the perturbation velocities in the  $x$ ,  $y$  and  $z$  direction,  $u_d$ ,  $v_d$  and  $w_d$  respectively,

$$\tilde{u}_{i,d}(k_1, k_2, z) = \frac{\tilde{f}(k_1, k_2) k_1^2 |k_1|}{k_{12}^2} U_0. \quad (3.15)$$

In Equation 3.15,  $U_0 = U(h_m)$ , where  $U_0$  is the unperturbed wind speed which has a value of  $U(h_m)$  at the top of the middle layer and,

$$k_{12} = \sqrt{k_1^2 + k_2^2}. \quad (3.16)$$

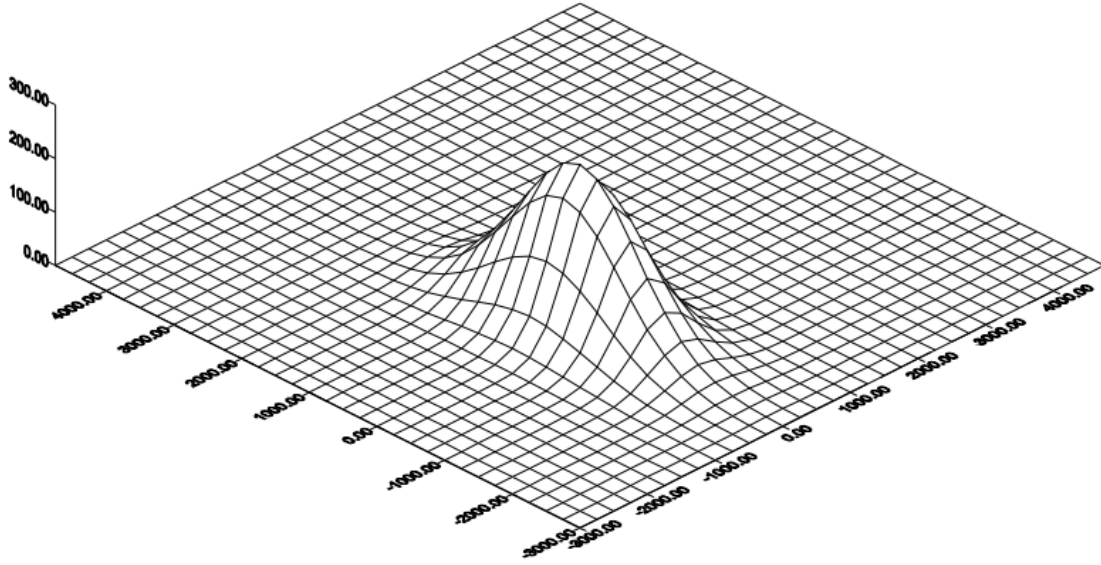


Figure 3.1: FLOWSTAR regularly spaced grid over an isolated hill with domain boundaries defined by wind-aligned rectangle (CERC Ltd, 2011).

Whilst this simplified resolution of the flow-field has the advantage of relatively short computational time, it is limited to terrain gradients under 1:3, where the assumptions of small perturbation theory hold true. It becomes evident that for steeper topographies, a more rigorous solution of the Navier-Stokes equations is required. Moreover, FLOWSTAR only considers recirculation flows when the emission source is fully entrained within the recirculation zone. This severely limits the ability of the model to predict dispersion in the wake of steep hills and in valleys, especially where the plume is partially entrained in these recirculation region.

### 3.3 Numerical Modelling Using CFD

CFD models can offer a more robust treatment of the Navier-Stokes equations of fluid flow to simulate pollutant dispersion than conventional Gaussian numerical methods. However, as has been highlighted in Chapter 2, the computational resource demands of CFD methods are substantially greater than that of conventional Gaussian models. In terms of CPU demand, DNS methods are currently well outside the practical range for non-academic CFD applications involving high Reynolds number flows over complex geometries (Spalart, 2000; Fransen et al., 2011). Whilst LES models are more economical than DNS, due to the fact that only the large scale turbulent motions are resolved, LES can also incur high

CPU costs, which may be up to six orders of magnitude higher than that of steady RANS models (Fransen et al., 2011; Eggenspieler, 2011). Furthermore, Spalart (2000) note that for wall-bounded flows LES results may be inconsistent in the near wall region even when grid refinement and sub-grid scale modelling have been optimized to offer the best treatment of the filtered turbulence scales near the wall. Boersma et al. (1997) have highlighted the inconsistencies of sub-grid scale modelling, noting that whilst these are ordinarily offset by the negligible effect of filtered motions on the resolved large eddies, the contribution of microscale turbulence to total energy of the flow increases in wall bounded flows, where a larger proportion of the flow in the wall-normal direction is occupied by smaller turbulent motions. In these instances, Boersma et al. (1997) advise that the deficiencies of sub-grid scale modelling may be overcome by refining the computational grid such that the cut-off length scale of filtered turbulence is reduced, thus allowing resolution of the smaller motions. Unfortunately, such an undertaking will further increase the demand on CPU resources, making LES methods even less feasible for non-academic atmospheric boundary layer applications. Table 3.1 compares the relative CPU resource demands of LES methods and their transient RANS counterpart - unsteady RANS (URANS). It is seen that LES requires a computational grid which is up to three orders of magnitude finer than that required for URANS solution.

Table 3.1: Comparison of grid size and CPU resource demands for URANS and LES treatment of wall-bounded flow problem (Eggenspieler, 2011).

| Turbulence Model | Cells  | Time steps | CPU ratio |
|------------------|--------|------------|-----------|
| RANS             | $10^6$ | $10^2$     | 1         |
| LES              | $10^9$ | $10^4$     | $10^6$    |

Hybrid Detached Eddy Simulation (DES) models have been proposed to overcome the inconsistencies in modelling the wall stresses experienced with LES sub-grid filtering. For DES models, only separated regions of the flow are resolved and the attached flows which impinge on the wall are subject to RANS treatment. DES solvers require about four times less CPU time than pure LES solvers and can be an ideal option in thin boundary layer flows, where a significant proportion of the energy containing eddies are detached from the wall (Nikitin et al., 2000; Kawai and Larsson, 2012). The formation of an artificial buffer region between the RANS and LES regions of DES due to a mismatch of the log-layer profiles predicted by the RANS and LES solver respectively is observed in work by Piomelli et al. (2003) and has been identified as a persistent problem in DES models (Spalart, 2000). The error associated with this buffer region is not insubstantial, accounting for a 15-20% under-prediction of the wall stresses (Nikitin et al., 2000; Larsson and Kawai, 2010).

Both the LES and DES modelling approaches resolve large scale transient motions and are by definition unsteady solvers. However, a reduction in CPU resource requirements and compatibility with hourly-averaged meteorological data formats are desirable for pollutant

dispersion models. Therefore, CFD modelling for industrial air pollution problems is best served by steady RANS models, which solve the time-averaged flow-field (Huber et al., 2004), offering reasonably robust solutions of turbulent flow regimes (Launder et al., 2002). On this basis, a steady RANS numerical model has been adopted in this work.

### 3.3.1 Selection of a RANS Turbulence Closure Model

Here, the flow has been assumed to be incompressible based on the relatively low velocity of the ambient air and blast cloud velocity estimations reported in work by Silvester et al. (2009). These estimates indicated a maximum blast cloud velocity of approximately  $25 \text{ ms}^{-1}$ , resulting in a Mach number well below the critical value of 0.3 for compressible flows (Ferziger and Peric, 2002). Therefore the differential forms of the steady-state RANS equations for incompressible flow will be adopted and the incompressible RANS equation for continuity and momentum are taken as,

$$\rho \frac{\partial}{\partial x_j}(u_j) = 0, \quad (3.17)$$

and,

$$\rho \frac{\partial}{\partial x_j}(u_i u_j) = -\frac{\partial P}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + S_{u_i}. \quad (3.18)$$

where,  $\tau_{ij}$  represents the stress tensor,

$$\tau_{ij} = \mu \frac{\partial u_i}{\partial x_j} - \overline{\rho u'_i u'_j}, \quad (3.19)$$

The Boussinesq Hypothesis establishes a proportionality relationship between the Reynolds stress tensor and the mean rate of strain through the use of an isotropic turbulent eddy viscosity,  $\mu_t$  which is several orders of magnitude larger than the molecular viscosity  $\mu$  (Launder et al., 2002),

$$\overline{\rho u'_i u'_j} = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right). \quad (3.20)$$

The Reynolds stress terms appear in the energy equation and correspond to the dispersion of heat due to turbulent mixing. For an incompressible flow with constant fluid properties and no radiative heat transfer, the viscous heating and potential energy terms are negligible relative to internal energy of the fluid. Here, the energy equation is expressed in terms of the transport of temperature (Libby, 1996),

$$\frac{\partial}{\partial x_j}[u_j(\rho c_p T)] = \frac{\partial}{\partial x_j} \left[ u_j \tau_{ij} + \frac{c_p \mu_t}{\sigma_T} \left( \frac{\partial T}{\partial x_j} \right) \right] + \rho u_i g_i + S_h, \quad (3.21)$$

where  $\sigma_T$  is the turbulent Prandtl number which is the ratio of turbulent heat diffusivity to  $\mu_t$  and  $S_h$  is an internal energy source term.

As a consequence of Reynolds averaging, additional equations are required to solve for the Reynolds stresses, hence the closure problem associated with RANS models. The most popular linear RANS closure models are based on the Boussinesq Hypothesis, whilst non-linear models employ polynomial representations of the Reynolds stresses to arrive at a system of equations which must be solved concurrently with the RANS equations. The coefficients of the polynomials are routinely derived from calibration with results from experimental flows or previous numerical studies (Launder et al., 2002).

The simplest linear closure models use the Prandtl mixing length theory and apply algebraic expressions to directly relate the eddy viscosity to the mean rate of strain and a characteristic mixing length  $l_m$  (Versteeg and Malalasekera, 1995), resulting in a relation of the form,

$$\mu_t = \rho l_m^2 \sqrt{\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)^2}. \quad (3.22)$$

In wall-bounded flows, the mixing length is dependent on the wall normal distance, which can prove problematic for unstructured grids and separated flows (Launder et al., 2002). Therefore, the more complex two equation models which employ two additional transport equations to determine the fluctuating velocity components and turbulent length scale are generally preferred over mixing length and one equation models because they are not hindered by dependency on wall normal distance. Moreover, one cannot overlook the fact that the use of two-equation models, particularly the standard  $k - \varepsilon$  model, has been well documented in the literature (Alinot and Masson, 2005; Blocken et al., 2007b,a; Gorlé et al., 2009). In the  $k - \varepsilon$  model an extended form of the Boussinesq Hypothesis is used to include the normal Reynolds stresses (Versteeg and Malalasekera, 1995),

$$\overline{\rho u'_i u'_j} = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij}. \quad (3.23)$$

where the turbulent energy  $k$  is defined as,

$$k = \frac{1}{2} \overline{u'_i u'_i}. \quad (3.24)$$

The transport equation for turbulent kinetic energy  $k$  and its dissipation rate  $\varepsilon$  are expressed as,

$$\frac{\partial}{\partial x_j} [u_j (\rho k)] = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon, \quad (3.25)$$

$$\frac{\partial}{\partial x_j} [u_j (\rho \varepsilon)] = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{\varepsilon 1} \frac{\varepsilon}{k} (G_k + (1 - C_{\varepsilon 3}) G_b) - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k}, \quad (3.26)$$

$G_k$  and  $G_b$  are the shear and buoyancy contributions to the production or removal of turbulent kinetic energy, respectively and are expressed by,

$$G_k = -\overline{\rho u_i u'_j} \frac{\partial u_i}{\partial x_j}, \quad (3.27)$$

$$G_b = \beta g_i \frac{\mu_t}{\sigma_t} \left( \frac{\partial T}{\partial x_i} - \frac{g_i}{c_p} \right). \quad (3.28)$$

$C_{\varepsilon 1}$ ,  $C_{\varepsilon 2}$ ,  $C_{\varepsilon 3}$ ,  $C_\mu$ ,  $\sigma_k$  and  $\sigma_\varepsilon$  are the  $k - \varepsilon$  model closure coefficients. The eddy viscosity is computed from the  $k$  and  $\varepsilon$  turbulent velocity and length scale relation,

$$\mu_t = \rho C_\mu \frac{k}{\varepsilon}. \quad (3.29)$$

Alinot and Masson (2005) have demonstrated that the  $k - \varepsilon$  model offers flexibility, both in terms of the configuration of model coefficients and the inclusion of source terms to adapt the model to Monin-Obukhov similarity scaling of the atmospheric surface layer. The relative ease of use and the comparatively low computational expense of the  $k - \varepsilon$  model may also hold strong appeal for surface quarry operators and planners. Thus, the standard  $k - \varepsilon$  model has been selected for turbulence closure of the RANS equations in this work because it presents a good compromise between model accuracy and computational resource demand for engineering applications (Versteeg and Malalasekera, 1995).

### 3.3.2 Finite Volume Discretization of the Calculation Domain

CFD methods compute approximate solutions to the Navier-Stokes equations by first discretizing the fluid continuum into a set of finite locations in space and time, where each element of the grid retains all the macroscopic properties of the fluid continuum (Ferziger and Peric, 2002). Discretization replaces the continuous Navier-Stokes distribution of dependent variables with discrete functions which approximate the variation of these variables at fixed locations in the calculation domain (Patankar, 1980). Most commercial codes apply the finite volume approach because it can accommodate non-uniform and unstructured grids making the approach amenable to complex geometries. Figure 3.2, demonstrates the two-dimensional finite volume discretization as well as the node locations where the discretized equations are defined.

The finite volume method discretizes the flow domain into a series of non-overlapping control volumes. Hexahedral cells are generally preferred because they offer more computationally efficient discretization than tetrahedral cells (Labovsk and Jelemenski, 2011) as they can produce more accurate solutions of the discretized equations for the same number of edges compared to tetrahedral elements (Biswas and Strawn, 1998). On the other hand, tetrahedral cells may be better suited for complex geometries where structured meshing schemes may be difficult to implement and hexahedrons cannot be fitted to the geometry without computationally expensive grid manipulation (Biswas and Strawn, 1998; Yee et al., 2009). Complex domains consisting of unstructured tetrahedral meshes typically contain an inflation layer comprised of triangular prismatic elements applied near the wall to improve flow-field resolution in the near-wall region.

Finite difference approximations based on truncated Taylor series expansions are substituted into the Navier-Stokes equations to represent the partial derivatives in the convective, diffusive and source terms which contribute to the variation of each flow variable throughout the

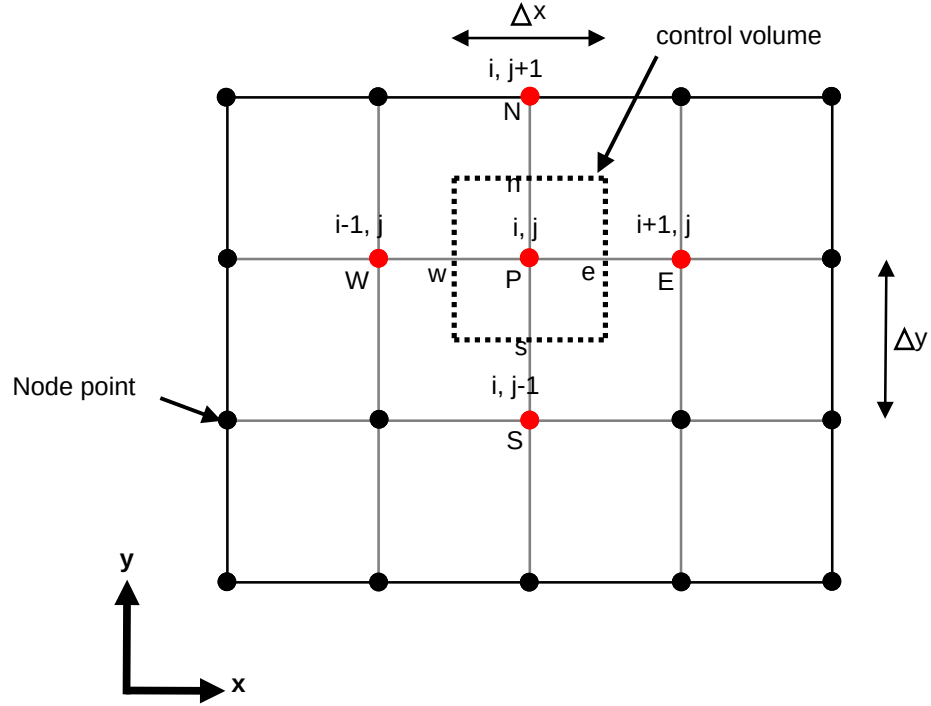


Figure 3.2: Illustration of finite volume discretization for a 2-dimensional structured grid.

calculation domain (Ferziger and Peric, 2002; Versteeg and Malalasekera, 1995). Higher-order terms in the Taylor series expansion are neglected, giving rise to a truncation error in the approximations. The resulting discretized equations are solved iteratively for each control volume to produce an approximate solution of the flow variables at the centroid of the control volume. Interpolation can be performed to obtain the value of flow variables at intermediate locations between the centroids of adjacent cells.

The proprietary ANSYS CFD meshing packages, GAMBIT 2.4.6 and ICEM CFD 14.5 have been used at various stages of this research project to construct computational domain geometry and produce optimized meshes for export to the CFD solver. GAMBIT 2.4.6 has been used to construct meshes for the homogeneous profile tests discussed in Section 3.4 of this chapter as well as the wind variability and idealized terrain studies in Chapters 4 and 5 respectively. GAMBIT 2.4.6 is best suited for a top-down modelling approach in which primitive 3D solids are used to construct the domain geometry, the software supports hexahedral, tetrahedral, pyramid and prism elements. ICEM CFD has been used for the considerably more complex geometry of the case study quarry in Chapter 6; it can produce meshes using faceted geometry from Stereolithographic (STL) terrain files and offers efficient meshing and diagnostic tools to create a mesh which satisfies the mesh quality criteria of the CFD solver.

### 3.3.3 Numerical Errors and RANS Limitations

Finite volume discretization of the fluid continuum invariably contributes to errors in the solution of the flow-field. Therefore, for a steady state RANS problem, discretization error represents the difference between the exact solution of the discretized equations and the analytical solution of the RANS partial differential equations (Zikanov, 2010), and only vanishes for an infinitesimally small grid spacing where the mesh most closely approximates the fluid continuum. Hence, a sufficiently fine grid must be constructed to minimise numerical uncertainty due to finite volume discretization. Consequently, it is important to verify grid independence of the solution by ensuring that there are no appreciable changes in the converged solution for incremental changes in grid refinement. Naturally, a converged numerical solution, in which appropriate convergence criteria have been defined and the normalized residuals have decayed by at least three orders of magnitude is required for demonstrating grid independence (Ferziger and Peric, 1996; Roache, 1997).

Roache (1997) presents a protocol involving the systematic refinement of the computational grid to evaluate grid independence in which grid refinement indices such as the Richardson error estimator may be used to estimate grid-convergence error. By comparing the solutions obtained using a coarse and a fine computational grid of similar geometric properties and cell height ratios no less than 1.3, the grid-convergence error in the solution can be estimated for the fine grid from,

$$E_{fine} = \frac{f_2 - f_1}{1 - r^p}, \quad (3.30)$$

where  $f_1$  and  $f_2$  are fine and coarse grid solutions of a variable,  $r$  is the grid refinement ratio given by,

$$r = h_2/h_1 > 1, \quad (3.31)$$

where  $h_2$  and  $h_1$  are the grid spacings of the coarse and fine meshes respectively and  $p$  is the formal order of accuracy of the solution algorithm which is dependent on the highest order of differencing terms included in the truncated Taylor series expansions. The coarse grid error is given by,

$$E_{coarse} = \frac{r^p(f_2 - f_1)}{1 - r^p}. \quad (3.32)$$

Additionally, Roache (1997) and Phillips and Roy (2011) recommend the use of a Grid Convergence Index (GCI) which accounts for uncertainty in the Richardson estimators through the use of a safety factor. The GCI is defined as,

$$GCI_{fine,coarse} = F_s |E_{fine,coarse}|, \quad (3.33)$$

where  $F_s$  is a safety factor usually equal to 3 (Roache, 1997).

Apart from discretization error, other sources of error and uncertainty in CFD simulations arise from simplifications made in the mathematical representation of the flow as well as numerical approximations and structural limitations contained in the CFD code (Franke et al., 2007). Modelling errors are typically associated with an imprecise mathematical model, for example the use of inappropriate boundary conditions and poor initialization of

the flow. Numerical sources of error, with the exception of those due to a failure to ensure iterative convergence, are due to the innate limitations of the selected CFD code such as computer round-off and, are outside the control of the modeller (Ferziger and Peric, 1996; Franke et al., 2007).

Various recommendations have been put forward to improve the overall performance of the  $k - \varepsilon$  mathematical model and minimize computational error. Apsley and Castro (1997) recommended grid refinement near the pollutant source to improve model predictions of pollutant transport, whilst the studies of Franke et al. (2007), Riddle et al. (2004), Gorlé et al. (2009) and Pontiggia et al. (2009) have applied grid refinement near the wall to permit resolution of the near-wall region, where steep gradients in flow variables are observed. Alinot and Masson (2005) explored the representation of various turbulent states of the atmospheric surface layer in order to accurately characterize the wind regime under different meteorological conditions. Suffice to say, the successful replication of incompressible ABL flows is contingent upon the use of solver settings and boundary conditions which are compatible with the physics of the flow.

### **3.4 Obtaining Homogeneous ABL Profiles using the ANSYS FLUENT $k - \varepsilon$ model**

The ANSYS FLUENT version 14.5  $k - \varepsilon$  model, subsequently referred to as the FLUENT  $k - \varepsilon$  has been employed throughout this work to model the atmospheric flow-field. ANSYS FLUENT is a commercial CFD package that is extensively used for both industrial and academic fluid flow applications. ANSYS Inc., the proprietor of FLUENT, distributes the software for both HPC (High Performance Computing) and desktop use. The FLUENT package offers a comprehensive suite of CFD modelling tools, including LES, DES, the Reynolds Stress Model, two equation turbulence models such as the  $k - \varepsilon$  and  $k - \omega$  closure models and the Spalart-Allmaras one equation turbulence model. FLUENT provides various customization options and model configuration settings which permit the simulation of single or multiphase turbulent flows coupled with physical phenomena such as heat transfer, species transport, particulate dispersion, acoustic transmission and combustion.

FLUENT offers the choice of either a pressure-based or a density-based solver. The latter option uses the continuity equation to calculate the density field and the equation of state to calculate the pressure field, and is preferred for compressible, high speed flows in which shock waves may develop (ANSYS, 2009a). The pressure-based solver computes the pressure field from a sequence of pressure and velocity correction steps, involving the continuity and momentum equations. The pressure-based solver is more suitable for low speed, incompressible or moderately compressible flows (Mach Number  $< 0.3$ ). In addition to these solver settings, FLUENT RANS models can accommodate both transient and stationary flows. Furthermore, FLUENT permits the user to change the velocity formulation from an absolute to a relative frame of reference for rotating flows.

The capabilities of the FLUENT solver can be expanded through the use of User Defined Function (UDF) The UDF structure conforms to general C syntax rules and is comprised

of functions and macros which can perform the aforementioned operations. Pre-defined functions and macros are provided by FLUENT in a built-in *udf.h* header file which is accessed in the UDF through the use of an include directive.

In addition to ensuring adequate refinement of the computational grid, it is also important to verify that the mesh is of sufficient quality to allow the solver to converge to the correct solution of the flow-field. FLUENT uses the following criteria to assess the quality of a mesh:

1. The cell squish index ranges from 0 to 1 and measures non-orthogonality of a cell. It is computed using a vector from a cell centroid to each of its faces and the corresponding face area vector. Values close to 1 indicate poor quality, however FLUENT is able to tolerate cells with squish index values up to 0.95.
2. The aspect ratio quantifies the stretching of a cell, and is evaluated using the ratio of the maximum to minimum distance of either the cell centroid to any of the face centroids or the cell centroid to any node. It is recommended that the aspect ratio be restricted to a maximum of 5:1 in the bulk flow away from the walls and 35:1 in boundary layer regions.
3. Cell skewness is a measure of the distortion of a cell, computed as the difference between the actual cell shape and that of an equilateral shape of equivalent volume. For FLUENT simulations, average skewness should be limited to 0.33 for the entire mesh and 0.95 for any individual element.

### 3.4.1 $k - \varepsilon$ Model Solver Settings

The solver settings for ANSYS FLUENT version 14.5  $k - \varepsilon$  code have been selected in accordance with work by Alinot and Masson (2005), to optimize the model for ABL flow under different atmospheric stability classes. Firstly, the pressure-based solver which was developed for incompressible, low velocity flows has been used in conjunction with a Pressure-Velocity coupling algorithm. Although the modeller is afforded the option of solving the discretized RANS equations sequentially using the segregated pressure-based solver, the coupled solver is routinely employed because it provides faster solution convergence (ANSYS, 2009a). Unlike the density-based solver which determines the pressure field from the ideal gas equation, the coupled pressure-based solver calculates the pressure field from an iterative pressure correction routine which links the solution of the momentum and continuity equations (Versteeg and Malalasekera, 1995; ANSYS, 2009a).

The SIMPLEC (Semi-Implicit Method for Pressure Linked Equations-Consistent) algorithm has been chosen for pressure-velocity coupling. SIMPLEC is a variant of the default SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm, with fewer approximations in the derivation of the pressure and velocity corrections (Versteeg and Malalasekera, 1995). SIMPLEC uses an initial, guessed pressure field to compute the velocity field from the discretized momentum equations. The algorithm then proceeds to substitute the velocity components into the continuity equation, to produce a pressure correction term

which is subsequently applied to adjust the pressure field in the momentum equations. The pressure and velocity field are corrected iteratively until the solution converges. The pressure field is corrected according to the relation,

$$P = P^* + \alpha_P P', \quad (3.34)$$

where  $P^*$  represents the initial pressure estimate and  $P'$  is the pressure correction term. The coefficient  $\alpha_P$  denotes an under-relaxation factor which is applied to moderate large values of the correction term so that solution convergence is possible even when there is a significant difference between the estimated pressure field and the corrected pressure (Versteeg and Malalasekera, 1995). The corresponding velocity field is corrected in a similar fashion. The steps of the SIMPLEC pressure-velocity coupling algorithm are illustrated in detail in Figure 3.3, where the discretized equations are displayed and the terms  $d_{i,j}$  represent the under-relaxation factors.

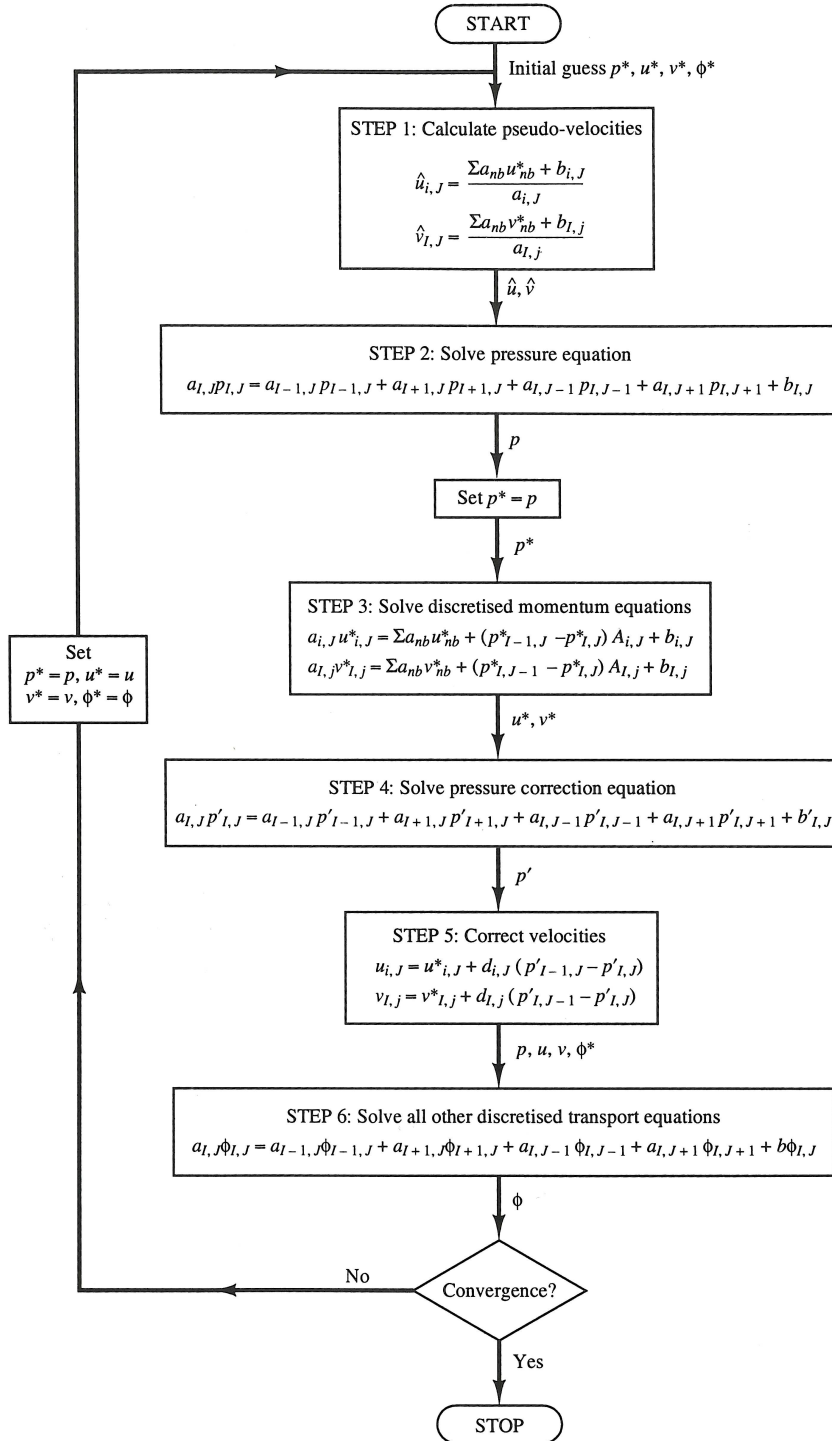


Figure 3.3: SIMPLEC pressure-velocity coupling algorithm iterative steps to solve the discretized equations using initial guessed field for pressure, velocity and transported variables from Versteeg and Malalasekera (1995).

Alinot and Masson (2005) developed their CFD model for aerodynamic analysis of rotational flows associated with wind turbines, and selected the Pressure Staggered Option (PRESTO) for pressure interpolations. The PRESTO scheme is indicated for flows with large pressure variations such as high speed, swirling flows (ANSYS, 2009a), where interpolation of nodal values of velocity to estimate the pressure gradient at the cell faces yields non-physical results. PRESTO implements a staggered grid which allows direct evaluation of the pressure gradient on the cell faces. Since swirling flows do not feature in the current study, the standard pressure interpolation scheme is retained. The second order upwind differencing

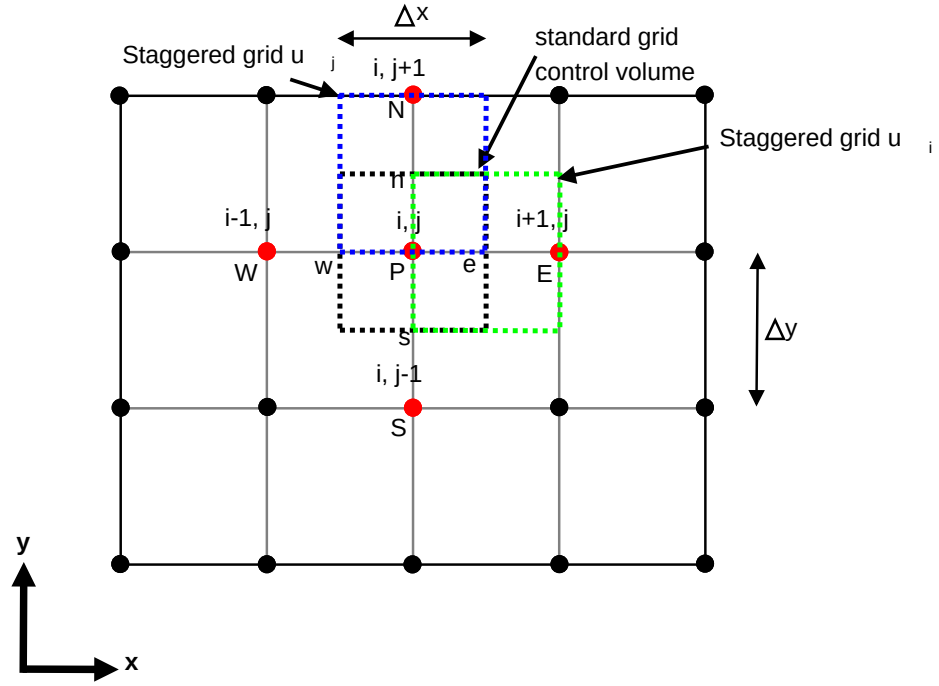


Figure 3.4: Illustration of staggered grid system to allow evaluation of velocity components on alternate grid for pressure interpolation.

scheme has been selected to compute the advection terms in the discretized RANS equations. The scheme preserves the direction of propagation of transported properties when the flow vector between two adjacent cells is not normal to the faces of the downwind cell. A least-squares cell based approach has been adopted to evaluate gradients required for computation of derivatives in the diffusion and advection terms.

### 3.4.2 Appropriate Boundary Conditions

Appropriate initial and boundary conditions are imposed on the computational domain to constrain the solution of the general Navier-Stokes equations to a particular flow-field (Anderson Jr, 1995; Versteeg and Malalasekera, 1995). Boundary conditions demarcate solid

and fluid regions of the domain, specify the fluxes of mass, momentum and heat entering the domain and indicate the direction of the incoming flow and its initial turbulence characteristics (Ashgriz and Mostaghimi, 2002). Consequently, the definition of appropriate boundary conditions in CFD models follows a two-pronged approach. It is seen that the physical implementation of a particular type of domain boundary is coupled with specification of numerical constraints on the values of variables at the boundary in mathematical forms which correspond to Dirichlet, Neumann or mixed boundary conditions (Ferziger and Peric, 2002; Ashgriz and Mostaghimi, 2002).

The boundary conditions must be compatible with the physics of the flow problem. For instance, in wall-bounded viscous flows, the enforcement of the no-slip condition at the wall acts to constrain the velocity and temperature in the wall-adjacent layer of fluid to that of the wall. Correct reproduction of the ABL flows in CFD models depends on the definition of fully developed velocity and turbulence profiles at the domain inlet, such as those proposed by Richards and Hoxey (1993). These inlet profiles represent the influence of an upstream fetch not modelled in the computational domain (Franke et al., 2007). Hargreaves and Wright (2007) used a symmetry boundary at the top of the domain in order to test the ability of unmodified CFD wall functions to produce sustained ABL profiles across their domain, based upon the modelling approach proposed by Richards and Hoxey (1993). Hargreaves and Wright (2007) and Franke et al. (2007) suggest the application of a constant shear stress corresponding to the velocity profiles at the top of the domain, to prevent decay of the velocity profile when a symmetry condition is enforced at the top boundary. Alternatively, Franke et al. (2007), Blocken et al. (2007a) recommend the use of fixed values for the flow variables in the layer of cells adjacent to the top of the domain in conjunction with the symmetry boundary. Alinot and Masson (2005) specified velocity inlets at the upwind and top boundaries of their computational domain, which is illustrated by Figure 3.5. The velocity inlet boundary is prescribed for incompressible flows, and allows for the specification of velocity and scalar profiles which are used to compute the fluxes of mass, momentum and energy entering the domain (ANSYS, 2009a).

The stability modified profiles for  $\mathbf{u}$ ,  $T$ ,  $k$  and  $\varepsilon$  presented in Chapter 2 were imposed at the domain inlet through the use of User-Defined Functions (UDFs) which serve to extend the functionality of the FLUENT  $k - \varepsilon$  turbulence model. From the  $\varepsilon$  profile equation,

$$\varepsilon(z) = \frac{u_*^3}{\kappa z} \phi_\varepsilon, \quad (3.35)$$

an expression for the turbulent kinetic energy can be derived by substituting the model equation for turbulent viscosity, Equation 3.29 into the mixing length relation (Alinot and Masson, 2005),

$$\mu_t = \frac{\rho k u_* z}{\phi_m} \quad (3.36)$$

resulting in the stability modified Richards and Hoxey (1993) profile for the turbulent kinetic energy,

$$k(z) = \sqrt{\frac{\mu_t \varepsilon}{\rho C_\mu}} = 5.48 u_*^2 \left[ \frac{\phi_\varepsilon}{\phi_m} \right]^{1/2}. \quad (3.37)$$

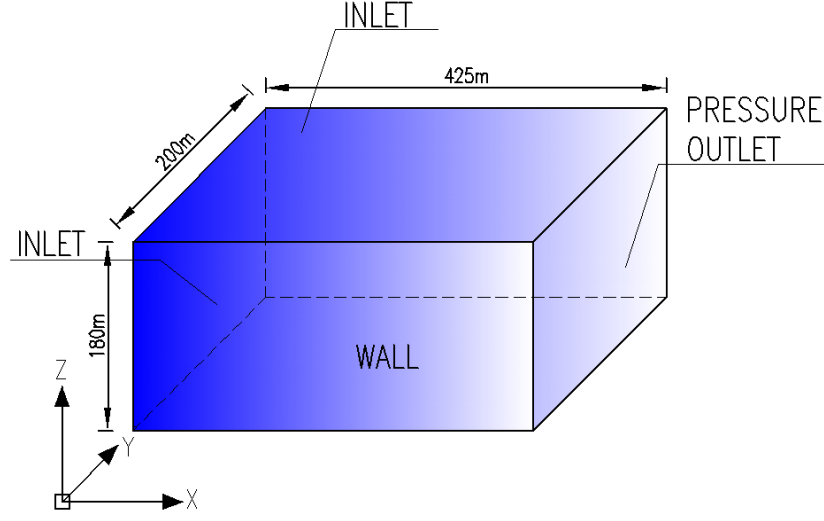


Figure 3.5: Diagram of flat terrain modelling domain.

Pontiggia et al. (2009) noted that when a velocity inlet condition is applied at the top of the computational domain, the vertical profiles of velocity and temperature are preserved at the expense of the fluxes of turbulent kinetic energy and its dissipation rate. The turbulence profiles are brought to zero because the component of velocity normal to the boundary is zero. Fortunately, this does not interfere with solution values in the near-surface region if the computational domain is sufficiently high (Blocken et al., 2007a).

Alinot and Masson (2005) based their use of an outflow condition at the downwind boundary of their domain on the recommendations of Patankar (1980), which prescribe the use of an outflow where the flow is fully developed and the outflow boundary can be positioned far away from zones of interest in the calculation domain to avoid propagating errors due to forcing of the diffusive flux to zero at the outflow. Consequently, a pressure outlet boundary condition is preferred in this study where the flow behaviour in the downwind fetch is significant. Symmetry boundary conditions were imposed on the lateral boundaries of the computational domain.

### 3.4.3 Stream-wise Gradients in the Undisturbed ABL and the Role of Wall Functions

Wall functions are implemented in the FLUENT  $k - \varepsilon$  model to resolve the flow-field in the viscosity affected near-wall region where the flow profiles may not be accurately captured by the turbulence model (Craft et al., 2004; ANSYS, 2009b). The near-wall region consists of three parts as shown in Figure 3.6, an inner viscous sub-layer where the flow is approximately

laminar, an outer layer where the log-law is applied and an intermediate buffer region (Blocken et al., 2007b).

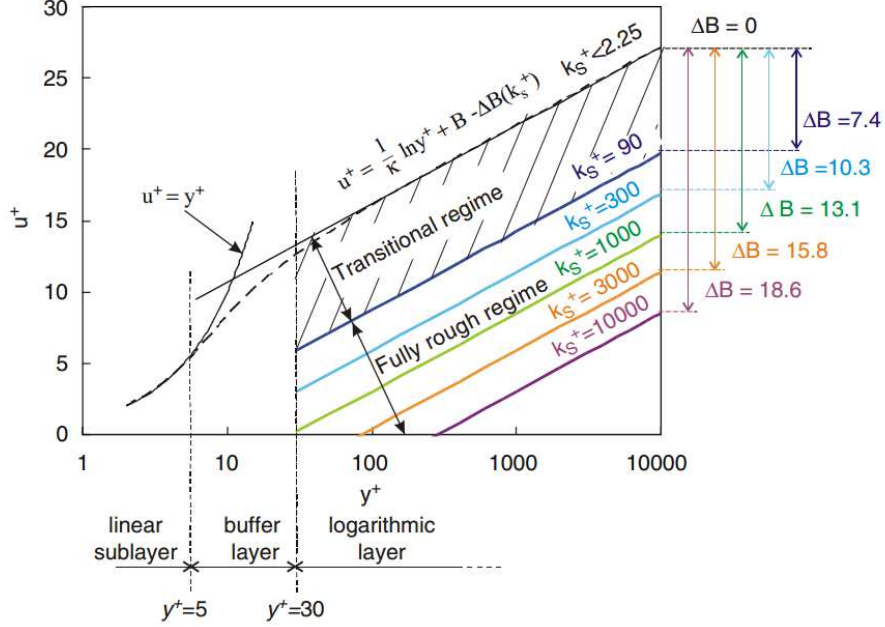


Figure 3.6: Law of the wall for smooth and sand-grained roughened surfaces showing law of the wall for the viscous sublayer, buffer layer and log region (Blocken et al., 2007b).

Consequently, stream-wise gradients may develop along the flow in the empty computational domain as a result of incompatibility between the wall function and the boundary layer profiles imposed at the inlet (Hargreaves and Wright, 2007; Blocken et al., 2007b,a). In order to assess the severity of stream-wise gradients in the flow profiles, Blocken et al. (2007b) recommends simulation of the atmospheric boundary layer in an empty fetch before any complex terrain features are introduced.

Considering a two dimensional flow in which the  $y$  coordinate is vertical and synonymous with the  $z$  coordinate in a three dimensional flow, the standard rough wall log-law for mean velocity in FLUENT is expressed as,

$$\frac{u}{u_*} = \frac{1}{\kappa} \ln \left( \frac{E k_s y^+}{C_{k_s} k_s^+} \right), \quad (3.38)$$

$$y^+ = \frac{\rho y_p u_*}{\mu}, \quad (3.39)$$

$$k_s^+ = \frac{\rho k_s u_*}{\mu}, \quad (3.40)$$

$$u_* = C_\mu^{1/4} k_p^{1/2}, \quad (3.41)$$

where  $y^+$  and  $k_s^+$  represent the dimensionless wall distance and dimensionless equivalent roughness respectively.  $E_{ks}$  is an empirical model constant with a value of 9.793 and  $C_{ks}$  is a roughness constant usually taken as 0.5. The distance from the wall to the centroid of the wall adjacent cell is represented by  $y_p$  and  $k_s$  is the equivalent sand-grain roughness height.  $k_p$  is the turbulent kinetic energy in the wall adjacent cell, which along with the dissipation rate  $\varepsilon_p$  are estimated by the wall functions,

$$k_p = \frac{u_*^2}{\sqrt{C_\mu}}, \quad (3.42)$$

$$\varepsilon_p = \frac{u_*^3}{\kappa y_p} \quad (3.43)$$

The dimensionless equivalent sand-grain roughness is derived from the shift in the  $y$ -intercept of the smooth wall log-law which is required to accommodate rough-wall flows. The log-law is employed when  $y^+ > 11.225$ , below this value, the linear relation  $u^+ = y^+$  is used to model the laminar viscous sub-layer.

Wall functions implicitly model the effects of roughness elements outside the boundaries of the computational domain, therefore horizontal inhomogeneity of the undisturbed ABL profiles can also be caused by incorrect specification of ABL roughness height in the  $k - \varepsilon$  model (Hargreaves and Wright, 2007). In particular, an equivalent sand-grain roughness height  $k_s$  must be defined for the ABL, to match the effects of aerodynamic roughness  $z_0$  to that of the equivalent roughness in the law of the wall (Hargreaves and Wright, 2007; Blocken et al., 2007b),

$$k_s = \frac{E_{ks} z_0}{C_{ks}}. \quad (3.44)$$

As illustrated in Figure 3.7, the law of the wall is implemented to bridge the solution between the centroid of the wall-adjacent cell and the wall. Therefore, it is necessary to ensure that the condition  $y_p > k_s$  is satisfied. For rough terrain, where values of  $z_0 > 0.1$  m are typical, it is difficult to simultaneously maintain this condition and the requirement for adequate resolution of the near wall ABL, which necessitates high vertical grid refinement near the wall, starting with a first cell height of less than 1 m (Blocken et al., 2007a). Moreover, values of  $y^+$  which lie within the limit  $30 < y^+ < 500$  are required for consistent application of the rough wall functions however, for ABL flows,  $y^+$  values in excess of 10000 are not uncommon, due to the  $y_p$  restrictions and characteristic  $u_*$  values of the ABL (Hargreaves and Wright, 2007). To overcome this problem Blocken et al. (2007b) have suggested that the FLUENT code should be modified to accommodate  $z_0$  dependent wall functions instead of  $k_s$  dependent wall functions. Chavez et al. (2012) and Gromke et al. (2008) adopted the less onerous option of using a shorter upstream domain to minimize stream-wise gradients as they were unable to implement  $k_s$  geometric roughness whilst maintaining a sufficiently fine vertical mesh. They concluded that effects of explicitly modelled large scale obstacles would significantly outweigh the effects of stream-wise gradients attributable to an ABL roughness specification which did not uphold Equation 3.44.

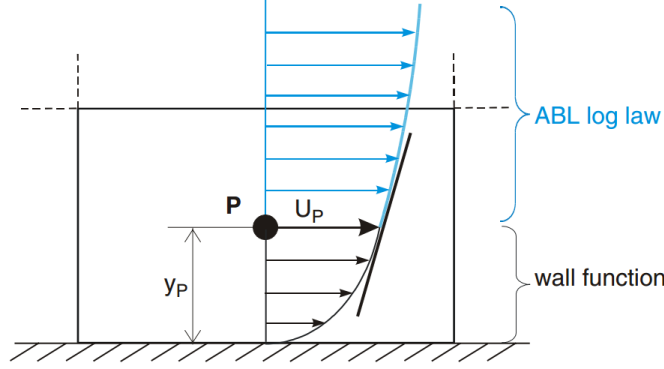


Figure 3.7: Wall function fitting of logarithmic inlet velocity profile at centre of wall adjacent cell Blocken et al. (2007b).

#### 3.4.4 Model Coefficients and the Inclusion of Buoyancy Effects

Crespo and Hernandez (1996) and Alinot and Masson (2005) modified the default  $k - \varepsilon$  coefficients in order to make the closure equations compatible with Monin-Obukhov similarity theory. Significant efforts were made by Alinot and Masson (2005) to present robust mathematical models of the atmospheric boundary layer which could replicate the stable, neutral and unstable ABL.

Alinot and Masson (2005) deduced that appropriate values of  $C_{\varepsilon 3}$  were required in order to obtain congruence between the Monin-Obukhov theory and the  $k - \varepsilon$  turbulence model when the effects of thermal buoyancy were significant, therefore an expression for  $C_{\varepsilon 3}$  was derived from the  $\varepsilon$  equation,

$$C_{\varepsilon 3} = 1 - \frac{\mu_T \left( \frac{\partial u}{\partial z} \right)^2}{G_b} + \frac{C_{\varepsilon 2} \rho \epsilon}{C_{\varepsilon 1} G_b} - \frac{k}{G_b \epsilon C_{\varepsilon 1}} \left[ \frac{\partial}{\partial z} \left( \frac{\mu_T}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial z} \right) \right] \quad (3.45)$$

Subsequently the curve fitting expression, Equation 3.46 was obtained, where  $C_{\varepsilon 3}$  is represented as a function of the stability parameter,  $z/L$ ,

$$C_{\varepsilon 3} = \sum_{n=0}^5 a_n \left( \frac{z}{L} \right)^n, \quad (3.46)$$

where the values of  $a_n$  are stability dependent coefficients of the curve fitting expression. Table 3.3, summarizes the modifications to the coefficients  $C_\mu$ ,  $C_{\varepsilon 1}$ ,  $C_{\varepsilon 2}$  and  $C_{\varepsilon 3}$  of the  $k - \varepsilon$  model adopted by various researchers over the decades since the original model was proposed by Jones and Launder (1972). In these studies, values of  $\kappa = 0.42$ ,  $\sigma_T = 1.0$ ,  $\sigma_k = 1.0$  and  $\sigma_\epsilon = 1.3$  were adopted.

Table 3.2: Alinot and Masson (2005)  $C_{\varepsilon 3}$  curve fitting expression coefficients

| $a_n$ | $L > 0$              |                      | $L < 0$                           |                                   |
|-------|----------------------|----------------------|-----------------------------------|-----------------------------------|
|       | $\frac{z}{L} < 0.33$ | $\frac{z}{L} > 0.33$ | $\left \frac{z}{L}\right  < 0.25$ | $\left \frac{z}{L}\right  > 0.25$ |
| $a_0$ | 4.181                | 5.225                | -0.0609                           | 1.765                             |
| $a_1$ | 33.994               | -5.269               | -33.672                           | 17.1346                           |
| $a_2$ | -442.398             | 5.115                | -546.880                          | 19.165                            |
| $a_3$ | 2368.12              | -2.406               | -3234.06                          | 11.912                            |
| $a_4$ | -6043.544            | 0.435                | -9490.792                         | 3.821                             |
| $a_5$ | 5970.776             | 0.000                | -11163.202                        | 0.492                             |

 Table 3.3:  $k - \varepsilon$  turbulence closure model constants

| Researchers            | $C_\mu$ | $C_{\varepsilon 1}$ | $C_{\varepsilon 2}$ | $C_{\varepsilon 3}$                |
|------------------------|---------|---------------------|---------------------|------------------------------------|
| Jones and Launder 1972 | 0.09    | 1.44                | 1.92                | 1.0                                |
| Crespo et al 1985      | 0.0333  | 1.176               | 1.92                | 0.8                                |
| Alinot and Masson 2005 | 0.0333  | 1.176               | 1.92                | $\sum_{n=0}^5 a_n (\frac{z}{L})^n$ |

### 3.4.5 The Boussinesq Approximation

In flows influenced by buoyancy, solution of the energy equation is required to enable coupling of the temperature field and the flow equations (Libby, 1996). The Boussinesq approximation has been adopted to simplify the effects of density variations in the flow which accompany changes in temperature. The approximation is based on the assumption that density variations in the lower ABL are sufficiently small to be neglected in the continuity and momentum equations except when the density appears along with gravitational acceleration in the body force term for buoyancy (Spiegel and Veronis, 1960). Utilizing the Boussinesq approximation,  $\rho = \rho_0(1 - \beta\Delta T)$ , the gravity term in the momentum equation is computed from,

$$(\rho - \rho_0)g \approx -\rho_0\beta(T - T_0)g, \quad (3.47)$$

where  $\beta$  is the thermal volumetric expansion coefficient of air,  $\Delta T = T - T_0$ ,  $T_0$  is a reference operating temperature and  $\rho_0$  is a constant density of the flow at  $T_0$ .

## 3.5 Replicating the Alinot and Masson (2005) ABL Profiles

A structured mesh of length 425 m, height 180 m and width 200 m consisting of 360800 hexahedral cells was used to model the undisturbed ABL as shown in Figure 3.8, with cell heights ranging from 0.6 m for the wall adjacent cells to 5.6 m for the cells adjacent to the top

boundary. Consequently, 110 cells were used to discretize the vertical height. The 3D mesh employed here was essentially a 20 cell  $y$ -direction extrusion of the 2D mesh constructed by Alinot and Masson (2005). Mesh independence tests were conducted by Alinot and Masson (2005), in accordance with recommendations by Roache (1997), to arrive at this final mesh size. It was considered necessary to use a 3D mesh from the onset, to ensure that the Alinot and Masson (2005) modifications to the standard  $k - \varepsilon$  model could be consistently applied to simulate the 3D flow phenomena considered in this research. An extruded cell width of 10 m was considered to be appropriate because the gradients of flow variables in the  $y$  direction were zero. The stream-wise direction was uniformly discretized using 164 cells of approximately 2.6 m length.

The simulations in this chapter, Chapter 4 and Chapter 5 were conducted on a parallel cluster consisting of Dell Poweredge R410 servers with dual Xeon 4-core processors running at 2.8GHz, and an 8 Mbyte cache. The system was comprised of 8 nodes with 8 cores per node resulting in a total of 64 cores overall. On a single core, the average run time per simulation using the domain in Figure 3.8 was 3 hours.

In addition to the under-relaxation factor for pressure field computations discussed in Section 3.4.1, under-relaxation factors are also present to control updating of other flow variables listed in Table 3.4. The default under-relaxation factors provided by FLUENT have been found to be suitable for a wide range of CFD problems and it is generally recommended that these are not modified except in the event that the solution iterations appear to be unstable or divergent (ANSYS, 2009b). Furthermore, to achieve qualitative convergence, FLUENT requires that the scaled residuals decrease by at least three orders of magnitude in accordance with the convergence criteria in Table 3.4. A point-surface monitor was defined at the midpoint of the domain,  $(x, y, z) = (0, 212.5, 90)$ , to assess changes in the computed turbulent kinetic energy as the solution progressed, thus allowing appraisal of quantitative convergence. The default limits for the flow properties were maintained, with the exception of the turbulent viscosity to laminar viscosity ratio, where the maximum limit was increased from  $1 \times 10^5 \text{ kgm}^{-1} \text{ s}^{-1}$  to  $1 \times 10^7 \text{ kgm}^{-1} \text{ s}^{-1}$  after estimating  $\mu_t$  from the initial turbulence variables.

Table 3.4: Under-relaxation factors and convergence criteria for the computation of flow variables.

| Variable               | under-relaxation | convergence criteria |
|------------------------|------------------|----------------------|
| Pressure               | 0.3              | -                    |
| Density                | 1.0              | -                    |
| Continuity             | -                | $1 \times 10^{-3}$   |
| Momentum ( $u, v, w$ ) | 0.7              | $1 \times 10^{-3}$   |
| $k$                    | 0.8              | $1 \times 10^{-3}$   |
| $\varepsilon$          | 0.8              | $1 \times 10^{-3}$   |
| $\mu_t$                | 1.0              | -                    |
| Energy                 | 1                | $1 \times 10^{-6}$   |

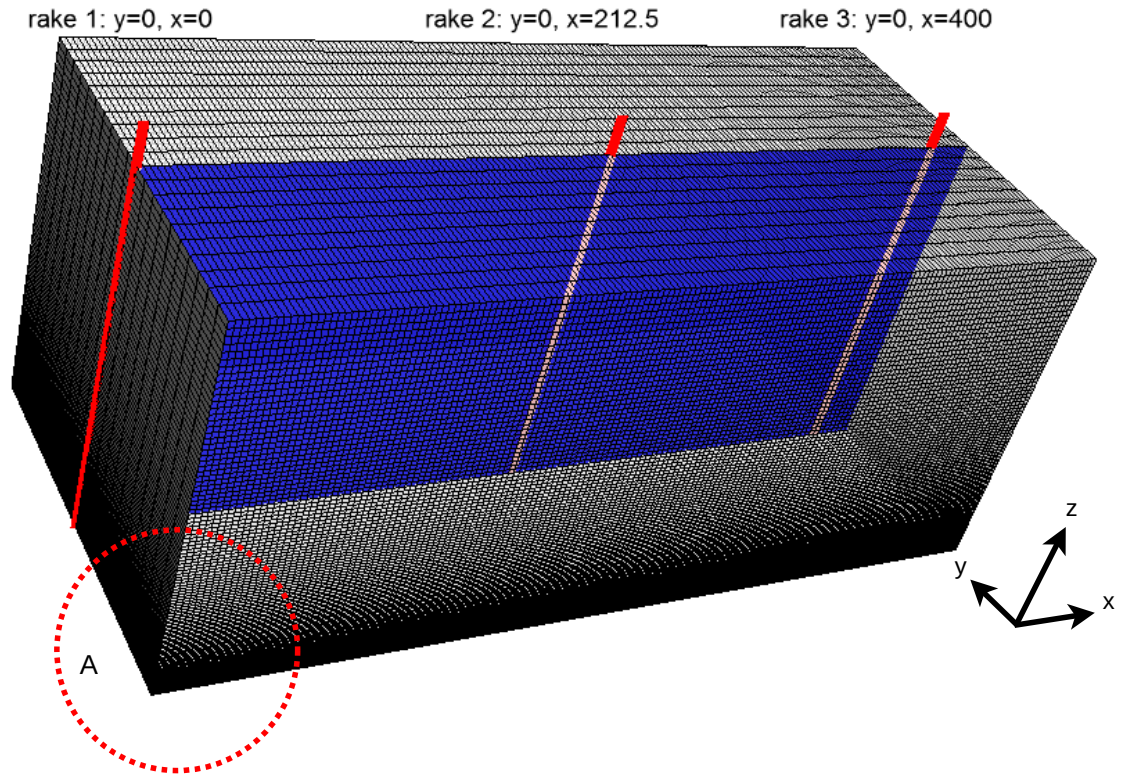


Figure 3.8: Image of the hexahedral mesh used to discretize the empty computational domain. Flow variable were plotted on vertical rakes at positions indicated on the  $y=0$  plane, highlighted in blue. The region encircled in the dashed red circle is magnified to show geometric cell growth in the vertical direction.

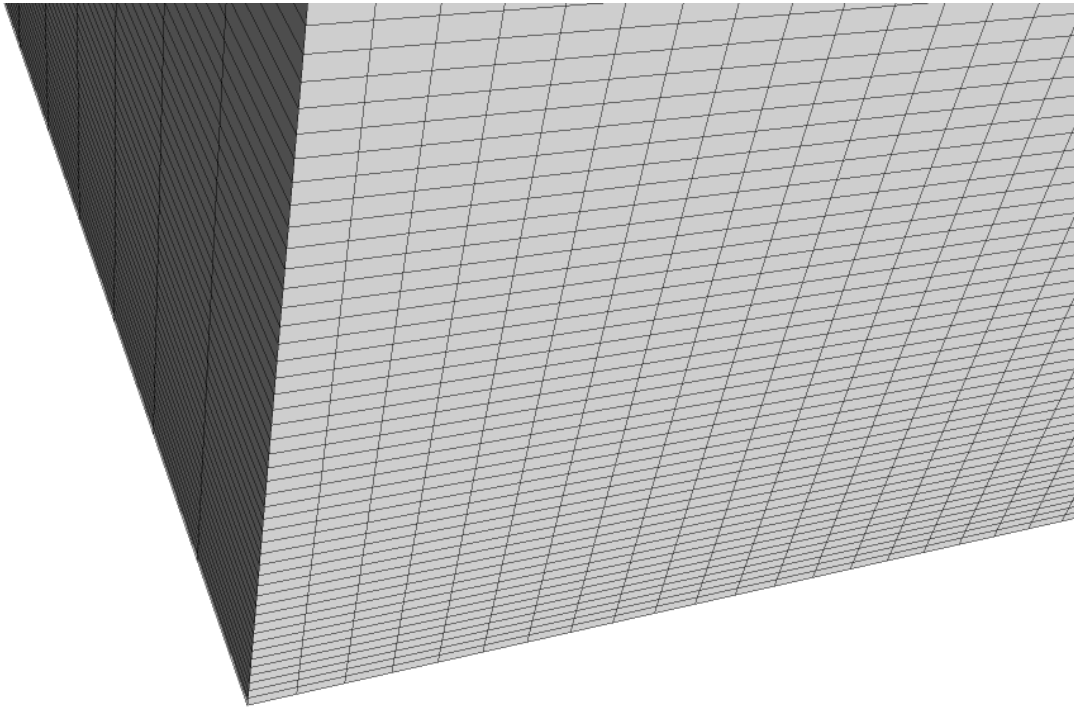


Figure 3.9: Magnified region of the empty computational domain, showing cells of uniform width and length, with geometric growth of cell heights in  $z$ -direction to capture large variations of flow variables in near-wall region.

The fully developed ABL was simulated for three thermal stability classes (Table 3.5) and for the physical properties of air under standard conditions adopted by Alinot and Masson (2005), where  $\rho = 1.225 \text{ kgm}^{-3}$ ,  $\mu = 1.8 \times 10^{-5} \text{ kgm}^{-1} \text{ s}^{-1}$  and  $c_p = 1006.43 \text{ Jkg}^{-1} \text{ K}^{-1}$ . Values of the reference wind velocity,  $u_h$ , and turbulent intensity,  $I$ , at a reference height  $h_{ref} = 35 \text{ m}$  were prescribed as  $10 \text{ ms}^{-1}$  and  $10\%$  respectively, with initial values of  $k$  and  $\varepsilon$  computed from,

$$k = \frac{3}{2}(u_h \cdot I)^2, \quad (3.48)$$

$$\epsilon = (C_\mu)^{(3/4)} k^{(3/2)} / \ell, \quad (3.49)$$

$$\ell = 0.07L. \quad (3.50)$$

where  $\ell$  is the characteristic eddy length scale and  $L$  is the height of the domain. The wall temperature,  $T_w$ , for each of the stability classes was deduced from non-dimensional temperature profiles given in the paper by Alinot and Masson (2005), as shown in Figure 3.10,

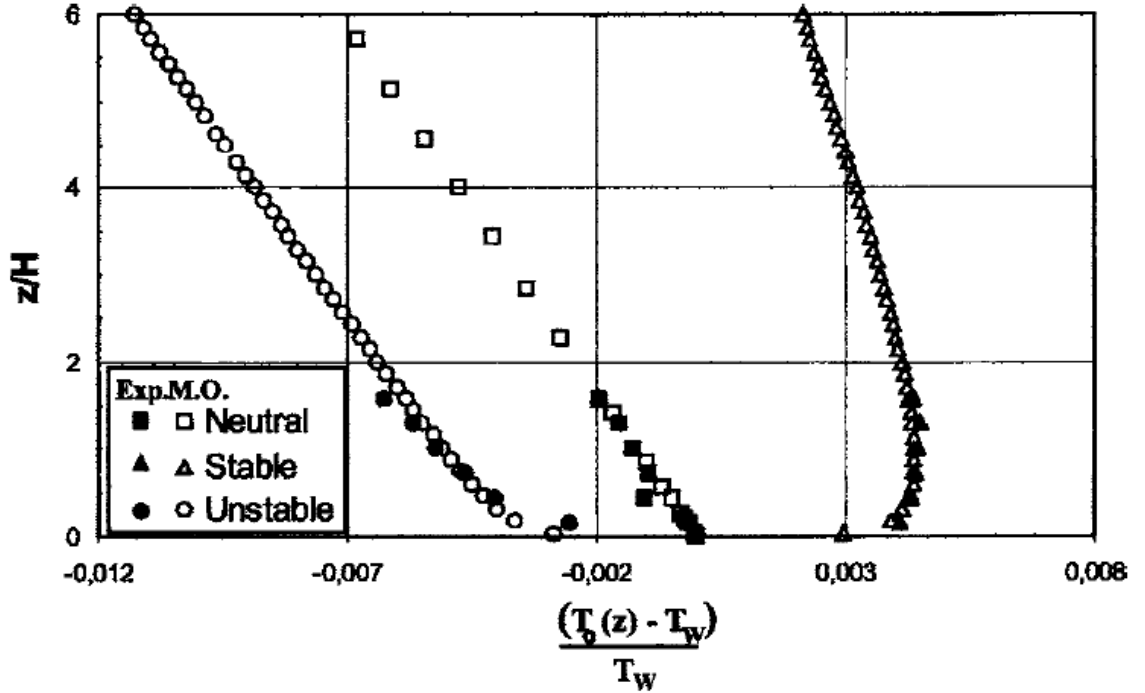


Figure 3.10: Non-dimensional temperature profiles for the neutral, stable and unstable test cases (Alinot and Masson, 2005).

Using  $U_h$ ,  $T_w$ , and  $L_{MO}$  given in Table 3.5, values for the heat flux,  $Q_w$  and  $z_0$  were computed. The values of  $z_0$  were sufficiently low to allow the criterion  $y_p > k_s$  to be satisfied.

Table 3.5: Alinot and Masson (2005) flow properties for the stable, neutral and unstable ABL.

| Stability Class | $L_{MO}$ (m) | $Q_w$ ( $\text{Wm}^{-2}$ ) | $z_0$ (m) |
|-----------------|--------------|----------------------------|-----------|
| Stable          | 191          | -37.9                      | 0.006     |
| Neutral         | $>  10^5 $   | 0                          | 0.00188   |
| Unstable        | -231         | 20.73                      | 0.0004    |

### 3.5.1 Formulation of $k$ , $\varepsilon$ and Energy Source Terms

In FLUENT, when a non-zero gravity field is specified and the energy equation is enabled, a term,

$$\beta g_i \frac{\mu_T}{\sigma_T} \left( \frac{\partial T}{\partial x_i} \right) \quad (3.51)$$

is automatically used to incorporate the effects of thermal buoyancy in the  $k$  equation (Eggenspieler, 2011). The incorporation of buoyancy in the FLUENT  $\varepsilon$  equation is more obscure, because the default value of  $C_{\varepsilon 3}$  is 1.0 in FLUENT; corresponding to an absence of buoyancy contribution to the transport of  $\varepsilon$ . Therefore, source terms were formulated in accordance with Alinot and Masson (2005), to introduce the thermal buoyancy production term to the transport equations,

$$S_E = \frac{\partial}{\partial x_i} \left[ \frac{c_p \mu_T}{\sigma_T} \left( \frac{-g_i}{c_p} \right) \right] \quad (3.52)$$

$$S_k = \beta g_i \frac{\mu_T}{\sigma_T} \left( \frac{-g_i}{c_p} \right) \quad (3.53)$$

$$S_\varepsilon = C_{\varepsilon 1} \frac{\varepsilon}{k} (1 - C_{\varepsilon 3}) \beta g_i \frac{\mu_T}{\sigma_T} \left( \frac{\partial T}{\partial x_i} - \frac{g_i}{c_p} \right) \quad (3.54)$$

where  $S_E$ ,  $S_k$  and  $S_\varepsilon$  are unit source terms for energy,  $k$  and  $\varepsilon$  respectively. The source term for  $k$  only contain a dry adiabatic lapse rate correction to the buoyant energy production term, Equation 3.51, defined in FLUENT, because fluent partially accounts for buoyancy in the  $k$  transport equation. An adiabatic lapse rate correction term is also introduced to the energy equation, which already considers thermal effects through the temperature gradient diffusion term. Since buoyancy is not accounted for in the  $\varepsilon$  transport equation, the full Alinot and Masson (2005) buoyancy term is defined in the  $\varepsilon$  source term. The User Defined Function (UDF) in Appendix A has been written in C and compiled to expand the capabilities of the FLUENT CFD model. This UDF was used to define the modified Richards and Hoxey (1993) flow and turbulence profiles at the domain inlet, introduce the buoyancy source terms given in Equations 3.52 to 3.54 to their relevant transport equations and create scalars and user defined memory locations for manipulating and storing field data. The UDF structure conforms to general C syntax rules and is comprised of functions and macros which can perform the aforementioned operations. Pre-defined functions and

macros are provided by FLUENT in a built-in *udf.h* header file which is accessed in the UDF through the use of an include directive.

### 3.5.2 Testing the homogeneity of the ABL Profiles

The non-dimensionalized profiles of  $u$ ,  $T$ ,  $k$  and  $\varepsilon$  were plotted along vertical rakes positioned at  $(x, y)=(0,0)$ ,  $(x, y)=(212.5,0)$  and  $(x, y)=(400,0)$  for the three stability cases in order to assess the severity of any stream-wise gradients occurring along the domain. Figure 3.11 to Figure 3.13 show that the profiles do in fact remain approximately homogeneous. Some decay of the turbulent kinetic energy, approximately 10%, is observed in the top 30 m of the domain for the unstable ABL in Figure 3.13. Figure 3.11 appears to also show a relatively slight decay in  $k$  for the stable ABL. The neutral profiles appear to be the most consistent in terms of horizontal homogeneity along the domain. On average, the changes in the profiles amounted to less than 2% of the inlet values.

Based on these observations, it is likely that the stream-wise gradient in the unstable  $k$  profile has arisen as a consequence of the specification of the velocity inlet condition at the top of the domain, and the modifications to the model coefficients and turbulence closure equations. As mentioned previously, the velocity inlet top boundary condition has a tendency to affect the turbulent fluxes. Furthermore, it is entirely possible that the modifications to the original model constants and the inclusion of buoyancy effects in the model equations may lead to discrepancies between the wall functions and turbulence model. However, these inhomogeneities only begin to be manifested at a height of  $4h_{ref}$  above the wall, therefore it is apparent that the stream-wise gradients do not adversely affect computational results in the region of interest near the wall.

The homogeneous profiles also reveal the characteristic flow-field behaviour for the three stability classes. In the stable ABL, illustrated on Figure 3.11, thermal stratification effects contribute to the removal of  $k$  from the flow, producing a profile which displays a decrease in  $k$  with increasing vertical height and a lower wind shear than the other classes. The turbulent dissipation rate is also the highest for the stable ABL, relative to the other stability classes. An examination of the neutral ABL profiles in Figure 3.12, exhibit a constant  $k$  throughout the height of the domain. This is expected considering that the normalized  $k$  profile reduces to a constant in the absence of thermal buoyancy effects, where  $k/u_*^2 = 5.48$  according to Equation 3.37. In contrast to the stable ABL case, the highest wind shear is experienced in the unstable ABL illustrated in Figure 3.13. This is accompanied by an increase in turbulent kinetic energy with height which corresponds to the positive contribution of thermal buoyancy to the turbulent kinetic energy of the flow. In all three atmospheric stability cases, a spike in turbulent kinetic energy was observed near the ground, Hargreaves and Wright (2007) attributed this to over-prediction of the kinetic energy production term,  $G_k$  in the wall-adjacent cells due to the assumption of a local equilibrium of  $k$  and  $\varepsilon$  parameters in the standard wall function.

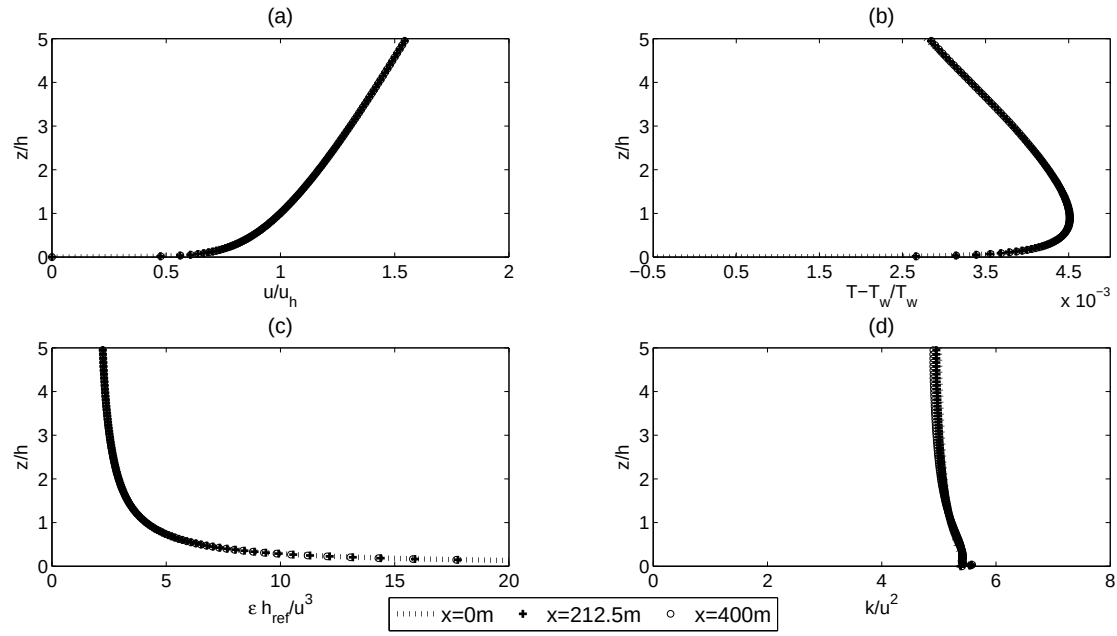


Figure 3.11: Stable ABL profiles of non-dimensionalized a)  $u$ , b)  $T$ , c)  $\varepsilon$  and d)  $k$ , from vertical rakes located at  $x=0$  m (dashed line),  $x=212.5$  m (crosses) and  $x=400$  m (circles).

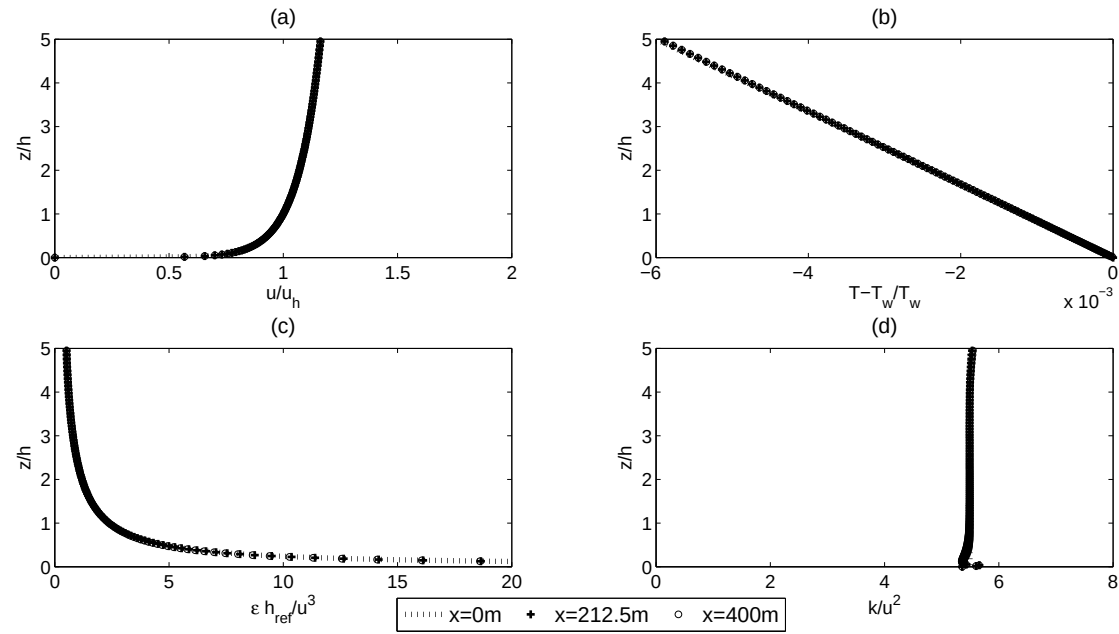


Figure 3.12: Neutral ABL profiles of non-dimensionalized a)  $u$ , b)  $T$  c)  $\epsilon$  and d)  $k$ , from vertical rakes located at  $x=0$  m (dashed line),  $x=212.5$  m (crosses) and  $x=400$  m (circles).

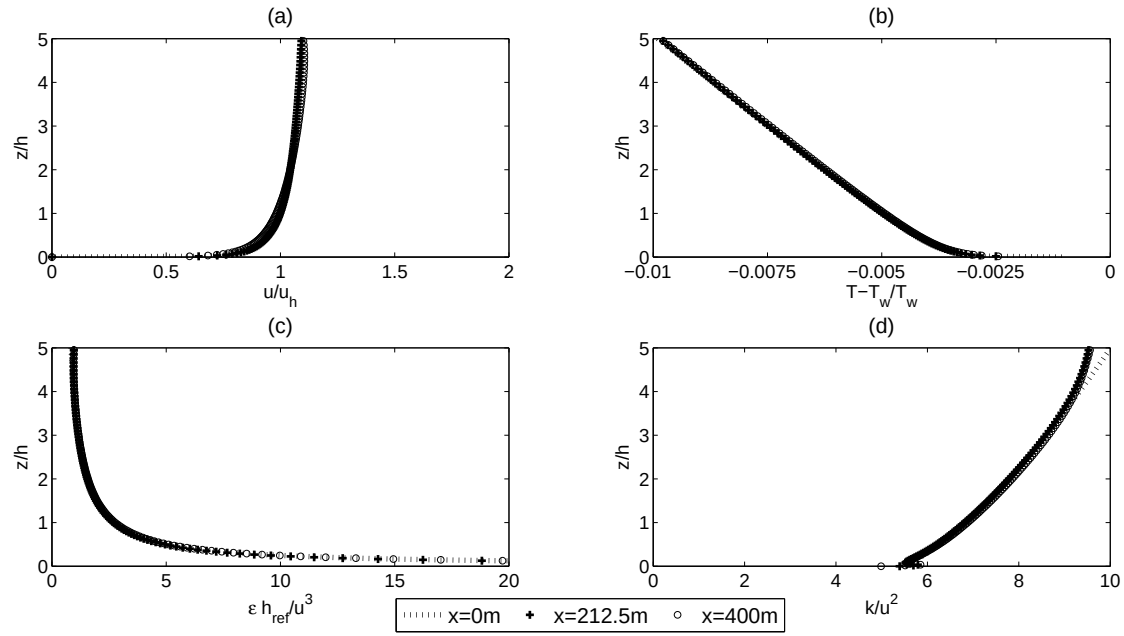


Figure 3.13: Unstable ABL profiles of non-dimensionalized a)  $u$ , b)  $T$ , c)  $\epsilon$  and d)  $k$ , from vertical rakes located at  $x=0$  m (dashed line),  $x=212.5$  m (crosses) and  $x=400$  m (circles).

### 3.5.3 Comparison with Alinot and Masson (2005) Results and Monin-Obukhov Similarity profiles

The stream-wise velocity, temperature and turbulence profiles obtained at  $(x, y) = (212.5, 0)$  have been compared to the results obtained by Alinot and Masson (2005) and also with empirical solutions based on Monin-Obukhov Similarity theory (M-O profiles). Firstly, a non-dimensionalization of the profiles was performed out with appropriate powers of the friction velocity for the velocity and turbulence profiles, resulting in the following normalizations,

$$\hat{u} = \frac{u}{2u_*} \quad (3.55)$$

$$\hat{k} = \frac{k}{u_*^2} \quad (3.56)$$

$$\hat{\varepsilon}_{stable, unstable} = \frac{|\varepsilon L_{MO}|}{u_*^3} \quad (3.57)$$

$$\hat{\varepsilon}_{neutral} = \frac{\varepsilon h_{ref}}{u_*^3}. \quad (3.58)$$

Similarly, the scaling temperature was used to non-dimensionalize the temperature profiles for the stable and unstable cases. Alinot and Masson (2005) employed the principles of dimensional analysis to deduce a scaling parameter for the neutral temperature profile based on temperature lapse at the top of constant shear layer,

$$\hat{T}_{stable} = \frac{(T - T_w)}{2T_*} \quad (3.59)$$

$$\hat{T}_{neutral} = \frac{c_p(T_w - T)}{5000gz_0} \quad (3.60)$$

$$\hat{T}_{unstable} = \frac{(T_w - T)}{3T_*} \quad (3.61)$$

These parameter normalization procedures allow the profiles for each of the stability classes to be presented on the same set of axes, as shown in Figures 3.14 to 3.16.

The simulations closely match both the Alinot and Masson (2005) and empirical Monin-Obukhov profiles for all three atmospheric stability classes. For the unstable profile, the decay in  $k$  near the top of the domain results in a departure of the  $k$  predictions from both the Monin-Obukhov empirical profiles and the (Alinot and Masson, 2005) profiles. However since the turbulence model will be subsequently employed to predict dust dispersion from quarry blasts emissions, it is unlikely that discrepancies near the top of the computational domain will significantly influence particle trajectory from blast emissions, since these are near ground releases which inject particulates within the lowest 50 m to 100 m of the computational domain.

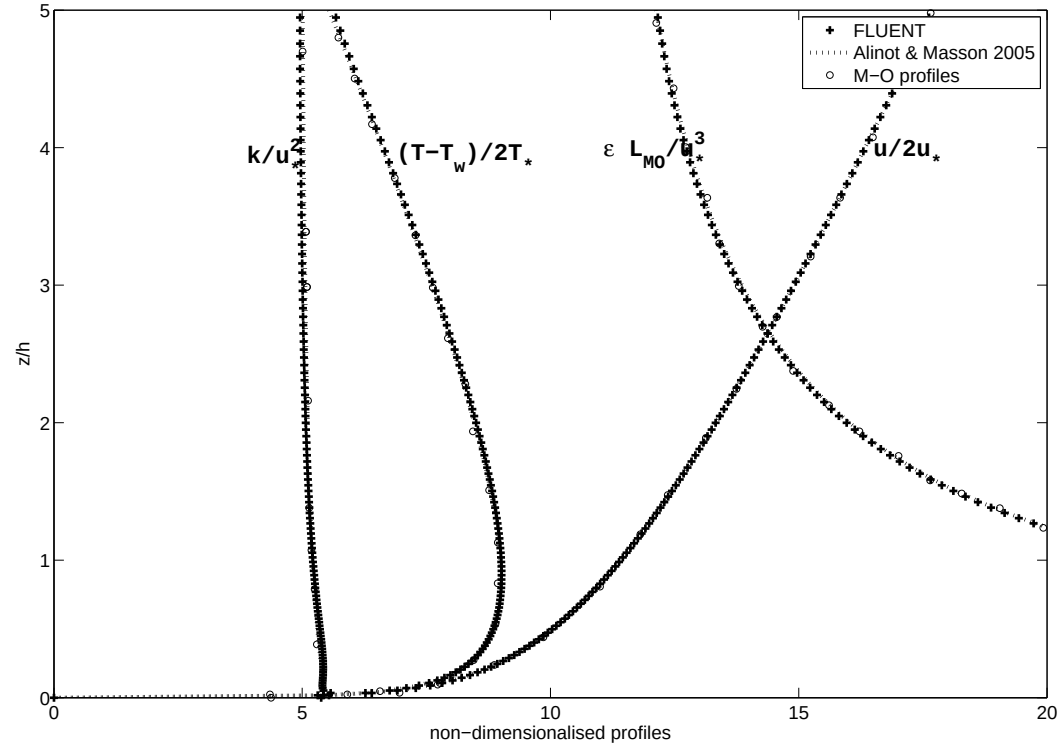


Figure 3.14: Comparison of Fluent test, Alinot and Masson (2005) and M-O normalized flow and turbulence profiles for the stable ABL,  $u(h)=10 \text{ ms}^{-1}$ ,  $I(h) = 8\%$ ,  $h_{ref}=35 \text{ m}$ .

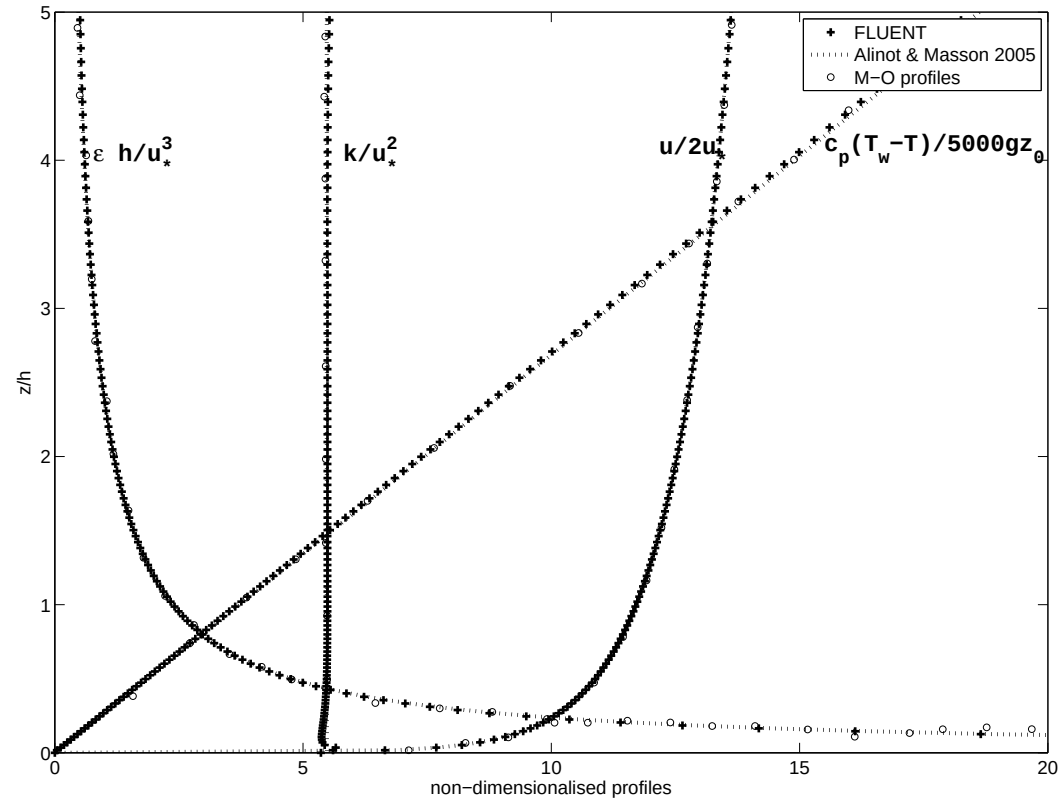


Figure 3.15: Comparison of Fluent test, Alinot and Masson (2005) and M-O normalized flow and turbulence profiles for the neutral ABL,  $u(h)=10\text{ ms}^{-1}$ ,  $I(h) = 8\%$ ,  $h_{ref}=35\text{ m}$ .

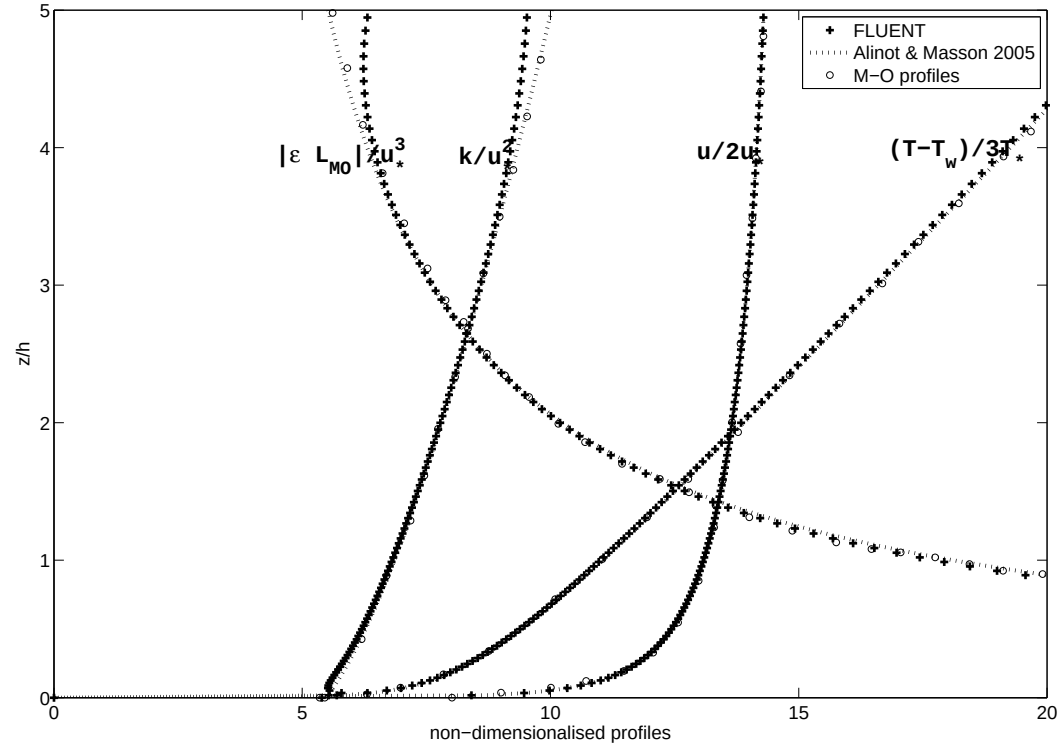


Figure 3.16: Comparison of Fluent test, Alinot and Masson (2005) and M-O normalized flow and turbulence profiles for the unstable ABL,  $u(h)=10 \text{ ms}^{-1}$ ,  $I(h) = 8\%$ ,  $h_{ref}=35 \text{ m}$ .

### 3.6 Summary

This chapter has presented an overview of the numerical methods which may be employed to obtain solutions to the governing Navier-Stokes equations of turbulent boundary layer flows. The features of various CFD numerical models, namely DNS, LES, DES, RANS, have been discussed to ascertain their suitability for industrial quarry dust dispersion applications. Due to their computational efficiency and ability to produce stable, reasonably accurate solutions of the atmospheric flow-field, RANS models have been found to be the most appropriate for modelling the wind field in which fugitive dust is transported and dispersed. It was demonstrated that the RANS  $k - \varepsilon$  model can be used to simulate the undisturbed atmospheric boundary layer under different stability conditions through the optimization of its solver settings and modification of its coefficients and turbulence closure equations based on the findings of Alinot and Masson (2005). These modifications serve to incorporate the effects of thermal buoyancy in the  $k - \varepsilon$  model and make the model equations compatible with Monin-Obukhov Similarity Theory. The problem of horizontal inhomogeneity of the undisturbed profiles identified in work by Hargreaves and Wright (2007) has been addressed. Therefore, the Alinot and Masson (2005) profiles obtained for the undisturbed ABL under stable, neutral and unstable conditions were replicated to demonstrate how the modifications could be used in conjunction with modified Richards and Hoxey (1993) inlet profiles and appropriate solver settings to obtain horizontally homogeneous profiles of the ABL.

In the ensuing chapter, the Lagrangian Discrete Phase Model (DPM) will be coupled with the Eulerian solution of the flow-field provided by the buoyancy modified  $k - \varepsilon$  presented here. This will enable stochastic tracking of particulates emitted from a representative blast emission.

## Accounting for Wind Direction Variability in Lagrangian Particle Dispersion Simulations

### 4.1 Past Studies of Wind Direction Variability

This Chapter addresses the under-prediction of lateral spreading of the pollutant plume observed in CFD simulations conducted by Riddle et al. (2004). A probability weighted averaging procedure has been implemented here to incorporate the lateral plume spread effects of wind direction variability into dust dispersion simulation results obtained by coupling the FLUENT  $k - \varepsilon$  turbulence and Discrete Phase models. The Moore (1976) formulation, applied in the UK-ADMS plume spread module, has been presented in Chapter 2 and is used in this work to parametrize wind variability in terms of the standard deviation of the horizontal wind direction over a one hour averaging time. Work by Quinn et al. (2001) has proposed a methodology to incorporate wind direction variability in CFD simulations of the neutral ABL, in which wind direction fluctuations were represented by nine CFD simulations, each corresponding to  $5^\circ$  angular increments of wind direction within a range of  $-20^\circ$  to  $20^\circ$ . Probability weighted summations of the simulations were subsequently used to account for the effects of wind direction variability on plume dispersion.

A more recent paper by Vervecken et al. (2013), builds on the Quinn et al. (2001) methodology by proposing a decomposition of total wind direction variability,  $\sigma_\alpha$ , into one component due to boundary layer turbulence  $\sigma_{\theta t}$  and another due to external causes of wind direction variability  $\sigma_\theta$ ,

$$\sigma_\alpha = \sigma_\theta + \sigma_{\theta t}. \quad (4.1)$$

They assert that  $\sigma_\theta$  can be derived from field measurements, once  $\sigma_{\theta t}$  is deduced from the turbulence closure equations because variability due to boundary layer turbulence is already represented in the turbulence model. Thus from the  $k - \varepsilon$  model equations,

$$\sigma_{\theta t} = \frac{2}{3} \frac{u_*^2}{U^2 \sqrt{C_\mu}}, \quad (4.2)$$

where  $U$  is the mean wind speed at a given height. Their reasoning appears to be in line with the premise of the empirically derived equation by Moore (1976), Equation 2.62, which results from decoupling wind direction variability due to boundary layer turbulence from that due to larger scale atmospheric motions.

The current study is distinct from previous studies by Quinn et al. (2001) and Vervecken et al. (2013) because in addition to the neutral ABL, the stable and unstable ABL are also considered, thus the methodology is shown to be applicable to all three stability classes. Moreover, unlike work by Quinn et al. (2001) and Vervecken et al. (2013), this study pertains to the dispersion of a particulate plume consisting of four particle size fractions representative of typical total suspended particle (TSP) emissions. The steady-state solution of the flow-field obtained using the FLUENT  $k-\varepsilon$  model has been coupled with the Discrete Phase Model (DPM) which is available in FLUENT for stochastic tracking of particulates injected into the computational domain. Thus, whilst the flow-field has been modelled in a Eulerian reference frame, the trajectory of individual particulates is computed in a Lagrangian reference frame centred on the individual particles. Quinn et al. (2001) and Riddle et al. (2004) have noted that predictions of gaseous dispersion obtained using massless particles in the Lagrangian DPM were superior to those obtained using the Advection-Diffusion (AD) model. Moreover, Thomson (1987) indicated that stochastic models are more appropriate tools for modelling near-source dispersion of particles entrained in complex flow regimes.

In the stochastic model, simulations of particle-eddy interactions are influenced by the Lagrangian integral time, which the user is able to modify through the time scale constant  $c_L$ , which has a function analogous to the turbulent Schmidt number,  $Sc_t$  used in the Advection-Diffusion equation. By reducing the value of  $c_L$ , the effect of turbulence on particle trajectory may be dampened, thereby altering the dispersive characteristics of the FLUENT plume. Consequently,  $c_L$  has been calibrated in this work through comparison to UK-ADMS lateral plume spread predictions.

The proposed methodology for incorporating wind direction variability into the CFD model, relies on parametrisation of the standard deviation of wind direction in a manner which captures the dependency of wind direction variability on the mean wind velocity and the averaging time. This methodology will ultimately be applied to account for the effects of wind direction variability on quarry dust dispersion, where the meteorological dataset does not include measurements of wind direction variability.

## 4.2 Parametrizing Wind Direction Variability

Quinn et al. (2001) used a Gaussian probability density function to describe the frequency of wind direction variability in the near-wake of buildings. Field measurements of wind direction variability in the nocturnal ABL by Mahrt (2007) lend support to the assumption that the frequency distribution of wind variability is strongly Gaussian, both when the wind direction changes are measured directly and when they are correlated to the wind speed, as illustrated in Figures 4.1 and 4.2 respectively.

Based on these wind variability frequency observations by Mahrt (2010), a Gaussian prob-

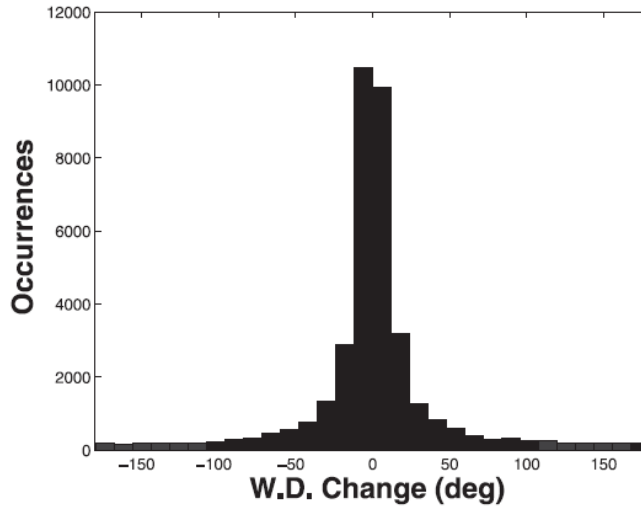


Figure 4.1: Frequency distribution of wind direction variability angles measured at a height of 2 m at 1 minute intervals in the nocturnal ABL, for a 4 month observation a period, from Mahrt (2010).

ability density function has also been adopted to describe wind direction variability in this work, for which the Moore (1976) generalisation, (Equation 2.62 presented in Chapter 2) has been selected for parametrisation of the standard deviation of wind variability.

It was mentioned in Chapter 2 that UK-ADMS has been extensively validated using datasets from the Kinkaid, Indianapolis and Prairie Grass field experiments, which each contain large datasets of sufficient quality for validation of regulatory dispersion models, ergo, the Kinkaid and Indianapolis datasets are used by the European Initiative on *Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes* in their Model Validation Toolkit, whilst the Prairie Grass measurements are used in American Society for Testing materials (ASTM) model validation (CERC, 2013).

Under meteorological conditions ranging from the neutral to the convective ABL, the Kinkaid experiments measured the concentration field of  $\text{SF}_6$  emitted from a 187 m stack surrounded by flat, rural terrain. In Indianapolis,  $\text{SF}_6$  tracer gas was released from a stack height of 83.8 m over flat terrain of urban roughness classification and concentration measurements were subsequently obtained for both diurnal and nocturnal meteorological conditions. The Prairie Grass experiments measured the concentration of  $\text{SO}_2$  emitted from a near-ground source surrounded by flat grassland. These experimental campaigns provide conclusive evidence that UK-ADMS concentration predictions correlate well with field measurements for emissions from elevated sources surrounded by flat terrain.

UK-ADMS predictions appeared to be most strongly correlated to the field measurements for the Prairie Grass dataset, in which the site topography was almost entirely homogeneous with an aerodynamic roughness height corresponding to that of flat, open terrain. For this dispersion site, 65% of the predictions were within a factor of two of the measurements and

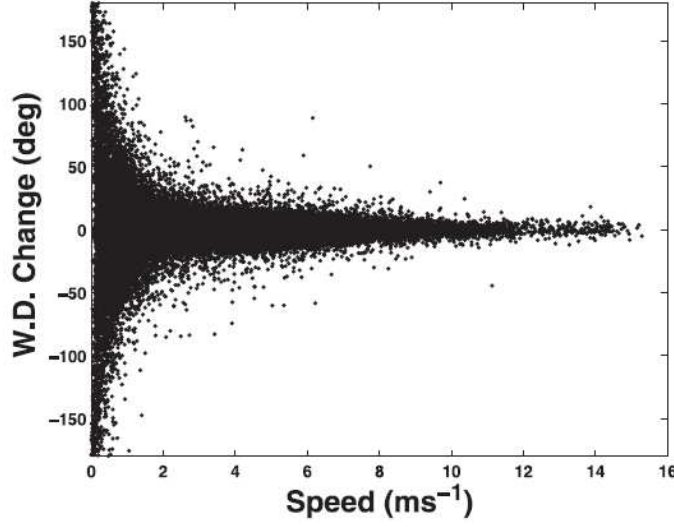


Figure 4.2: Wind direction variability angular changes as a function of wind speed, measured at a height of 2 m at 1 minute intervals in the nocturnal ABL, for a 4 month observation a period, from Mahrt (2010).

the mean concentration predicted by UK-ADMS was 70% of the measured mean concentration. On the basis of these model evaluation studies, and since the Moore (1976) equation is applied in the plume spread module of UK-ADMS (Version 5.0), the UK-ADMS model is used as a baseline for assessing the improvements in lateral plume spreading obtained using the proposed CFD modelling methodology to predict particulate concentration over flat terrain of low aerodynamic roughness - dispersion site conditions for which UK-ADMS is known to perform well.

In the methodology which follows, a limit of  $\sigma_\theta < \pi/6$  is imposed, to constrain the wind direction angles to realistic values, such that the angle subtended by the range  $-3\sigma_\theta$  to  $3\sigma_\theta$ , within which 99% of the observations lie, is no greater than  $\pi$ . This is in keeping with the findings of Mahrt (2010), illustrated in Figures 4.1 and 4.2. A limit of  $\sigma_\theta < \pi/6$  is also used in UK-ADMS.

It has been demonstrated in work by Mahrt (2010) and Davies and Thomson (1999), that  $\sigma_\theta$  remains approximately constant with increasing wind speed above a threshold of  $5 \text{ ms}^{-1}$  for both the nocturnal and diurnal ABL. Joffre and Laurila (1988) proposed characterisation of the wind variability according to the equations,

$$\sigma_\theta (\text{rad}) = \begin{cases} \frac{0.32 \text{ ms}^{-1}}{U_{10}} & U_{10} \leq 5 \text{ ms}^{-1} \\ 0.065 & U_{10} > 5 \text{ ms}^{-1} \end{cases}, \quad (4.3)$$

which specify a constant value of  $\sigma_\theta$  for winds above  $5 \text{ ms}^{-1}$ . Hanna (1983) adopted the

formula,

$$\sigma_{\theta} (rad) = \frac{0.5 \text{ ms}^{-1}}{U_{10}}, \quad (4.4)$$

for light winds below  $5 \text{ ms}^{-1}$ , which produces a less conservative estimate of  $\sigma_{\theta}$ . Equations 4.3, and 4.4 result in  $\sigma_{\theta}$  values of  $3.7^{\circ}$  and  $5.7^{\circ}$  respectively for mean wind speeds above  $5 \text{ ms}^{-1}$ , whilst Davies and Thomson (1999) obtained a value of  $\sigma_{\theta} = 6.3^{\circ}$  for their field data set illustrated in Figure 4.3. Therefore, a constant value of  $\sigma_{\theta} = 5^{\circ}$  has been applied in the current study for wind speeds  $\geq 5 \text{ ms}^{-1}$ . This value is based on the averages of the minimum wind variability specified in Davies and Thomson (1999), Joffre and Laurila (1988) and Hanna (1983).

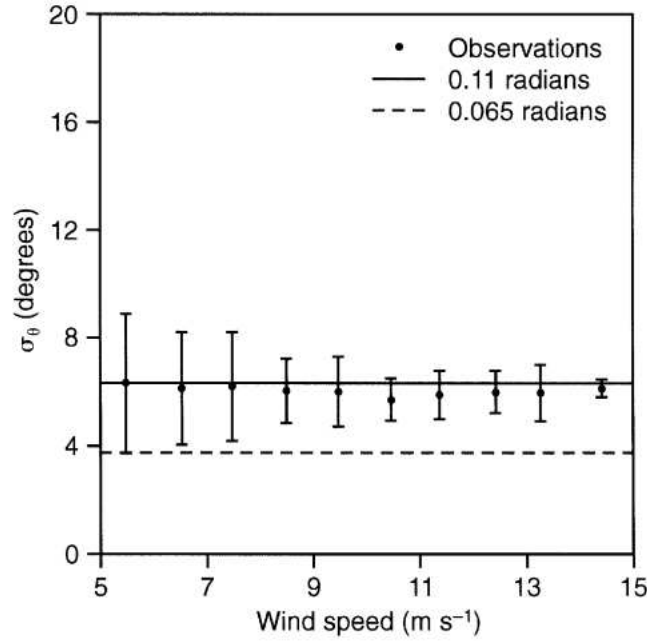


Figure 4.3: Variation of  $\sigma_{\theta}$  with wind speed, for Cardington field observations reproduced from Davies and Thomson (1999).

### 4.3 Methodology

In FLUENT, the Eulerian solver for the continuous phase is coupled with the DPM to simulate the dispersion of a discrete second phase consisting of spherical particles entrained in the fluid (ANSYS, 2009b). The DPM is valid for systems in which the discrete phase occupies less than 10% of the volume of the continuous phase, although it is acceptable for the total mass of the discrete phase to be greater than that of continuous phase due to the significantly larger density of the particles. Coupling of the continuous and discrete phases may be two way - allowing for the transfer of heat, mass and momentum between both phases, or one way - permitting only uni-directional transfer of these quantities. The one-way coupling option has been selected here to model the particulates injected into the computational domain as a passive emission with negligible effect on the continuous phase. The DPM determines the trajectory of injected particles by integrating the particle force balance equation according to Newton's Second Law of motion, written in a Lagrangian reference frame,

$$\frac{du_p}{dt} = F_D(u - u_p) + \frac{g_i(\rho_p - \rho)}{\rho_p}, \quad (4.5)$$

where  $u$  is the fluid velocity,  $u_p$  is the velocity of the particle,  $F_D(u - u_p)$  is the specific drag force acting on the particle, with the specific drag per unit velocity,  $F_D$ , given by,

$$F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D \text{Re}_p}{24}. \quad (4.6)$$

The acceleration due to gravity in the  $i^{\text{th}}$  direction is represented by  $g_i$ , with the second term on the right hand side of Equation 4.5 representing the net acceleration of the particle in the direction of the gravity vector.  $\rho$  and  $\rho_p$  are the fluid and particle densities respectively and the equivalent spherical diameter of the particle is denoted by  $d_p$ .  $C_D$  is the dimensionless drag coefficient calculated as,

$$C_D = a_1 + \frac{a_2}{\text{Re}_p} + \frac{a_3}{\text{Re}_p^2} \quad (4.7)$$

where the drag law constants  $a_1$ ,  $a_2$  and  $a_3$  apply to smooth spherical particles and are given by Morsi and Alexander (1972) for various ranges of particle relative Reynolds number  $\text{Re}_p$ ,

$$\text{Re}_p = \frac{\rho d_p |u_p - u|}{\mu}. \quad (4.8)$$

In the DPM, the stochastic tracking option can be enabled to calculate the trajectories of individual particulates using a Discrete Random Walk (DRW) approach, which uses the instantaneous flow velocity,  $\bar{u} + u'(t)$ , instead of the mean component of the flow velocity  $\bar{u}$  in the integration of Equation 4.5 over discrete time intervals (ANSYS, 2009b). Therefore, each particle path consists of a series of random steps and possesses the statistical properties of a discrete-time Markov chain, such that each successive step along the particle path is

strongly correlated to the particle position at the current step, but independent of the previous steps (Lawler and Limic, 2010).

The particle must be specified as either *inert*, *droplet* or *combusting* to allow FLUENT to activate the appropriate physical laws applicable to the particle type. For instance, vaporization, boiling and devolatilization laws are activated for droplets, whilst inert particles, such as those considered in this work, are only subject to heating and cooling laws by way of a heat balance equation.

Having specified the particle type, the modeller must consider the manner in which the particles are to be introduced into the domain. Several pre-defined injection options are available, such as single, group, cone, surface and various atomizer configurations. Alternatively, the modeller can create an external injection file to describe the distribution of particles in the injection, as has been done in this work. This approach offers more flexibility to define a particle size distribution with varying mass flow rates for each size range than the built-in Rosin-Rammler diameter distribution method which uses an exponential function to fit a mass fraction to each particle size range. An injection file is also a more practical approach for performing preliminary computations of particle distribution throughout a volume source and specifying the initial conditions of an injection consisting of a large number of particles. For all classes of injection, the initial position of the particles must be specified using Cartesian coordinates, as well as values of  $d_p$  representative of each size range, the velocity vector, initial temperature and particle mass flow rate.

Before commencing the simulation, discrete phase boundary conditions must be defined at each boundary of the computational domain to allow the DPM solver to determine the fate of the particles at the boundaries (ANSYS, 2009b). The *trap* boundary condition allows the mass of the particle to be retained in the cell adjacent to the point of collision on a boundary - typically a wall. An *escape* condition is generally applied at inlets and outlets to simulate the particle mass exiting the domain. Both of these boundary conditions cause the DPM to terminate particle trajectory computations. The *reflect* condition allows the particle to rebound off the boundary with a change in its momentum, whilst an *interior* condition, as the name suggest, can only be applied at an internal boundary which is transparent to the particles.

#### 4.3.1 The Computational Domain

The computational domain and solver settings discussed in Chapter 3 are also utilized here. The discretization of the computational domain remains the same, consisting of a structured mesh of 360,800 hexahedral cells and a first cell height of 0.6 m. This yielded a total of 110 node points, with a successive cell height ratio of approximately 1.2 in the vertical direction.

#### 4.3.2 DPM Boundary Conditions and Injection Parameters

The specification of the domain inlet, top and outlet boundary conditions remains unchanged from that employed in Chapter 3, with velocity inlets imposed at the domain inlet

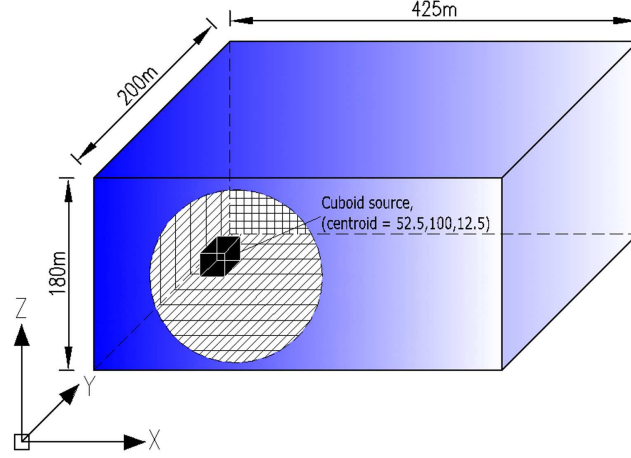


Figure 4.4: The computational domain, showing position of cuboid volume source.

and top boundaries. The stability-modified profiles for velocity, temperature and turbulence have been used to characterise the equilibrium boundary layer at the inlets. However, instead of symmetry boundary conditions, velocity inlets have been used at the lateral boundaries of the domain to allow specification of the velocity components since the incoming wind is no longer strictly normal to the domain inlet for the wind variability simulations. Consequently, profiles for the  $u$  and  $v$ , components of the flow velocity, have been specified at all the velocity inlets. The standard rough wall treatment was retained for the wall boundary as well as the aerodynamic roughness length of  $z_o = 0.01$  m.

In the DPM, an injection file, given in Appendix B, was used to introduce a particulate emissions source represented by a  $5\text{ m} \times 5\text{ m} \times 5\text{ m}$  cuboid volume source with its centroid positioned at Cartesian coordinates  $x, y, z = 52.5, 100, 12.5$ . The particle size distribution for Total Suspended Particulates (TSP) defined in Chapter 2 was applied in the injection file to create particulate injection points which were regularly distributed at spacings of 0.2 m throughout the volume, resulting in a total of 62500 particles. Riddle et al. (2004) used a total of 10000 inert particles to define a single injection in their inter-comparison study of UK-ADMS and the FLUENT DPM. Other studies by Kallio and Reeks (1989) and Greenfield and Quarini (1998) used between 500 to 10000 particles to define their injections. Dehbi (2008) advised that due to the computationally expensive nature of Lagrangian particle tracking, the number of particles should be large enough to compute a sufficient number of particle trajectories to adequately account for turbulent fluctuations on particle dispersion. They used 10000 particle tracks in their study to define a uniformly distributed injection occupying 50% of their domain, but noted that there was no significant change in particle deposition rate between injections comprising of 5000 and 10000 particles. The comparatively larger number of particulates used here is representative of the lower range used to define a blast injection. Including Lagrangian particle tracking of 62500 particles

in the simulation increased the run time of each simulation by approximately one hour. The total mass flow rate of all the fugitive dust particles injected into the domain was computed for a representative quarry blast which liberated 25000 tonnes of limestone rock. The MDEQ (2004) PM<sub>10</sub> blast emission factor of 0.036 kg/tonne was used to derive a TSP emission rate of 0.568 kgs<sup>-1</sup> for the blast event. The particles were assigned the density of the parent rock, which was taken as 2600 kgm<sup>-3</sup> for limestone. The initial velocity of injected particulates was 0 ms<sup>-1</sup>. The injection file assigns an individual flow rate to each of the particles so that computations of particle concentration and accretion can be performed through a summation of the total number of particles entering a cell or impacting on a wall boundary respectively.

A trap boundary condition was assigned to the wall so that particle trajectory calculations are terminated for particles which collide with the wall (ANSYS, 2009b). Accretion settings have been enabled at the wall to allow calculation of the mass flux of particles impacting on the wall boundary face,

$$R_{\text{accretion}} = \sum_{p=1}^{N_{\text{particles}}} \frac{\dot{m}_p}{A_{\text{face}}} \quad (4.9)$$

The accretion rates of the particulates at the wall boundary were used to assess lateral plume spread, these were compared to dry deposition rates from the UK-ADMS model. Escape boundary conditions were imposed at the flow boundaries for the discrete phase, where any particle impacting the boundary was reported as having escaped the domain and the trajectory calculations are terminated (ANSYS, 2009b).

### 4.3.3 Meteorological Conditions

The meteorological conditions adopted in this study are those of the three stability classes listed in Table 4.1. Values of the Monin-Obukhov length have been selected to coincide with the middle of the ranges suggested by Barthelmie (1999) and Woodward (1999) for the stable and unstable atmosphere respectively. Characteristic wind speeds at a reference height of 10 m were derived from the Pasquill-Gifford-Turner (PGT) scheme for the three stability classes. Values of the surface heat flux were calculated using the equation for the Monin-Obukhov Length scale. The wind variability  $\sigma_\theta$ , was computed from Equation 2.62, and for  $u_{10} \geq 5 \text{ ms}^{-1}$ ,  $\sigma_\theta$  was taken as  $5^\circ$ .

Table 4.1: Meteorological parameters used to define the three stability classes in the wind variability simulations.

| Stability | PGT class | $u_{10}$<br>(ms <sup>-1</sup> ) | $\sigma_\theta$<br>(°) | $L_{MO}$<br>(m) | $Q_w$<br>(Wm <sup>-2</sup> ) | $T_w$<br>(K) |
|-----------|-----------|---------------------------------|------------------------|-----------------|------------------------------|--------------|
| Unstable  | A         | 5                               | 5.0                    | -100            | 28.41                        | 298          |
| Neutral   | D         | 8                               | 5.0                    | $>  10^5 $      | 0                            | 285          |
| Stable    | F         | 3                               | 5.7                    | 100             | -4.17                        | 283          |

A relatively low reference wind speed of 3 ms<sup>-1</sup> has been chosen to represent the stable

case. Thus, the wind velocity profile is representative of the lower wind conditions generally experienced in the stable ABL, because as the wind speed increases above  $5 \text{ ms}^{-1}$  with a corresponding increase in mechanical turbulence, the atmospheric stability tends towards the neutral case. The value of  $3 \text{ ms}^{-1}$  is also sufficiently high so as not to challenge the reliability of the Gaussian model.

#### 4.3.4 Wind Variability Simulations

Zanetti (1990) notes that whilst instantaneous plume concentrations may be irregular, the time-averaged concentration profiles can be approximated by a Gaussian distribution in horizontal direction, thus the probability density function of wind direction variability was assumed to be Gaussian, an assumption which is also supported by the frequency distribution of field measurements of wind direction change in Mahrt (2010).

The mean wind direction,  $\mu_\theta$  was allocated a value of zero, since the fetch represents a flat homogeneous terrain, and changes in direction of the mean wind would translate to an equivalent rotation of the plume about a vertical axis centred on the domain inlet, with the plume dispersion parameters remaining unchanged. The limits of the directional variability were taken to be  $\mu_\theta - 3\sigma_\theta$  and  $\mu_\theta + 3\sigma_\theta$  respectively, since over 99% of the area under a Gaussian distribution will fall within three standard deviations of the mean. Thus CFD simulations were carried out for evenly spaced angular increments within this range.

Quinn et al. (2001) noted that their use of nine values of wind direction fluctuations may not have been sufficient, thus in the present work, sensitivity tests were carried out to determine an optimal number of simulations required to adequately account for directional variability, thereby improving the robustness of the weighting method without requiring an excessive number of simulations. Wind variation increments of  $\sigma_\theta$ ,  $\sigma_\theta/2$  and  $\sigma_\theta/4$  were used to produce resultant plumes from the weighted summations of 7, 13 and 25 sets of simulations respectively. At the largest angular increment, corresponding to  $\sigma_\theta$ , the scatter of accretion results was more pronounced as can be seen in Figure 4.5(c). All increments appeared to produce results that were closely matched in terms of accretion predictions. Upon inspection, a variation of approximately 7% was observed between the weighted results of the  $\sigma_\theta$  set and the  $\sigma_\theta/2$  set beyond the accretion maxima. However the difference between the weighted results of the  $\sigma_\theta/2$  set and  $\sigma_\theta/4$  set was appreciably smaller at 1%.

The difference between the locations of the concentration maxima was negligible for all increments and did not appear to be dependent on the size of the angular increments used to represent the wind variability for a given value of  $\sigma_\theta$ . This sensitivity test was only carried out for the neutral boundary layer, because the calculated standard deviations for all three stability classes were of similar magnitudes ( $5^\circ$  to  $5.7^\circ$ ). For larger standard deviations, of a higher order of magnitude, increments of  $\sigma_\theta/8$  may prove to be more appropriate.

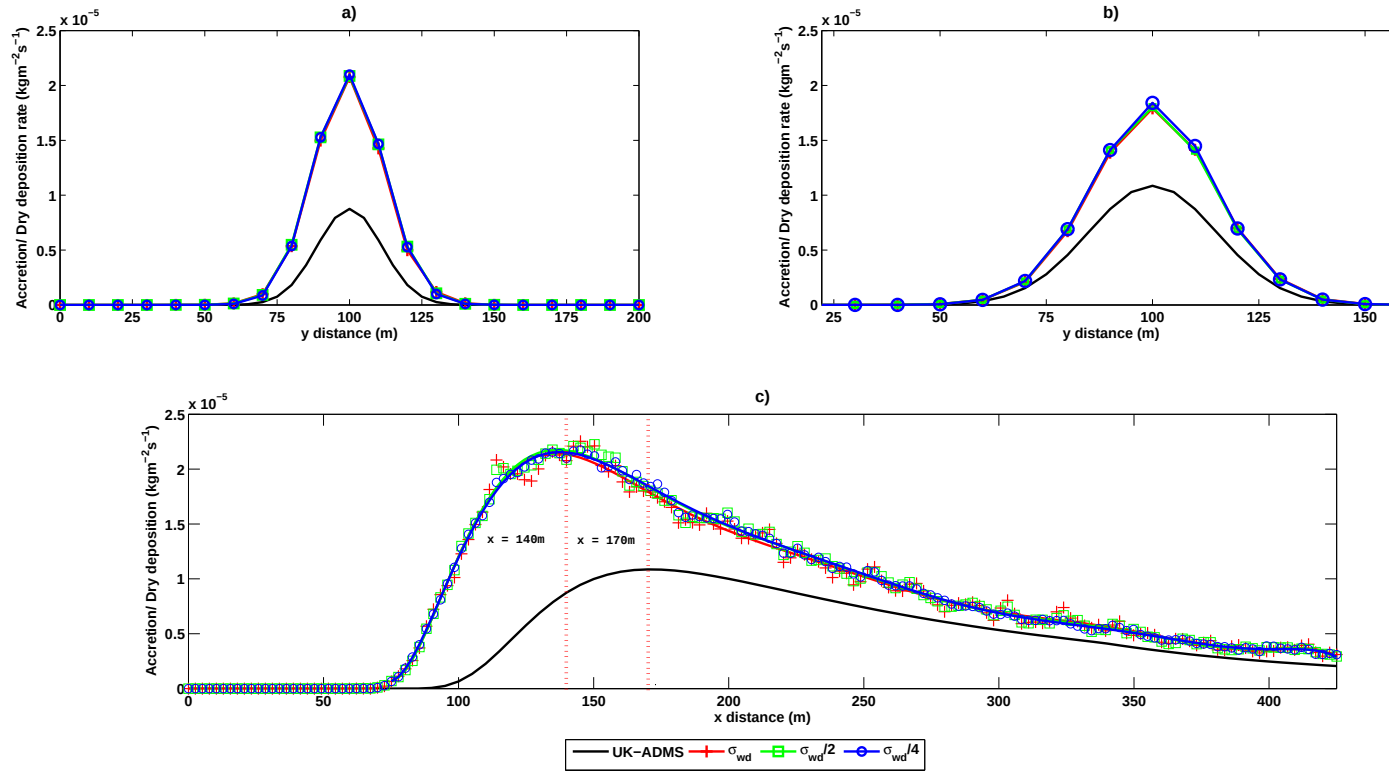


Figure 4.5: Wind variability method at different  $\sigma_\theta$  increments, neutral ABL  $c_L = 0.15$ ,  $\sigma_\theta = 5^\circ$  at a)  $x = 140$  m, b)  $x = 170$  m, c)  $y = 100$  m.

To produce the results seen in Figure 4.5, the FLUENT accretion rate for each of the directional variations and the mean wind direction were exported to MATLAB, where the process of weighting the contribution of each of the wind directions to the resultant plume was carried out according to the following equation:

$$\bar{A} = \frac{\sum_{i=0}^n p_i A_i}{\sum_{i=0}^n p_i}, \quad (4.10)$$

where  $\bar{A}$  is the weighted average accretion rate,  $i$  is an integer corresponding to the simulation number,  $n$  is the total number of simulations and  $p$  is the probability of occurrence of the  $i^{th}$  wind direction variation. In equation 4.10, the weighted values were normalised using the total probability of the limits  $-3\sigma_\theta$  to  $3\sigma_\theta$ , given by  $\sum_{i=0}^n p_i$  which was approximately equal to one.

A quadrature method was used to evaluate the definite integral of the Gaussian function at intervals corresponding to  $\sigma_\theta/2$ , thus determining the probability of occurrence of each wind direction variation from the following expression,

$$p(\theta) = \frac{1}{\sigma_\theta \sqrt{2\pi}} \int_{\theta-\sigma_\theta/4}^{\theta+\sigma_\theta/4} \exp \left[ -\frac{(\theta - \mu_\theta)^2}{2\sigma_\theta^2} \right] d\theta, \quad (4.11)$$

here  $\theta$  is taken to be the angular value of the wind direction variation.

#### 4.3.5 The Influence of the Lagrangian Integral Time Scale Constant

To predict the particle trajectory, the DRW model uses the instantaneous fluid phase velocity in the integration of Equation 4.5 where the fluctuating velocity component  $u'(t)$  is a discrete piecewise constant function of time. Under the assumption of turbulence isotropy, the value of the fluctuating velocity component at each discrete time interval is computed from,

$$u' = v' = w' = \zeta \sqrt{2k/3} \quad (4.12)$$

where  $\zeta$  is a normally distributed random number between -1 and 1, representing the Gaussian distribution of the fluctuating velocity components. The value of  $\zeta$  is held constant over a time scale representing the duration of particle interactions with turbulent eddies in the flow. A particle may interact with eddies over the duration of their lifetime or the particle may cross one eddy and interact with another. Therefore the particle-eddy interaction time scale is taken as the shorter of the characteristic eddy lifetime or the particle crossing time. The characteristic eddy lifetime,

$$\tau_e = -T_L \log(r) \quad (4.13)$$

is a function of the Lagrangian integral time, where  $r$  is a uniformly distributed random number which allows the characteristic eddy lifetime to also vary randomly. The Lagrangian Integral time is correlated to the Eulerian integral time of the continuous phase, hence,

$$T_L = c_L \frac{k}{\varepsilon}, \quad (4.14)$$

where  $c_L$  is a correlation coefficient known as the Lagrangian integral time scale constant. The particle eddy crossing time is calculated from,

$$t_{cross} = -\tau \ln \left[ 1 - \left( \frac{L_e}{\tau|u - u_p|} \right) \right], \quad (4.15)$$

where  $\tau$  is the particle relaxation time,

$$\tau = \frac{\rho d_p^2}{18\mu}. \quad (4.16)$$

In Equation 4.15,  $L_e$  is the eddy length scale and  $|u - u_p|$  is the relative velocity of the particle.

The default value of the Lagrangian integral time scale constant  $c_L$ , is set to 0.15 in the FLUENT standard  $k - \varepsilon$  model, and values of turbulent kinetic energy and its dissipation rate in Equation 4.14 are obtained from the solution of the flow-field. The FLUENT DPM guide indicates that the precise value of  $c_L$  is not well known, however Gorlé et al. (2009) observed that the value of this constant may have an important effect on predictions of concentration which utilise the stochastic model. In fact, from Equation 4.14 and 4.13 it is seen that variations to the value of  $c_L$  can be used to modify the characteristic eddy lifetime, thereby modulating the influence of turbulent fluctuations on the trajectory of a particle throughout its residence time in the computational domain (Tian et al., 2006). Therefore, this work adopts recommendations by Gorlé et al. (2009) to perform sensitivity test to calibrate  $c_L$ .

According to Du et al. (1995), the Lagrangian integral time scale is correlated to the turbulent dissipation rate for turbulent eddies in the inertial sub-range according to,

$$T_L = \frac{2\sigma_u^2}{C_o\varepsilon}, \quad (4.17)$$

where  $\sigma_u^2$  is the u-velocity variance component in the isotropic turbulence model and  $C_o$  represents the inertial sub-range Kolmogorov constant which is important for determining the Lagrangian velocity structure function and the influence of velocity fluctuations on turbulent diffusion of particles (Rizza et al., 2010). Values of  $C_o$  ranging between 3 and 10 have been proposed in the literature for high Reynolds number flows (Du et al., 1995; Degrazia and Anfossi, 1998; Rizza et al., 2010). Furthermore, Degrazia and Anfossi (1998) has derived values of  $C_o$  for the three velocity components under different atmospheric stability conditions.

The turbulent kinetic energy can be written in terms of the velocity variances as,

$$k = \frac{1}{2}(\sigma_u^2 + \sigma_v^2 + \sigma_w^2) \quad (4.18)$$

In accordance with the assumption of isotropic turbulence which underpins the  $k - \varepsilon$  model,  $\sigma_u^2 = \sigma_v^2 = \sigma_w^2$ , resulting in,

$$k = 1.5\sigma_u^2. \quad (4.19)$$

Table 4.2: Values of the Kolmogorov constant proposed by Degrazia and Anfossi (1998) for different atmospheric stability conditions.

| Variable        | $C_o$ range     |
|-----------------|-----------------|
| Unstable $u$    | $2.23 \pm 0.89$ |
| Unstable $v, w$ | $3.44 \pm 1.38$ |
| Stable $u$      | $4.53 \pm 1.81$ |
| Stable $v, w$   | $6.98 \pm 2.79$ |

Thus equation 4.17 can be rearranged to give  $T_L$  in terms of turbulent kinetic energy and its dissipation rate,

$$T_L = \frac{4}{3C_o} \frac{k}{\varepsilon}, \quad (4.20)$$

and an equation for the time scale constant can be deduced by relating Equations 4.14 and 4.20,

$$c_L = \frac{4}{3C_o}. \quad (4.21)$$

In the FLUENT DPM, the default  $c_L$  value of 0.15 correlates to a  $C_o$  value of 8.9 and falls within the range recommended by Degrazia and Anfossi (1998) in Table 4.3. It is seen in Table 4.3, that there is no general consensus on appropriate values of  $C_o$ , since the constant appears to exhibit a dependence on the Reynolds number and some of the underlying physics of Lagrangian stochastic tracking are not fully resolved (Yeung, 2002).

Table 4.3: Values of the time scale constant derived from values of the Kolmogorov constant proposed in the literature

| Researchers          | $C_o$ range   | $c_{Lmin}$ | $c_{Lavg}$ | $c_{Lmax}$ |
|----------------------|---------------|------------|------------|------------|
| Thompson 1987        | $4.0 \pm 2.0$ | 0.22       | 0.33       | 0.67       |
| Yeung 2002           | 6.4           | -          | 0.21       | -          |
| Biferale et al. 2005 | $5.2 \pm 0.8$ | 0.22       | 0.26       | 0.30       |
| Du et al. 1995       | $3.0 \pm 0.5$ | 0.38       | 0.44       | 0.53       |
| Degrazia et al. 1998 | 1.34-9.77     | 0.14       | 0.57       | 0.99       |

The characteristic lifetime of turbulent eddies which interact with the particles can be adjusted through modifications to the time scale constant,  $c_L$ . Here,  $c_L$  has been reduced to 0.05 through calibration of the FLUENT model with UK-ADMS. On this basis, it can be deduced that a damping of the effects of turbulent diffusion on particle trajectory is necessary to bring the  $k - \varepsilon$  model predictions in line with those of UK-ADMS, which is not surprising given that the Gaussian model is a special solution of the Advection-diffusion equation which is derived under the assumption that the downwind dispersion of pollutants is dominated by advective transport.

## 4.4 Results and Discussion

### 4.4.1 Homogenous ABL Profiles

In Figure 4.6, profiles of normalized velocity  $u$ , turbulent kinetic energy  $k$ , turbulent dissipation rate,  $\varepsilon$ , and temperature,  $T$  along vertical rakes positioned at  $(x, y) = (212.5, 100)$  have been plotted for the stable, neutral and unstable ABL using the modifications to the

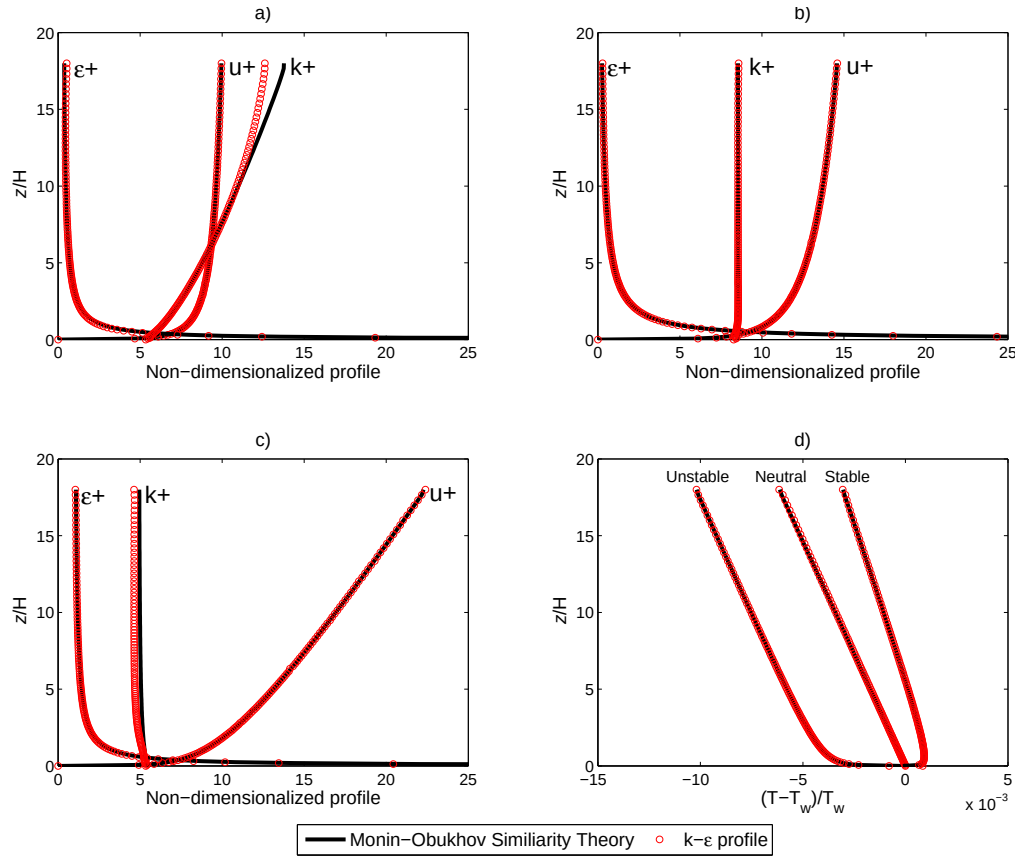


Figure 4.6: Homogenous turbulence profiles, a) Unstable ABL, b) Neutral ABL, c) Stable ABL, d) Normalized Temperature for the stability classes used in the wind variability simulations

$k-\varepsilon$  model and the modified Richards and Hoxey (1993) inlet profile equations proposed by Alinot and Masson (2005). The flow variables  $u$ ,  $k$  and  $\varepsilon$  were normalized using appropriate

powers of the scaling velocity  $u_*$ , whilst  $T$  was normalized using the wall temperature,  $T_w$ ,

$$\hat{u} = \frac{u}{u_*}, \quad (4.22)$$

$$\hat{k} = \frac{k}{u_*^2}, \quad (4.23)$$

$$\hat{\varepsilon} = \frac{\varepsilon h_{ref}}{u_*^3}, \quad (4.24)$$

$$\hat{T} = \frac{(T - T_w)}{T_w}. \quad (4.25)$$

In Equations 4.22 to 4.25,  $h_{ref}$  represents the reference height of 10 m and  $T_w$  is the temperature at the wall. These plots display the results of a check to ensure that the profiles remain homogeneous and consistent with the empirical Monin-Obukhov profiles imposed at the inlet when the reference meteorological conditions used by Alinot and Masson (2005) are replaced with those in Table 4.1. The unstable  $\hat{k}$  profile in Figure 4.6 a) experience decay beyond a height of 100 m, with a maximum decay in  $\hat{k}$  of approximately 8% at the top of the domain. The neutral profiles of  $\hat{\varepsilon}$ ,  $\hat{u}$  and  $\hat{k}$  in Figure 4.6 b) show the best agreement with the Monin-Obukhov empirical profiles. In Figure 4.6 c), the stable non-dimensionalized  $k$  profile experience a decay of 10%. The normalized temperature profiles are shown to be consistent with Monin-Obukhov Similarity Theory in Figure 4.6 d). In general, the change in meteorological conditions results in turbulence profiles which show a similar degree of agreement the with Monin-Obukhov profiles as the original Alinot and Masson (2005) meteorological conditions.

#### 4.4.2 DPM Accretion Results

In UK-ADMS, dry deposition is modelled using a Eulerian approach which relies on the calculation of a deposition velocity that brings particles in contact with the wall. Therefore the dry deposition flux, which is defined as the rate of accumulation of particulate mass per unit wall surface area is calculated from,

$$F_{dry} = v_d C(x, y, 0), \quad (4.26)$$

where  $v_d$  is the deposition velocity and  $C(x, y, 0)$  is the near-surface concentration of particulates. The deposition velocity is a function of particle properties, surface characteristics and wind speed; its value is held constant throughout the calculation domain when the terrain is homogeneous.  $v_d$  consists of a diffusive part  $v'_d$ , which considers the effects of turbulence on particle transport and a gravitational part,  $v_t$ , which accounts for settling of the particle under the influence of gravity,

$$v_d = \frac{v_t}{1 - \exp(-v_t/v'_d)}. \quad (4.27)$$

The accretion rate is the DPM equivalent of the dry deposition flux, nevertheless salient differences arise between the two quantities due to the stochastic treatment of turbulent

diffusion employed by the DRW model, in which turbulent fluctuations and particle-eddy interactions are directly accounted for in the computation of individual particle trajectories. Strictly speaking, UK-ADMS deposition velocity deals with the statistics of the mean flow and turbulent diffusion is implicitly accounted for through the particle diffusivity.

In UK-ADMS, the plume concentration field is attenuated through the application of a depletion factor as material is removed at the deposition surface. This surface is assumed to act as a perfect sink for particulates such that dry deposition is irreversible and particles cannot be re-suspended (Aspley and CERC, 2012; Sehmel, 1970). This treatment is consistent with the trap boundary condition applied at the wall in the FLUENT DPM.

Accretion results obtained from the FLUENT DPM have been compared to UK-ADMS dry deposition predictions in Figures 4.8 to 4.10. The plots are of dust accretion on the ground ( $\text{kgm}^{-2}\text{s}^{-1}$ ) plotted variously against distance in the along-wind direction and the cross-wind direction, below the plume centreline. In the ensuing discussion and the accompanying figures, FLUENT results with wind variability modifications will be identified by the abbreviation WVM as well as the value of  $c_L$  used for each of these simulations. FLUENT simulations using the default value of  $c_L$  without wind variability considerations will henceforth be referred to as base FLUENT and UK-ADMS deposition profiles will be identified as such.

A preliminary examination of the plume profiles confirms that both FLUENT and UK-ADMS predictions follow the well known trends in plume behaviour expected for the three stability classes. The relatively high wind speed of the neutral case generated the highest levels of mechanical turbulence, leading to enhanced dispersion of the dust particles and consequently it was seen that the lowest deposition was observed for this case. This scenario matches that expected in physical conditions, where the advective transport of particulates due to higher winds ensures that particles are entrained for longer residence times in the airflow and are thus dispersed further from the source. The stable ABL is the least dispersive case and exhibits the highest near-source deposition flux of all the stability classes. This result can be attributed to turbulence suppression due to thermal stability and accordingly particle trajectories predicted by the stochastic model will be affected to a lesser extent by turbulent fluctuations. Mechanically generated turbulence which was more significant than that of the stable case and buoyancy induced turbulence as a result of thermal instability ensured that dust dispersion in the unstable case is observably higher than that of the stable case, producing a lower deposition maximum.

In keeping with work by Riddle et al. (2004), this study observed that the lateral extent of the dust deposition plume was underestimated by the base FLUENT results compared to UK-ADMS predictions. In order to improve the lateral plume spread predictions of the FLUENT DPM, this work has systematically undertaken to explore the implications of the following modifications on model predictions, relative to the base FLUENT case:

1. FLUENT with  $c_L=0.05$
2. FLUENT WVM with  $c_L=0.15$
3. FLUENT WVM with  $c_L=0.05$ ,

To arrive at the value of  $c_L=0.05$ , FLUENT results were calibrated against UK-ADMS predictions using the wind variability method and various values of  $c_L$  ranging from 0.15 to 0.0375. This value of  $c_L$  yielded accretion predictions which were on average, 30% higher than UK-ADMS predictions for the three stability classes and locations of the accretion maxima predicted using this value of the constant were within 10 m of UK-ADMS peak deposition predictions. Predictions of maximum accretion which were in better agreement with UK-ADMS results were obtained by reducing  $c_L$  to 0.0375, but this improvement is offset by decreases in lateral spreading and elongation of the plume in the downwind direction.

In trial simulations with  $c_L$  increased to 0.30, the plume initially encountered the ground nearer to the source than in the default  $c_L=0.15$  case, this is also notably closer to the source than UK-ADMS predictions. Dry deposition and accretion rate along the longitudinal axis of the plume and also in the transverse direction have been plotted for the stable case in Figure 4.7. The stable case is regarded here as the most critical case, because as mentioned in Section 2, wind variability is likely to be the dominant dispersive mechanism in stable, low wind conditions. Figure 4.7 illustrates that an increase in the time scale constant does not improve FLUENT predictions relative to UK-ADMS, in terms of comparability of accretion rates and lateral plume spread.

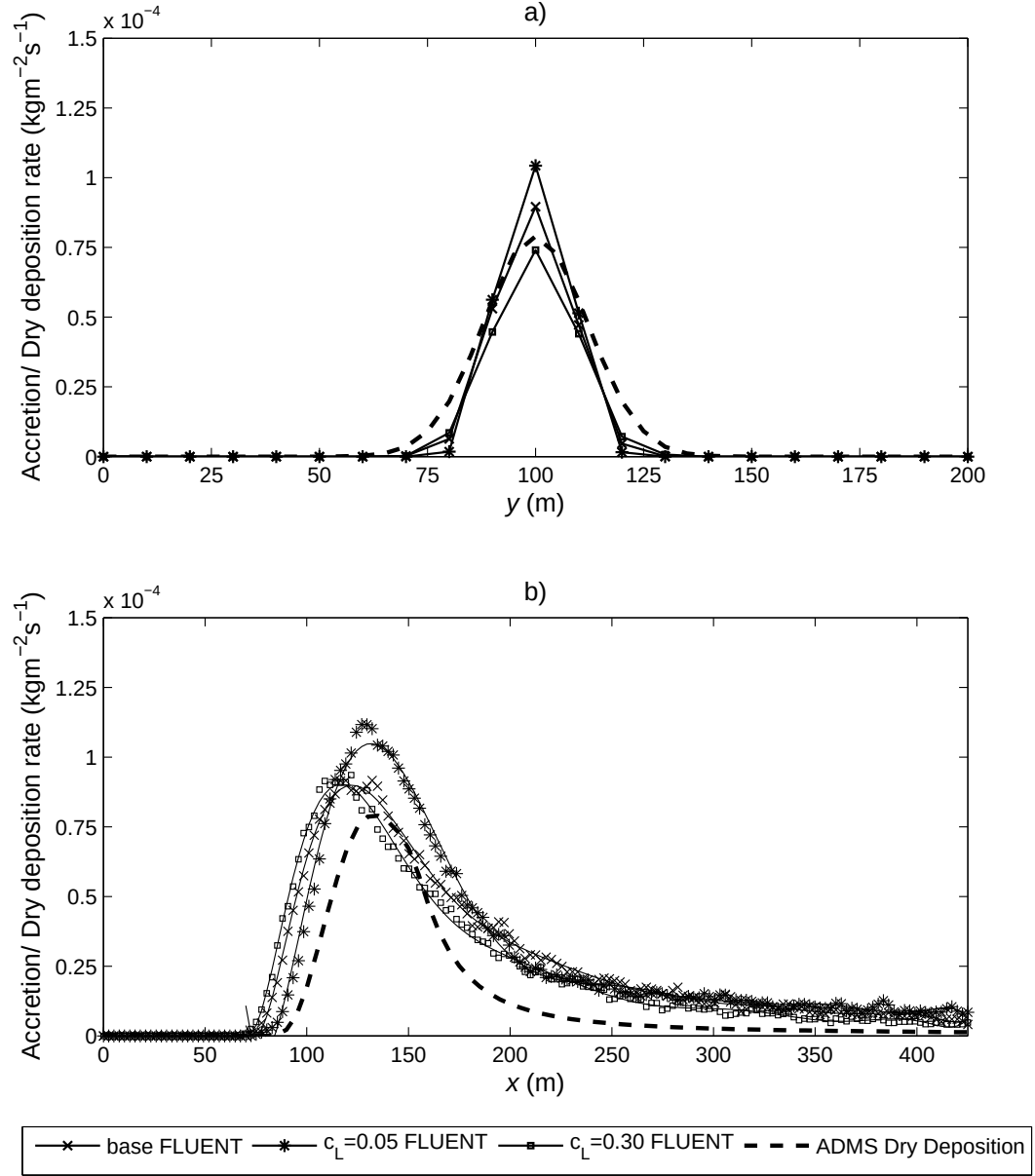


Figure 4.7: Stable DPM accretion plots with different  $c_L$  values,  $\sigma_\theta = 5.7^\circ$ , a)  $x=135$  m, b)  $y=100$  m

On the other hand, when  $c_L$  is reduced to 0.05, particle accretion begins further from the emission source. Moreover, the accretion levels decrease below those experienced using  $c_L = 0.15$ . Figures 4.8 to 4.10 show that a reduction from the default value of the time-scale constant on its own, did not produce any marked improvements in the prediction of lateral plume spread. Thus, it becomes apparent that the problem of under-prediction of lateral plume spread cannot be rectified solely by modifying the value of  $c_L$ . It is seen that  $c_L$  is a blunt instrument for improving the lateral spreading of the plume, because due to the model assumption of turbulent isotropy, modifying the value of  $c_L$  alters the dispersive characteristics of the plume in all three directions.

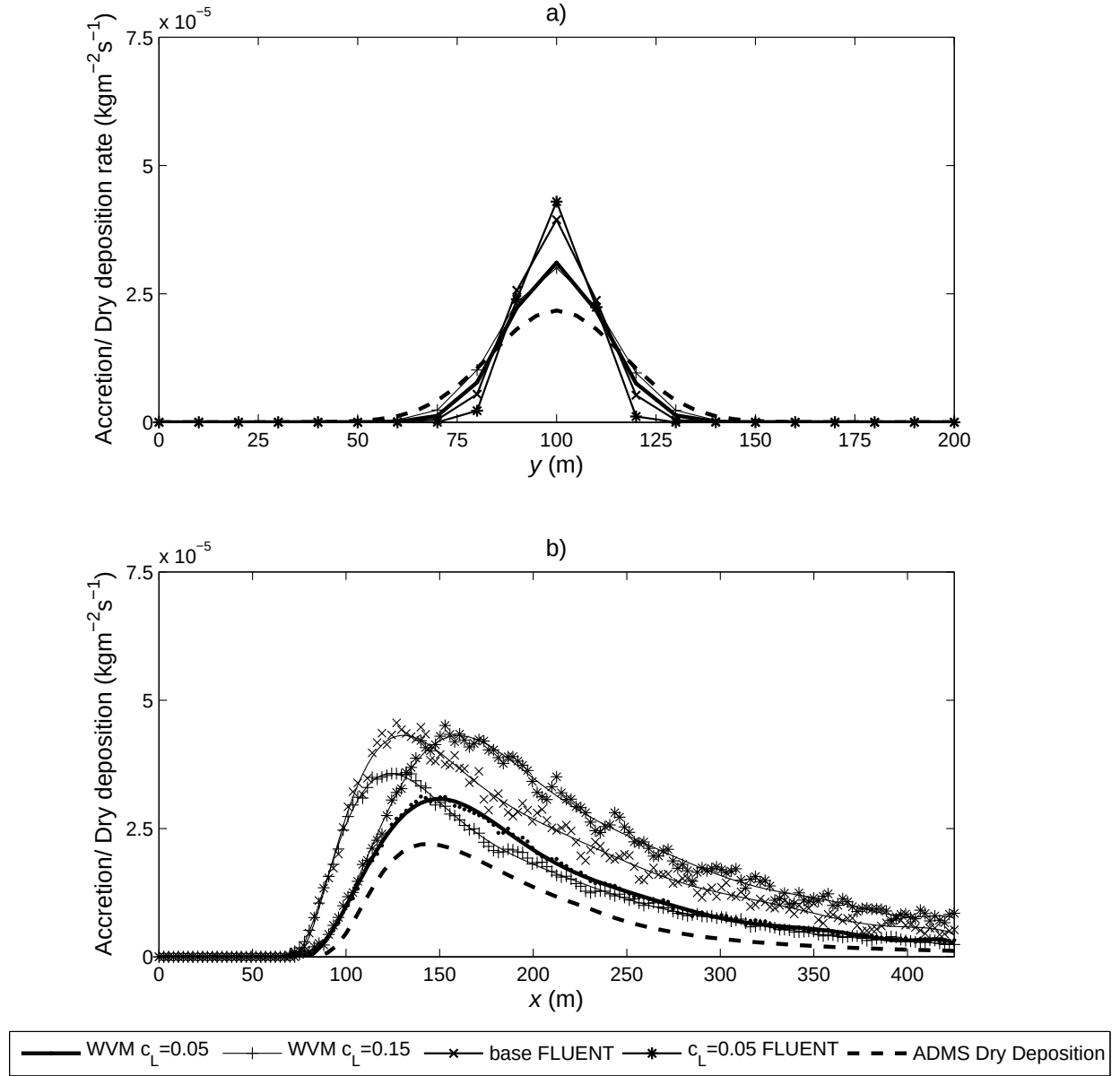


Figure 4.8: Unstable DPM accretion and UK-ADMS 5.0 plots,  $\sigma_\theta = 5.0^\circ$ , a)  $x=135$  m, b)  $y=100$  m

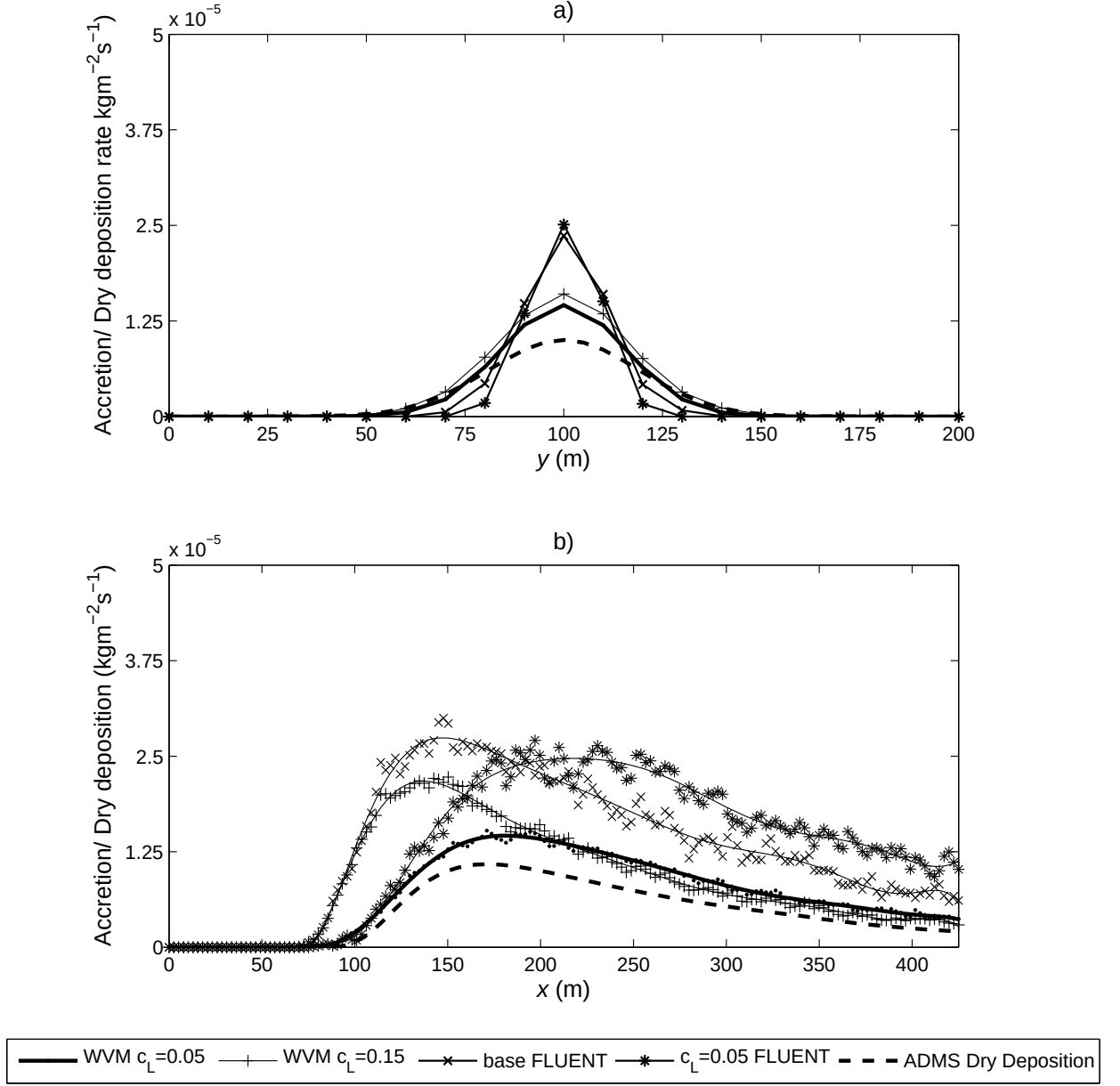


Figure 4.9: Neutral DPM accretion and UK-ADMS 5.0 plots,  $\sigma_\theta = 5^\circ$ , a)  $x=135$  m, b)  $y=100$  m

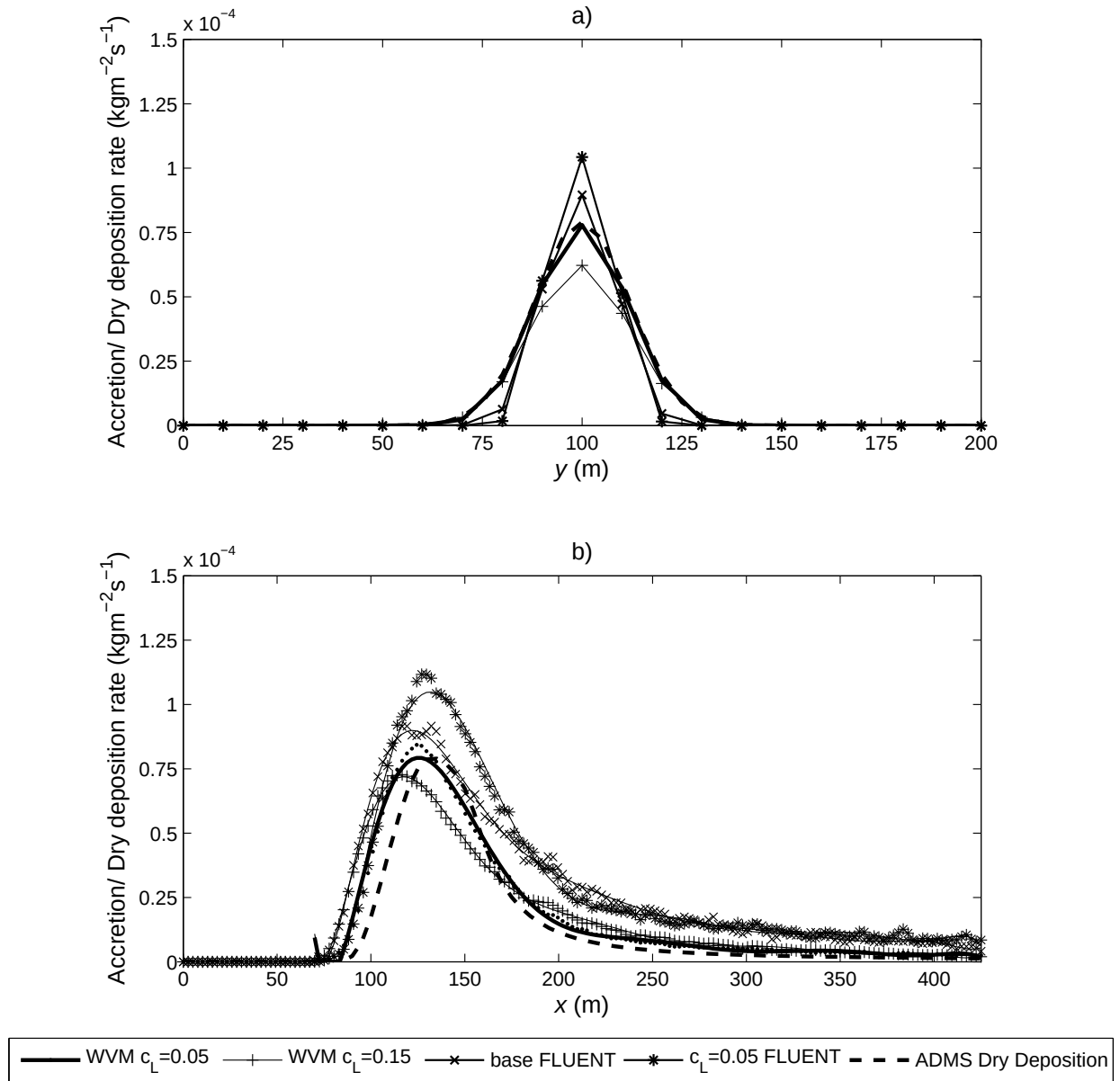


Figure 4.10: Stable DPM accretion and UK-ADMS 5.0 plots,  $\sigma_\theta = 5.7^\circ$ , a)  $x=135$  m, b)  $y=100$  m

Improvements in the predictions of lateral dispersion for the three stability classes were achieved by incorporating wind direction variability into the FLUENT simulations, with the stable ABL simulations exhibiting the most significant improvements. This is evidenced by the plots in Figures 4.8(b) to 4.10(b). Lateral plume spread predictions have been quantified in Table 4.4 using the lateral width of the plume about the centreline to the distance where the accretion rate has decayed to zero. This width is evaluated from Figures 4.8(a), 4.9(a) and 4.10(a), at the same  $x$  distance corresponding to the UK-ADMS deposition maxima. Results indicate that FLUENT predictions of lateral spread across the location of the peak deposition now fall within 15% of UK-ADMS predictions for the simulations which include wind variability modifications. Similarly, the contour plots in Figures 4.11(c) to 4.13(c) also show improved lateral spread compared to their base FLUENT counterparts in Figures 4.11(b) to 4.13(b). This improvement in lateral spread predictions occurs in the WVM case where the default value of  $c_L$  is retained and also the case where  $c_L=0.05$ . However, it is seen that combining the wind variability method with the reduced  $c_L$  value of 0.05 is the most effective approach to obtaining FLUENT results which are a reasonable approximation of UK-ADMS results.

Table 4.4: Lateral Plume Spread Predictions

| Stability | Lateral Spread (m) |              |              |                 |              |
|-----------|--------------------|--------------|--------------|-----------------|--------------|
|           | ADMS               | FLUENT       |              | FLUENT with WVM |              |
|           |                    | $c_L = 0.15$ | $c_L = 0.05$ | $c_L = 0.15$    | $c_L = 0.05$ |
| Unstable  | 90                 | 65           | 60           | 80              | 80           |
| Neutral   | 100                | 80           | 60           | 100             | 100          |
| Stable    | 80                 | 60           | 60           | 80              | 80           |

Riddle et al. (2004) also make mention of the tendency of the DPM to predict elevated deposition fluxes at distances further downwind of the emission source than UK-ADMS. The FLUENT DPM guide (ANSYS, 2009b), identifies this as an anomaly which arises in non-homogeneous turbulence fields, where the DPM random walk model tends to accumulate the particles in low turbulence regions. However, the contour plots, Figures 4.11(c) to 4.13(b), have been included to show that this is somewhat alleviated by the wind-direction variability method, because the elevated fluxes are moderated by probability averaging of simulation results.

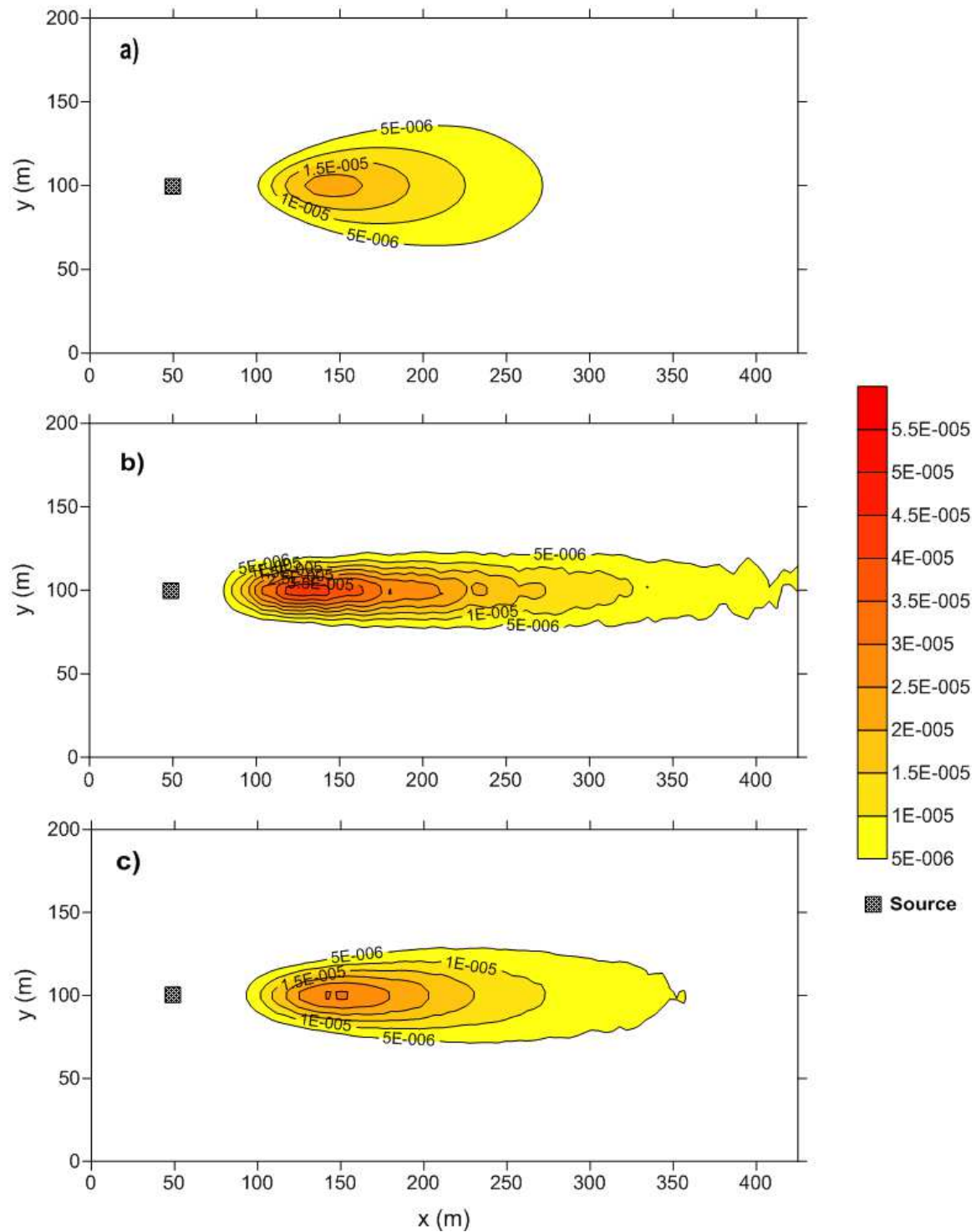


Figure 4.11: Dry deposition contours (kgm<sup>-2</sup>s<sup>-1</sup>) for an unstable ABL, a) UK-ADMS, b) base FLUENT, and c) FLUENT WMV  $c_L = 0.05$ .

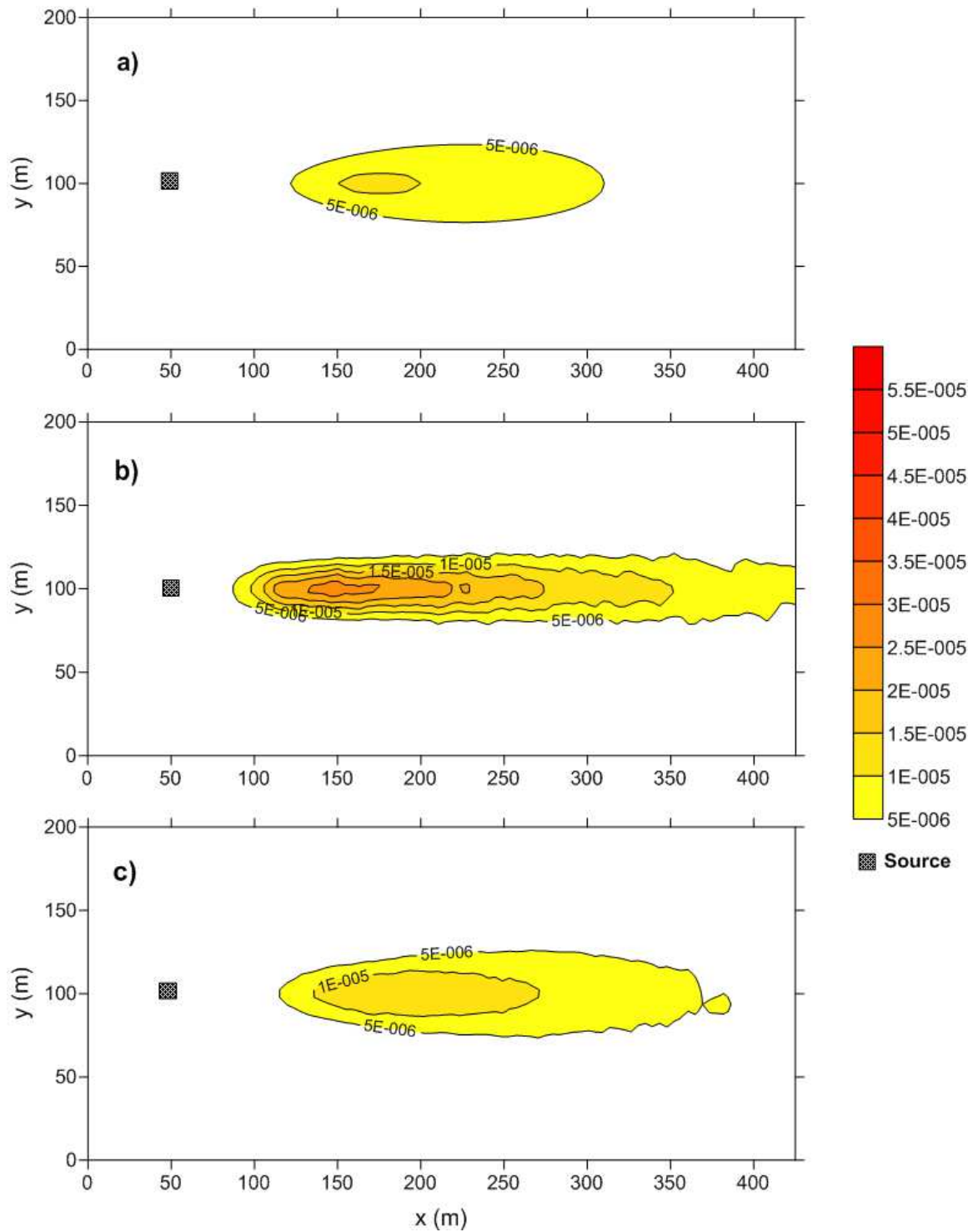


Figure 4.12: Dry deposition contours (kgm<sup>-2</sup>s<sup>-1</sup>) for a neutral ABL, a) UK-ADMS, b) base FLUENT and c) FLUENT WMV  $c_L = 0.05$

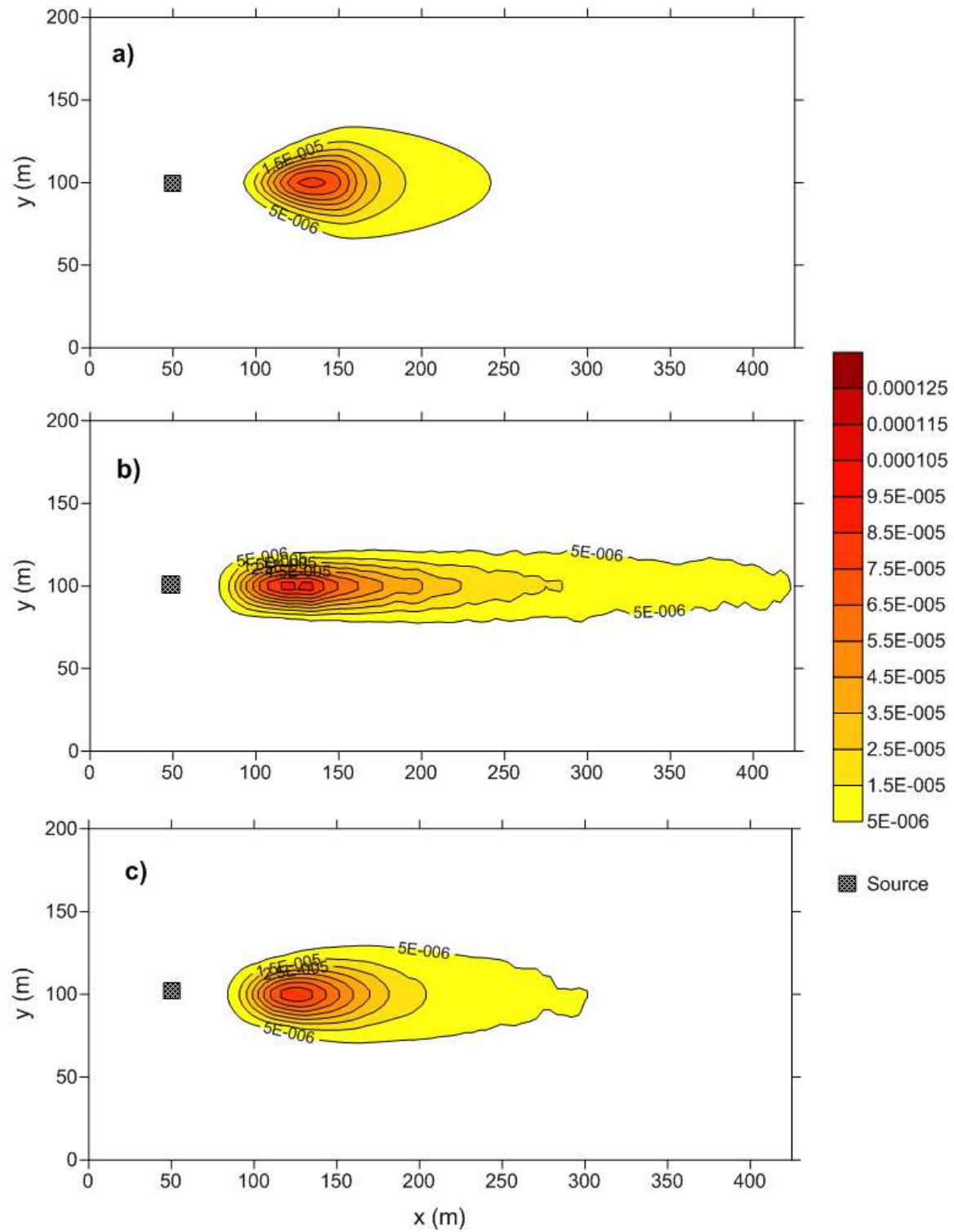


Figure 4.13: Dry deposition contours ( $\text{kgm}^{-2}\text{s}^{-1}$ ) for a stable ABL, a) UK-ADMS, b) base FLUENT and c) FLUENT WMV  $c_L = 0.05$

## 4.5 Summary

In this chapter the DPM has been coupled to  $k - \varepsilon$  turbulence model to provide stochastic tracking of dust particles emitted from an elevated volumetric emission source surrounded by flat terrain of aerodynamic roughness height  $z_0 = 0.01$ . A methodology has been presented to incorporate the effects of wind direction variability in the buoyancy modified  $k - \varepsilon$  model. The proposed modelling strategy has adopted the Moore (1976) empirical formulation to parametrize mesoscale wind variability in terms of the standard deviation of the wind direction. Subsequently, resultant plumes were computed using Gaussian-probability weighted averaging of the accretion predictions of a series of CFD simulations run at various wind angles within three standard deviations of the mean wind direction. For unstable, neutral and stable atmospheric conditions, comparison of the resultant accretion rate profiles to UK-ADMS dry deposition predictions has demonstrated that the proposed methodology has produced improvements in the lateral spreading of the CFD predictions, such that, FLUENT predictions of lateral plume spread are within 15% of UK-ADMS predictions.

The calibration of the Lagrangian integral time scale constant,  $c_L$ , has also been explored as a means to improve lateral plume spread predictions in the  $k - \varepsilon$  model, however, modification of  $c_L$  indiscriminately alters the dispersion characteristics of the plume in all three directions due to the homogeneous treatment of turbulence in the  $k - \varepsilon$  model. Therefore it was concluded that whilst  $c_L$  can be used to moderate the influence of turbulence on particulate dispersion, the wind variability probability averaging procedure presented in this chapter was necessary to improve FLUENT predictions of the lateral spreading of the plume.

## Flow and Dispersion over Idealised Depressions

### 5.1 Flow within Valleys

In this study, the numerical model developed in Chapter 3 is applied to simulate the atmospheric flow field over a series of circular depressions of cosine profile of aspect ratios 8, 4, 2.67 and 2 respectively. The aspect ratio,  $\alpha$ , describes the geometric shape of a valley and is defined as the ratio of the valley half-width  $L/2$  to its depth  $D$ ,

$$\alpha = \frac{L}{2D}. \quad (5.1)$$

The effects of varying the depression depth are examined in conjunction with variations in atmospheric stability. Moreover, particulates are injected into the computational domain above the centre of the depression, in order to illustrate the effects of the terrain and the corresponding flow field perturbations on the dispersion of particulates. This study is a precursor to the case study in Chapter 6, which will simulate the the wind field and fugitive dust dispersion over a UK quarry (Old Moor Quarry). Thus the results obtained from the numerical model are compared to those obtained using the Gaussian dust dispersion model UK-ADMS which is routinely applied for predicting dust dispersion from quarries.

Snyder et al. (1991) used wind tunnel experiments and numerical simulations to study the effects of two dimensional valley topography on the flow and the dispersion of a tracer gas. In their study, three different aspect ratios 3, 5 and 8, were considered. These corresponded to steep, medium and gentle-sided valleys, illustrated in Figure 5.1.

Snyder et al. (1991) indicated that a well-defined recirculation zone occurred in the steepest valley, occupying a region approximately  $0.5x/a$  upwind of the valley centre to  $0.5x/a$  downwind. They described the occurrence of incipient separation of the boundary layer in the medium-sloped valley, where the mean flow remained in the positive downwind direction, with localised, instantaneous flow reversals observed near the ground as a consequence of wall friction. In the gentle valley, the boundary layer remained attached to the ground and there was no flow reversal. These flow phenomena are illustrated in Figure 5.2. Snyder

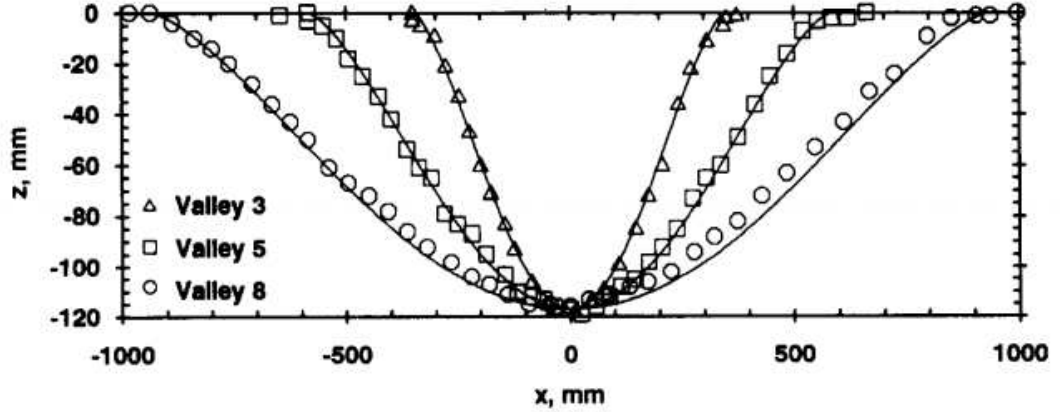


Figure 5.1: 2D valley profiles for 3, 5 and 8 aspect ratio valleys used in wind tunnel study by Snyder et al. (1991). Solid lines correspond to ideal shapes, whilst markers represent measured shapes.

et al. (1991) were also able to demonstrate that the perturbations to the flow field in plot (a) of Figures 5.2 and 5.3, due to the presence of a steep valley, can amplify downwind concentrations of pollutants by as much as 1400% as a result of the plume becoming entrained in recirculation regions of the flow. Profiles of non-dimensionalized velocity,  $u/U_\infty$ , and turbulence intensity  $\sigma_u/U_\infty$  are displayed in Figure 5.2 and 5.3. Where  $U_\infty$  is the free stream wind velocity in the Snyder et al. (1991) study and  $\sigma_u$  is the normal stress component in the along-wind direction.

Snyder et al. (1991) did not consider the effects of thermal buoyancy, however the work presented herein uses a modified  $k - \varepsilon$  model to examine both buoyant and non-buoyant flow fields over a series of idealised circular depressions with cosine profiles. As was done in Chapter 4, particulate matter will be injected into the flow fields and the particle trajectories will be predicted using the Discrete Phase Model, in order to assess the impact of topography and stability class on dispersion.

Other field and laboratory investigations have indicated that flow within, and in the immediate vicinity of, an isolated valley is analogous but opposite to flow over isolated hills (Garvey et al., 2005; Wiggs et al., 2002). Due to pioneering studies such as Jackson and Hunt (1975), it is widely accepted that winds perpendicular to the valley's longitudinal axis experience initial acceleration upwind of the valley, followed by deceleration down the side walls. Upon exiting the valley, the flow again accelerates up the side walls to a maximum at the downwind edge of the valley (Garvey et al., 2005). Separation of the boundary layer, may occur within the valley depending on the valley geometry and the prevailing atmospheric conditions. Snyder et al. (1991) observed that the initial boundary layer profile was recovered some distance downwind, ranging from  $2D$  downwind to  $8D$  depending on the aspect ratio of the valley. In the current study, the emphasis is on the perturbations to the atmospheric boundary layer (ABL) which occur within and immediately downwind of the valley.

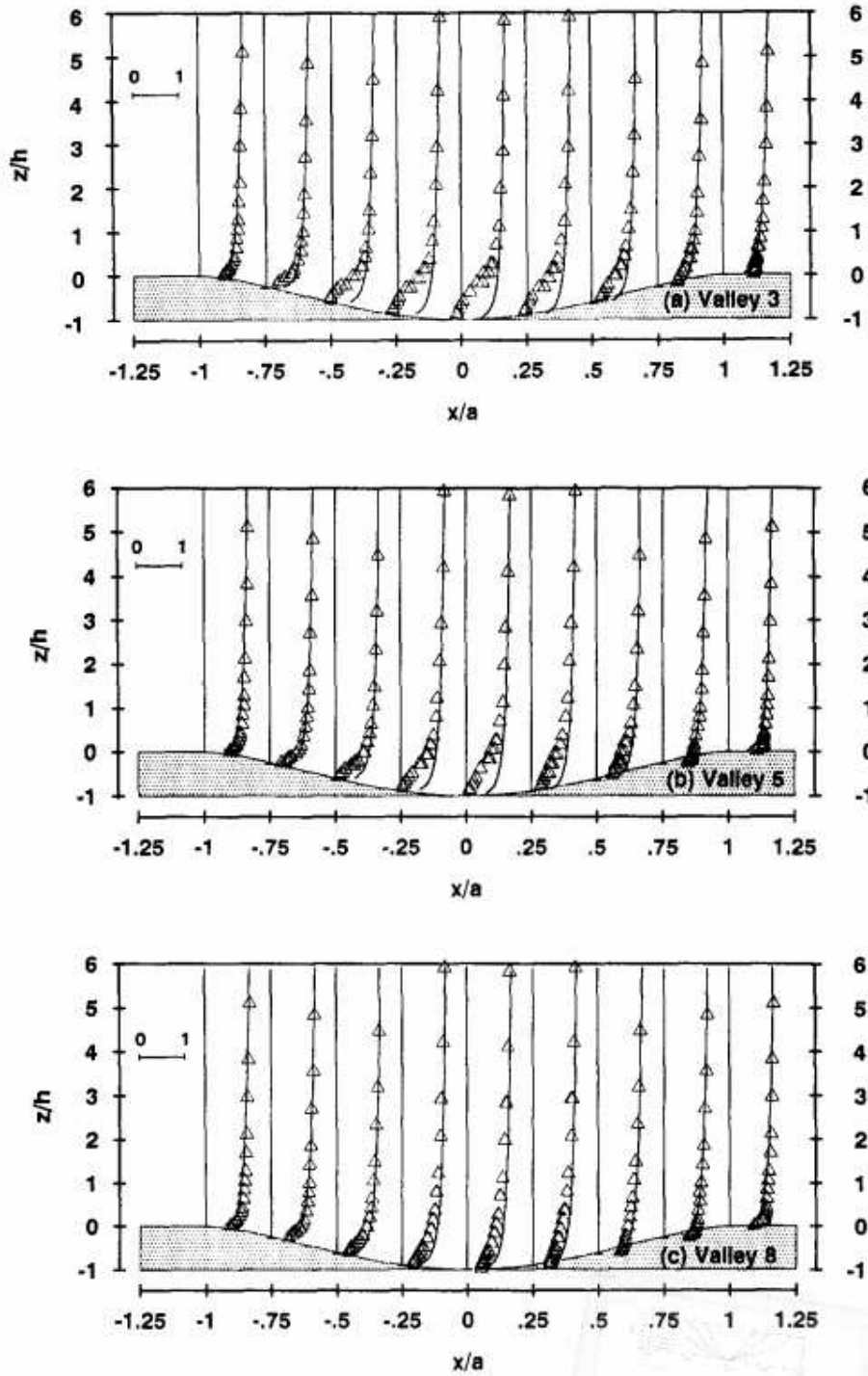


Figure 5.2: Profiles of  $u/U_\infty$  for (a) 3, (b) 5 and (c) 8 aspect ratio valleys from Snyder et al. (1991), the solid lines indicate results from numerical simulations, whilst the triangular markers represent wind tunnel measurements.

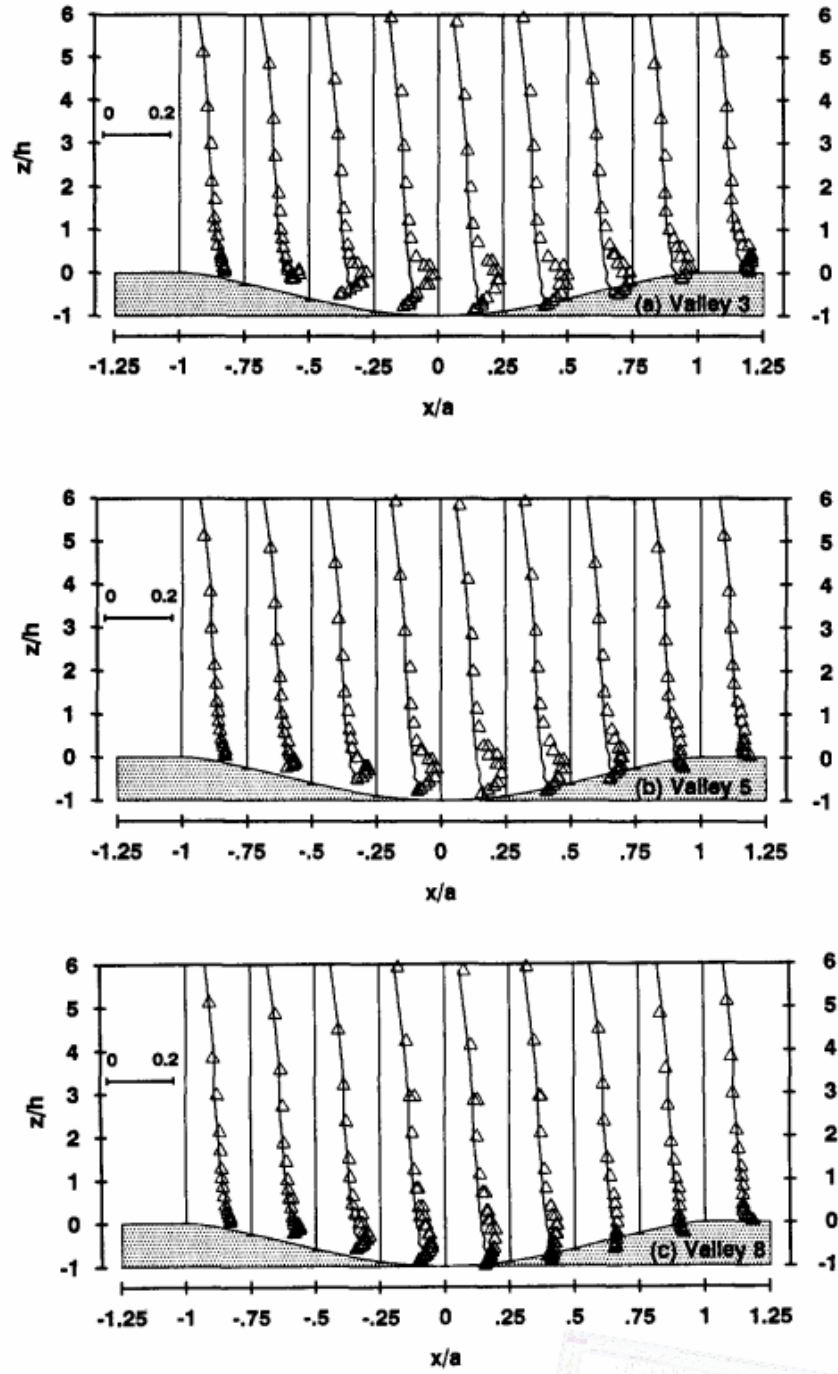


Figure 5.3: Profiles of  $I = \sigma_u / U_\infty$  for (a) 3, (b) 5 and (c) 8 aspect ratio valleys from Snyder et al. (1991), the solid lines indicate results from numerical simulations, whilst the triangular markers represent wind tunnel measurements.

### 5.1.1 Numerical Simulation of Valley Flows

Maurizi (2000) compared the simulation results of flow over a series of 2D valleys of increasing aspect ratio using three RANS models, namely the standard  $k - \varepsilon$  model, the Re-Normalization group (RNG) model and a variant of the standard  $k - \varepsilon$  model which included a turbulent dissipation source term to act as a sink for excess turbulent kinetic energy. As expected, their results indicated good agreement between all three models and the experimental results for the valleys without boundary layer separation. For the steep valley, of aspect ratio 3, the standard  $k - \varepsilon$  model predictions were in good agreement with the experimental results for the first half of the valley, however beyond the valley centre-line, the turbulent kinetic energy was over-predicted by the standard model. They attribute the modelling deficiencies of the standard  $k - \varepsilon$  model to limitations of the flux-gradient approach to modelling the Reynolds stresses in the recirculation region. Maurizi (2000) recommend adaptation of  $k - \varepsilon$  models for atmospheric flows to improve the predictions obtained using these models.

Despite their limitations, RANS models offer a considerably more rigorous treatment of the complex atmospheric flow regimes than the UK-ADMS FLOWSTAR model. As discussed in Chapter 3, the UK-ADMS complex terrain model FLOWSTAR only provides a rudimentary resolution of flow recirculation, however the FLOWSTAR model has been extensively validated for terrain with gradients under 1:3, and in these cases the model predictions have been found to be in good agreement with field measurements. Therefore, the flow-field and particle dispersion results obtained using the the  $k - \varepsilon$  model have been compared to UK-ADMS results, to determine whether there is good agreement between the  $k - \varepsilon$  and UK-ADMS flow-fields for the cases where the depression aspect ratio is greater than 3.

## 5.2 Methodology

### 5.2.1 Introduction of a Wall Distance Scalar in the Numerical Model

The model setting discussed in Chapter 3 to configure the FLUENT  $k - \varepsilon$  model for simulating the atmospheric surface layer, have also been implemented in the idealised terrain studies documented in this chapter. Thus, the modifications to the coefficients of the standard  $k - \varepsilon$  model and the addition of buoyancy source terms to the energy and turbulence closure equations have been maintained in order that thermal stability effects are adequately accounted for by the model. However, since the ground surface is not flat, an additional modification of the numerical model is required, in which a wall distance scalar is implemented to produce profiles of the field variables which conform to the shape of the wall. The wall distance,  $z'$  has been used in the profile and transport equations instead of the absolute value of elevation  $z$ , allowing the model to consistently apply the logarithmic profile equations when the ground level is non-zero. A user-defined scalar field,  $\varphi$ , has been introduced in the FLUENT UDF (Appendix A) to enable computations of the wall distance at any point in the domain, with a Dirichlet boundary condition of  $\varphi = 0$  imposed at the wall (Tucker, 1998; Xu et al., 2011). Since only the diffusive flux of the scalar in the  $z$

direction is of concern, the transport equation for the scalar is a Poisson equation,

$$\frac{\partial^2 \varphi}{\partial z^2} = -1. \quad (5.2)$$

The general solution of Equation 5.2, is in the form of a quadratic expression,

$$az^2 + bz + c = 0 \quad (5.3)$$

to arrive at the solution, Equation 5.2 is integrated, yielding,

$$\frac{\partial \varphi}{\partial z} = -z + C_1, \quad (5.4)$$

$$\varphi = \frac{-z^2}{2} + C_1 z + C_2, \quad (5.5)$$

where  $C_1$  and  $C_2$  are the constants of each integration. Due to the boundary condition,  $\varphi = 0$ , imposed at the wall, where  $z = 0$ , then  $C_2 = 0$  and from Equation 5.4,

$$C_1 = \frac{\partial \varphi}{\partial z} + z. \quad (5.6)$$

By substituting Equation 5.6 into Equation 5.5, a quadratic equation for  $\varphi$  is obtained,

$$\varphi = z \frac{\partial \varphi}{\partial z} + \frac{z^2}{2}, \quad (5.7)$$

$$\frac{z^2}{2} + \frac{\partial \varphi}{\partial z} z - \varphi = 0, \quad (5.8)$$

thus the wall distance field can be determined by solving for the positive root of Equation 5.8, using the quadratic formula,

$$z = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}, \quad (5.9)$$

and is given by the following expression (Tucker, 1998),

$$z' = -\frac{\partial \varphi}{\partial z} + \sqrt{\left(\frac{\partial \varphi}{\partial z}\right)^2 + 2\varphi}. \quad (5.10)$$

The use of a wall distance scalar has not been previously documented in other studies concerned with atmospheric flows over complex terrain, therefore the implementation of  $z'$  in this work is a significant stage in the optimization of the RANS numerical model, which eradicates the need to enforce a baseline elevation of zero at the domain inlet by artificially extending the domain to include a flat terrain region upwind of the area of interest; a feature which will be necessary for simulating the flow-field over the case study quarry and its surrounding topography.

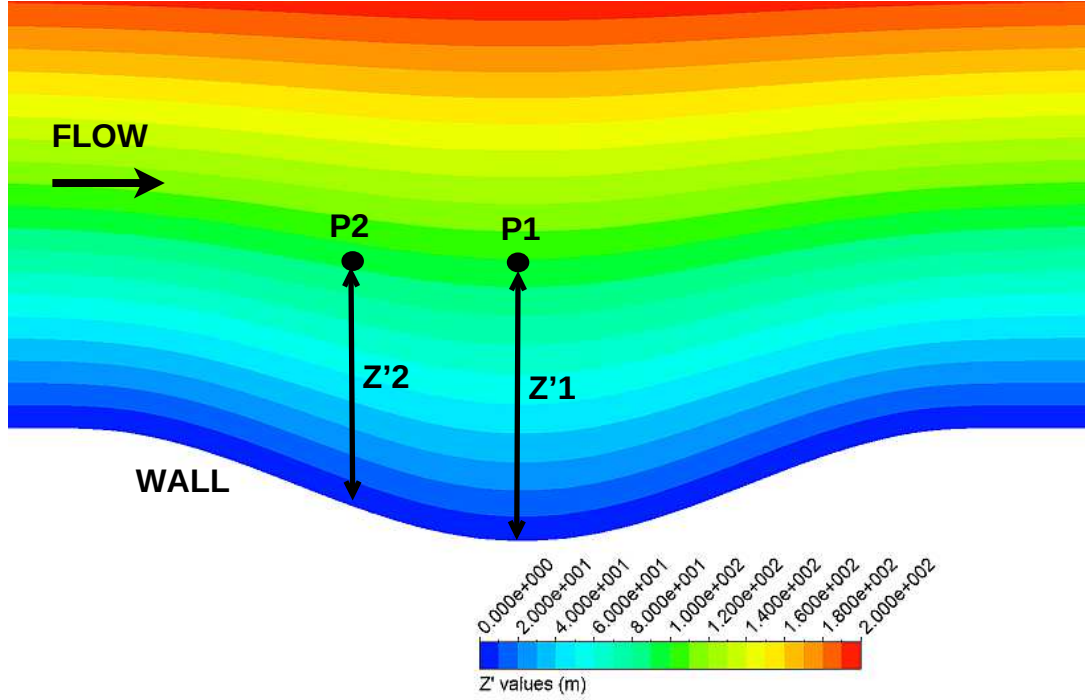


Figure 5.4: Plane at  $y = 0$  through  $\alpha = 4$  depression illustrating  $z'$  field and values for points P1 and P2.

### 5.2.2 Validation of the $k - \varepsilon$ Model with Wind Tunnel Results from Ishihara et al. (1999)

Ishihara et al. (1999) conducted a wind tunnel investigation of the flow over a 3D scale model of a circular hill of cosine squared cross-section, with a shape profile represented by

$$z_s(x, y) = h \cos^2 \left( \pi \frac{(x^2 + y^2)^{1/2}}{2L} \right), \quad (5.11)$$

where  $h$ , the height of the hill (40 mm), and  $L$ , the width of the hill, (200 mm) illustrated in Figure 5.5. Mean velocity and turbulence measurements were obtained using a split wire probe. The  $x$  component of the mean velocity was found to be well represented by the log velocity profile equation with  $u_* = 0.212 \text{ ms}^{-1}$ . The model surface roughness was  $z_0 = 0.01 \text{ mm}$ , which was characteristic of a grass covered hill. Since the simulated boundary layer was one thousandth of the full scale boundary layer, the equivalent full scale roughness was 0.01 m (Ishihara et al., 1999).

The wind profile recorded by Ishihara et al. (1999) indicated the following near surface behaviour of the flow-field;

1. slight deceleration at the windward base of the hill

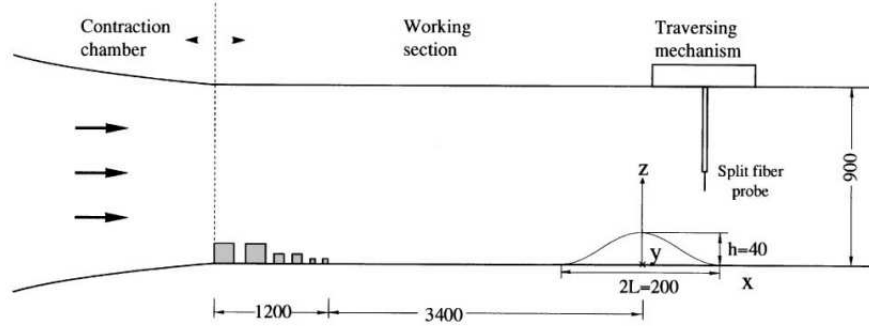


Figure 5.5: Experimental section of wind tunnel and cross-section of scale model of 3D cosine squared hill employed by Ishihara et al. (1999).

2. acceleration over the crest of the hill
3. separation of the flow on the leeward side of the hill near the crest, with the formation of a recirculation bubble which extended horizontally to the leeward base of the hill or approximately  $2.5h$  from the crest. In the vertical direction, perturbations to the turbulent field in the lee of the hill appeared to extend  $1.5h$  above the ground.

An attempt has been made to validate the modified  $k - \varepsilon$  numerical model presented in the current work using the wind tunnel measurements of Ishihara et al. (1999). Reynolds number independence is an underlying principle of the Monin-Obukhov similarity hypothesis and a necessary precondition which permits scale modelling of atmospheric flows (Neff and Meroney, 1996). According to Neff and Meroney (1996) and Petersen (2008), Reynolds number independence is satisfied for the experimental model when the flow Reynolds number exceeds the range 11000 to 15000. Conversely, Snyder (1992) have determined that Reynolds number independence may be assumed for complex terrain dispersion studies at  $Re > 4000$ , when the pollutant sources are located within the cavity wake region because of the dominance of wake effects on plume dispersion. Since Coriolis forces have been neglected in both the experimental and numerical models, establishing similarity of the Rossby Numbers as recommended by Sharma et al. (2005) is not applicable here. By default, Richardson number similarity exists between the models as a consequence of zero wall heat flux which gives rise to neutrally buoyant conditions in both instances where  $Ri = 0$ . A geometrically similar full scale mesh, Figure 5.6 has been constructed with boundary conditions intended to approximate those arising in the wind tunnel. Figures 5.7 and 5.8 show the mesh refinement applied horizontally and in the vertical direction in the vicinity of the hill. The scaling friction velocity and full scale roughness height defined by Ishihara et al. (1999) have been applied in the numerical simulations, thus the dimensionless quantities predicted by the numerical model can be compared to the wind tunnel results.

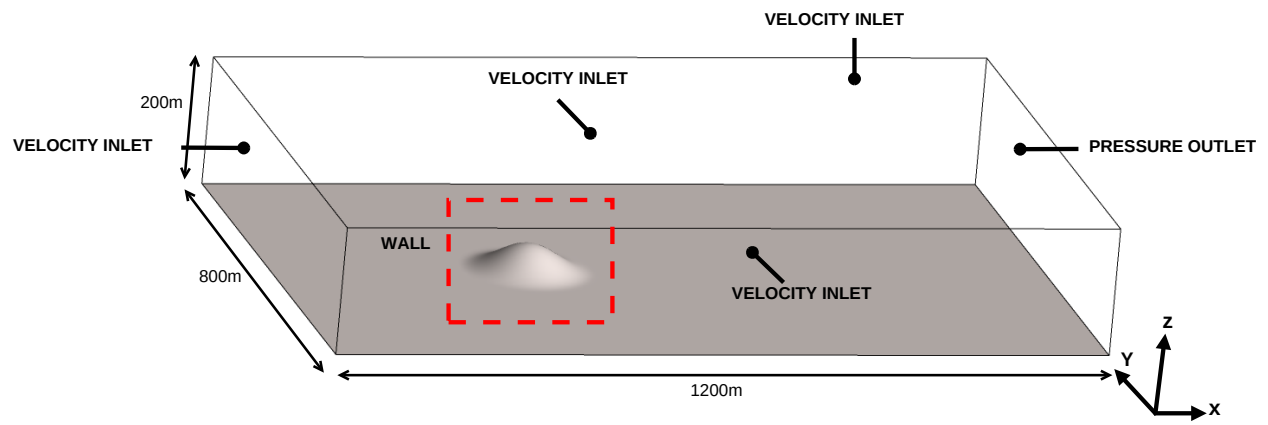


Figure 5.6: Computational domain and boundary conditions used to perform full scale simulations of the 3D hill in Ishihara et al. (1999)

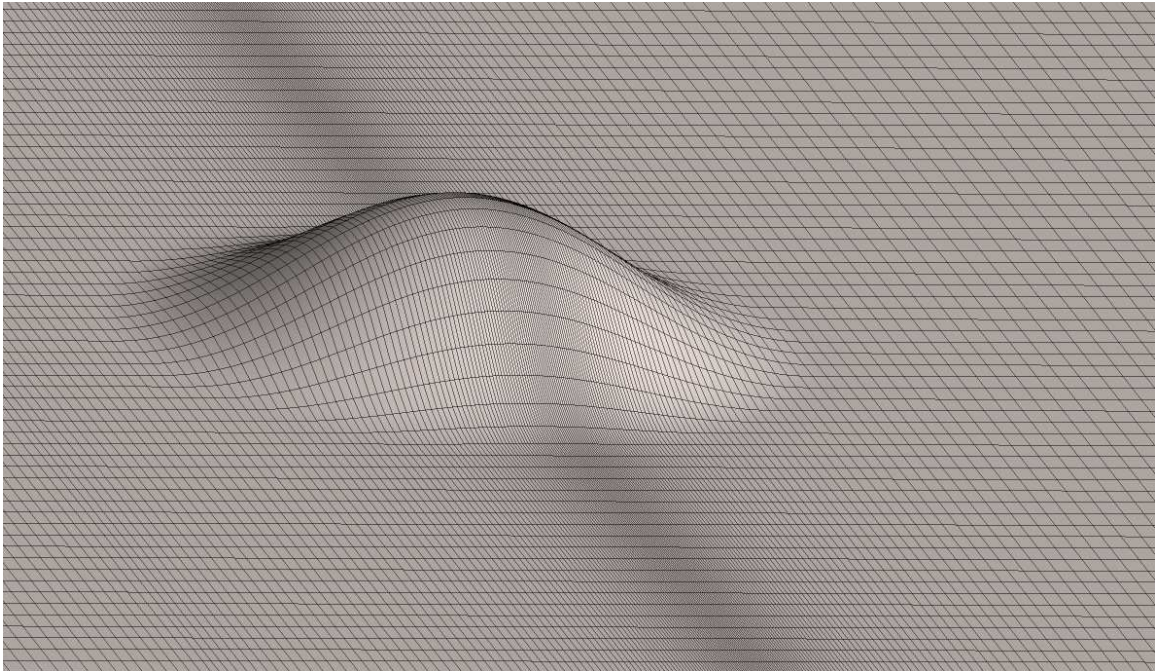


Figure 5.7: Enlargement of mesh region enclosed in red rectangle showing grid refinement near hill on ground surface Ishihara et al. (1999).

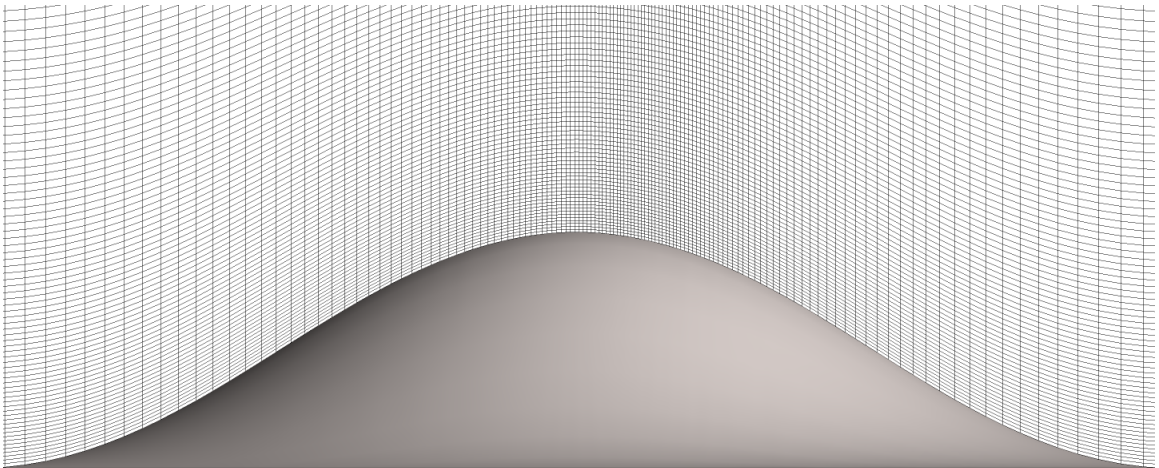


Figure 5.8: Cross-section of mesh showing vertical cell distribution above and around cosine squared hill.

Plot (a) of Figure 5.9 indicates that the numerical model can approximate the  $u$  component of the velocity field derived from the experiment. The respective locations of separation and reattachment points predicted by the model coincide with the wind tunnel observations. Additionally, the reverse flow velocity computed by the numerical model at  $1.25h$  downwind of the hill crest, is the same order of magnitude as that measured in the wind tunnel. The normal Reynolds stress components have been directly measured in the wind tunnel using a split wire probe, however, the  $k - \varepsilon$  model does not directly compute the normal stress components. Instead, these are derived from the turbulent kinetic energy, through application of the model assumption of turbulent isotropy, where  $\sigma_u = \sigma_v = \sigma_w$ . Therefore  $\sigma_u$  can be derived from the relation,

$$\sigma_u = \sqrt{\frac{2}{3}k}. \quad (5.12)$$

Comparison of the model and wind tunnel values of  $\sigma_u$  in Plot (b) of Figure 5.9 reveals good agreement between the simulated and measured values in the upwind half of the hill. Beyond the hill crest, the modified  $k - \varepsilon$  model appears to under-predict the vertical extent of the turbulent flow-field perturbations. Moreover, the peak  $\sigma_u$  predicted by the numerical model at  $1.25h$  is roughly two-thirds of the wind tunnel measurement. As the undisturbed profiles are recovered downwind of the obstacle, the discrepancies between the simulated and measured values become less pronounced. These discrepancies are likely to be due to the  $k - \varepsilon$  model assumption of turbulence isotropy - which is not corroborated by the experimental results. Measured peak values of  $\sigma_u/u_h$ ,  $\sigma_v/u_h$  and  $\sigma_w/u_h$  are 0.32, 0.18 and 0.22 respectively. Indeed, peak  $\sigma_u/u_h$  in the wake region may be more accurately approximated using,

$$\sigma_u = \sqrt{\frac{2k}{2.25}} \quad (5.13)$$

Furthermore, the friction Reynolds Number,

$$\text{Re}_* = \frac{u_* z_0}{\nu}, \quad (5.14)$$

of the scale model is 0.14, which is less than the critical value of 2.5 recommended by Neff and Meroney (1996) to ensure fully rough flow in the wind tunnel and Ishihara et al. (1999) have declared that Reynolds number independence has not been achieved in the near surface region of the experimental model.

The comparisons of the flow profiles show that whilst the modified  $k - \varepsilon$  model does not capture the full extent of the recirculation zone downwind of the hill, the model is capable of reproducing the general behaviour of the flow observed in the wind tunnel. The numerical model predictions are of the same order of magnitude as the experimental results and the simulated peak  $\sigma_u/u_h = 0.22$  is within a factor of 1.5 of the experimental measurements.

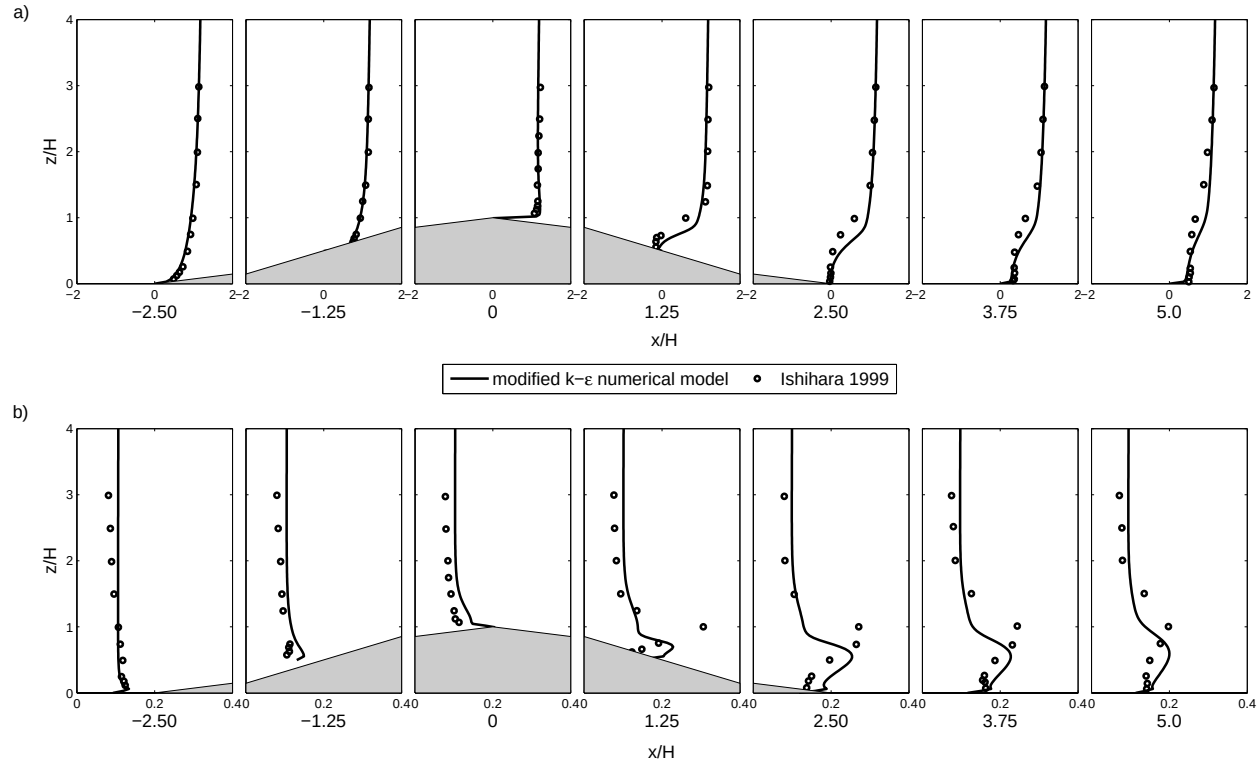


Figure 5.9: Comparison of a) normalized  $u$  component of velocity and b) normalized  $\sigma_u$  profiles over cosine squared hill computed by the modified  $k-\varepsilon$  to those obtained in wind tunnel experiments by Ishihara et al. (1999).

### 5.2.3 The Computational Domain for Flow over Cosine Depressions

The computational domain, shown in Figure 5.10, retains the boundary conditions imposed in the flat terrain domain employed in Chapter 4, where velocity inlets have been applied at the inlet, top and side boundaries and a pressure outlet has been imposed at the exit. The buoyancy modified turbulence profile equations proposed by Alinot and Masson (2005) have also been applied. With respect to particulates injected into the computational domain, trapped boundary conditions are enforced at the wall and escape conditions are specified at all other boundaries. Consequently, accretion of the particles at the wall can be computed and compared to UK-ADMS dry deposition predictions as has been done in Chapter 4.

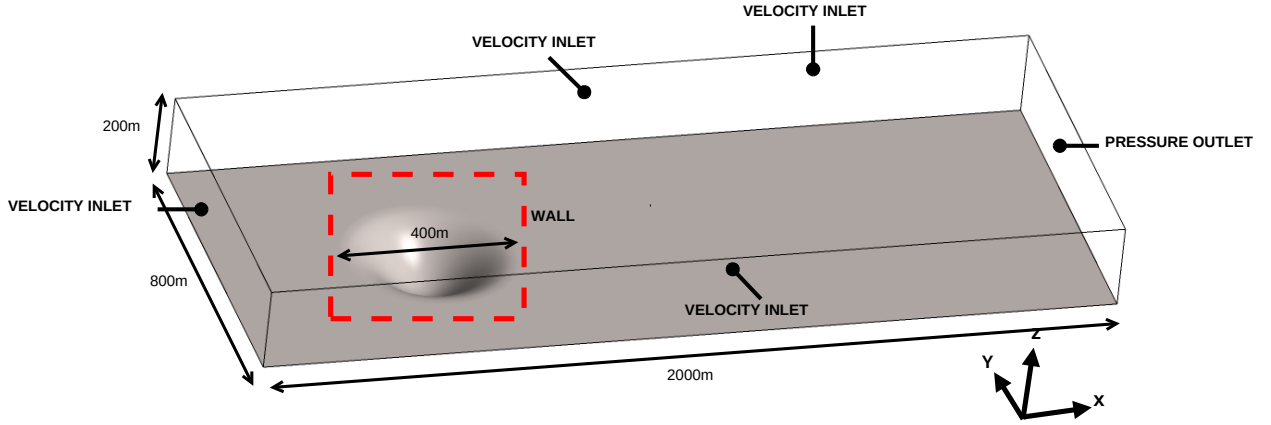


Figure 5.10: The computational domain, showing dimensions of the fetch and depression and imposed boundary conditions.

The atmospheric flow-field has been resolved for a series of circular depressions with cosine cross-section, where the terrain elevation  $z_r$ , is given by,

$$z_{r_d} = -\frac{D}{2} \left( \cos \frac{2\pi r}{L} + 1 \right), \quad (5.15)$$

where  $r_d$  is the radial distance from the centre of the depression  $(x_o, y_o)$ ,

$$r_d = \sqrt{(x - x_o)^2 + (y - y_o)^2}, \quad (5.16)$$

with  $x_o$  and  $y_o$  of 500 m and 0 m in this case. From Figure 5.10, the width of the depression can be seen to be 400 m and four models with depths of the depression of 25, 50, 75 and 100 m were built. These correspond to aspect ratios of 8, 4, 2.67 and 2 respectively. The leading edge is at a distance of 300 m downwind of the inlet, to allow sufficient distance for the dissipation of any upstream effects due to the presence of the depression. Table 5.1 shows the meteorological parameters used to define the three stability classes considered. Here  $u_{10}$  is the mean wind speed at a reference height  $h_{ref}$  of 10 m above flat terrain

Table 5.1: Meteorological Parameters

| Stability | PGT class | $u_{10}$ (ms <sup>-1</sup> ) | $L_{MO}$ (m) | $Q_w$ (Wm <sup>-2</sup> ) | $T_w$ (K) |
|-----------|-----------|------------------------------|--------------|---------------------------|-----------|
| Unstable  | A         | 5                            | -100         | 28.41                     | 298       |
| Neutral   | D         | 8                            | $>  10^5 $   | 0                         | 285       |
| Stable    | F         | 3                            | 100          | -4.17                     | 283       |

and  $z_0=0.01$  m. The DPM model has been applied for tracking of a continuous stream of tracer particles throughout the 125 m<sup>3</sup> cuboid volume source which has been described in Chapter 4. The centroid of the particulate source is located at 10 m above the geometric centre of the depression. This source elevation was selected to ensure that the particles are not injected too close to the wall, which would mean a large percentage would be immediately trapped. The particles have zero initial velocity and are passively transported by the flow field, thus individual particle trajectories are determined by balancing the gravitational and aerodynamic drag forces acting on each particle. The DPM model settings established in Chapter 4 have been used in this study, as well as the continuous total particulate emission rate of 0.586 kgs<sup>-1</sup>.

#### 5.2.4 Mesh Independence Study

The meshes for each of the depressions were constructed in GAMBIT, this consisted of paving the ground surface with an unstructured mesh of quadrilaterals using a size function to cluster most cells in and around the depression, as illustrated in Figure 5.11. This surface mesh was then swept in the  $z$ -direction to produce hexahedral elements, shown in Figure 5.12. The thickness of the mesh was increased with height using a successive cell growth ratio, thereby enabling resolution of the near-ground region where gradients of the flow variables are steepest.

Table 5.2: Mesh refinement parameters for fine, medium and coarse meshes.

| Parameter                  | Fine mesh | Medium mesh | Coarse mesh |
|----------------------------|-----------|-------------|-------------|
| Number of cells            | 2933002   | 1445950     | 868100      |
| Edge growth rate           | 1.01      | 1.02        | 1.02        |
| Edge count                 | 122       | 110         | 100         |
| Size function min size (m) | 3         | 4           | 5           |
| Size function growth ratio | 1.1       | 1.1         | 1.1         |
| Size function max size (m) | 10        | 15          | 20          |

Mesh sensitivity tests were performed for a representative case, the unstable case with  $\alpha = 4$  depression. The unstable case was selected because the effects of the buoyancy modifications are particularly dominant for this case. Fine, medium and course grids were constructed

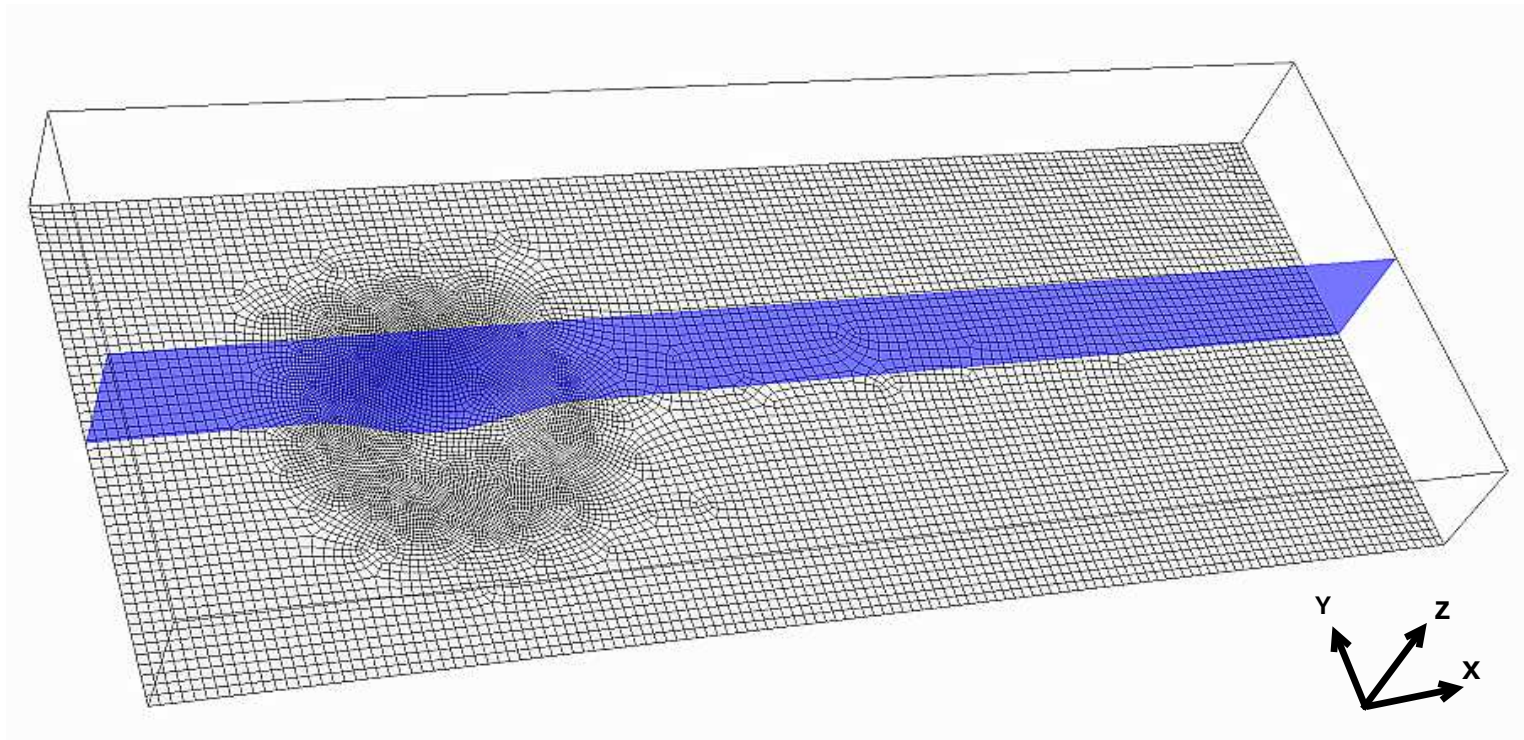


Figure 5.11: The unstructured face mesh on the ground surface showing the effects of the size function around the depression.

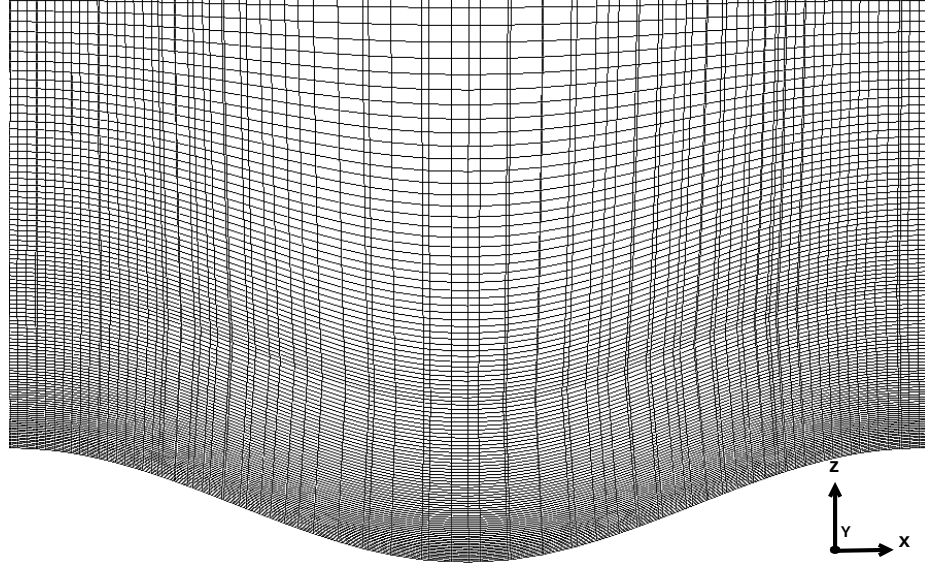


Figure 5.12: The mesh on a vertical slice through the centre of the depression, showing clearly the growth of cell size with height.

and the flow-field was solved for each of the three grids, the corresponding mesh parameters have been summarized in Table 5.2. In Figure 5.13, turbulent kinetic energy profiles are compared at different vertical rakes along  $y = 0$  for the three grids. The rake locations on the  $x$ -axis are given in terms of the depression width,

$$x' = \frac{2(x - x_o)}{L} \quad (5.17)$$

The mesh independence test results indicated that whilst good agreement of the turbulence profiles was obtained for the approach flow with all three meshes, there is some divergence between the predictions beyond the centreline of the depression. The coarsest mesh predicts the highest turbulence downwind of the depression. This result implies that insufficient refinement of the mesh may be partially responsible for the over-prediction of turbulent kinetic energy by the  $k - \epsilon$  model reported in some studies. Based on these observations, the medium mesh was selected for further computations, as this mesh presents an optimal balance between model run time and independence of the solution for the available computing resources. Using a single compute node and 8 cores on the parallel cluster described in Chapter 3 to run the simulations, the run times for the fine, medium and coarse grids were approximately 8.5, 5.5 and 4 hours respectively. The coarse-grid Richardson error,  $E_{\text{coarse}}$  for turbulent kinetic energy has been approximated for the medium mesh according to recommendations by Roache (1997),

$$E_{\text{coarse}} = \frac{r^p \epsilon}{1 - r^p}, \quad (5.18)$$

with

$$\epsilon = f_2 - f_1, \quad (5.19)$$

where  $f_2$  and  $f_1$  are the numerical solutions for turbulent kinetic energy obtained using the medium and fine density mesh respectively. These numerical solutions were recorded at a series of points along  $y = 0$ , located 25 m from the wall. The  $x$  coordinates of the points are  $x = 500$ ,  $x = 700$ , and  $x = 1000$  respectively. The refinement factor,  $r$ , is taken as the ratio of the number of cells of the fine mesh to the medium mesh.  $p$  is the formal order of accuracy of the solution algorithm which is 2 for a second order solution. The third column of Table 5.3 gives the Richardson error estimate between the medium and fine grid. It appears that grid refinement error has a greater influence on the turbulence predictions at the centre of the depression and on average, the error between the medium and fine mesh is approximate 4% of the turbulent kinetic energy.

Table 5.3: Coarse-grid Richardson error estimates

| $x$ (m) | $\epsilon_k$ | $E_{coarse}$ |
|---------|--------------|--------------|
| 500     | 0.0813       | -0.107       |
| 700     | 0.0312       | -0.041       |
| 1000    | 0.0379       | -0.093       |
| Average | 0.0701       | -0.0803      |

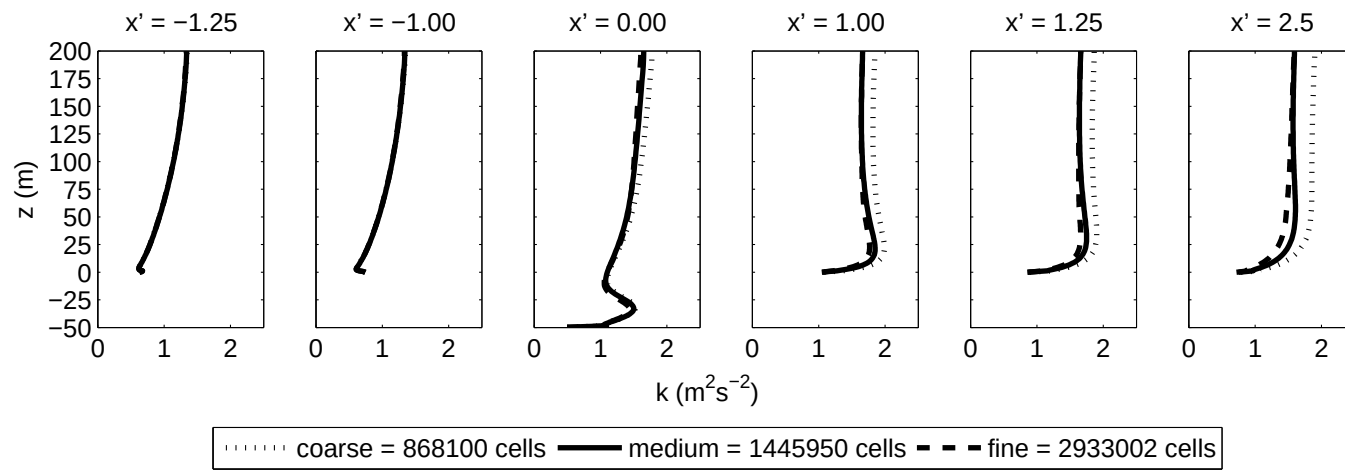


Figure 5.13: Comparison of unstable turbulent kinetic energy profiles over  $\alpha=4$  depression for coarse, medium and fine grids.

### 5.3 Results and Discussion

#### 5.3.1 The Influence of Idealized Terrain on the Flow-field

The vertical profiles plots are taken in the same way as the previous section, and the profiles have been normalised, with,

$$\hat{u} = \frac{u}{u_{10}}, \quad (5.20)$$

and,

$$I = \frac{(2/3k)^{1/2}}{u_{10}} \quad (5.21)$$

UK-ADMS parametrises turbulence in terms of the turbulent velocity fluctuations  $\sigma_u$ ,  $\sigma_v$  and  $\sigma_w$ . Therefore, the turbulence intensity in the UK-ADMS profiles has been computed using the following equation:

$$I = \frac{\sqrt{\frac{1}{3}(\sigma_u^2 + \sigma_v^2 + \sigma_w^2)}}{u_{10}} \quad (5.22)$$

The flow-fields of the four depression depths are characterised by non-dimensional stream-wise velocity and the turbulence intensity, as shown in Figures 5.14a to 5.17b on vertical rakes along the depression centreline,  $y = 0$ . Figures 5.14a and 5.15a indicate that the boundary layer remains attached for  $\alpha = 8$  and  $\alpha = 4$  respectively for all stability classes, although localised flow reversal occurs near the wall in the stable 4 aspect ratio valley which is characterised by weaker winds.

There is an increase in the turbulence intensity as the depression deepens. For  $\alpha = 2.67$ , separation of the boundary layer occurs in all three cases, characterised by flow reversal in the upwind half of the depression (Figure 5.17a). The magnitude of flow reversal is greater for the  $\alpha = 2$  case than for the  $\alpha = 2.67$  case. Moreover, when  $\alpha = 2.67$ , the flow separation begins to occur at  $x = -0.5$ ; conversely, in the  $\alpha = 2$  case, separation of the boundary layer starts further upwind at  $x = -0.75$ . It is observed that turbulence is generally affected in the near ground region corresponding to about one depression height in the 8, 4, 2.67 and 2 aspect ratio cases. However, at the centre of the  $\alpha = 2$  depression, Figure 5.17b, turbulent intensity perturbations extend into the above-ground boundary layer. The presence of an inflection point for the stable case in particular, appears to indicate the formation of a separation region within the depression where terrain effects supersede stability effects, this may indicate decoupling of the flow within the depression region from the boundary layer. For all cases, a spike in turbulent intensity is generated near the ground as a result of shear within the depression. In the unstable case, the turbulence generated near the ground is propagated upwards into the ABL. Thus the approach flow profiles quickly recover downwind of the depression. On the other hand, for the stable case, the spike in turbulence is confined to the near ground region, approximately one depression height from the wall, due to suppression of turbulent transport in the vertical direction.

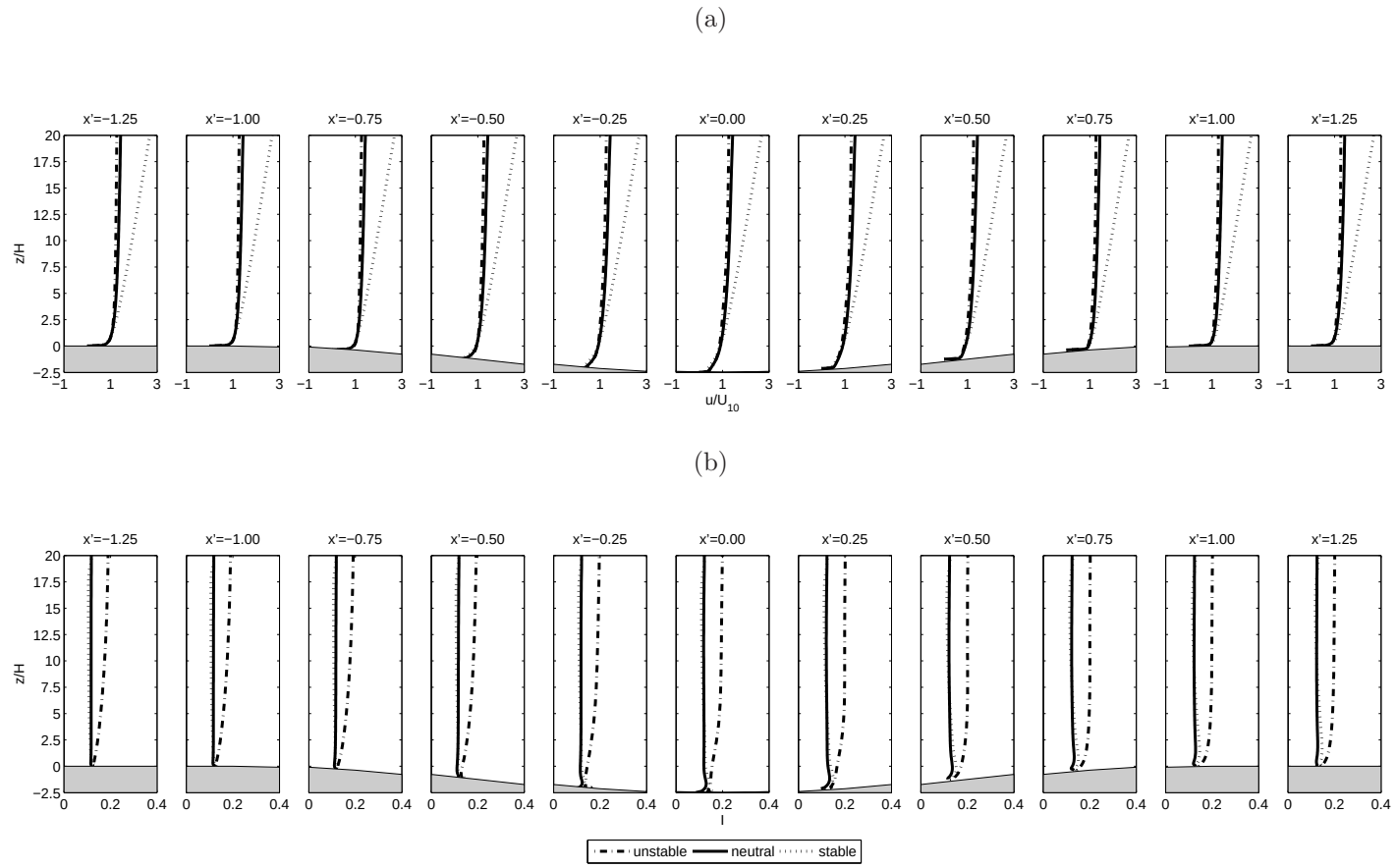


Figure 5.14: Flow profiles across  $\alpha=8$  depression at  $y = 0$  of a)  $\hat{u}$  and b)  $I$ .

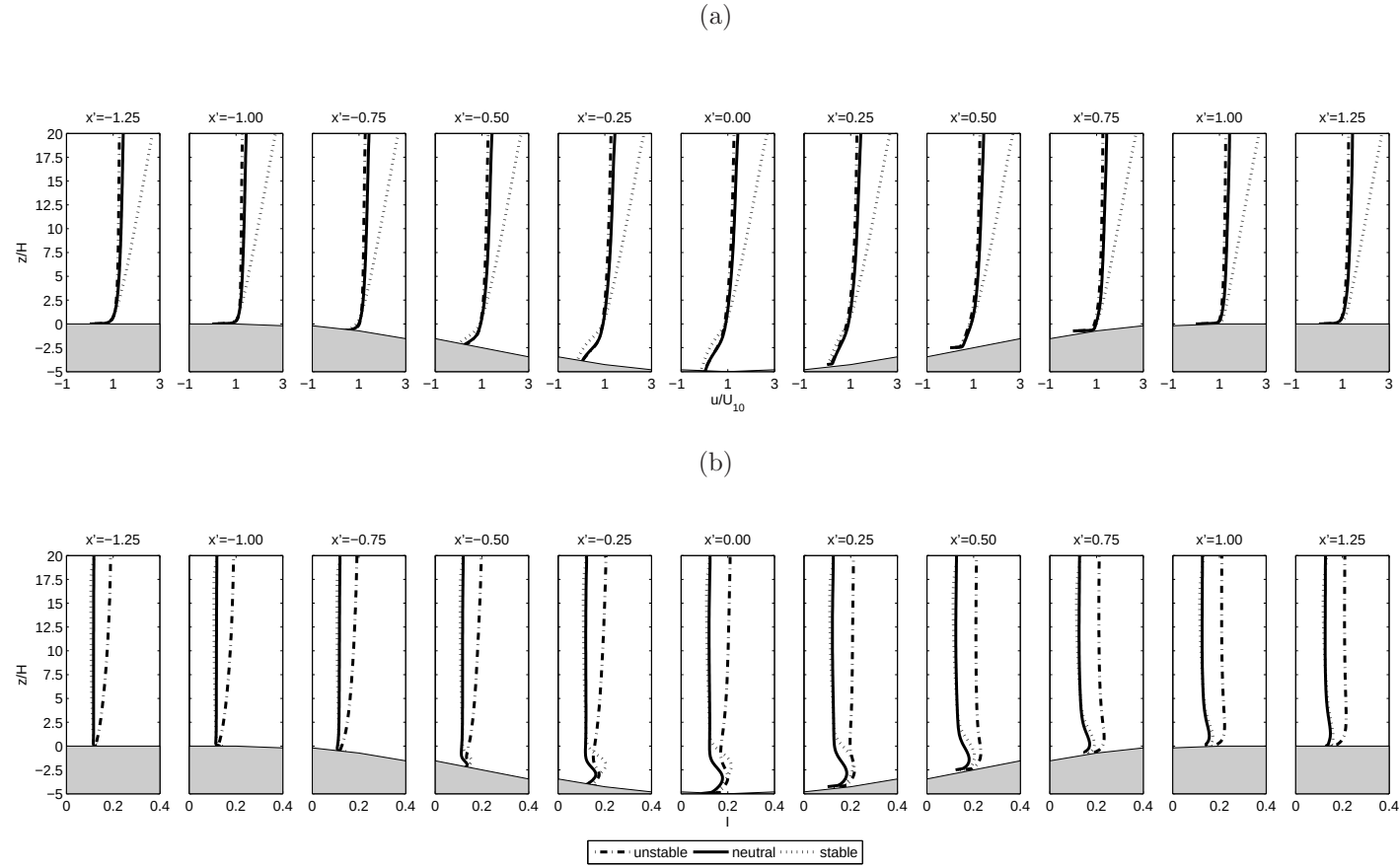


Figure 5.15: Flow profiles across  $\alpha=4$  depression at  $y = 0$  of a)  $\hat{u}$  and b)  $I$ .

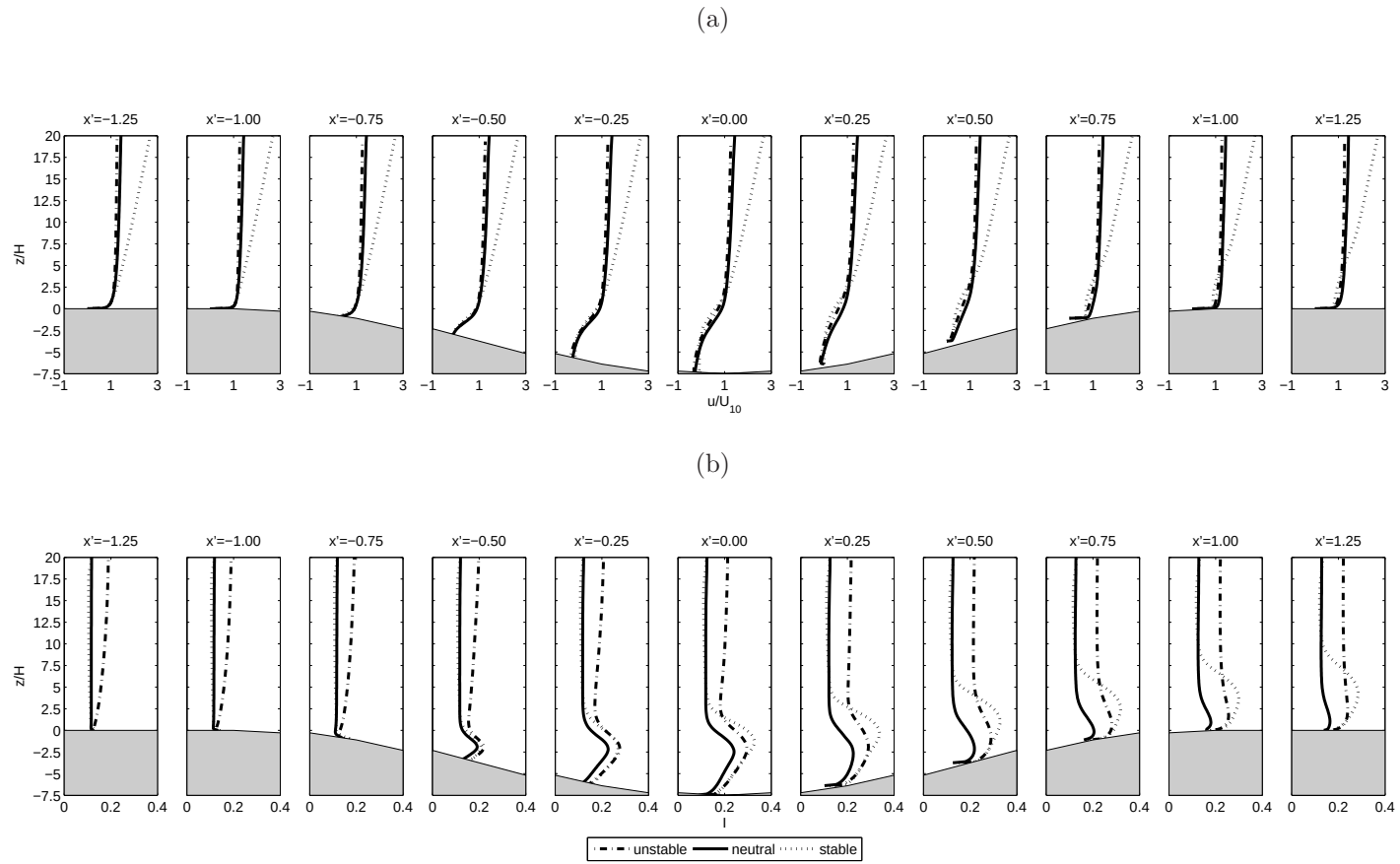


Figure 5.16: Flow profiles across  $\alpha=2.67$  depression at  $y = 0$  of a)  $\hat{u}$  and b)  $I$ .

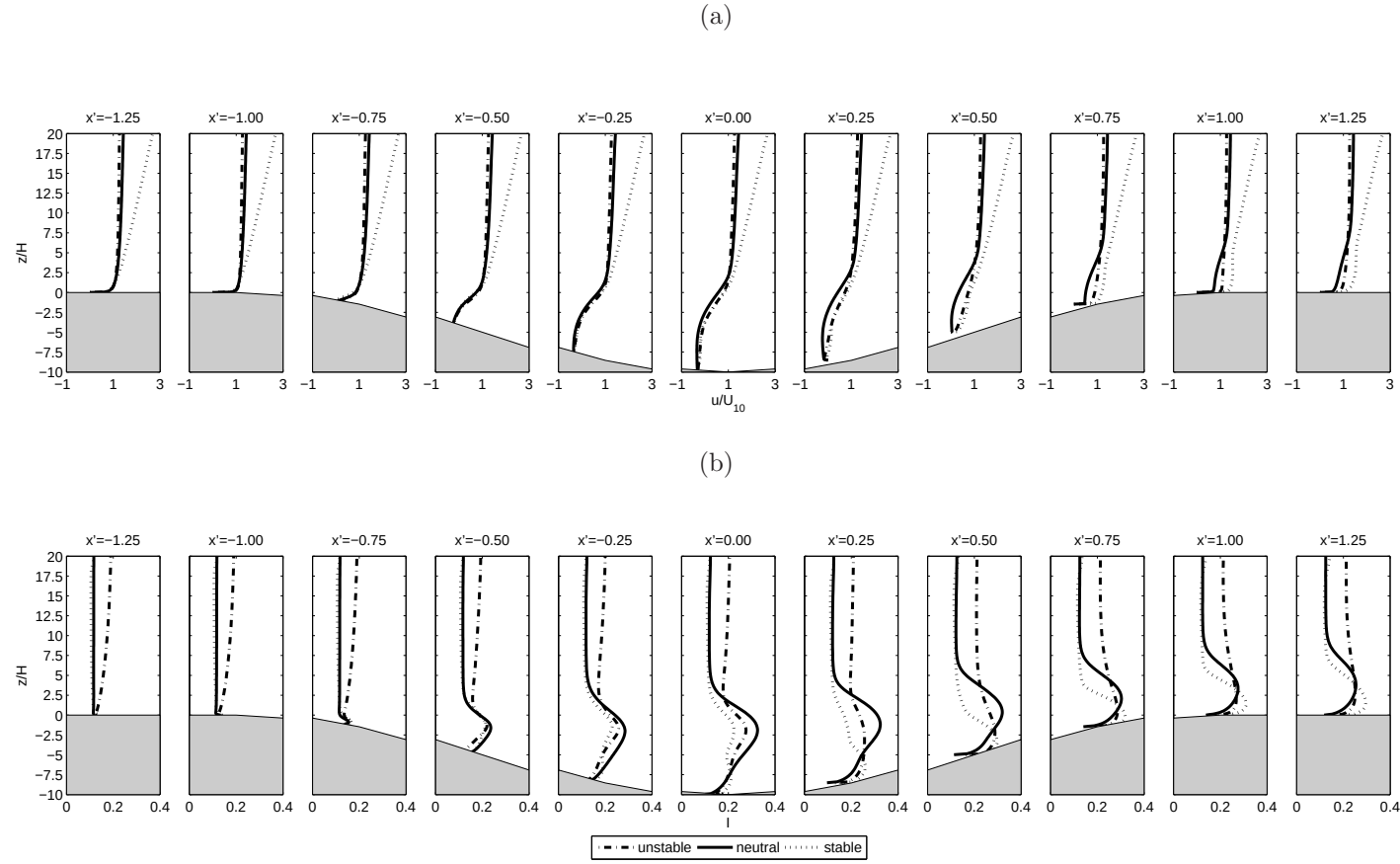


Figure 5.17: Flow profiles across  $\alpha=2$  depression at  $y = 0$  of a)  $\hat{u}$  and b)  $I$ .

Since there is no such constraint on turbulent transport in the horizontal direction, turbulence is transported in the stream-wise direction and the ABL perturbations are carried further downwind of the depression relative to the other stability cases.

In Figures 5.18 to 5.20, the velocity vectors give some insight into the extent of the recirculation bubble. The unstable case produces a better defined recirculation region. Re-attachment of the ABL also occurs further downwind for the unstable case, at  $x = 0.75$ , compared to  $x = 0.5$  for the stable case. Under stable conditions, a recirculation region develops for the aspect ratio 4 case, although this region is not as well established as that of the aspect ratio 2.67 and 2 cases. This result is in keeping with work by Bell and Thompson (1980) which indicated that the development of a recirculation zone is dependent on a critical Froude number and consequently boundary layer separation and accompanying recirculatory flows are more likely for the stability classes with characteristically lower wind speed.

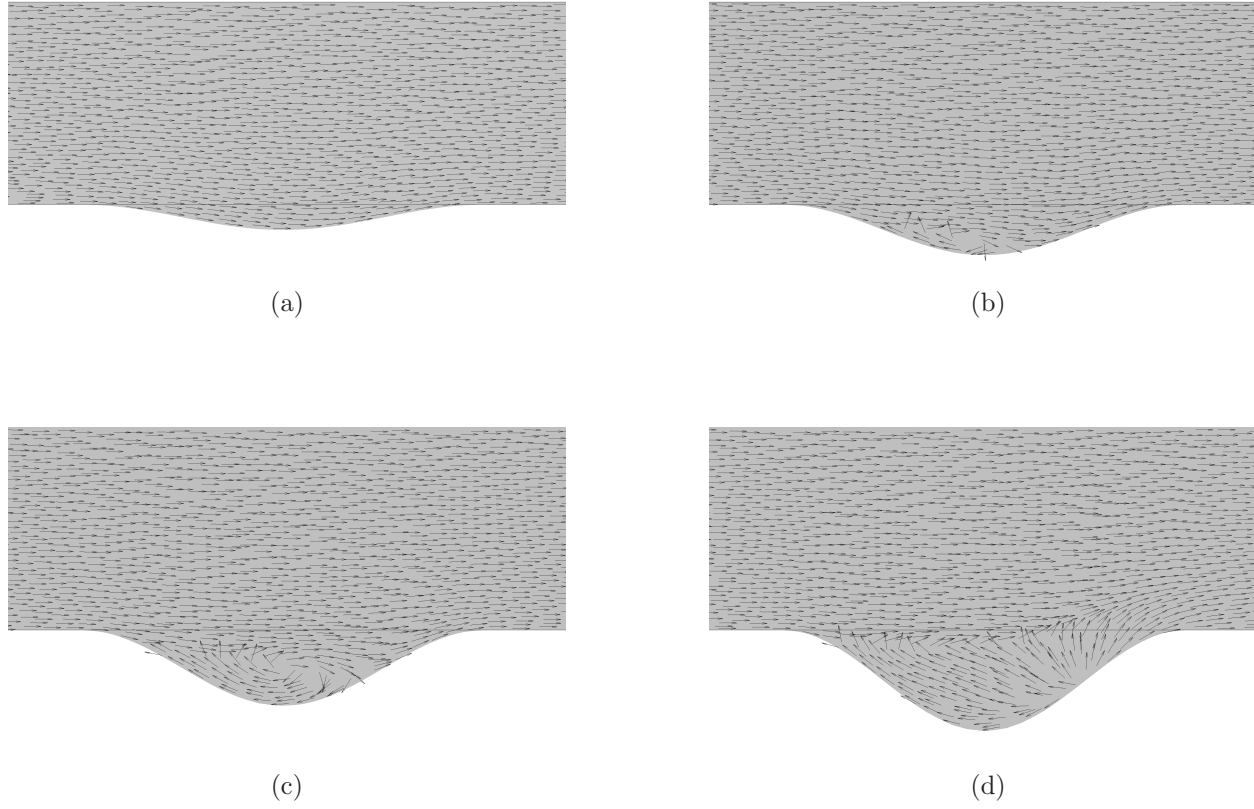


Figure 5.18: Velocity vector plots for the stable ABL on a central plane  $xz$  plane through the depression for aspect ratios (a) 8, (b) 4, (c) 2.67 and (d) 2.

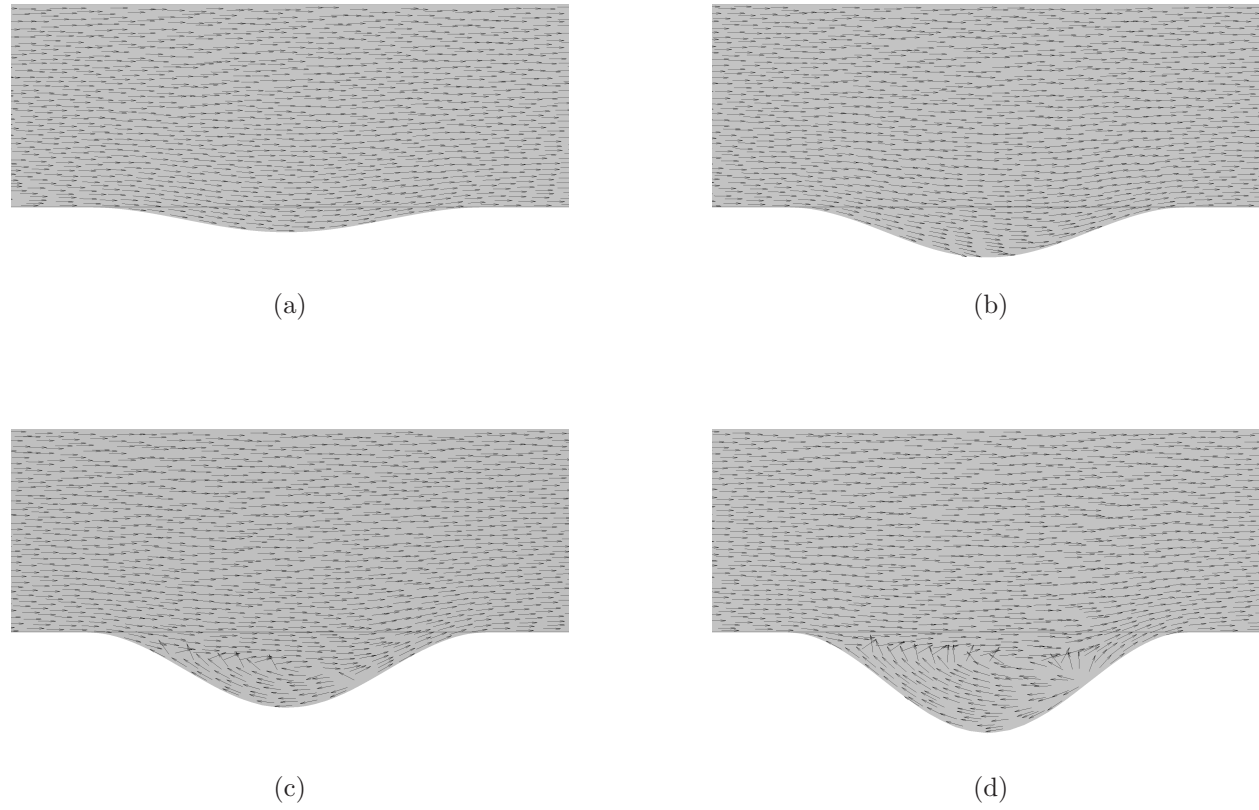


Figure 5.19: Velocity vector plots for the neutral ABL on a central plane  $xz$  plane through the depression for aspect ratios (a) 8, (b) 4, (c) 2.67 and (d) 2.

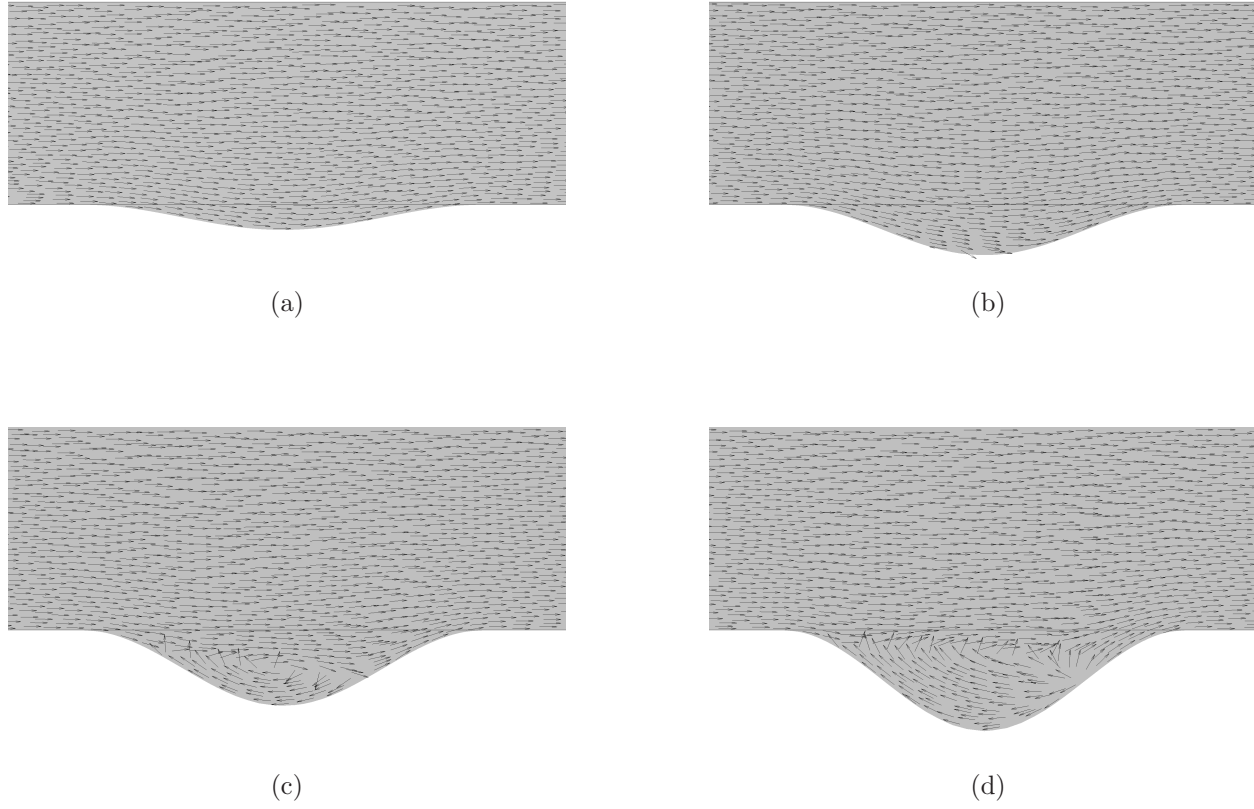


Figure 5.20: Velocity vector plots for the unstable ABL on a central plane  $xz$  plane through the depression for aspect ratios (a) 8, (b) 4, (c) 2.67 and (d) 2.

### 5.3.2 Correlation of the Froude Number to Flow Separation

In the numerical model of flow over an isolated cosine depression, it is seen that the downward displacement of the ABL into the depression produces a discontinuity in the atmospheric profiles. Large spikes in turbulent kinetic energy occur within the valley, particularly in the near wall region, this appears to be accompanied by increases in thermal energy and temperature to satisfy the energy conservation equation. This is most pronounced in the stable case of flow within the 100 m depression. The discontinuity in temperature profile within the valley corresponds to a strengthening of inversion conditions within the depression, as shown in Figure 5.21, this equates to a smaller lapse rate than that of the free atmosphere above the depression. The discontinuity in temperature profile numerically represents a ground-based temperature inversion which is exacerbated by the presence of the depression.

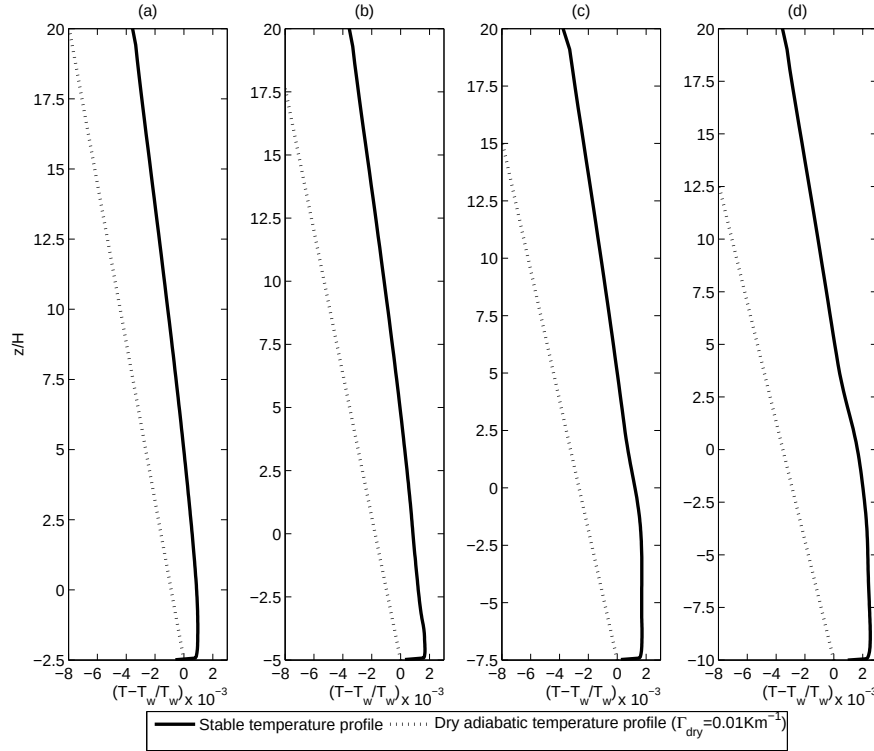


Figure 5.21: Stable temperature profiles at the depression centre  $(x_0, y_0)$  compared to the adiabatic temperature profile for depression aspect ratios of (a) 8, (b) 4, (c) 2.67, (d) 2.

Table 5.4 gives the moduli of the buoyancy frequency and corresponding Froude number at the valley crest for the stable atmosphere over the succession of depressions. The critical values of the Froude number which can be used to characterise a valley flow regime were

Table 5.4: Buoyancy frequency and Froude number values for the stable ABL over the depressions.

| $\alpha$ | $N \text{ (s}^{-1}\text{)}$ | Fr   |
|----------|-----------------------------|------|
| 8        | 0.0186                      | 5.90 |
| 4        | 0.0144                      | 3.81 |
| 2.67     | 0.0186                      | 1.43 |
| 2        | 0.0167                      | 0.75 |

introduced in Chapter 2. According to Grainger and Meroney (1993), the range  $1.3 < \text{Fr} < 1.6$  corresponds to a flow regime in which the air within the valley remains coupled to the free atmosphere above. For  $\text{Fr} < 1.3$ , a separate internal flow regime develops within the valley, whilst at the other end of the range, when  $\text{Fr} > 1.6$ , ventilating flows are likely to arise (Grainger and Meroney, 1993). The Froude number computations to show the progression of the flow from a ventilating regime to a decoupled flow when the Froude number is below the critical value as the depression deepens,

$$\text{Fr} = \bar{u} \left[ \frac{gD(T_D - T_0)}{T_0} \right]^{-1/2}, \quad (5.23)$$

where  $\bar{u}$  is the mean wind velocity at the valley crest, and  $T_D$  and  $T_0$  are the temperatures at the valley edge and wall respectively. The estimated values of the Froude number correlate reasonably well with the development of reverse flow detailed in the turbulence profile graphs and the expected flow behaviour described by Grainger and Meroney (1993).

### 5.3.3 The Influence of the Depressions on Particle Dispersion

In Figure 5.22a to Figure 5.24d, the normalised particle mass concentration field,  $\hat{C}(x, y, z)$ , has been computed according to,

$$\hat{C}(x, y, z) = \frac{C(x, y, z)U_{10} (h_{ref})^2}{Q}, \quad (5.24)$$

and its contours have been plotted on a  $xz$  plane positioned at  $y = 0$  m using a logarithmic scale to permit visualisation of the recirculation zones and also demonstrate the influence of depressions of varying aspect ratio on particle dispersion. In Equation 5.24,  $Q$  is the emission rate,  $C(x, y, z)$  is the concentration and  $h_{ref}$  is the reference height of 10 m. In Figures 5.22a, 5.23a and 5.24a, the particles are dispersed downwind of the source and a receptor located in the downwind region from  $x' = 0$  to  $x' = 0.5$  would experience the highest concentration,  $\hat{C}(x, y, z) = 2$ . This correlates with the flow-field results in Section 5.3.1, where it is seen that no recirculation occurs in the aspect ratio 8 depression for all three stability classes. Figure 5.24a shows that the concentration plume is visibly more dispersed in the vertical direction under unstable atmospheric conditions, whilst neutral conditions appear to elongate the high concentration region in Figure 5.23a as a result of increased advection of particulates from the source due to the characteristically higher wind speed in this stability class.

As the depression aspect ratio decreases to 4, localized recirculation begins to occur particularly in the stable and unstable cases which are characterized by lower wind speeds and Froude numbers. In Figure reffig:50scstar, the particulate plume is dispersed both upwind and downwind of the source, although the plume concentration field is more heavily weighted in the downwind direction. The maximum concentration is experienced symmetrically about the source. This result implies that flow and dispersion in the depression is not entirely dominated by recirculation structures at this aspect ratio and some of the particulates escape the confines of the depression. Figure 5.23b indicates that at an aspect ratio of 4, flow reversal is extremely localized for the neutral case and the plume is predominantly dispersed downwind. Some of the particulate plume is dispersed upwind for the unstable case in Figure 5.24b up to a distance of  $x' = -0.25$  as opposed to  $x' = -0.50$  in the stable case. For all three cases, the plume is brought to the ground nearer to the source in the aspect ratio 4 depression than the aspect ratio 8 depression.

The particulate trajectories are more profoundly affected by flow reversal in the  $\alpha = 2.67$  and  $\alpha = 2$  cases. In Figures 5.22c, 5.23c and 5.24c, the concentration plume appears to be largely confined to the depression cavity, such that the peak concentration at the downwind edge of the valley is approximately three orders of magnitude less than the maximum concentration within the depression. For the depression of aspect ratio 2, recirculation appears to dominate the flow within the cavity, and few of the particulates escape the confines of the depression for all three stability classes. Figure 5.22d shows that dispersion is primarily upwind of the source under stable atmospheric conditions, the maximum  $\hat{C}$  approaches 1.24 near the wall within  $x' = -0.25$  and at the downwind edge of the valley the particulate concentration is very near background levels. In the neutral atmosphere,

Figure 5.23a, the simulation results suggest that the plume is more dispersed within the depression than under stable conditions, however unlike the  $\alpha = 8$  and  $\alpha = 4$  cases, higher concentration is predicted to occur upwind of the source.

The simulation results for an unstable atmosphere combined with the  $\alpha = 2$  depression have been presented in Figure 5.24d. The figure shows that relative to the stable and neutral cases, the plume is well mixed within the entire depression and penetrates further up into the overhead ABL. This implies that as in the  $\alpha = 8$ ,  $\alpha = 4$  and  $\alpha = 2.67$  depression, dispersion of the particulates, especially in the vertical direction is enhanced by unstable atmospheric conditions. In general, the normalized concentration contours of the particulate plume suggest that as recirculation within the depression becomes more prominent and dominates the flow, particulates are more likely to remain trapped within the depression. Furthermore, dispersion of the plume is enhanced by the buoyancy-generated turbulence in the unstable atmosphere.

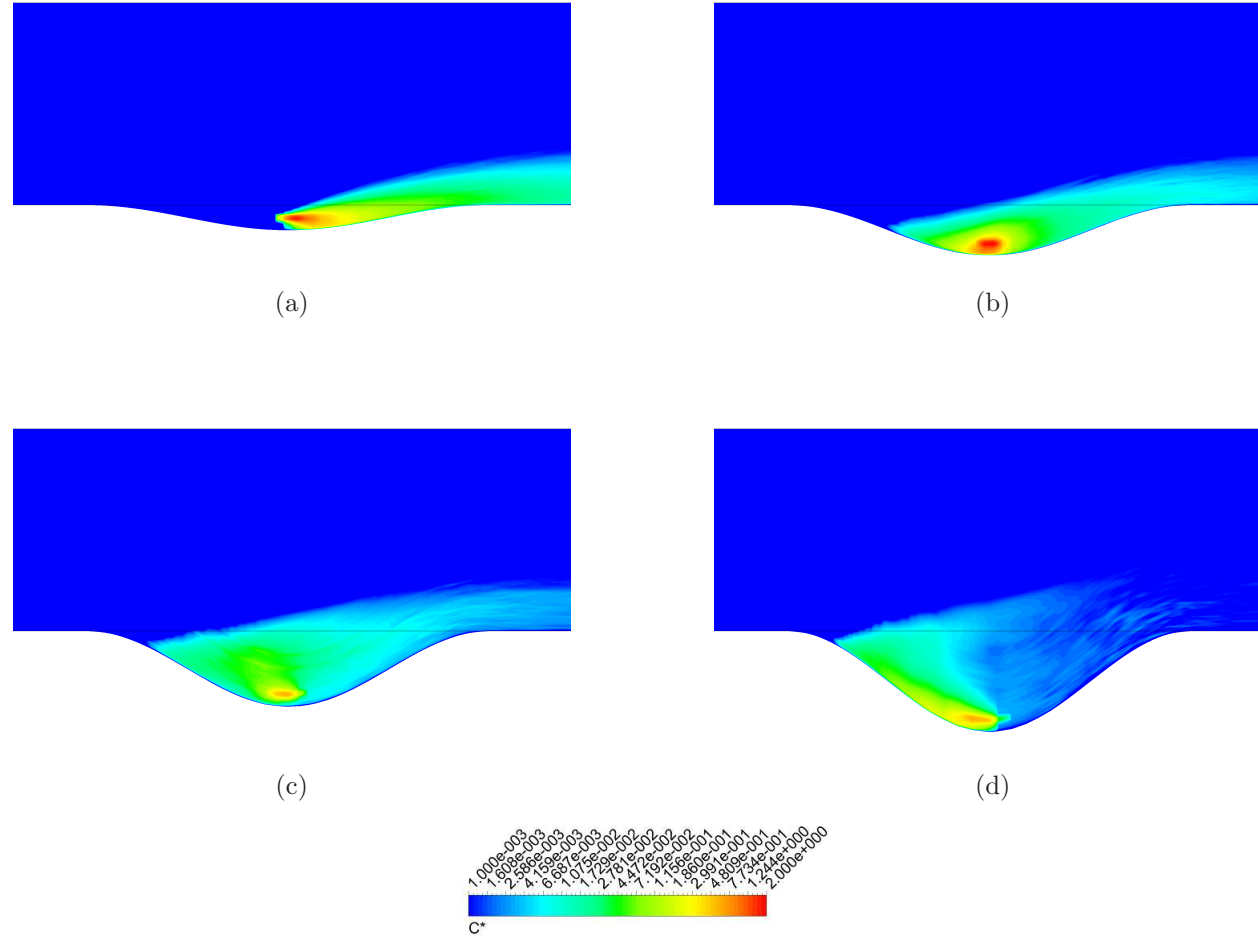


Figure 5.22: Non-dimensionalised concentration contour plots,  $\hat{C}$ , for the stable ABL, for depression of aspect ratio (a) 8, (b) 4, (c) 2.67, (d) 2.

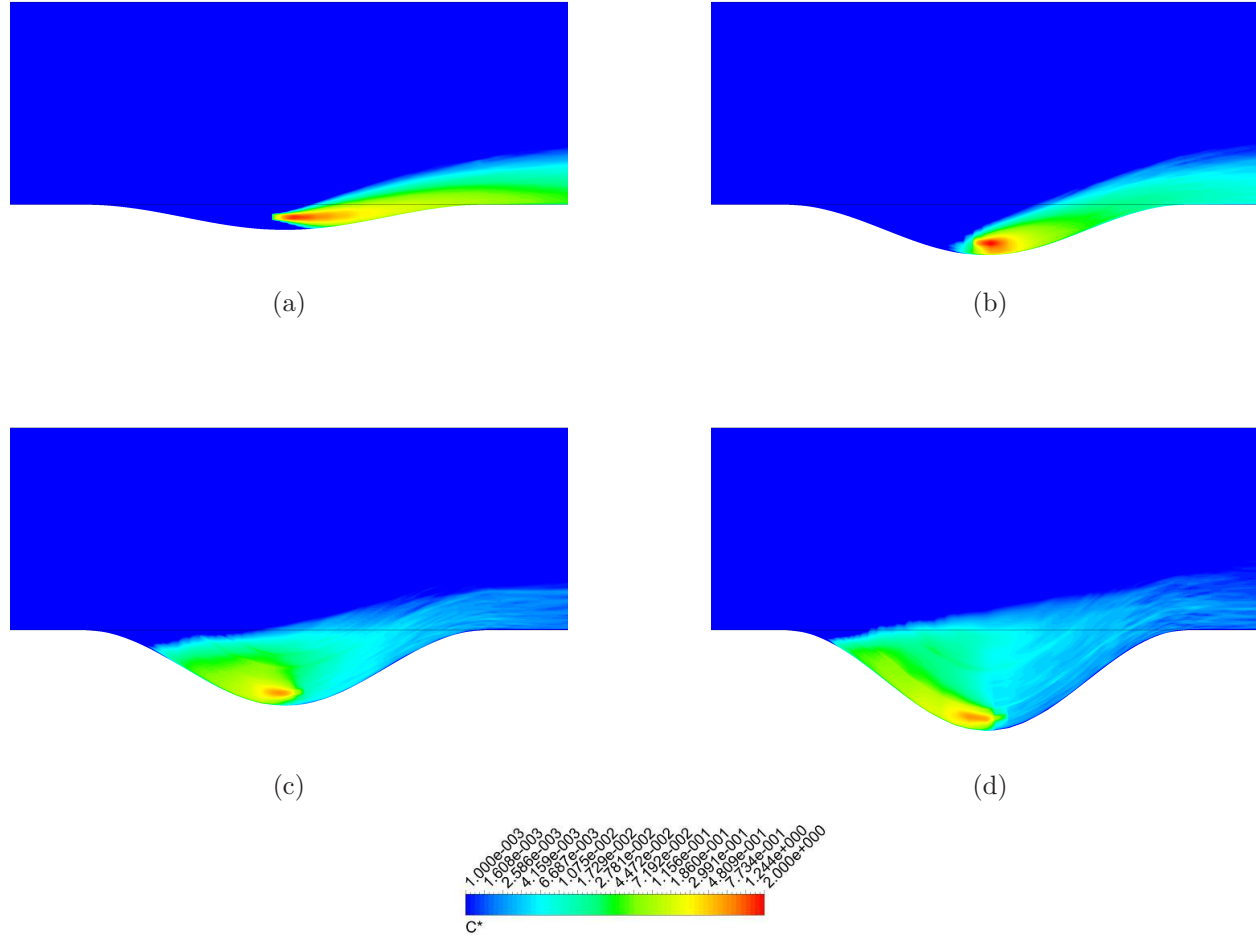


Figure 5.23: Non-dimensionalised concentration contour plots,  $\hat{C}$ , for the neutral ABL, for depression of aspect ratio (a) 8, (b) 4, (c) 2.67, (d) 2.

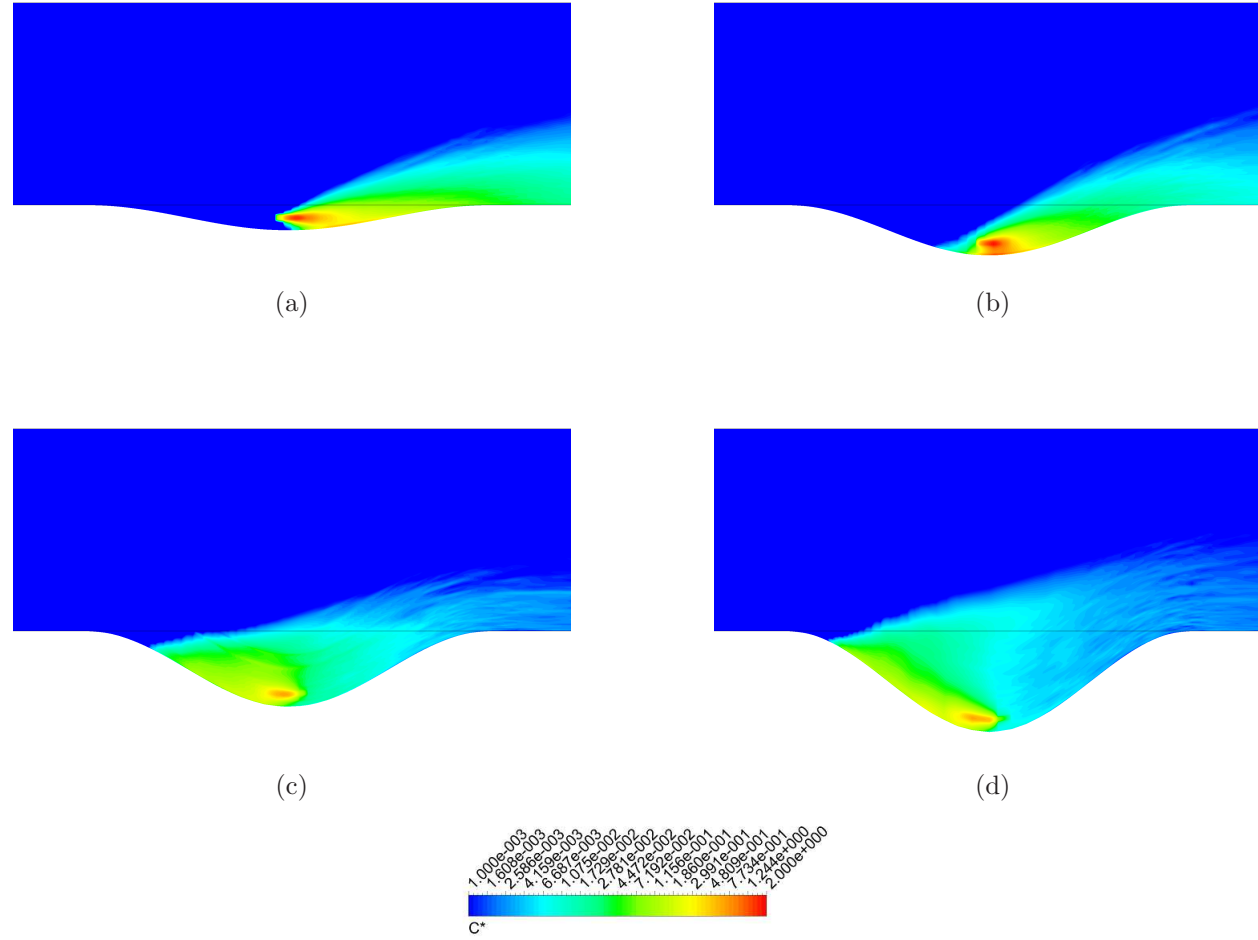


Figure 5.24: Non-dimensionalised concentration contour plots,  $\hat{C}$ , for the unstable ABL, for depression of aspect ratio (a) 8, (b) 4, (c) 2.67, (d) 2.

#### 5.3.4 Comparison of $k - \varepsilon$ and UK-ADMS Turbulence Profiles

For the depression of aspect ratio 8, the non-dimensionalised u-velocity and turbulence intensity profiles from the FLUENT model are in relatively good agreement with the UK-ADMS profiles for the stable and neutral stability classes as shown in Figures 5.25 to 5.26. For the stable and neutral ABL, the results from the two numerical models diverge as the depression depth increases and are substantially different from Figures 5.28 and 5.29 for the  $\alpha = 2$  depression. The small perturbation theory on which the UK-ADMS complex terrain module is based is no longer applicable for terrain with an aspect ratio exceeding 1:3 and so the results of UK-ADMS are not reliable beyond this gradient. It is observed that UK-ADMS fails to register any reverse flow within a height of  $1D$  off the ground for the  $\alpha = 2$  aspect ratio depression, nor does it predict the spike in turbulent intensity which occurs near the ground as a consequence of increasing shear within the depression. It is observed that FLUENT predicts a slightly greater deceleration of the flow over the valley than UK-ADMS. Overall, these observations imply that UK-ADMS is less sensitive than FLUENT to the presence of the valley even when the gradient is within the range covered by the small perturbation theory.

The best agreement of the two sets of profiles is generally observed for the neutral case of the depression with  $\alpha = 8$ , for both the non-dimensionalized velocity and the turbulent intensity profiles, Figure 5.26a) and Figure 5.26b) respectively. This is expressly related to the fact that thermal buoyancy effects are not a component of either model for the neutral case. Thus the implicit differences in the description of buoyancy in each model, which are likely to account for some of observed discrepancies between the unstable FLUENT and UK-ADMS profiles in Figure 5.27, do not factor in the neutral case. The stable profiles of turbulence intensity obtained from the FLUENT and UK-ADMS simulations, Figure 5.25b), also show good agreement for the  $\alpha = 8$  depression. This is likely to be due to the suppression of the buoyant generation term in FLUENT for stable ABL condition where the temperature gradient and  $L_{MO}$  are both positive. These results demonstrate that UK-ADMS produces a crude resolution of the flow-field due to its solution of analytical equations for continuity and momentum whereas the modified  $k - \varepsilon$  model considers the full system of non-linear RANS equations of the flow. Both models apply Monin-Obukhov Similarity scaling of the atmospheric surface layer, although UK-ADMS invokes mixed layer scaling for the computation of the velocity variances in the middle layer under convective conditions.

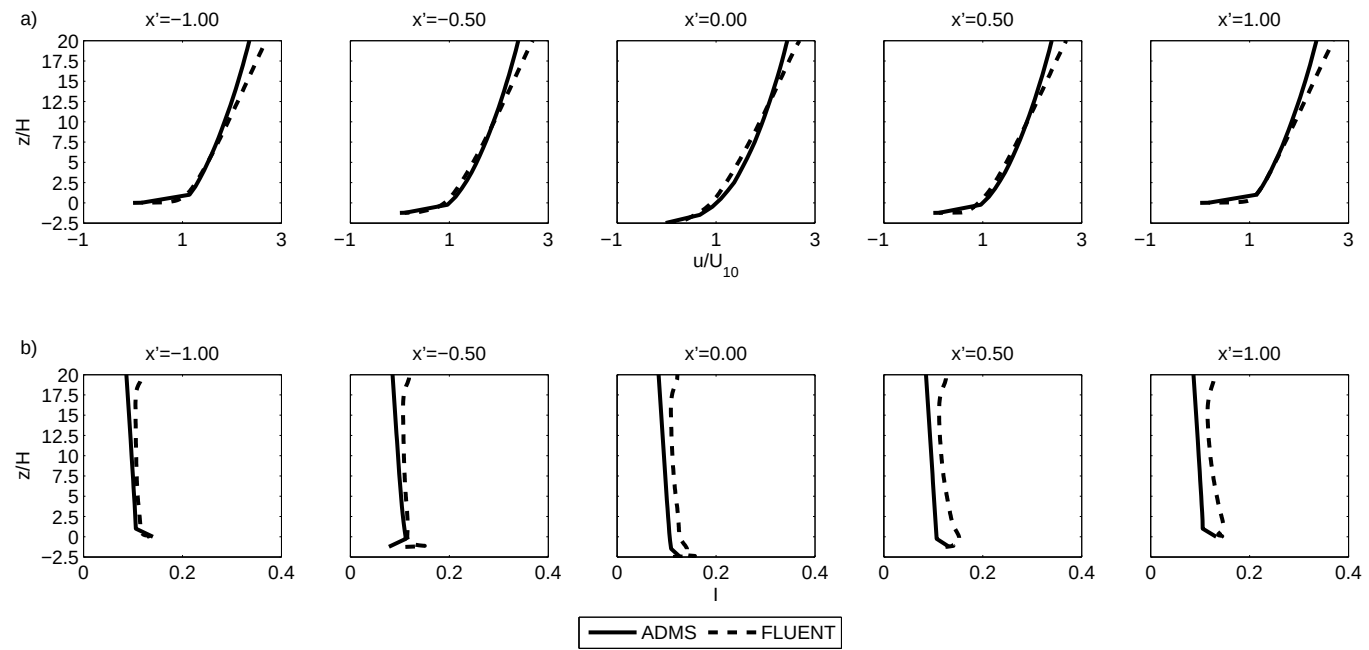


Figure 5.25: Comparison of UK-ADMS and FLUENT a)  $\hat{u}$  and b)  $I$  profiles for the stable ABL over the  $\alpha = 8$  depression.

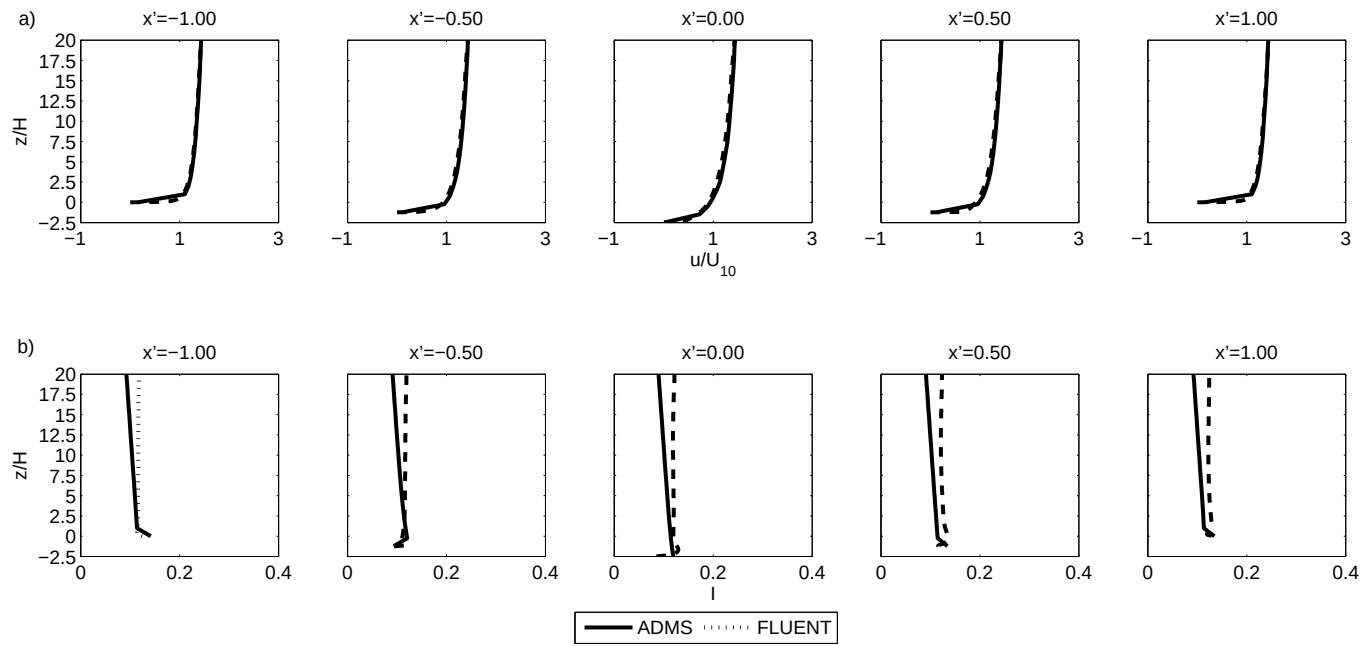


Figure 5.26: Comparison of UK-ADMS and FLUENT a)  $\hat{u}$  and b)  $I$  profiles for the neutral ABL over the  $\alpha = 8$  depression.

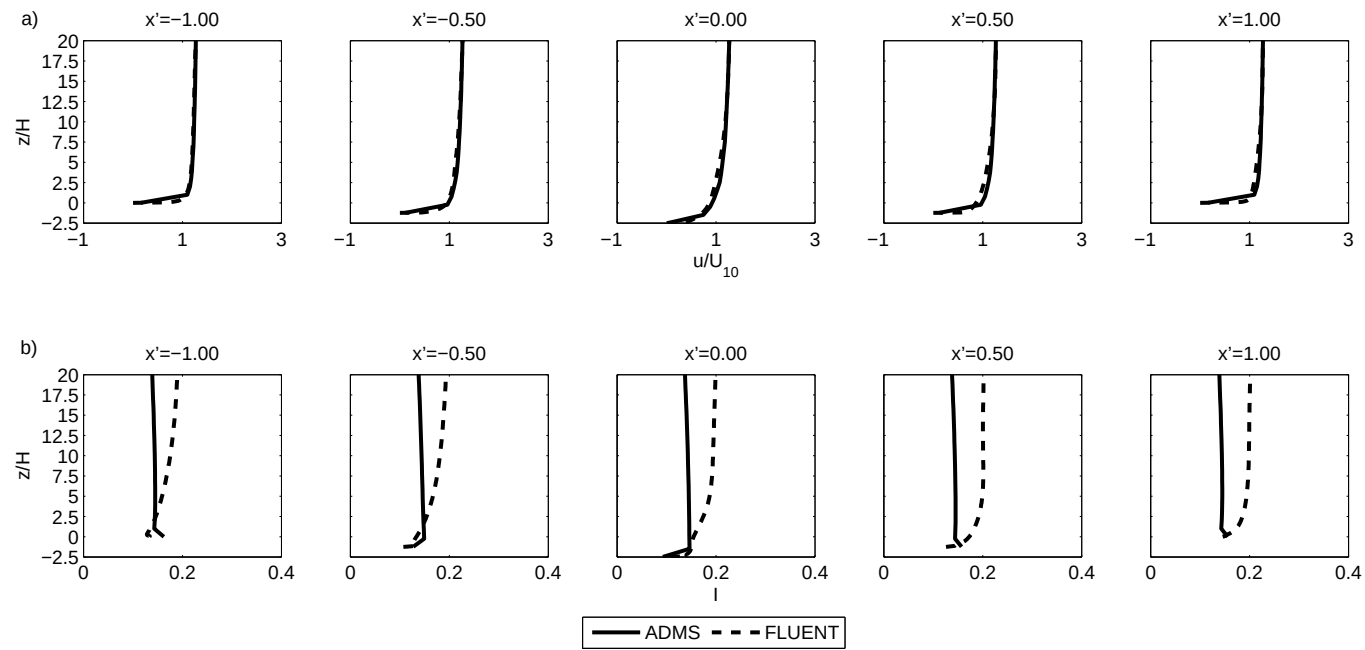


Figure 5.27: Comparison of UK-ADMS and FLUENT a)  $\hat{u}$  and b)  $I$  profiles for the unstable ABL over the  $\alpha = 8$  depression.

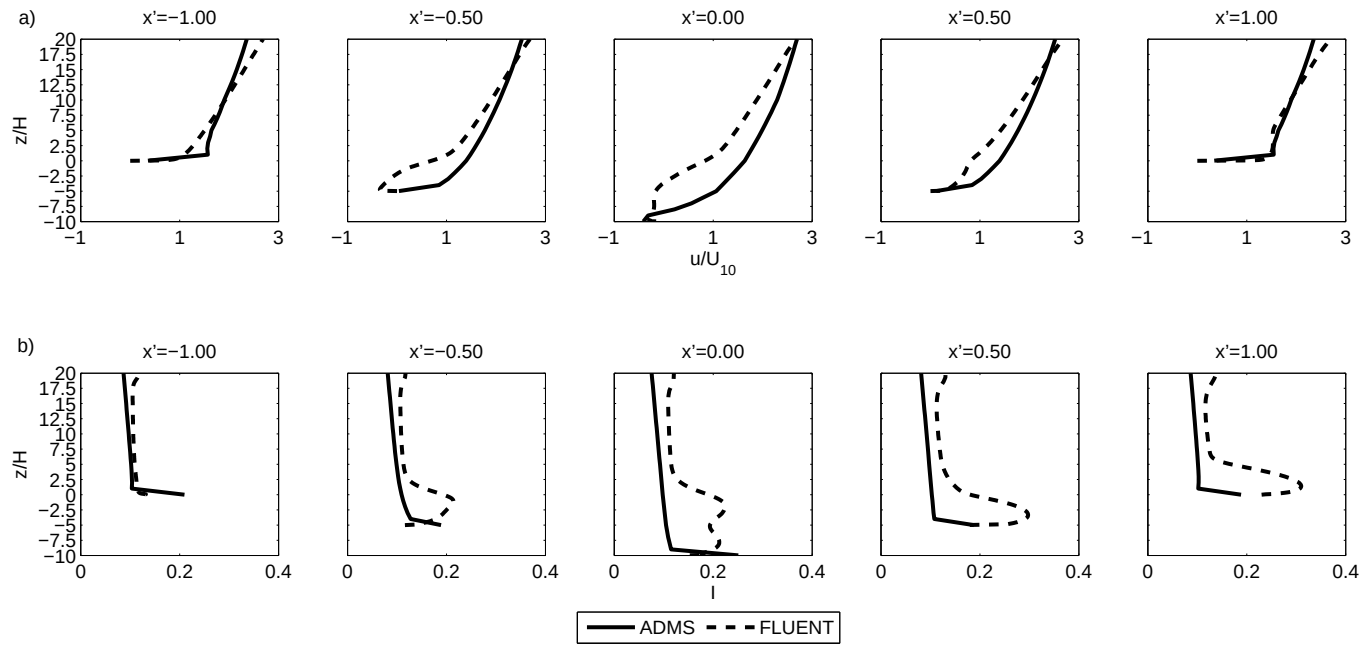


Figure 5.28: Comparison of UK-ADMS and FLUENT a)  $\hat{u}$  and b)  $I$  profiles for the stable ABL over the  $\alpha = 2$  depression.

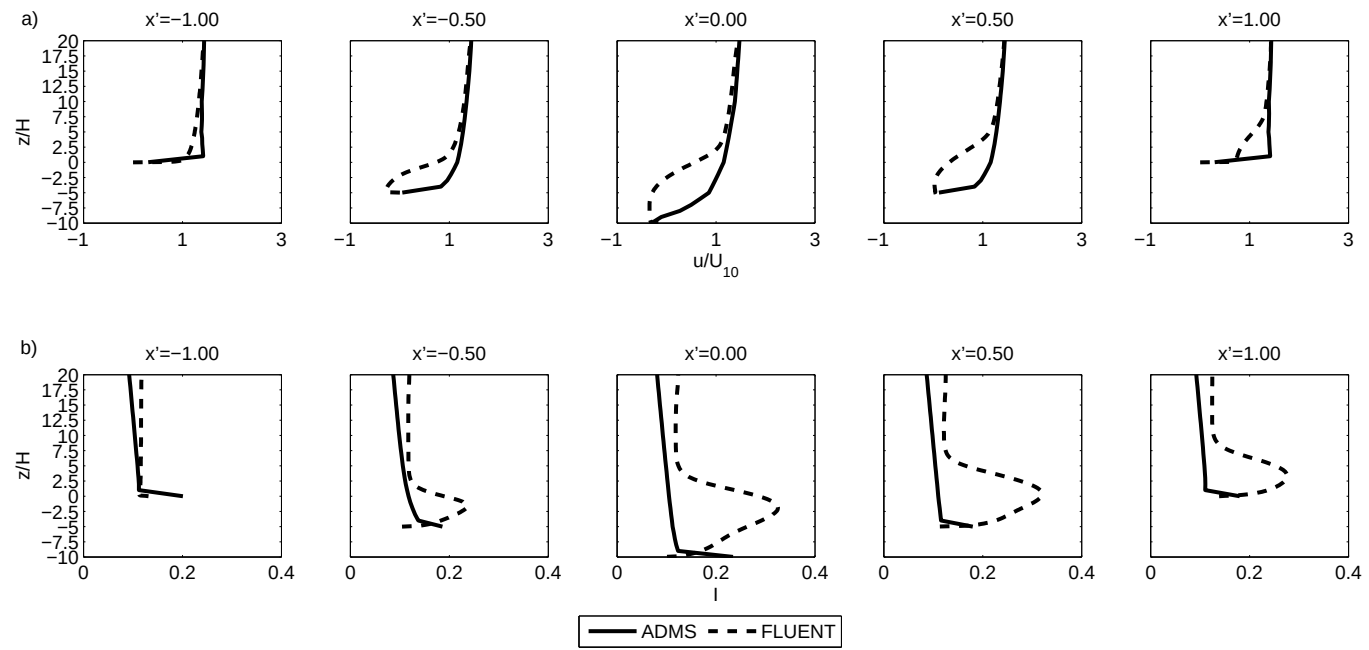


Figure 5.29: Comparison of UK-ADMS and FLUENT a)  $\hat{u}$  and b)  $I$  profiles for the neutral ABL over the  $\alpha = 2$  depression.

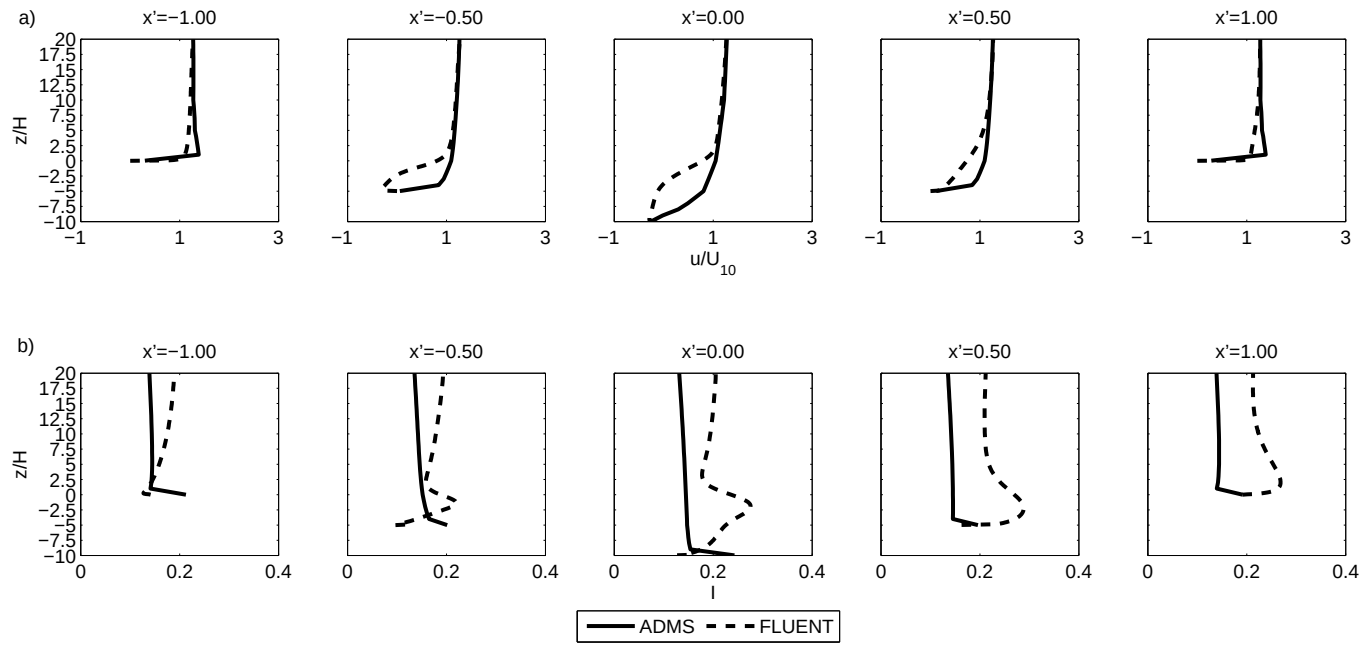


Figure 5.30: Comparison of UK-ADMS and FLUENT a)  $\hat{u}$  and b)  $I$  profiles for the unstable ABL over the  $\alpha = 2$  depression.

### 5.3.5 Comparison of $k - \varepsilon$ and UK-ADMS Dry Deposition Predictions

Chapter 4, discussed the quantification of the particulate mass flux at the wall in UK-ADMS and FLUENT as dry deposition flux and accretion rate respectively. Therefore in this section a comparative analysis of particle mass flux at the ground surface is conducted to assess how flow-field resolution in each model influences its predictions of particulate deposition at the ground surface.

For the  $\alpha = 8$  cases shown in Figure 5.31a, 5.31b and 5.31c, deposition of the particulates occurs downwind of the source due to the absence of recirculation flow. Peak deposition has been predicted to occur within  $L/4$  of the source. The FLUENT deposition plumes are more elongated than their UK-ADMS counterparts, and the underlying cause of this difference in plume shape was discussed extensively in Chapter 4, where it was established that wind direction variability is not an intrinsic component of the FLUENT  $k - \varepsilon$  model, consequently the deposition plumes generated by FLUENT will have smaller lateral extents relative to UK-ADMS plumes.

As the depression aspect ratio increases to 2, Figures 5.32a, 5.32b and 5.32a, the lateral extent of the deposition plume in the FLUENT results appears to be dominated by the increased turbulence and flow recirculation. Thus, it might indicate that for a source situated deep within a depression of aspect ratio  $\approx 2$ , the effects of turbulent fluctuations on the dispersion of particles outweigh mesoscale wind direction variability. Only the FLUENT simulations in Figures 5.32a, 5.32b and 5.32c show recirculation flow in the  $\alpha = 2$  depression; hence it is only in the FLUENT simulations that the particulates appear to be transported upwind of the source. Both the turbulence profiles and the dry deposition contours reveal that UK-ADMS fails to demonstrate this significant feature of the  $\alpha = 2$  case.

Under stable ABL conditions, both the UK-ADMS and FLUENT predict the largest values of dry deposition flux and accretion rate respectively in Figure 5.31a. In Figure 5.31b where reversed flow is not predicted by either model, the particulate plume is more elongated than the other two classes; this is likely to be due to the characteristically higher wind speed associated with the neutral ABL. For the deepest depression, with  $\alpha = 2$  in Figures 5.32a, 5.32b and 5.32a, conclusions on the deposition of particles can only be inferred from the FLUENT model predictions as UK-ADMS predictions are known to be unreliable at this value of terrain aspect ratio on account of the inability of the FLOWSTAR module to simulate atmospheric flow-fields perturbed by steep terrain. FLUENT predicts a maximum accretion rate which, on average, is about 4 times higher than UK-ADMS the UK-ADMS deposition flux and also predicts that the particles are generally deposited within the depression. In Figure 5.32c a more dispersed deposition flux profile relative to the other two atmospheric classes is observed for the unstable condition; this is likely to be an indicator of increased turbulent diffusion of the particulates brought about by the buoyancy generated turbulence which is characteristic of this case.

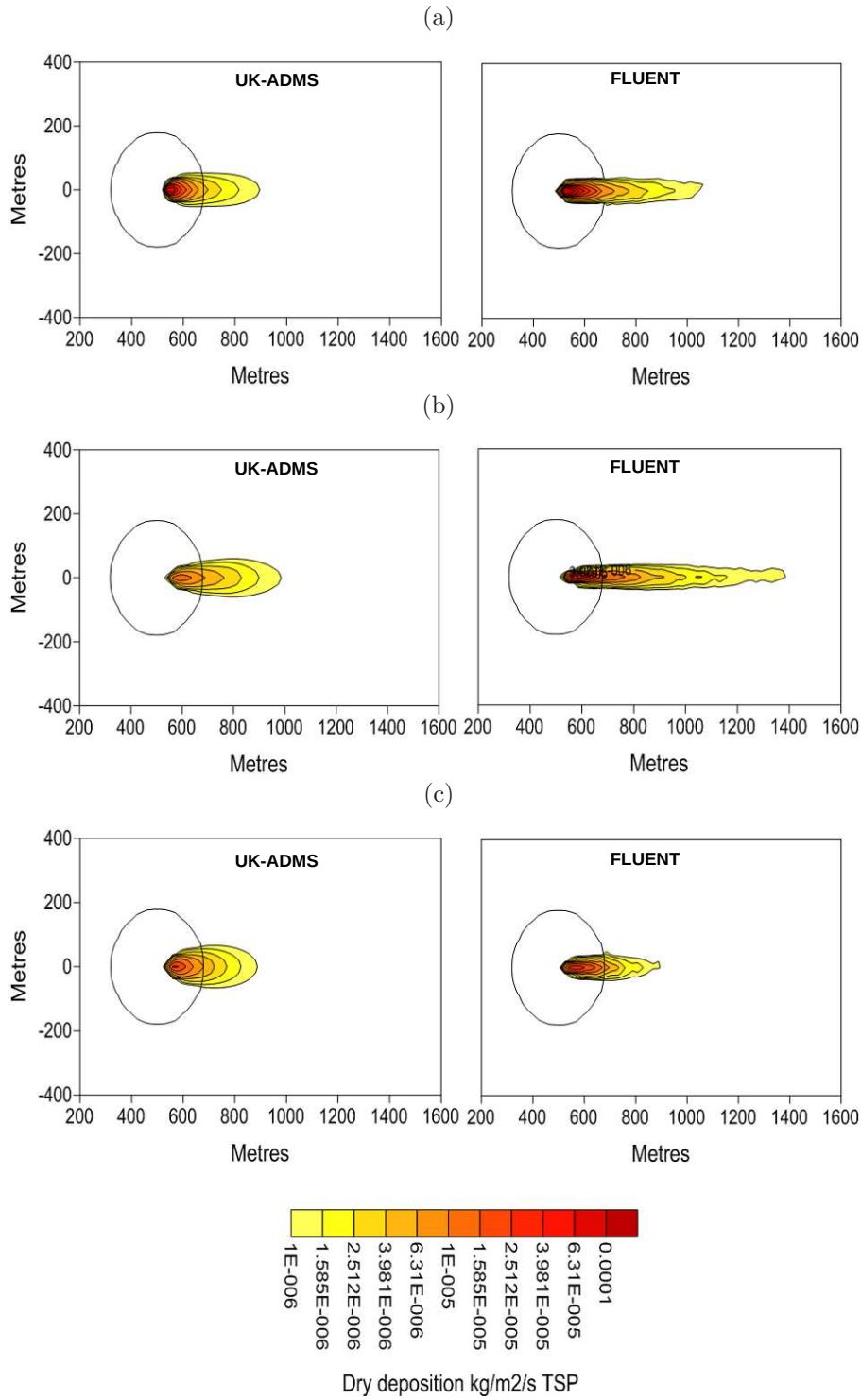


Figure 5.31: Comparison of UK-ADMS and FLUENT dry deposition contour plots for the  $\alpha = 8$  depression for a) stable, b) neutral and c) unstable atmospheric conditions.

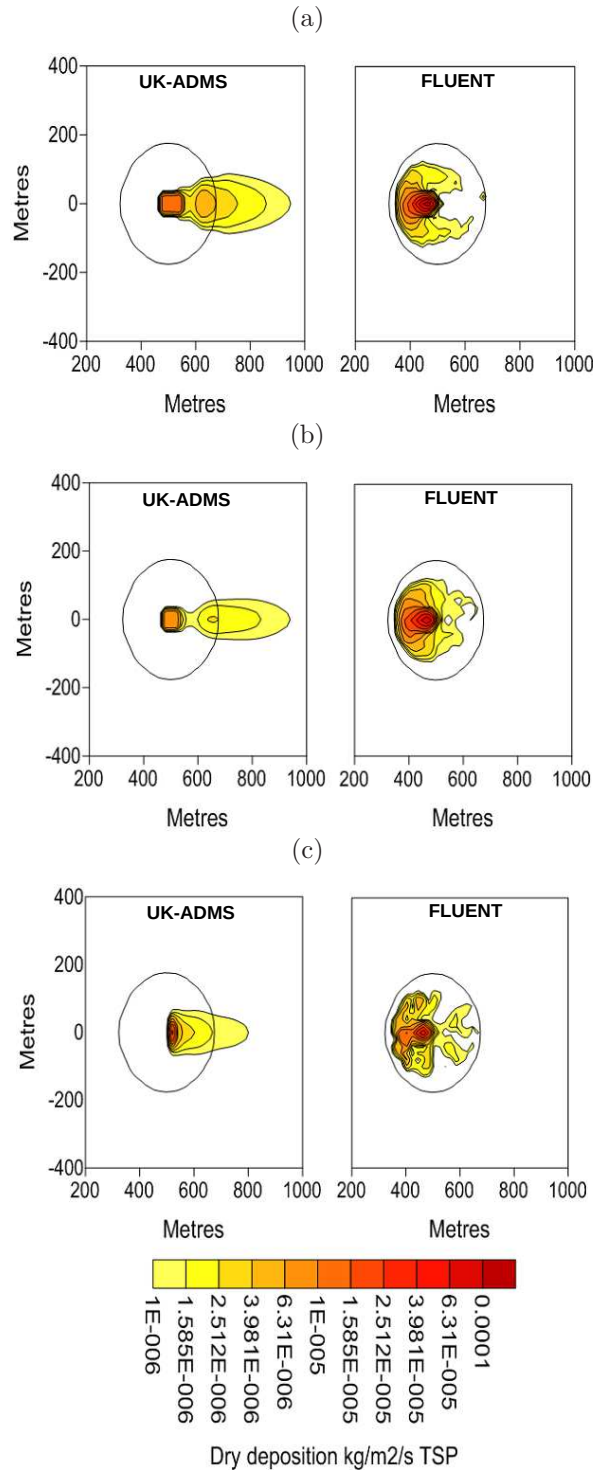


Figure 5.32: Comparison of UK-ADMS and FLUENT dry deposition contour plots for the  $\alpha = 2$  depression for a) stable, b) neutral and c) unstable atmospheric conditions.

## 5.4 Summary

This chapter has presented a study of the combined effects of varying aspect ratio and thermal stability on flow and dispersion within an idealized circular depression of cosine profile. In order to optimize the buoyancy modified  $k - \varepsilon$  model for the simulation of flow over variable terrain, a wall distance scalar,  $\varphi$ , was introduced, with a Dirichlet boundary condition of  $\varphi = 0$  imposed at the wall. This modification has allowed the model to generate profiles of the flow variables which conformed to the shape of the wall and were consistent with the depth of the boundary layer throughout the computational domain. Furthermore, the model predictions of neutral atmospheric flow have been validated using experimental data from a wind tunnel study by Ishihara et al. (1999), which has shown that the  $k - \varepsilon$  model under-predicts the Reynolds stress component in the lee of a cosine-squared hill by a factor of 1.5. This under-prediction was likely to be primarily due to isotropic treatment of turbulence in the model. Despite this limitation, the comparative analysis of FLUENT  $k - \varepsilon$  and UK-ADMS flow-field simulations have demonstrated that the proposed  $k - \varepsilon$  model is able to simulate flows which are outside the remit of the UK-ADMS complex terrain module, FLOWSTAR. In the depression of aspect ratio  $\alpha = 8$ , UK-ADMS flow-field prediction were found to be in good agreement with those of the  $k - \varepsilon$  turbulence model, however as the terrain steepness increased to  $\alpha = 2$ , the flow-field predictions of the two models were seen to differ considerably. In particular, UK-ADMS was unable to replicate the recirculation regime and the spike in turbulence occurring near the ground as a consequence of increased shear production as the flow encounters the depression.

The idealized terrain simulation results demonstrated that development of recirculation zones within a depression was contingent on the strength of the mean wind and the aspect ratio. Perturbation of the incoming flow became more pronounced as the depression depth increased, consequently recirculation zones were predicted nearer the leading edge of the depression with increasing aspect ratio. From the normalized velocity profiles, it was inferred that the characteristically low wind speed of the stable atmospheric regime was more likely to give rise to flow reversal in deep depressions. According to the normalized concentration plots, particles were entrained in the reverse flow region of the  $\alpha = 2$  depression, and transported upwind of the source for all three stability classes; however the neutral case displayed a tendency towards ventilating flows for  $\alpha = 8$  and  $\alpha = 4$  where the particulates are swept out of the depression. This observation was consistent with the higher wind speed and Froude numbers associated with this case.

Thermal buoyancy was seen to influence the recovery of the initial profiles downwind of the depressions; for the unstable regime, the flow profiles were recovered a shorter distance downwind of the depression implying that enhanced vertical mixing was responsible for the distribution of turbulence in the vertical direction. Conversely, the disturbances to the profiles due to the presence of the depression were transported further downwind for the stable case because vertical mixing is suppressed for this stability regime. An examination of the stable temperature profiles at the centre of each depression and the corresponding Froude numbers provided evidence that the strong recirculation regime of the  $\alpha = 2$  valley

correctly correlated to a Froude number of 0.75 which is below the critical value of 1.3 for decoupling of the flow within the depression.

## A Case Study of Old Moor Quarry

### 6.1 Overview of the Case Study

As reviewed in Chapter 2, Silvester et al. (2009) applied the standard  $k-\varepsilon$  model to simulate dust dispersion from a surface quarry under neutral atmospheric conditions. Their study demonstrated that even under idealized, neutrally buoyant conditions, three-dimensional CFD models produced a better approximation of the internal flow regimes which develop within the complex geometry of a surface quarry than the FLOWSTAR flow-field solver embedded in the UK-ADMS dispersion model. The principal aim of the current work is to further investigate the application of CFD models to quarry dust dispersion modelling. In particular, this study focuses on the fugitive dust emissions generated and observed during bench blasting operations under actual site meteorological conditions. The CFD models developed herein are validated against the actual dust deposition measured during field surveys at a case study quarry (Old Moor Quarry, Lafarge-Tarmac), located in the Peak District in the Derbyshire Dales, England. Consequently, the CFD models consider a range of atmospheric stability conditions including the neutral stability case. The stability modifications to the standard  $k-\varepsilon$  model proposed in Chapter 3 and the wall distance scalar function introduced in Chapter 5 have been implemented in the development of the CFD model to allow replication of the actual site meteorology and topography. The wind variability modifications have also been applied to incorporate the effects of mesoscale wind variability in the model predictions of fugitive dust deposition.

The proposed models are validated against dust deposition measurements recorded between June 9<sup>th</sup> to July 17<sup>th</sup> 2006 by a network of dust deposition gauges located downwind of a sequence of bench blasting events conducted at the quarry. The dust measurements were collected, computed and analysed during a measurement campaign conducted as part of the Mineral Industry Sustainable Aggregate (MIST) funded Dust Monitoring Research project. Here, a quantitative approach has been adopted to evaluate the model performance in accordance with dispersion model performance metrics described by Hanna et al. (2004). Cumulative dust deposition predictions from the model are compared against Frisbee gauge

dust deposition readings at Old Moor. The Frisbee gauges record the accumulation of dust over the entire monitoring period, therefore, cumulative dust deposition has been determined at positions in the domain corresponding to the gauge locations. The cumulative dust deposition is computed from a summation of the dust predictions for all bench blasts conducted within the monitoring period.

## 6.2 Old Moor Quarry Location

The Old Moor Quarry is located in the Borough of High Peak, Derbyshire and is approximately 4 km east of the town of Buxton and 1 km west of Tunstead village. The Ordnance Survey grid reference for Old Moor Quarry is SK100745 and the quarry is centred on longitude -1.8432, latitude 53.2653, or Easting 410557 and Northing 374269. Most of the excavated area lies within the Peak District National Park. At the time of the measurement campaign, the quarry boundaries extended to 835 m long, 785 m wide and depth of 69 m.

The quarry is operated under a joint venture between Lafarge UK and Tarmac Ltd. The Lafarge-Tarmac Tunstead operation consists of the Tunstead and Old Moor quarries and the adjoining Buxton lime and cement plant which is connected to Old Moor by a haul road causeway traversing the 50 m deep Great Rocks Dale Valley.

The stone crushing and processing plant for both quarries is located within Tunstead Quarry and a freight line runs within the Great Rocks Dale valley, serving Tunstead and other quarry operations in the local area (Tarmac, 2013). The combined Tunstead operations are the largest supplier of lime and lime-based products in the UK, extracting between 5 and 6 million tonnes of limestone per annum (Tarmac, 2013). Planning permission for extraction at Old Moor was first granted on the 30th of January 1980 and will expire in 2040 when the quarry is predicted to reach its final working depth of 108 m. Subsequent restoration plans will integrate the excavation into the surrounding landscape of the Peak District National Park.

The aerial photographs shown in Figure 6.2 and Figure 6.3 demonstrate how systematic extraction of minerals towards the permitted boundaries east of Great Rocks Dale Valley has led to continuous change in the land-form over a period of 14 months.

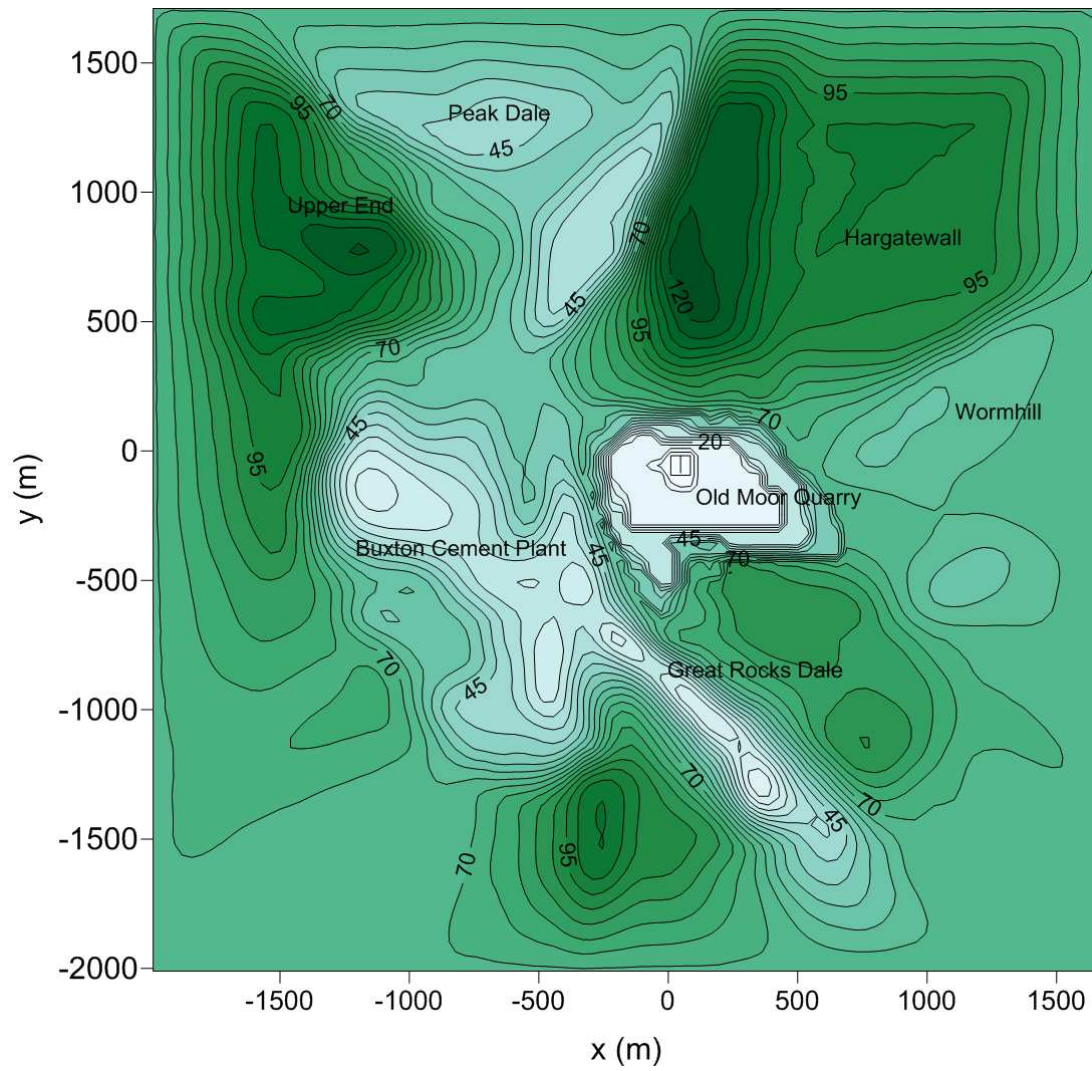


Figure 6.1: Contour map of Old Moor Quarry showing site elevations and surrounding areas.



Figure 6.2: Aerial view of Old Moor Quarry on 12<sup>th</sup> September 2005.



Figure 6.3: Aerial view of Old Moor Quarry on 31<sup>st</sup> December 2006.

### 6.3 Meteorological Pre-processing Routine

#### 6.3.1 Site Meteorological Measurements

Hourly averaged meteorological measurements were collected from a weather station located on site between June 9<sup>th</sup> 2006 to July 19<sup>th</sup> 2006. The meteorological station was installed and managed by the University of Nottingham and routine meteorological data was recorded including: the station code, date, time of day, hourly recordings of incoming solar radiation  $K^+$ , wind speed at a reference height of 10 m,  $U_{10}$ , mean wind direction,  $\theta$ , near surface air temperature  $T_a$ , relative humidity  $R_H$  and rainfall. The wind rose shown in Figure 6.4 shows that the prevailing wind direction for the measurement period was an Easterly wind at approximately  $\theta = 90^\circ$ , with average wind speed in excess of  $5.1 \text{ ms}^{-1}$ .

In the stability modified  $k - \varepsilon$  model, the ABL is parametrized in terms of the Monin-Obukhov length,  $L_{MO}$ , friction velocity,  $u_*$ , wall temperature,  $T_w$ , surface sensible heat flux  $Q_w$  and aerodynamic roughness height  $z_0$ . Furthermore, profiles of  $\mathbf{u}$ ,  $T$ ,  $k$  and  $\varepsilon$  have been defined at the domain inlets in accordance with Monin-Obukhov similarity scaling of the atmospheric surface layer. As is the case with many industrial operations, the meteorological station at the Old Moor site was not equipped with the specialist monitoring instruments required to directly measure these atmospheric parameters. Consequently, meteorological pre-processing is required. As mentioned in Chapter 2, the UK-ADMS meteorological pre-processing module adopts the boundary layer parametrization proposed in work by Holtslag and Van Ulden (1983), where a series of equations have been presented to allow computation of boundary layer input parameters for dispersion modelling from routinely measured meteorological variables. This approach has also been adopted in this chapter to derive the requisite ABL input variables for the  $k - \varepsilon$  model.

#### 6.3.2 Surface Radiation Balance

Bench blasting at the Old Moor quarry was carried out on specific days during monitoring period at approximately 11:00 hours. Consequently, the surface sensible heat flux may be determined by considering the balance of incoming and outgoing radiation at the ground surface under diurnal atmospheric conditions corresponding to this time. In Chapter 2, the equations of Holtslag and Van Ulden (1983), for net radiation at the surface,

$$Q^* = \frac{(1 - a)K^+ + c_1 T_a^6 - \sigma T_a^4 + c_2 N}{1 + c_3}, \quad (6.1)$$

and surface sensible heat flux,

$$Q^* = Q_w + \lambda E + G, \quad (6.2)$$

were introduced so that routine meteorological parameters such as the incoming solar radiation,  $K^+$  and near-surface temperature,  $T_a$ , can be used to establish the surface radiation balance and compute the surface sensible heat flux, which is required for the derivation of the Monin-Obukhov length and corresponding surface layer scaling parameters.

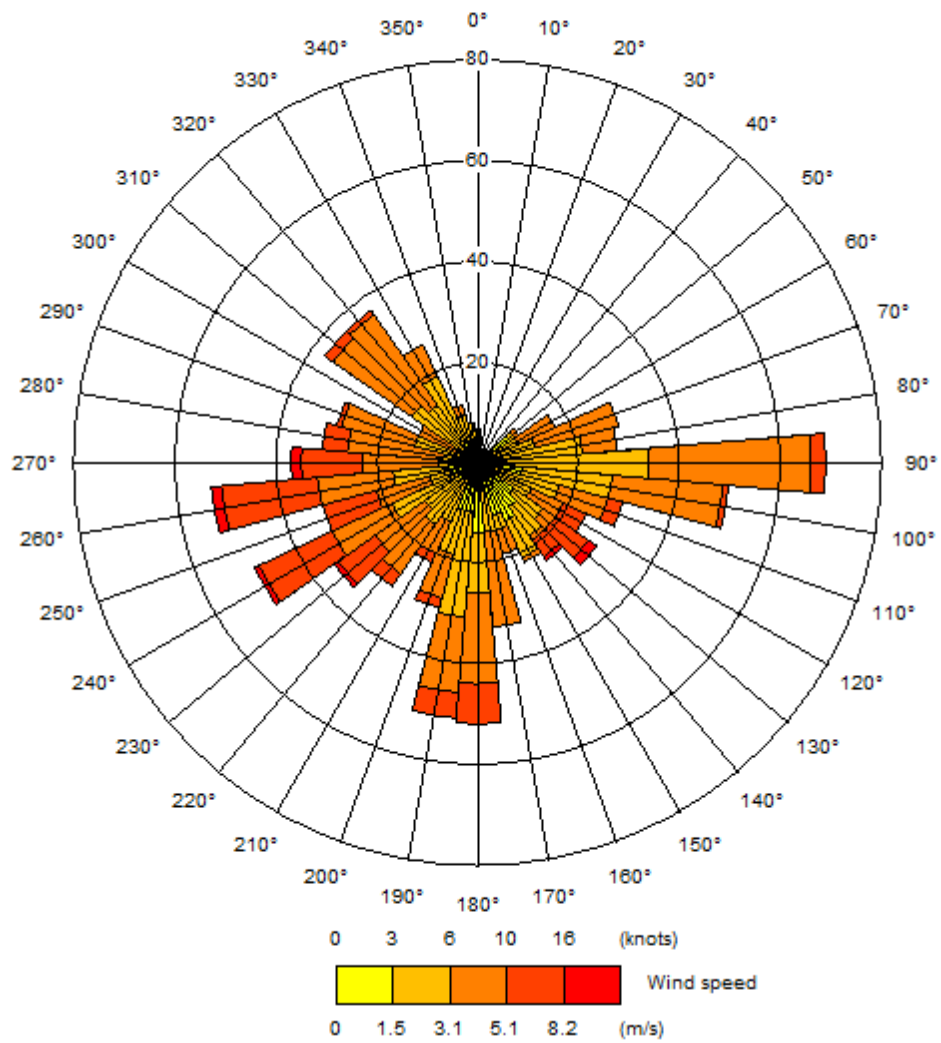


Figure 6.4: Old Moor wind speed and wind direction wind rose during measuring period

### 6.3.3 Fractional Cloud Cover

Representative ranges of fractional cloud cover from 0 to 1, in increments of 0.25 are used to compute the radiation budget estimates proposed by Holtslag and Van Ulden (1983). However, in practice, meteorological measurements of cloud cover are determined through visual observations of fractional cloud cover of the sky and are commonly estimated in terms of units called Oktas, where 1 Okta represents a fractional coverage of 1/8 of the sky. In the absence of meteorological measurements of cloud cover, the relative humidity may be used to determine the cloud cover. Walcek (1994) and Tompkins (2003) have established a correlation between cloud cover and relative humidity. Although temperature lapse rate, vertical velocity and wind-shear also exhibit weak correlation to cloud cover, Walcek (1994) concludes that the relative humidity is the best single atmospheric variable from which cloud cover can be determined in the lower troposphere. On this basis, Walcek (1994) have proposed the following equation to estimate cloud cover percentage,  $f\%$ ,

$$f\% = f_{100\%} \exp \left( \frac{RH - 1}{1 - RH_e} \right), \quad (6.3)$$

where  $f_{100\%}$  is the cloud cover at 100% relative humidity,  $RH$  is the measured relative humidity and  $RH_e$  is a critical value of relative humidity corresponding to a 37% reduction in the cloud cover fraction from that observed at  $RH=100\%$ .

Since there are no available historic measurements from which  $f_{100\%}$  and  $RH_e$  can be estimated for the Old Moor site, a conservative approach has been adopted for the computation of cloud cover fraction using the older scheme presented by Sundqvist et al. (1989),

$$f = 1 - \sqrt{\frac{1 - RH}{1 - RH_{crit}}}, \quad (6.4)$$

in which  $RH_{crit}$  is the threshold value of relative humidity at which clouds are likely to form, and is taken as 60%.

### 6.3.4 Surface Sensible Heat Flux Computations

In order to determine a value for the latent heat flux for substitution into Equation 6.2, the UK-ADMS model employs a simplification of the Penman-Monteith equation devised by Holtslag and Van Ulden (1983),

$$\lambda E = \frac{\alpha_{PT}}{1 + (\gamma/s)} (Q^* - G) + \alpha_{PT} \beta'. \quad (6.5)$$

In Equation 6.5,  $\alpha_{PT}$  is the Priestley-Taylor evaporation parameter, a default value of 1.0 is set within the UK-ADMS model. For the range of atmospheric conditions studied, an intermediate value between  $\alpha_{PT}=1.12$  for short grass and  $\alpha_{PT}=1.26$  for strongly advective conditions (Flint and Childs, 1991) is used. This is considered to be a reasonable estimate of the Priestley-Taylor parameter, since 50% of the wind observations at the site for the measurement period are greater than  $5 \text{ ms}^{-1}$  and a higher value of  $\alpha_{PT}$  is recommended by

Flint and Childs (1991) to account for increased evaporation from the surface due to high winds. It should be noted that variations in the evaporation parameter occur throughout the day. However, in the absence of continuous measurements of the Priestley-Taylor parameter, a constant value of  $\alpha_{PT}$  has been assumed for all the meteorological computations.

In Equation 6.5,  $\gamma$  is the psychrometric constant, which is the ratio of the specific heat capacity of water at constant pressure to its latent heat of vaporization,  $s$  is the slope of the saturation specific humidity-temperature curve and  $\beta'$  is a surface moisture constant which is equal to  $20 \text{ Wm}^{-2}$ . The ratio  $\gamma/s$  decays exponentially with increasing temperature.

Table 6.1: Values of  $T$  and  $\gamma/s$  at  $P=1000 \text{ mb}$ , Holtslag and Van Ulden (1983)

| $T_a$ ( $^{\circ}\text{C}$ ) | $\gamma/s$ | $\ln(\gamma/s)$ |
|------------------------------|------------|-----------------|
| -5                           | 2.01       | 0.698           |
| 0                            | 1.44       | 0.365           |
| 5                            | 1.06       | 0.058           |
| 10                           | 0.79       | 0.236           |
| 15                           | 0.60       | 0.511           |
| 20                           | 0.45       | 0.799           |
| 25                           | 0.35       | -1.050          |
| 30                           | 0.27       | -1.309          |
| 35                           | 0.21       | -1.561          |

By plotting the temperature,  $T_a$  in degrees, against  $\ln(\gamma/s)$ , a straight line is obtained in Figure 6.5 and an equation can be derived to determine the value of  $\gamma/s$  at any temperature,

$$\gamma/s = \exp(0.36 - 0.056T_a). \quad (6.6)$$

The surface sensible heat flux can subsequently be determined from,

$$Q_w = \frac{(1 - \alpha_{PT}) + (\gamma/s)}{1 + (\gamma/s)}(Q^* - G) - \alpha_{PT}\beta'. \quad (6.7)$$

Both Holtslag and Van Ulden (1983) and Su (1999) express the ground heat flux  $G$  as a fraction of the net radiation  $Q^*$ , which depends on the vegetation cover on the surface, thereby arriving at,

$$G = c_G Q^*. \quad (6.8)$$

Whilst Holtslag and Van Ulden (1983) apply a constant value of  $c_G=0.1$ , corresponding to a surface covering of short grass, Su (1999) recommends determining the ground cover coefficient by interpolating between the value for dense vegetation canopy and bare soil based on the fractional vegetation cover of the site under consideration,

$$c_G = \Gamma_c + (1 - f_c)(\Gamma_s - \Gamma_c) \quad (6.9)$$

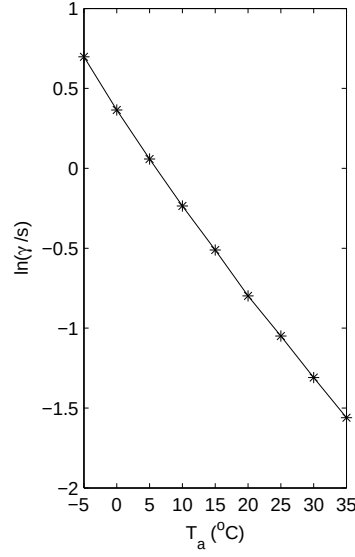


Figure 6.5: Psychrometric curve according to Holtslag and Van Ulden (1983)

where  $\Gamma_c=0.05$ , is the full vegetation canopy coverage coefficient,  $f_c$  is the fractional canopy coverage and  $\Gamma_s=0.315$  is the bare soil coefficient. In the UK-ADMS model a fixed value of  $c_G=0.1$  is used based on the Holtslag and Van Ulden (1983) evaluation that the ground heat flux is generally a small percentage of the net radiation over land surfaces and varying the value of  $c_G$  between 0.05 and 0.315 has a negligible effect.

### 6.3.5 Calculating the Monin-Obukhov Length

Once values of surface sensible heat flux and near-surface temperature have been computed from the routine meteorological data, it is possible to estimate the Monin-Obukhov length using an iterative method which requires approximation of the surface roughness length. For quarry and strip mine operations, USEPA (2008b) recommends a surface roughness length of 0.3 m in AERMET, the meteorological pre-processor which accompanies AERMOD. As has been explained in Chapter 2, this roughness length accounts for the presence of surface features of the excavation such as benches and slopes, however since the case study quarry topography has been explicitly modelled, a roughness length corresponding to the land cover classification of the surrounding terrain has been adopted. The quarry is predominantly surrounded by grasslands and low vegetation, thus, a surface roughness length of  $z_0 = 0.1$  m has been assumed.

The first iteration is carried out for neutral atmospheric conditions, such that the Bussinger-Dyer non-dimensional wind shear,  $\phi_m$  has the value of unity, and  $u_*$  is computed from substitution of the reference wind speed  $u_h$  into the logarithmic velocity profile equation for the adiabatic atmosphere. The resultant value of  $u_*$  is used to calculate an initial  $L_{MO}$ ,

hence for the subsequent iterations, corrected values of the non-dimensional wind shear can be determined from the Businger-Dyer functions. Additional iterations are performed until the values of  $u_*$ ,  $L_{MO}$  and  $\phi_m$  converge.

The Pasquill-Guifford-Turner (PGT) stability classifications are assigned to each line of meteorological data based on the computed values for  $L_{MO}$  and the ranges specified in Chapter 2. This enabled grouping and averaging of the data so that representative meteorology could be computed for each observed stability class. Table 6.2 lists the average values of the meteorological variables for observations falling under each stability class.

Table 6.2: Average values of  $L_{MO}$  corresponding to each PGT stability class for all meteorological data

| PGT class                     | A     | B     | C     | D       |
|-------------------------------|-------|-------|-------|---------|
| $L_{MO}$ (m)                  | -65   | -281  | -1113 | -125415 |
| $Q_W$ ( $\text{Wm}^{-2}$ )    | 58    | 58    | 24    | 0.4     |
| $T_W$ (K)                     | 293   | 293   | 289   | 283     |
| $u_*$ ( $\text{ms}^{-1}$ )    | 0.351 | 0.570 | 0.680 | 0.799   |
| $\phi_m$                      | 0.73  | 0.89  | 0.97  | 1.00    |
| $U_{10}$ ( $\text{ms}^{-1}$ ) | 3.5   | 6.1   | 7.4   | 9.2     |

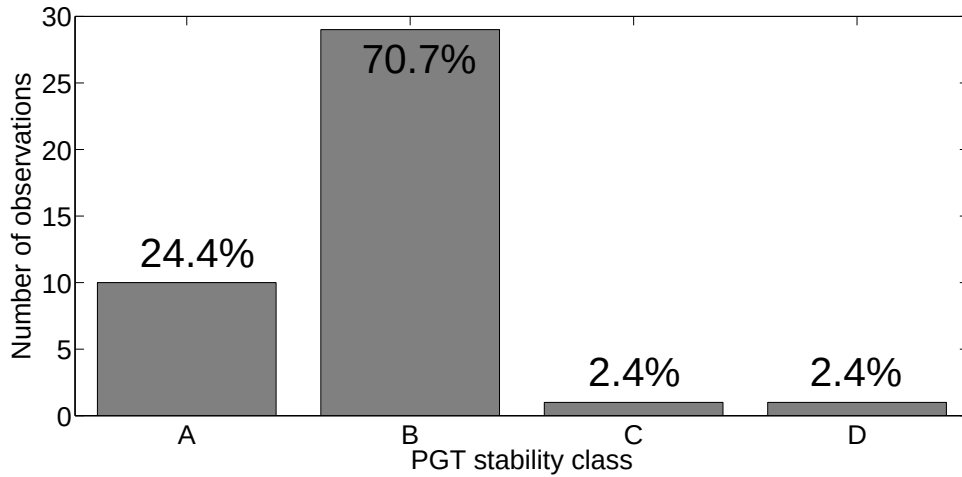


Figure 6.6: Frequency distribution of PGT stability classes at Old Moor quarry at the time of blasting for the measurement period from June 9<sup>th</sup> to July 19<sup>th</sup>.

As is typical of diurnal summertime atmospheric conditions, only four PGT stability classes are required to represent the data contained in Table 6.2, ranging from class A (strongly unstable) to class D (neutral). The strongly unstable observations appear to be associated with low wind speeds and relatively high values of surface sensible heat flux and near surface temperature. The ABL stability tends towards the neutral case as the wind speed increases and surface sensible heat flux decreases, since more heat is lost to evapo-transpiration pro-

cesses under these strongly advective conditions. In Figure 6.6, the frequency distribution of stability classes over the observation period at 11:00 hours (blast time) indicate that the site meteorology is largely dominated by unstable atmospheric conditions, with over 90% of observations falling into either the very unstable or unstable categories. Average values of  $Q_w$  and  $T_w$  have also been calculated for each of the observed stability classes and these have been used to determine corresponding values of  $u_*$  and  $T_*$ .

### 6.3.6 Treatment of the Convective Mixed Layer

The very unstable ABL is associated with large variations in ABL parameters due to enhanced mixing arising from the buoyant production of turbulence. Under strongly convective conditions, the application of Monin-Obukhov Similarity scaling is confined to a thin surface layer of thickness generally of the order of  $|L_{MO}|$ , or up to  $2|L_{MO}|$ , to include the transition region between the surface layer and the fully-mixed layer, where thermal forcing does not yet dominate the flow. As illustrated in Figure 6.6, the majority of meteorological measurements recorded on site during the monitoring period fall under stability class B and have  $|L_{MO}| > 100$  m, therefore, although Monin-Obukhov Similarity scaling may not be applicable throughout the full depth of the computational domain, useful information regarding dispersion in the near-ground region up to a height of 100 m can be obtained using the proposed standard  $k - \varepsilon$  modifications even for the very unstable cases.

## 6.4 Characterization of Blast Emissions

The Michigan Department of Environmental Quality (MDEQ, 2004), provides guidance on the calculation of particulate emission rates from various fugitive dust generating processes within the mineral industries. In the absence of site specific emission factors, generic emission factor estimates compiled by the USEPA AP-42 (USEPA, 1998) for application to fugitive dust emissions from surface coal mining operations in the western United States are recommended for use. These emission factors have been computed using long-term averages of all available data of acceptable quality to estimate particulate emissions for a given source category (USEPA, 1998), based on the assumption that the quantity of fugitive dust liberated by a dust generating activity is directly proportional to the mineral throughput levels of the activity (MDEQ, 2004). For instance, in the case of bench blasting, MDEQ (2004) use USEPA AP-42 methods to establish that the tonnage of extracted rock is directly proportional to the fugitive dust emission factor. Despite their usefulness, emission factor equations for bench blasting do not account for short-term variability in dust emissions between individual blasts, nor do they account for fluctuations in meteorology or site specific operating conditions. Therefore, they are preferred for estimating continuous releases over relatively long averaging times ranging from one to 24 hours. Consequently, the total emission has been modelled as a continuous release occurring over the meteorological averaging time of one hour.

MDEQ (2004) recommends the use of a constant fugitive dust emission factor for  $PM_{10}$  of 0.038 kg per tonne of blasted rock for the calculation of fugitive dust emissions from

bench blasting. The studies of Appleton et al. (2006) and Silvester et al. (2006) employ this emission factor to estimate the total suspended particulate emissions from representative blasts recorded at Old Moor quarry. In Chapter 2, fugitive dust has been defined in terms of the inhalable dust fraction consisting of particulates of aerodynamic diameter ranging from  $2.5\text{ }\mu\text{m}$  to  $75\text{ }\mu\text{m}$ , and this definition of fugitive dust has been maintained throughout this thesis. Since  $\text{PM}_{10}$  particulates account for 50% of the mass of Total Suspended Particulates (TSP) as defined by the size distribution, the MDEQ (2004) estimate is doubled to give an emission factor of 0.076 kg per tonne for total suspended particulates.

By performing an analysis of the video stills recorded during a single blast, Silvester et al. (2006) determined that the dust cloud generated by a blast could be approximated by a cuboid of length 100 m, width 60 m and height equal to that of the bench. In Chapters 4 and 5, a volumetric emission source consisting of uniformly distributed points was used to define an injection source in the Discrete Phase Model which introduced particles into the computational domain. This method of seeding particles in the resolved flow-field is maintained in the case study and a volumetric source with TSP injection points at 5 m spacing throughout a cuboid of dimension corresponding to that of the dust cloud has been defined in the Lagrangian particle tracking model. The same blast dimensions have been assumed throughout in order to simplify the model set-up, on the basis that a similar configuration of explosive charges was used for all of the blast events monitored at the Old Moor Quarry.

In Table 6.3, the Easting and Northing coordinates of the centres of the bench faces have been obtained from the blast logs and converted to Cartesian coordinates relative to an origin positioned at Eastings 410557, Northings 374269 and  $z = -37.00$ , to facilitate positioning of the volume emission sources in the computational domain. The average emission rate  $\dot{m}_{avg}$ , associated with each blast is given in Table 6.4 and a classification scheme has been devised to group blasts within close proximity of each other and to identify the blasts according to the benches from which they occur.

Table 6.4 lists the Cartesian coordinates of the bounding vertices of the cuboid volume source regions and the associated dust emission rates for the blast clouds occurring at the bench locations listed in Table 6.3. The source regions are illustrated in Figure 6.7 and it can be seen that some are within close proximity of each other, such that there is an overlap of the volume sources used to define the initial blast clouds. Therefore, the blasts clouds in these clusters may be effectively represented by average blasts as shown in Figure 6.8. The bounding vertices and average emission rates of these average blasts are listed in Table 6.5.

Table 6.3: Coordinates of the centre point of the bench faces.

| Location | Eastings | Northings | $x$<br>(m) | $y$<br>(m) | $z$<br>(m) | $h_{bench}$<br>(m) |
|----------|----------|-----------|------------|------------|------------|--------------------|
| 1        | 410913   | 373911    | 356        | -358       | -25.625    | 22.75              |
| 2        | 411093   | 373852    | 536        | -417       | -9.25      | 15.50              |
| 3        | 410995   | 373840    | 438        | -429       | -10.25     | 13.50              |
| 4        | 411256   | 373963    | 699        | -306       | -8.00      | 18.00              |
| 5        | 410585   | 373984    | 28         | -285       | -47.50     | 17.00              |
| 6        | 411292   | 373899    | 735        | -370       | -8.1       | 16.20              |
| 7        | 410661   | 373984    | 104        | -285       | -47.75     | 16.50              |
| 8        | 411206   | 374039    | 649        | -230       | -8.00      | 18.00              |
| 9        | 410509   | 373984    | -48        | -285       | -47.75     | 16.50              |
| 10       | 410625   | 373996    | 68         | -273       | -45.45     | 21.10              |
| 11       | 410990   | 374226    | 433        | -43        | -27        | 20.00              |
| 12       | 411169   | 373852    | 612        | -417       | -9.5       | 15.00              |

Table 6.4: Coordinates of blast bounding vertices and the average emission rate for each blast.

| Location | $x_{min}$<br>(m) | $x_{max}$<br>(m) | $y_{min}$<br>(m) | $y_{max}$<br>(m) | $z_{min}$<br>(m) | $z_{max}$<br>(m) | $\dot{m}_{avg}$<br>(kgs <sup>-1</sup> ) |
|----------|------------------|------------------|------------------|------------------|------------------|------------------|-----------------------------------------|
| 1        | 306              | 406              | -358             | -298             | -37.00           | -14.25           | 0.0438                                  |
| 2        | 486              | 568              | -417             | -357             | -17.00           | -1.50            | 0.3738                                  |
| 3        | 388              | 488              | -420             | -360             | -17.00           | -3.50            | 0.2080                                  |
| 4        | 572              | 632              | -363             | -263             | -17.00           | 1.00             | 0.2739                                  |
| 5        | -22              | 78               | -285             | -225             | -56.00           | -39.00           | 0.2934                                  |
| 6        | 595              | 655              | -420             | -320             | -17.00           | 0.80             | 0.4725                                  |
| 7        | 54               | 154              | -285             | -225             | -56.00           | -39.50           | 0.4680                                  |
| 8        | 560              | 620              | -230             | -130             | -17.00           | 1.00             | 0.3038                                  |
| 9        | -98              | 2                | -285             | -225             | -56.00           | -39.50           | 0.3201                                  |
| 10       | 18               | 108              | -275             | -213             | -56.00           | -34.90           | 0.4581                                  |
| 11       | 338              | 398              | -103             | -3               | -37.00           | -17.00           | 0.4372                                  |
| 12       | 562              | 662              | -417             | -357             | -17.00           | -2.00            | 0.2292                                  |

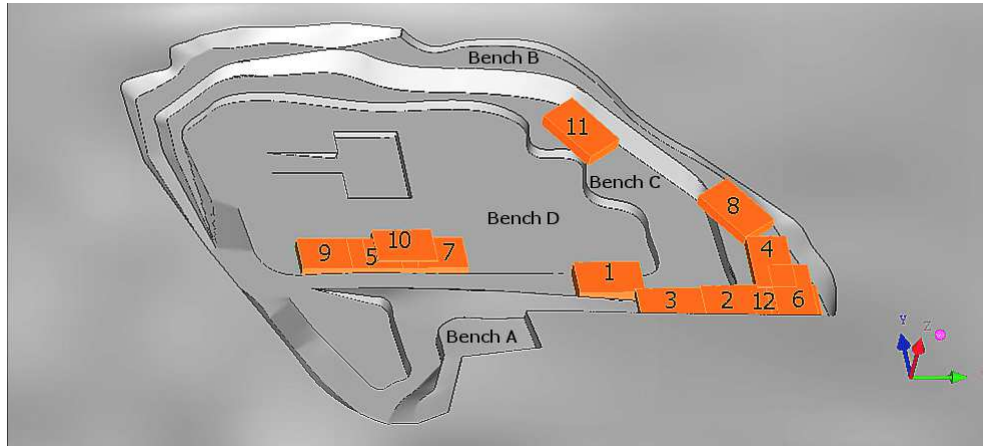


Figure 6.7: All initial blast cloud locations for bench blasting conducted during the measurement period.

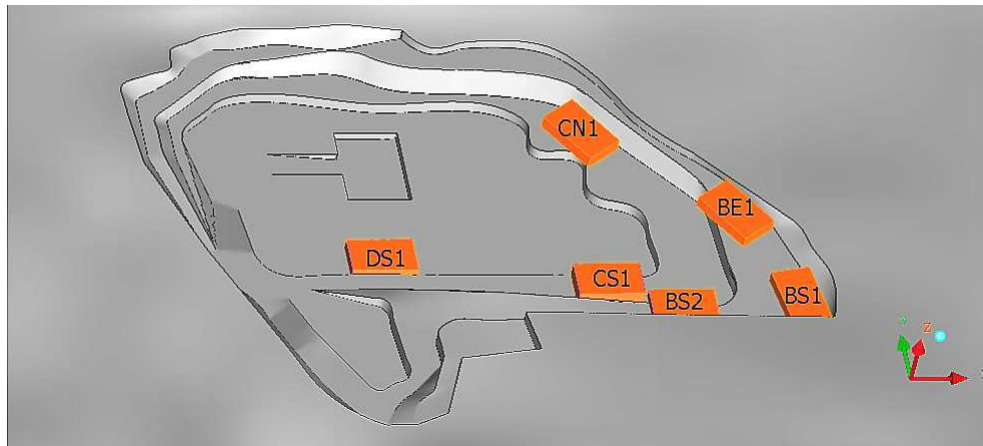


Figure 6.8: Representative blast locations, from averaging groups of blasts in close proximity of each other.

Table 6.5: Bounding vertices and average emission rate of representative blast calculated from averaging groups of overlapping blast.

| Location | $x_{min}$<br>(m) | $x_{max}$<br>(m) | $y_{min}$<br>(m) | $y_{max}$<br>(m) | $z_{min}$<br>(m) | $z_{max}$<br>(m) | $\dot{m}_{avg}$<br>( $\text{kg s}^{-1}$ ) |
|----------|------------------|------------------|------------------|------------------|------------------|------------------|-------------------------------------------|
| BS1      | 595              | 655              | -420             | -320             | -17.00           | 0.90             | 0.3732                                    |
| BS2      | 486              | 568              | -417             | -357             | -17.00           | -1.50            | 0.270                                     |
| BE1      | 560              | 620              | -230             | -130             | -17.00           | 1.00             | 0.3038                                    |
| CS1      | 306              | 406              | -358             | -298             | -37.00           | -14.25           | 0.0438                                    |
| CN1      | 338              | 398              | -103             | -3               | -37.00           | -17.00           | 0.4372                                    |
| DS1      | -22              | 78               | -285             | -225             | -56.00           | -39.00           | 0.3849                                    |

## 6.5 Artificial Terrain Simulations

The case study simulations which used the actual site topography were preceded by trial simulations where the computational domain included only the pit topography. Thus, the influence of the quarry topography on the flow-field can be isolated from that of the external orography. This scenario is considered to be representative of a quarry excavation surrounded by relatively flat terrain. These cases are subsequently referred to as the *Artificial Terrain* cases, and are used to perform preliminary investigations of dust dispersion from Blast B1 under the average meteorological parameters listed in Table 6.2. This blast was sited at the south-eastern corner of the quarry and has been used for all the Artificial Terrain simulations, primarily because the blast logs for the measurement period indicated that blasting occurred most frequently at or near BS1. The Artificial Terrain simulations have considered four stability classes from A to D and two wind directions. The first wind direction is the prevailing easterly at  $\theta = 90^\circ$  and the second is in the opposite direction at  $\theta = 270^\circ$ . Due to the positioning of the dust monitoring network outside the south-eastern boundary of the pit and the higher frequency of blasts from the eastern quadrant of the quarry, the gauge locations were likely to register the most deposition with a  $270^\circ$  wind.

### 6.5.1 Discretizing the Computational Domain

The computational domain boundaries were defined as illustrated in Figure 6.9 for  $\theta = 90^\circ$ , enclosing a plan area of approximately  $1750 \text{ m} \times 1750 \text{ m}$ . The Artificial Terrain mesh was created in ICEM CFD by first extracting the ground surface geometry from a Stereolithographic (STL) file of the quarry terrain, the Octree algorithm was then used to discretize the computational domain by creating an initial volume mesh consisting of tetrahedral elements of maximum length 16 m. An inflation layer comprised of prismatic elements was applied at the ground to resolve the flow in the near-wall region. This prism layer was allowed to grow geometrically from a first cell height of 0.6 m to a maximum prism height of 0.7 times

the tetrahedra base width. Within the quarry pit, a maximum surface mesh size of 2 m was enforced on the bench faces and tetrahedra size was constrained to a maximum of 8 m by a spherical density region centred on the pit and of diameter equal to the maximum pit length. This refinement region was created to capture small-scale features of the in-pit flow. External to the pit, tetrahedra were permitted to grow upward from their interface with the inflation layer towards the top boundary at a growth rate of 1.2, until the global maximum tetrahedra size of 16 m was reached. The final mesh was obtained after re-generation of the Octree mesh using the Delaunay mesher to produce a tetrahedral mesh with smoother volume transitions, consisting of a total of 5468438 cells. Figure 6.10 shows the surface mesh including the prismatic boundary layer. The region inside the rectangle is magnified in Figure 6.11 to better illustrate the prismatic boundary layer applied near the wall.

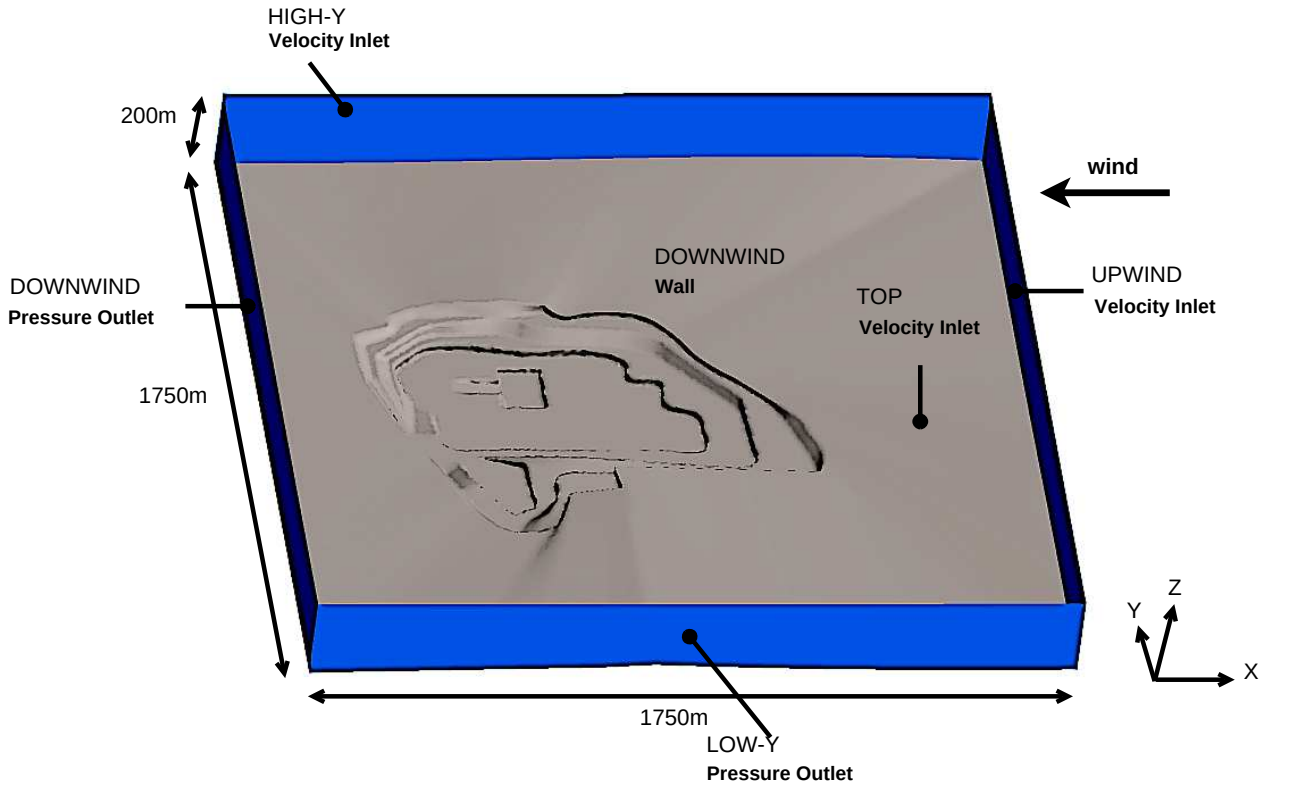


Figure 6.9: Specification of domain boundaries for prevailing wind direction,  $\theta = 90^\circ$ .

The case study simulations were performed on the University of Nottingham High Performance Beowolf-Class Computing Cluster, Minerva. The system consists of 166 Dell C6220 compute nodes, each containing  $2 \times 8$  core Intel Sandy bridge E5-2670 2.6 GHz processors and offering 32 GB of RAM. A further 10 compute nodes were classed as enhanced and offer 128 GB RAM. The system is able to perform  $46^{12}$  calculations per second, with 12 GPU accelerators which can increase the calculation rate by an additional  $1^{12}$  calculations per second. Distributing the computation across 8 cores on one compute node, and requesting 32GB of RAM, the average run time for the artificial terrain simulations High Performance Computing cluster was 4.5 hours.

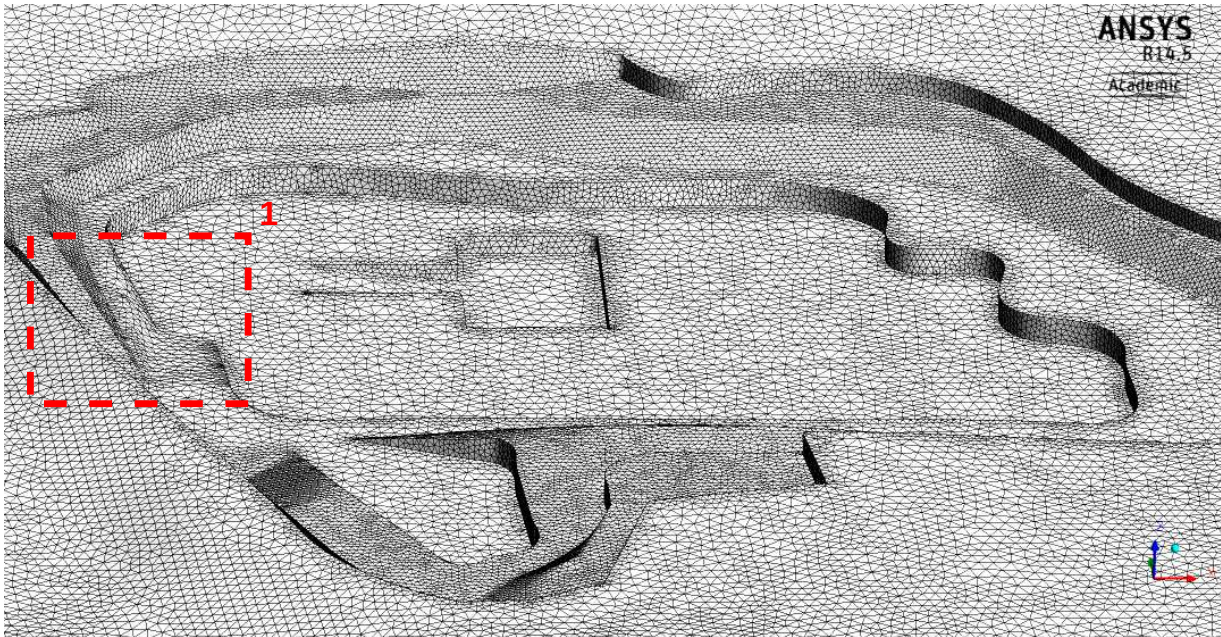


Figure 6.10: Plan view of surface mesh on the quarry bench floors and bench faces.

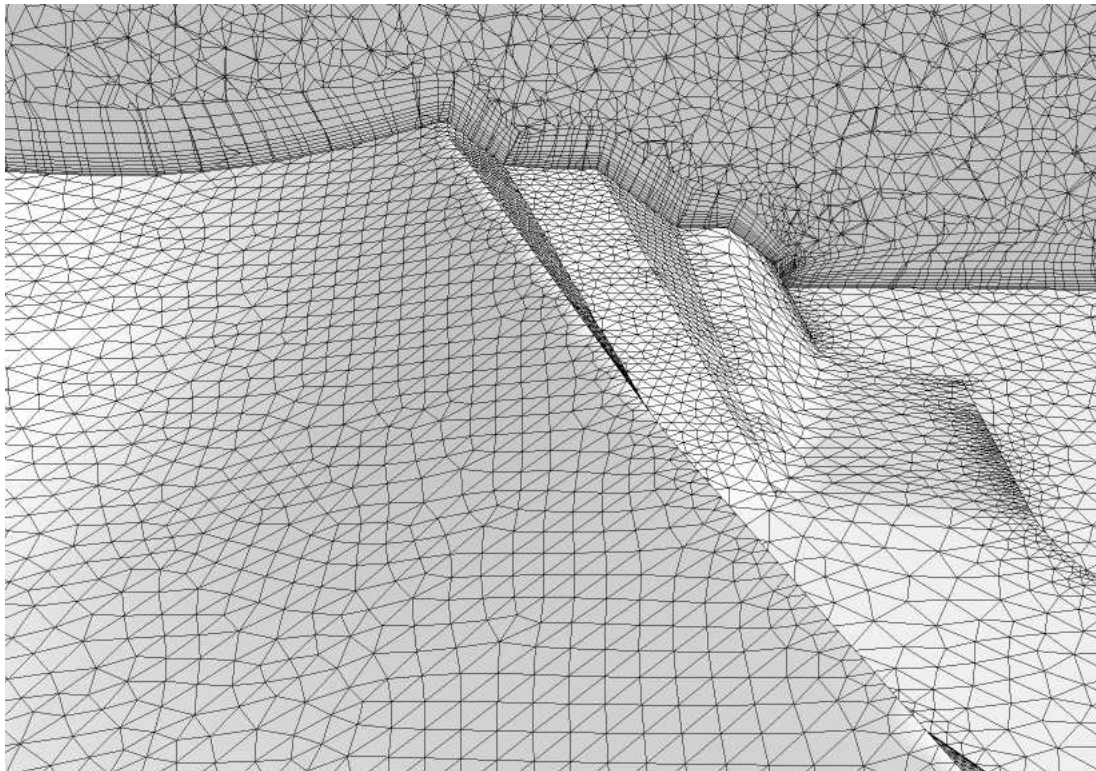


Figure 6.11: Prismatic layer near the wall in region 1 and cell refinement imposed on benches.

### 6.5.2 Specification of the Initial Blast Velocity

From their examination and analysis of video stills recorded for a single blast event at Old Moor Quarry, Silvester et al. (2009) found that the forward velocity of the blast dust cloud quickly decayed to that of the background flow as the blast was entrained in the ambient air. The horizontal profile of the blast cloud measured in the Silvester et al. (2009) study was introduced in Chapter 2, Figure 2.4. In the current study, parametric tests have been conducted for the Artificial Terrain cases to determine an appropriate value of initial particle injection velocity for a blast emission. The accretion rates of dust particles at the wall predicted using blast front velocities of  $25 \text{ ms}^{-1}$ , the maximum value recorded by Silvester et al. (2009), and those of a static injection were compared. The results from these simulations are shown in Figures 6.12 and 6.13 respectively. The difference in accretion rate between Figure 6.12 and Figure 6.13 is given in Figure 6.14. The accretion profiles for both simulations are similar in shape, both in the along-wind and cross-wind directions and show a similar distribution of particles. A maximum accretion rate of approximately  $1.45 \times 10^{-6} \text{ kg m}^{-2} \text{ s}^{-1}$  was observed in both instances. The differences in the observed accretion rate between the two simulation results, illustrated in Figures 6.12 and 6.13, lie in the range  $\pm 2.5 \times 10^{-8} \text{ kg m}^{-2} \text{ s}^{-1}$ . These differences in accretion rate appear to occur in localised zones concentrated near the downwind quarry boundary, thus implying that they may be attributed to the stochastic nature of the particle tracking model. This suggests that the defining the initial injection as static in the DPM produces a negligible effect on the overall accretion profile compared to using the maximum blast front velocity from Silvester et al. (2009). The apparent insensitivity of the accretion predictions to the initial velocity of the particles can be related to the particle force balance equation employed in the Discrete Phase Model to predict the trajectory of individual particles. Viscous drag on the particles increases proportionally to their relative velocity, arresting the momentum of the particles and dissipating their energy to the surrounding fluid, such that in the absence of other external forces, they primarily settle due to the action of gravity.

### 6.5.3 Examination of the Wind-field and Dust Dispersion within the Quarry

The flow behaviour predicted by the model over the Artificial Terrain was examined to determine whether it was consistent with well-established complex terrain flow phenomenon observed in other studies and discussed extensively in Chapter 5. For this purpose, the graphs in Figures 6.15a to 6.20b have been plotted to show the interaction of the flow-field with the complex quarry topography at a series of regularly spaced vertical rakes along a plane parallel to the mean wind direction and passing through the centre of the deepest bench. The positions of the rakes relative to the centre of the bench have been specified in terms of the  $x$ -coordinate, non-dimensionalized by the maximum depth of the pit,  $D = 69 \text{ m}$ . As with the idealized terrain profiles in Chapter 5, the normalized velocity component and turbulence intensity were plotted.

The length to width ratio of the quarry was approximately 1. Furthermore, unlike the idealized, symmetrical cosine depressions investigated in Chapter 5, the actual case study

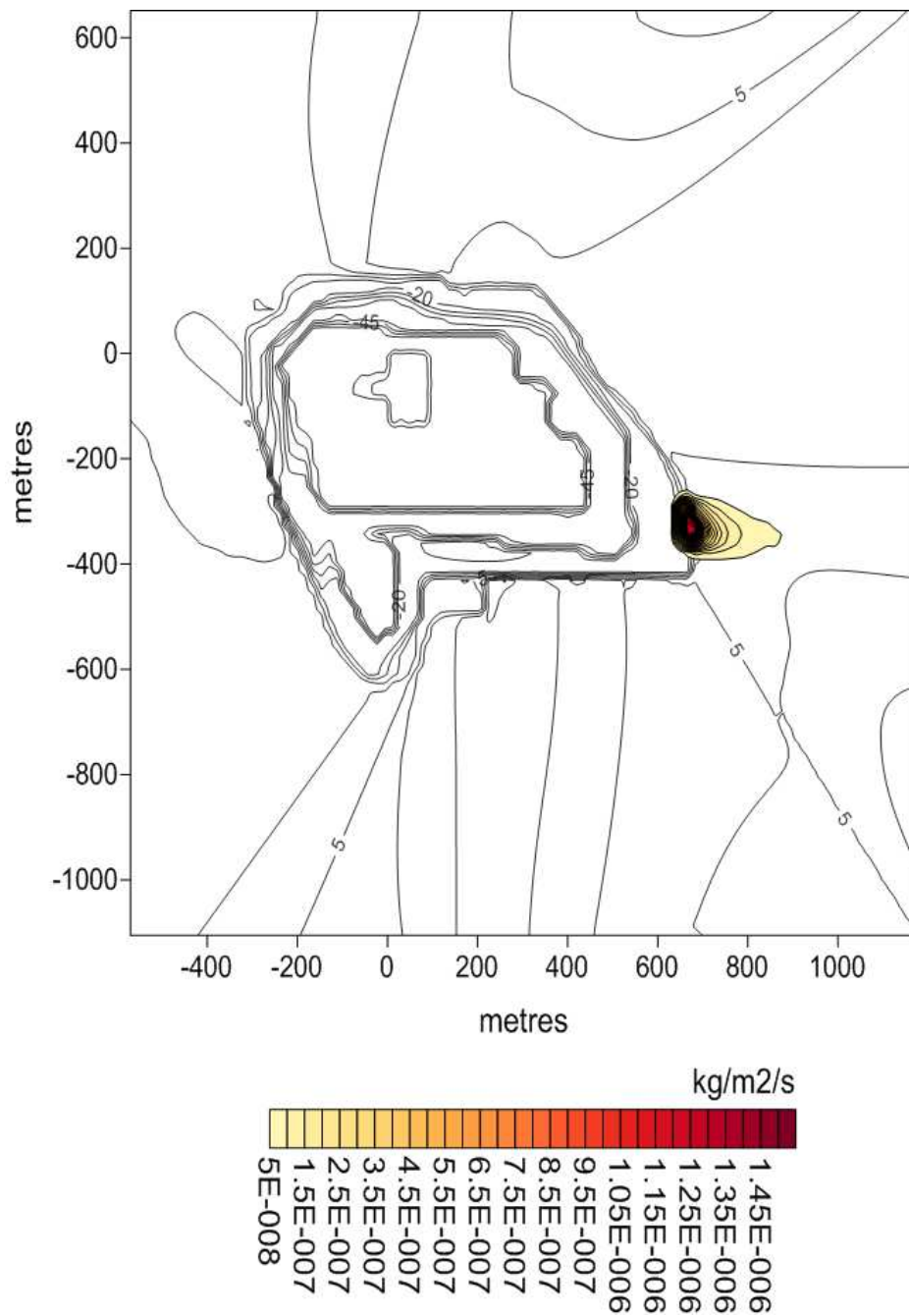


Figure 6.12: Dust accretion for static injection with initial particle injection velocity of  $0 \text{ ms}^{-1}$ .

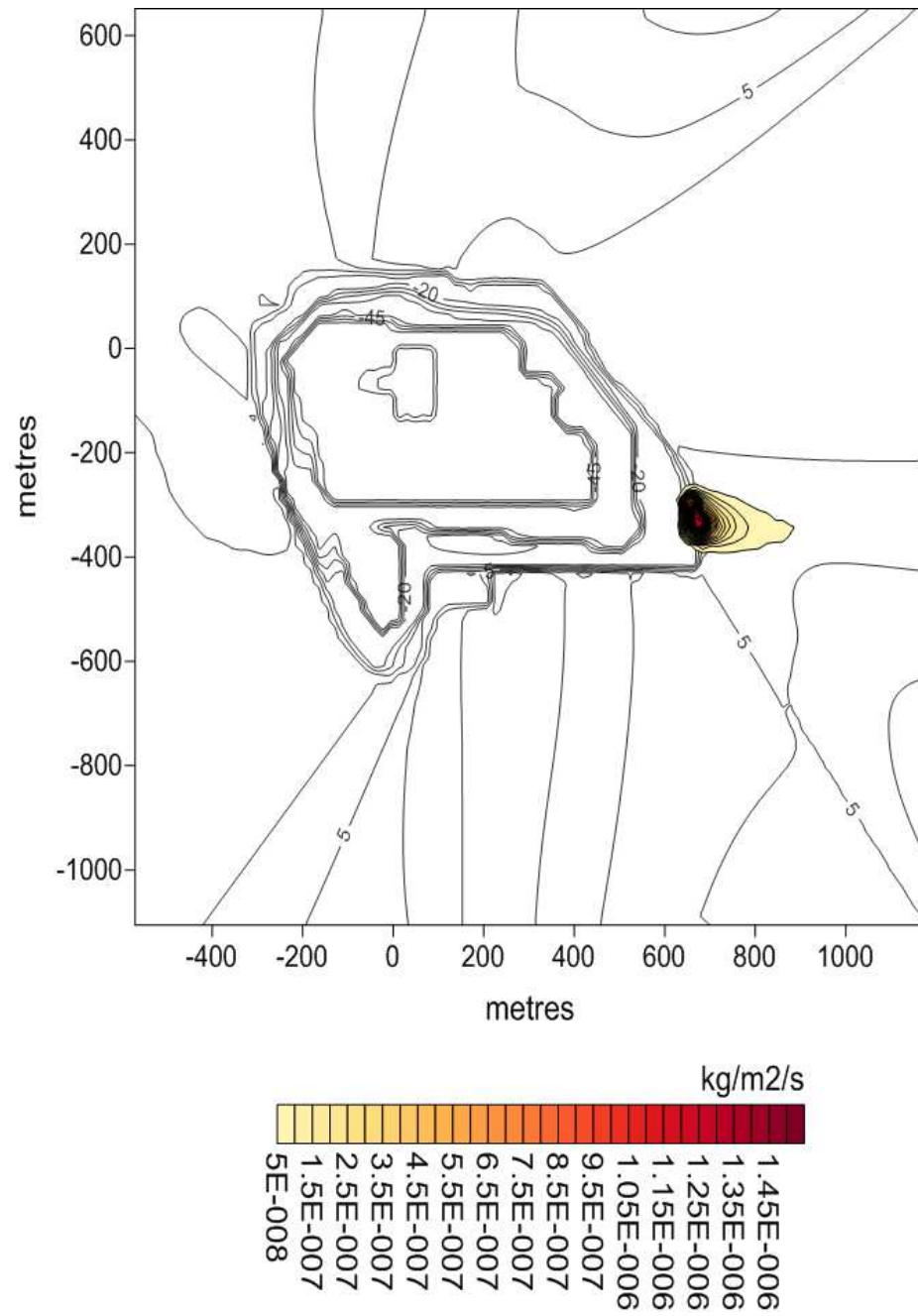


Figure 6.13: Dust accretion for initial particle injection velocity of  $25 \text{ ms}^{-1}$ .

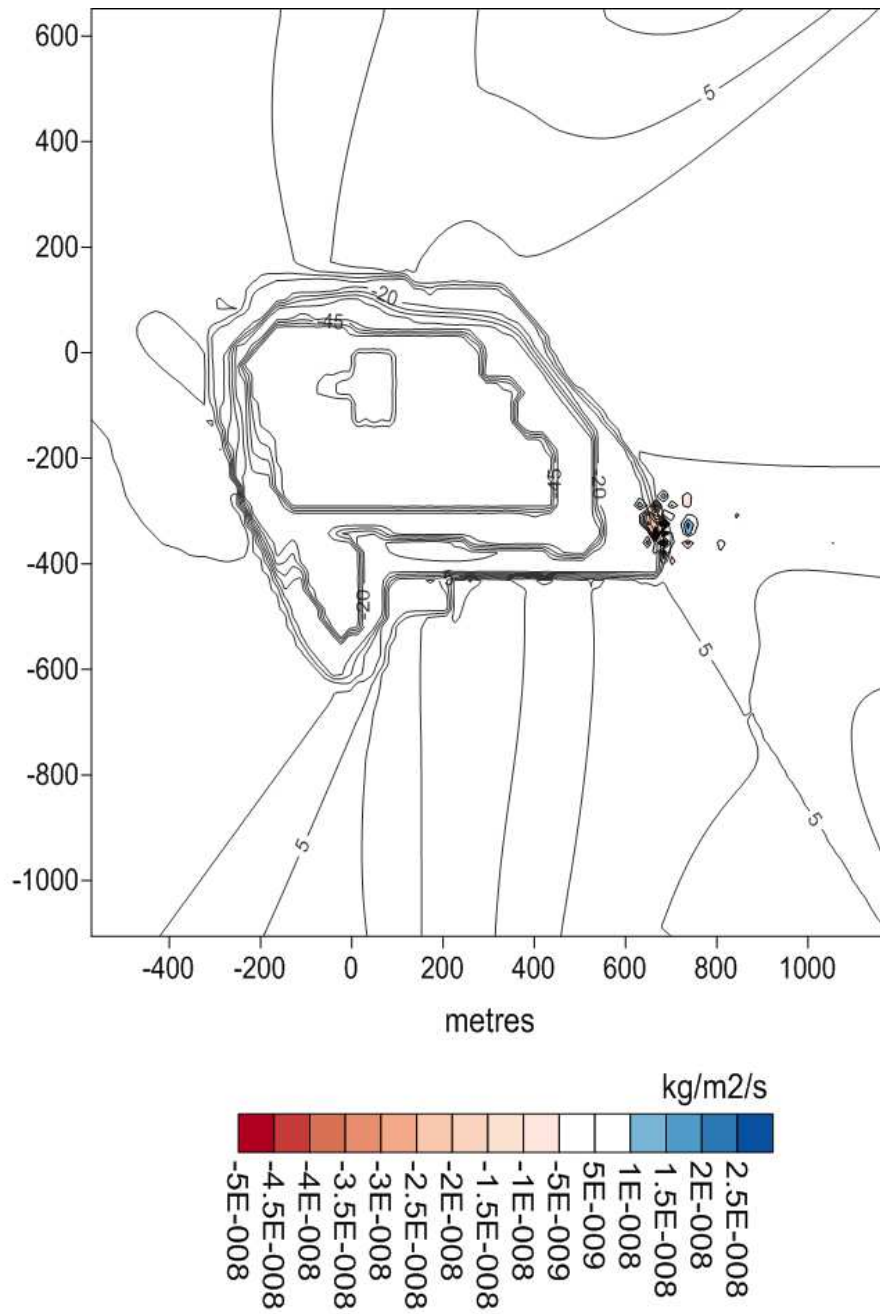


Figure 6.14: The difference between the  $0 \text{ ms}^{-1}$  and  $25 \text{ ms}^{-1}$  Accretion profiles.

quarry topography is asymmetric. In accordance with Chinthala and Khare (2011), who recommended consideration of the three-dimensionality of the flow when the length to width ratio is one, profile plots of the normalized  $u$ ,  $v$  and  $w$  velocity components have been included to examine how the pit terrain contributed to deviation of the flow represented by non-zero velocity components in the  $y$  and  $z$  directions. The normalized velocity components and turbulence intensity were calculated as follows,

$$\hat{u}_i = \frac{u_i}{|u_h|} \quad (6.10)$$

$$I = \frac{\sqrt{2/3k}}{|u_h|}, \quad (6.11)$$

the non-dimensional distance  $x'$  from the centre of the deepest bench is computed from,

$$x' = \frac{x - x_o}{D} \quad (6.12)$$

where  $x_o = 48$  is the  $x$  coordinate at the centre of the deepest bench.

In Figure 6.15a and Figure 6.15b, for both approach directions, in panels  $x' = 6.0$  and  $x' = -5.0$  respectively, it was seen that a separation region occurred as the flow entered the quarry excavation and encountered the face of Bench B. The characteristically lower wind velocities associated with increasing atmospheric instability are observed to result in slightly stronger flow reversal at this point for the strongly unstable case. Accordingly, the reverse flow magnitude at the topmost bench face B, was greatest for stability class A, where a reverse flow magnitude corresponding to  $0.3u_h$  was predicted by the model for either direction. Generally, the results showed that the wind-field of the near-neutral and neutral stability classes, C and D respectively, were least perturbed by the quarry terrain. A ventilating flow appeared to develop within the pit for these flow regimes, both of which were characterized by reference winds in excess of  $7 \text{ ms}^{-1}$  and relatively low surface sensible heat flux. As the flow progressed through the excavation, the profiles accelerated slightly over the flat terrain of the bench floors. The most pronounced flow reversals are observed for either direction as the flow descended onto the floor of the deepest bench.

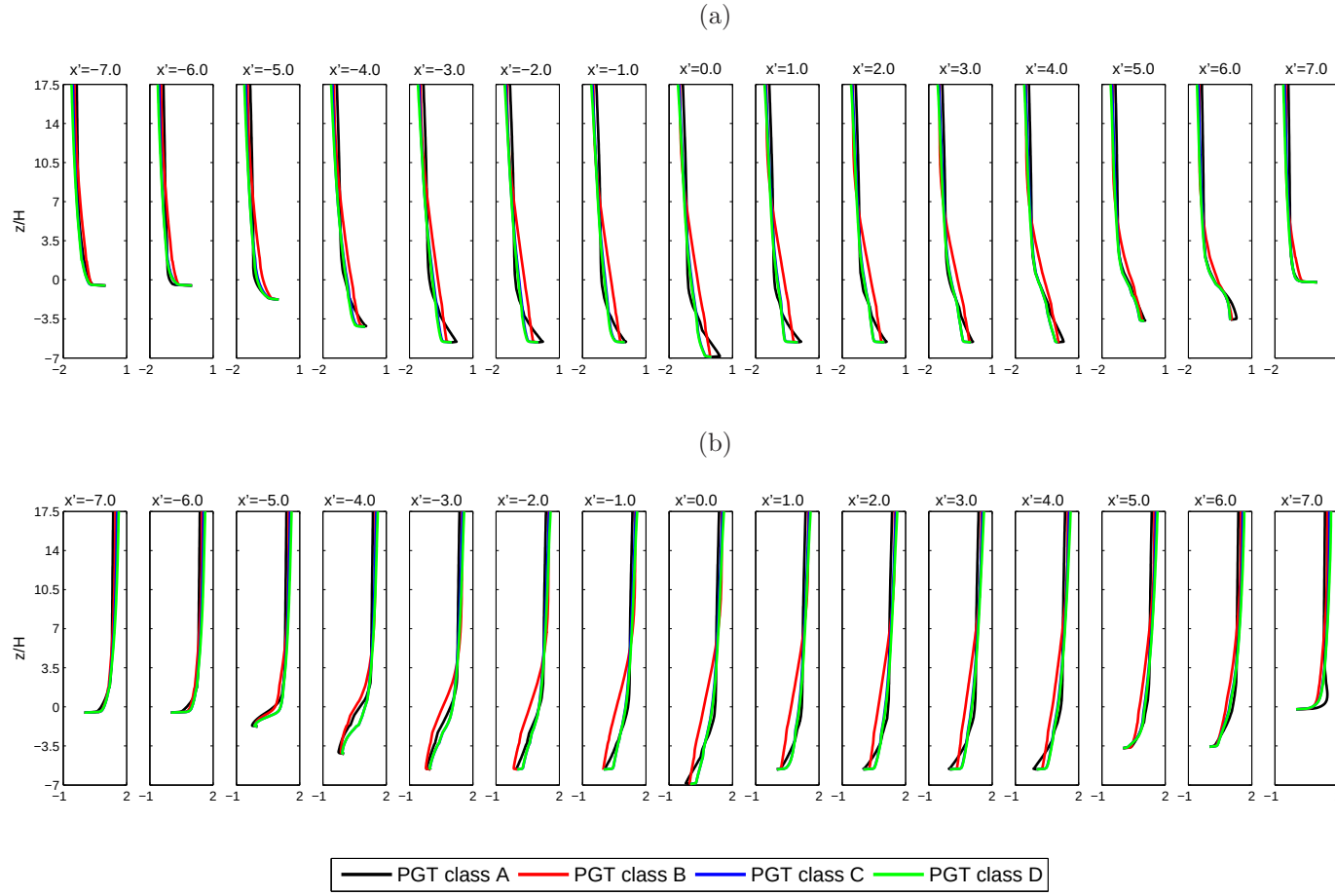


Figure 6.15: Comparison of normalized profiles of the  $u$ -velocity component for stability classes A, B, C and D for a)  $90^\circ$  prevailing wind direction and b)  $270^\circ$  counter-wind direction.

Figures 6.16a and 6.16b show the velocity contour plots predicted for the  $270^\circ$  wind direction to show a continuous distribution of the mean u-velocity component on a plane through  $y = -90$  m; this coincides with the locations of the velocity profile rakes. Two atmospheric stability classes, A and D, have been selected to illustrate the difference in the extent of the separation region between the very unstable and neutral atmospheres. The recirculation regions over the upwind benches of the quarry are larger for the unstable case and a clear demarcation is observed between the recirculating flow region within the pit cavity and the overhead skimming flow, which indicates a decoupling of the unstable ABL within the two deepest benches, C and D. A small recirculation flow bubble forms at the base of bench C as the flow exits the excavation. At the upwind face of the excavation, the flow behaviour indicated by the contours resembles the well-known flow in the vicinity of a backward-facing step, in which a recirculation flow region develops at the base of the step. Conversely, as the flow exits the quarry pit, a forward-facing step flow developed over the crest of bench C.

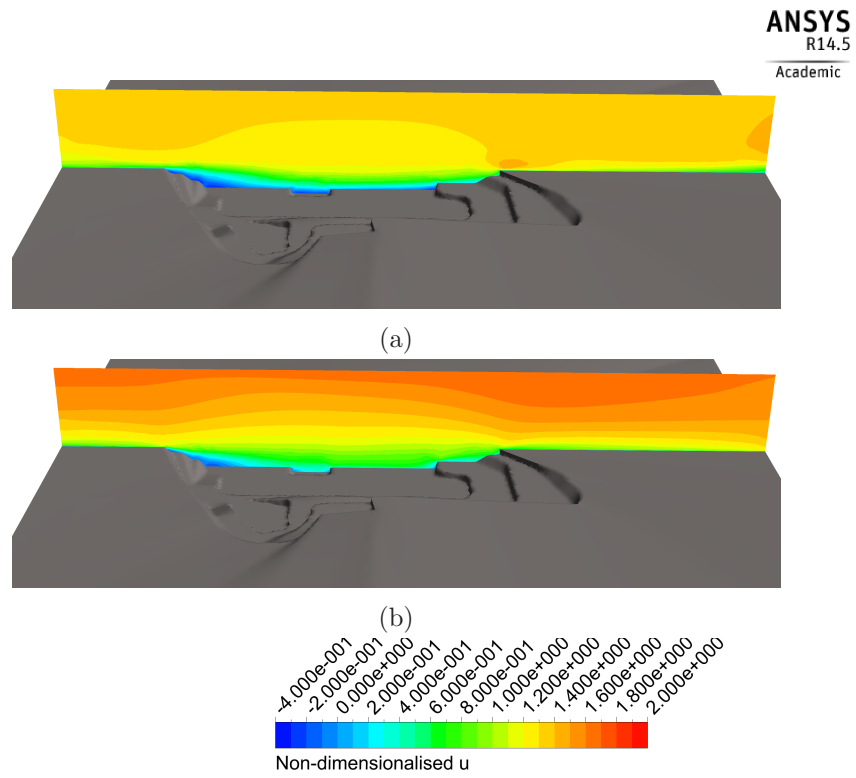


Figure 6.16: Normalized contour plots of  $u$  velocity component at  $y = -90$  m for  $270^\circ$  wind under a) stability class A and b) stability class D.

The turbulence plots generated for both wind directions, Figures 6.17a and 6.17b, show the characteristic near-ground spike in turbulence which was also predicted in the idealized terrain simulations described in Chapter 5. The imposition of stability classes A and B in the model produced the largest spikes in predicted turbulence, although the spike is more localised and confined to the near-wall region for class A. The turbulence spikes are observed where the flow enters and exits the excavation, indicating that this phenomenon is likely to accompany an increase in mechanical shear due to sudden changes in ground surface elevation.

The computed turbulence contour plots shown in Figure 6.18a and Figure 6.18b, are selected to exemplify the variation of the normalized turbulent kinetic energy between the strongly unstable and neutral atmospheres. As with the line graphs, the contours indicate near-wall peaks in the turbulent kinetic energy at the entry to the pit, which again approximates the turbulence characteristics of the flow-field over a backward facing step. Another, albeit smaller peak in turbulent kinetic energy is observed as the flow exits over the forward facing step at the downwind boundary of the pit. The observed increase in turbulent kinetic energy is induced by a combination of the interaction of the flow-field with the pit topography and the buoyancy generated turbulence. The spikes in turbulence are shown to be contained within the quarry excavation and are observed to quickly dissipate within two pit-depths downwind of the pit for stability class A. This is likely to be due to the enhanced vertical mixing associated with this case. The region of elevated turbulent kinetic energy in the upper ABL, above the pit was likely to be non-physical, indicating where the MO similarity modifications have reached the limit of their validity for the very unstable case. As with the idealized terrain cases in Chapter 5, compared to stability class A, the observed increase in near-ground turbulence due to complex terrain is propagated further downwind for a stability class D atmosphere, where the flow is dominated by advection. Compared to turbulence intensity over the flat terrain on the approach to pit an increase in turbulence intensity of about 100% is observed when the flow encounters the upwind face of the pit under stability class A atmospheric conditions. In contrast, a more modest increase of approximately 50% is observed in the vicinity of the benches for the stability class D atmosphere. This difference in turbulence intensity implies that the contribution of thermal buoyancy to the production of turbulence is significant.

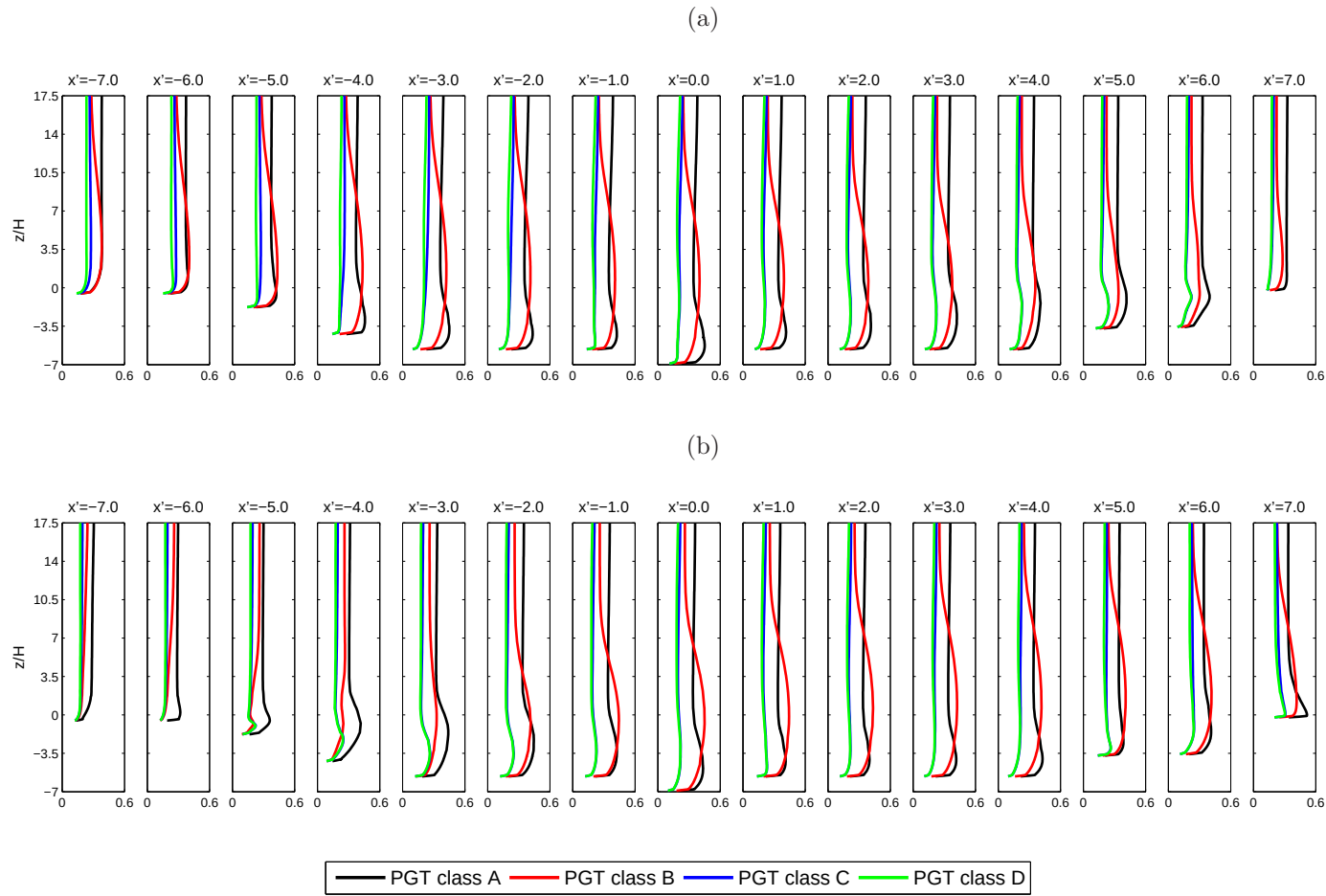


Figure 6.17: Comparison of turbulence intensity profiles for stability classes A, B, C and D for a)  $90^\circ$  prevailing wind direction and b)  $270^\circ$  counter-wind direction.

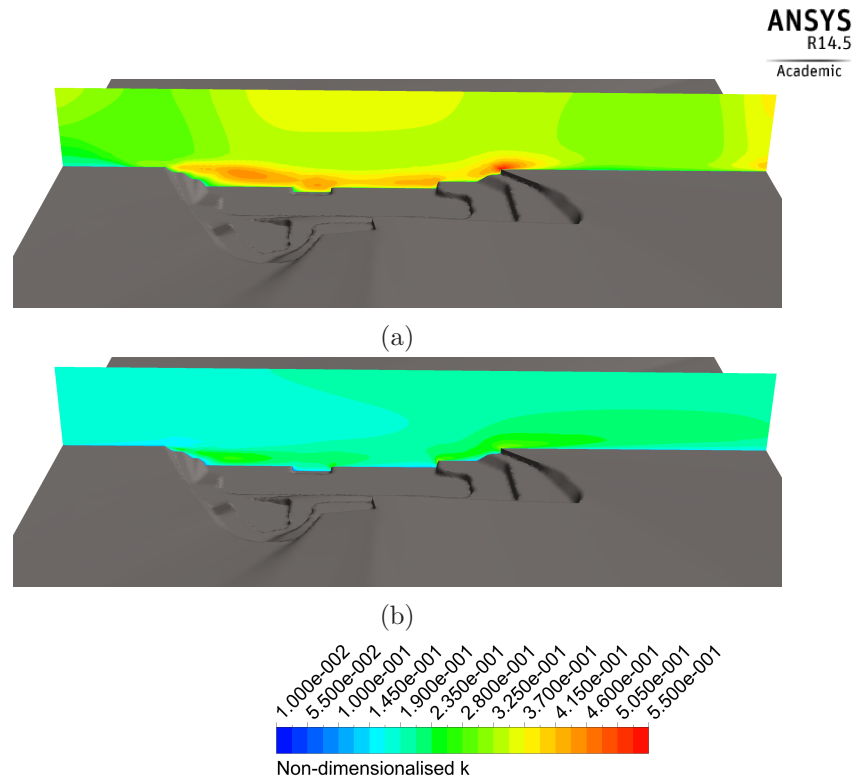


Figure 6.18: Contour plots of  $I = \sqrt{2/3k}/|u_h|$  at  $y = -90$  m for  $270^\circ$  wind under a) stability class A and b) stability class D.

The  $v$  and  $w$  velocity component plots in Figures 6.19a to 6.20b illustrate how the pit topography can cause deviation in the wind direction. The  $v$  and  $w$  components start off with negligible values at the inlet but experience pronounced peaks near the ground in locations which coincide with the formation of primary recirculation bubbles, where the flow enters and exits the excavation. An examination of the  $v$  profiles in particular, indicate how the flow is channelled laterally; in the case of a  $90^\circ$  wind direction, the flow-field is observed to deviate towards the positive  $y$  direction as it traverses the pit.

The non-dimensionalized dust concentration iso-volumes for each PGT stability class in Figure 6.21, show the combined effects of atmospheric instability and pit terrain on predicted plume dispersion. Stability classes A and B produce plumes which appear more dispersed than the other two stability classes investigated. Notably, the iso-volumes of cases A and B appeared to be almost identical in longitudinal extents; the same can be said of cases C and D. This suggests that the model predictions of dust dispersion is less sensitive to small changes in the meteorological variables, and a complete change of the stability regime, for example from unstable to neutral, is necessary to obtain predictions which register a significant change in the dispersive characteristics of the plume.

Due to the location of the blast relative to the identified  $90^\circ$  prevailing wind direction, the in-pit residence time computed for the particulates is greatest for this wind direction, and therefore the potential for in-pit retention increases. Conversely, there is less opportunity for in-pit retention with the counter-wind, as particles emitted near the edge of the pit are transported downwind. The dispersive effects of pit terrain were manifested in the occurrence of a wider, less elongated plume when the particulates were swept across the width of the pit.

In contrast to the  $90^\circ$  prevailing wind, which transports dust emissions across the pit excavation, the  $270^\circ$  wind direction shown in Figure 6.22 produces plumes that are smaller in width, which is indicative of less dispersion. This suggests that here, plume spread over the pit is influenced by a combination of factors, namely the in-pit residence time, the atmospheric stability class and the effects of pit topography on the transporting wind-field.

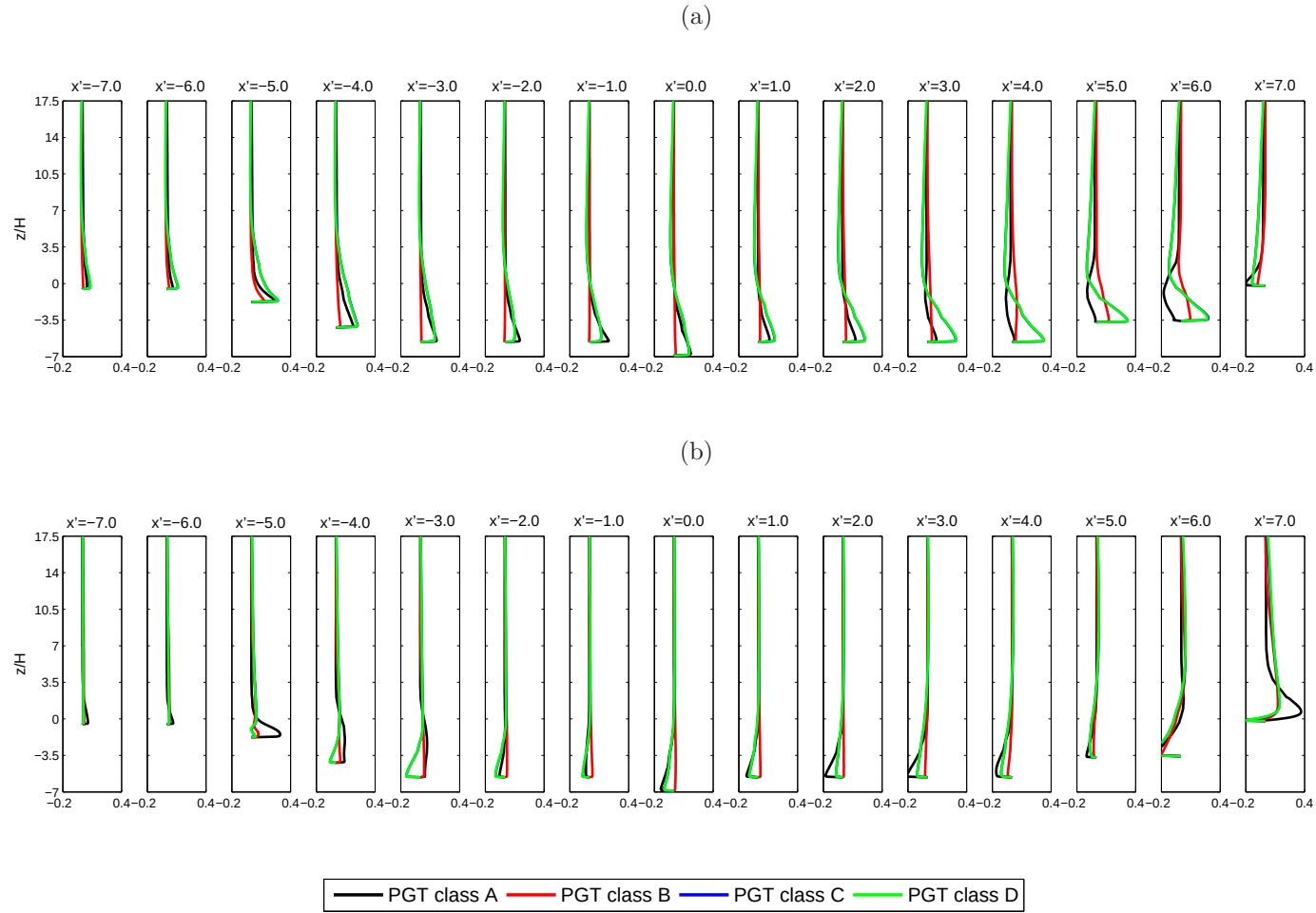


Figure 6.19: Comparison of normalized profiles of the  $v$ -velocity component for stability classes A, B, C and D for a)  $90^\circ$  prevailing wind direction and b)  $270^\circ$ .

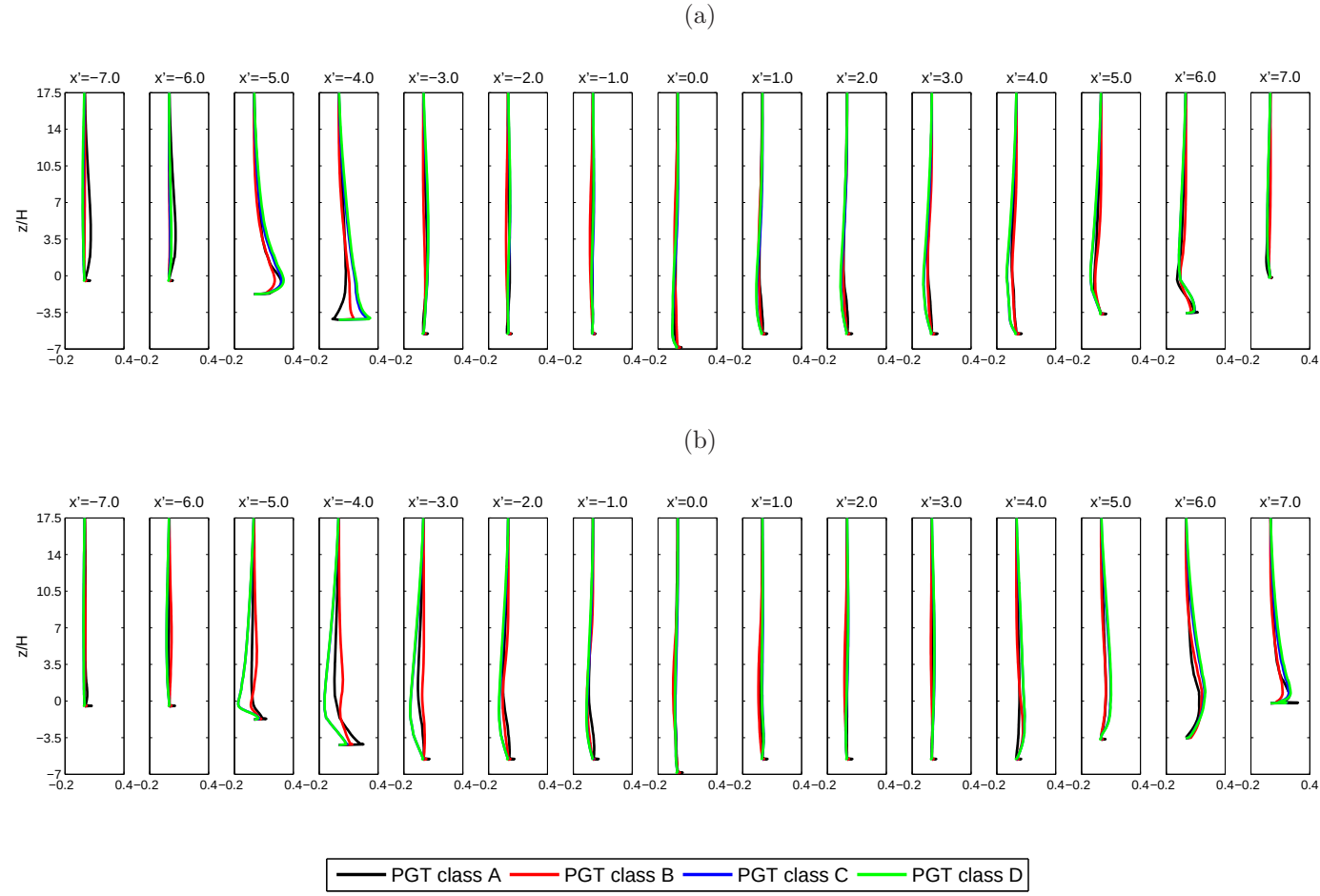


Figure 6.20: Comparison of normalized profiles of the  $w$ -velocity component for stability classes A, B, C and D for a)  $90^\circ$  prevailing wind direction and b)  $270^\circ$  counter-wind direction.

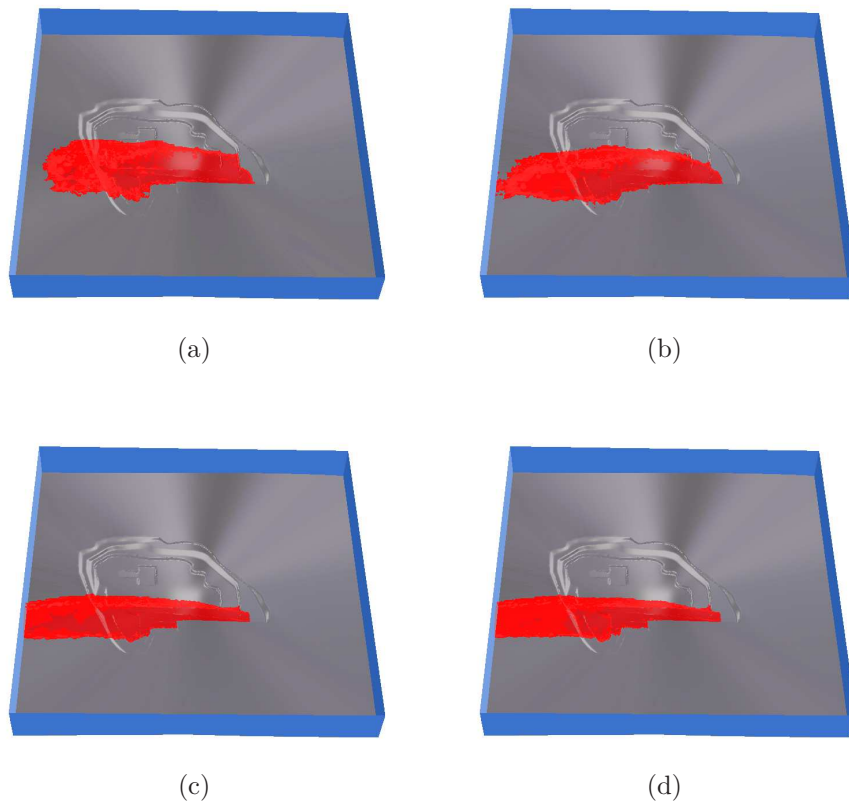


Figure 6.21: Hourly averaged particle mass concentration iso-volume for non-dimensionalized concentration greater than  $5 \times 10^{-4}$ ,  $90^\circ$  wind direction a) Stability class A, b) Stability class B, c) Stability class C and d) Stability class D.

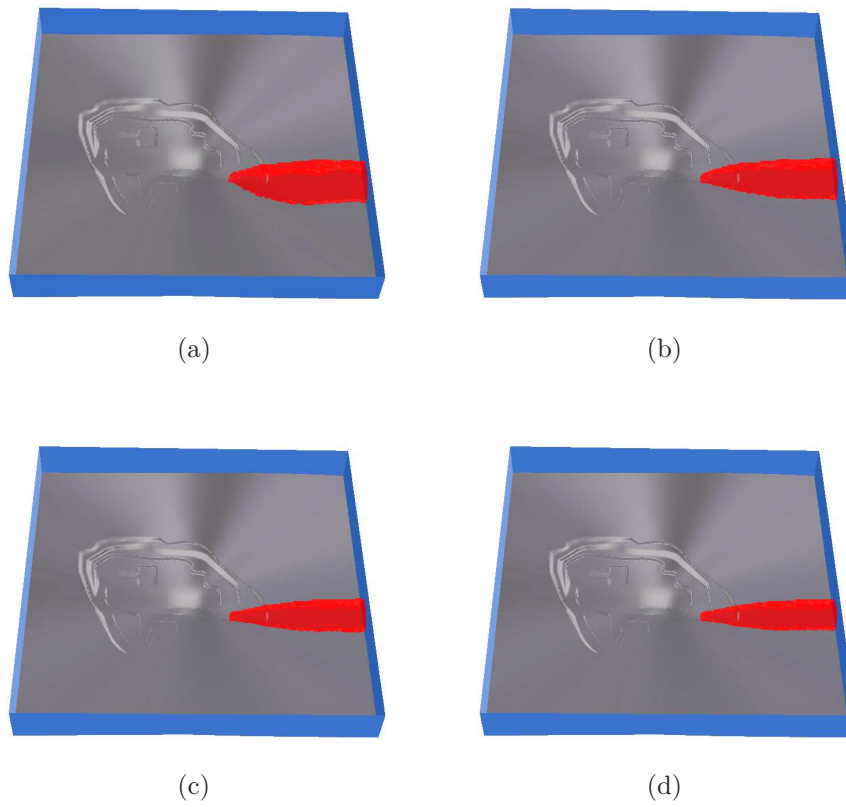


Figure 6.22: Hourly averaged particle mass concentration isovolume for non-dimensionalized concentration greater than  $5 \times 10^{-4}$ ,  $270^\circ$  wind direction a) Stability class A, b) Stability class B, c) Stability class C and d) Stability class D.

## 6.6 Actual Terrain Simulations

The performance of the buoyancy-modified  $k - \varepsilon$  model and its viability as a quarry dust dispersion modelling tool can be assessed through the use of a matching procedure as described by Derwent et al. (2010). This involves conducting a comparison of dust deposition field measurements obtained from the network of on-site Frisbee gauges to cumulative accretion predictions at the same locations in the computational domain. The evaluation of the degree of uncertainty associated with the dispersion model predictions is an integral part of the historic matching process and in this regard, a number of statistical performance metrics recommended by Hanna (1981) have been employed to quantify the uncertainty in model predictions. The general trends in the predicted dust accretion profiles were also examined to determine whether the model is capable of yielding results which satisfactorily approximate the actual dust deposition patterns and in-pit dust retention.

The domain of the actual terrain cases was extended to include the quarry pit and the surrounding landforms inclusive of the Great Rocks Dale Valley. The computational domain encompassed a total area of  $3750\text{ m} \times 3750\text{ m}$  and the top domain boundary is at a height of 400 m. Discretization of the domain was similar to the *Artificial Terrain* case, with the surface geometry of the quarry and surrounding landforms extracted from an STL file. The actual terrain mesh was comprised of 18811415 cells. Simulations using this mesh required distribution of the computations across 2 computed nodes using 16 cores each and 32 GB RAM per node on the University of Nottingham HPC. The run time for the artificial terrain simulations ranged from 8 to 10 hours. The coordinates of the triangle vertices in the STL file were used to generate an  $x, y, z$  terrain file in Comma Separated Values (CSV) format for importing into the UK-ADMS complex terrain utility, this enabled representation of the quarry topography in the UK-ADMS simulations through the use of the in-built FLOWSTAR model.

To accommodate the simulation of multiple wind directions and ensure that the dominant wind component is aligned with the inlet and outlet, the positioning of the pressure outlet has been varied as indicated in Figure 6.23 and accompanying Table 6.6. The top and side boundaries of the computational domain have been defined as velocity inlets.

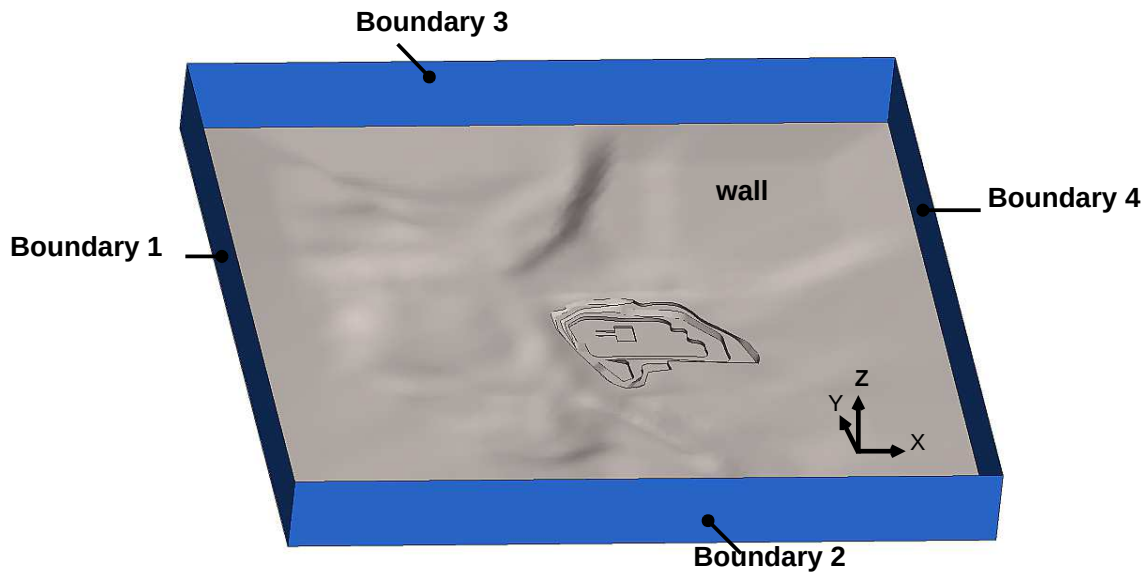


Figure 6.23: The boundaries of the computational domain used for the actual terrain simulations.

Table 6.6: Computational domain boundary conditions applied for different ranges of wind direction for the domain illustrated in Figure 6.23.

| Wind direction                         | Boundary type |            |            |            |
|----------------------------------------|---------------|------------|------------|------------|
|                                        | Boundary 1    | Boundary 2 | Boundary 3 | Boundary 4 |
| $45^\circ \leq \theta \leq 135^\circ$  | pressure      | velocity   | velocity   | velocity   |
|                                        | outlet        | inlet      | inlet      | inlet      |
| $135^\circ \leq \theta \leq 225^\circ$ | velocity      | velocity   | pressure   | velocity   |
|                                        | inlet         | inlet      | outlet     | inlet      |
| $225^\circ \leq \theta \leq 315^\circ$ | velocity      | velocity   | velocity   | pressure   |
|                                        | inlet         | inlet      | inlet      | outlet     |
| $315^\circ \leq \theta \leq 45^\circ$  | velocity      | pressure   | velocity   | velocity   |
|                                        | inlet         | outlet     | inlet      | inlet      |

### 6.6.1 The Influence of upwind topography

Due to the fact that the topographic complexity of the domain was increased in the *Actual Terrain* simulations, the structure of the wind-field over the quarry and upwind landforms was examined along a plane parallel to the wind direction passing through the deepest bench of the pit. The Great Rocks Dale Valley is situated upwind of the quarry and its effects on the approach flow are most prominent for the westerly winds. Here, contour plots of the non-dimensionalized wind-aligned velocity vector,  $u_\theta$ , on a plane aligned with the wind directions from  $245^\circ$  to  $315^\circ$  have been presented in Figures 6.24 to Figure 6.27 to illustrate differences in the in-pit flow regime between the artificial and actual terrain cases in Figure 6.16. The wind-aligned vector is obtained from the expression,

$$u_\theta = \frac{u \sin \theta + v \cos \theta}{u_{10}}. \quad (6.13)$$

Figures 6.16a and 6.16b show that the approach flow conforms to the logarithmic velocity profile upwind of the quarry pit for the Artificial Terrain cases. Recirculation flow is confined to the pit cavity, mainly in the wake of the backward facing step formed by the upwind benches and also over the deepest bench. In Figure 6.24, the wind vector is visualized on a plane aligned with the direction of the mean wind, indicated by the arrow, and traversing the deepest section of the Great Rocks Dale Valley. The flow decelerates within the Great Rocks Dale Valley and then accelerates up the valley ridge. Thus the initial inlet wind profile is disturbed by the valley and remains so before the flow encounters the pit terrain. Consequently, the in-pit flow regime is noticeably different from the artificial terrain scenario, as a separation zone does not develop on the backward facing step at the entrance to the pit. The other contour plots, Figures 6.25 to 6.28 show the progression as the wind direction changes until it is almost perpendicular to the long axis of the pit, where the wind approaches from the south west at the shallowest part of the valley. The plots show, that development of a separated flow region at the entrance to the pit, is dependent on the upwind topography. Where the approach flow is not significantly perturbed by the upwind topography, for example Figures 6.26, 6.27 and 6.28, the familiar backward facing step reverse flow regime develops at the upwind bench faces.

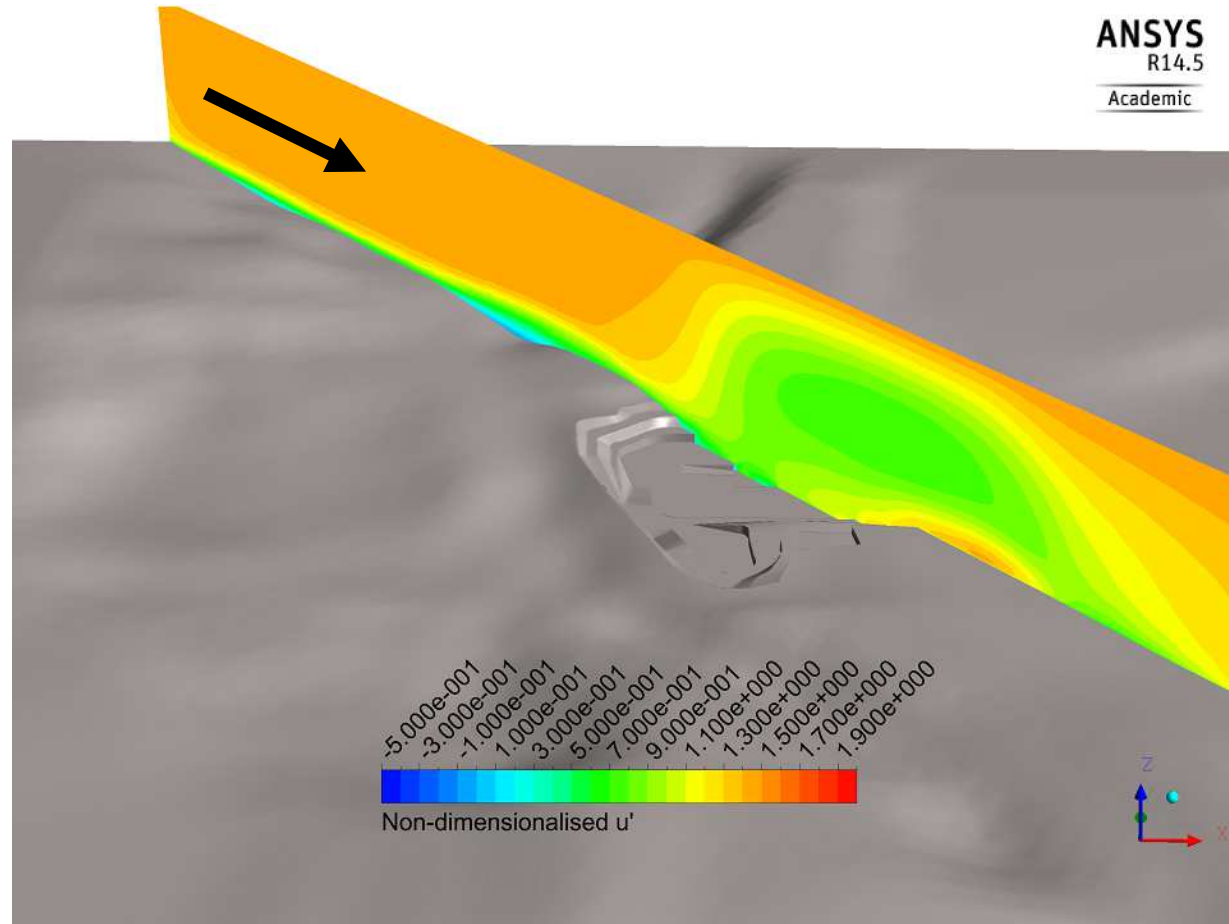


Figure 6.24: Non-dimensionalized  $u_\theta$  contour plots for  $\theta = 310.1^\circ$ , on 16<sup>th</sup> June.

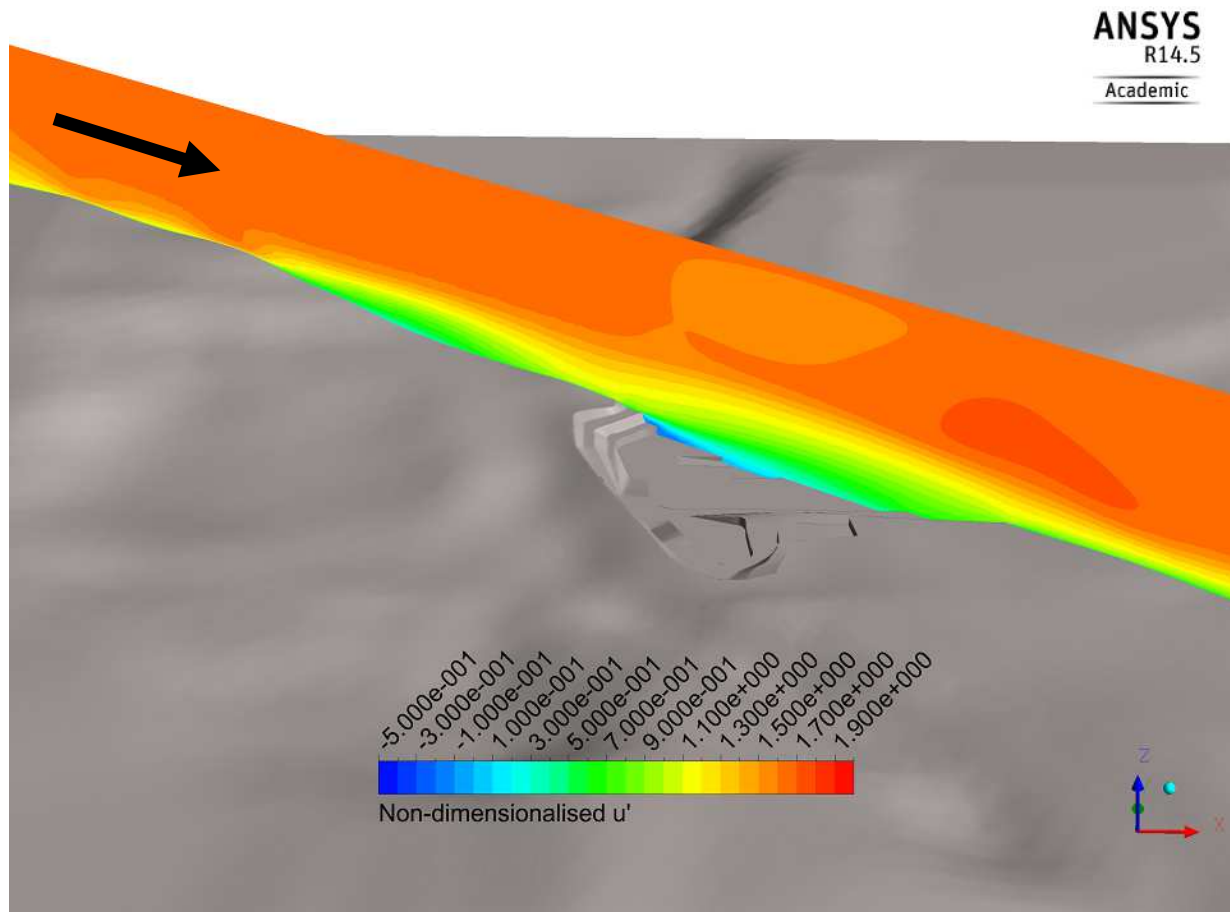


Figure 6.25: Non-dimensionalized  $u_\theta$  contour plots for  $\theta = 306.2^\circ$  on 6<sup>th</sup> July.

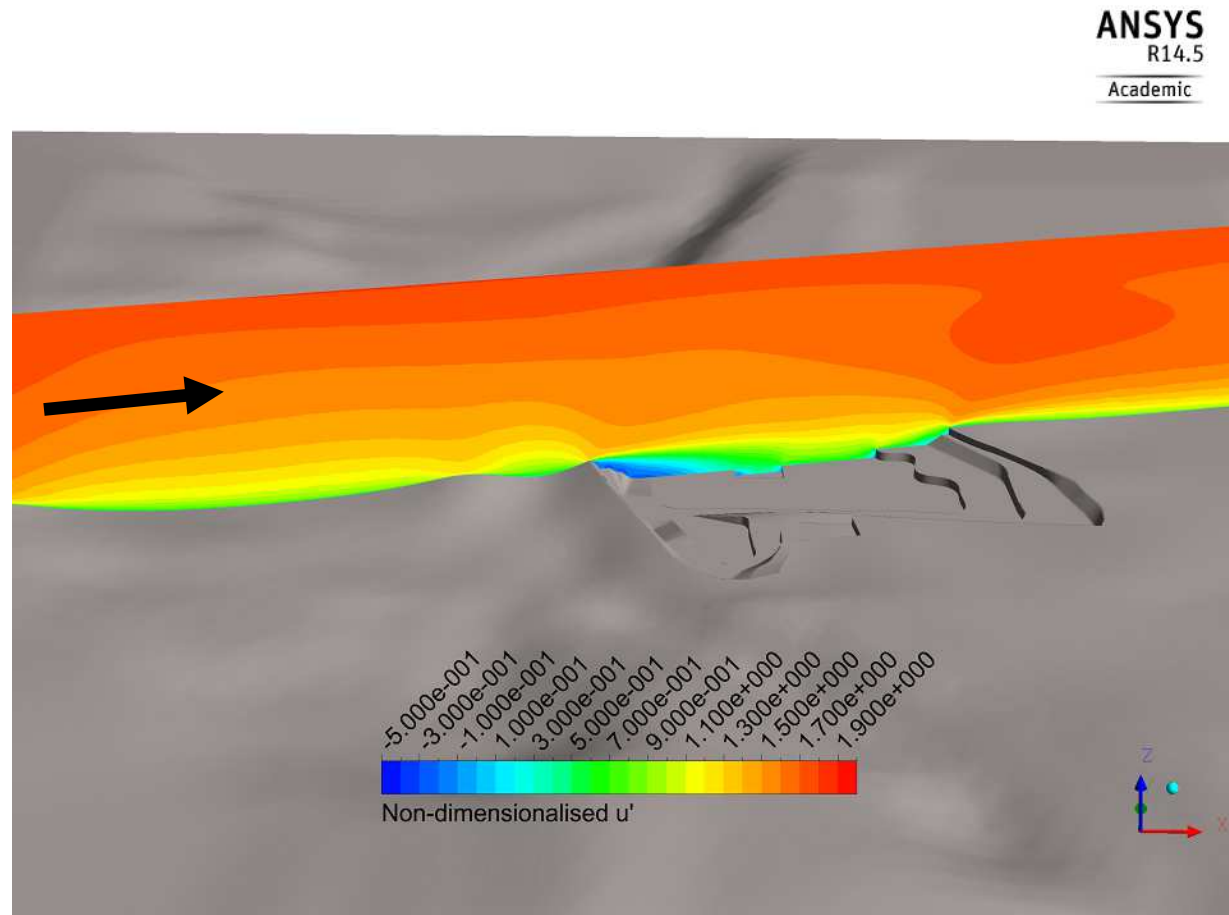


Figure 6.26: Non-dimensionalized  $u_\theta$  contour plots for  $\theta = 258.2^\circ$ , on 22<sup>nd</sup> June.

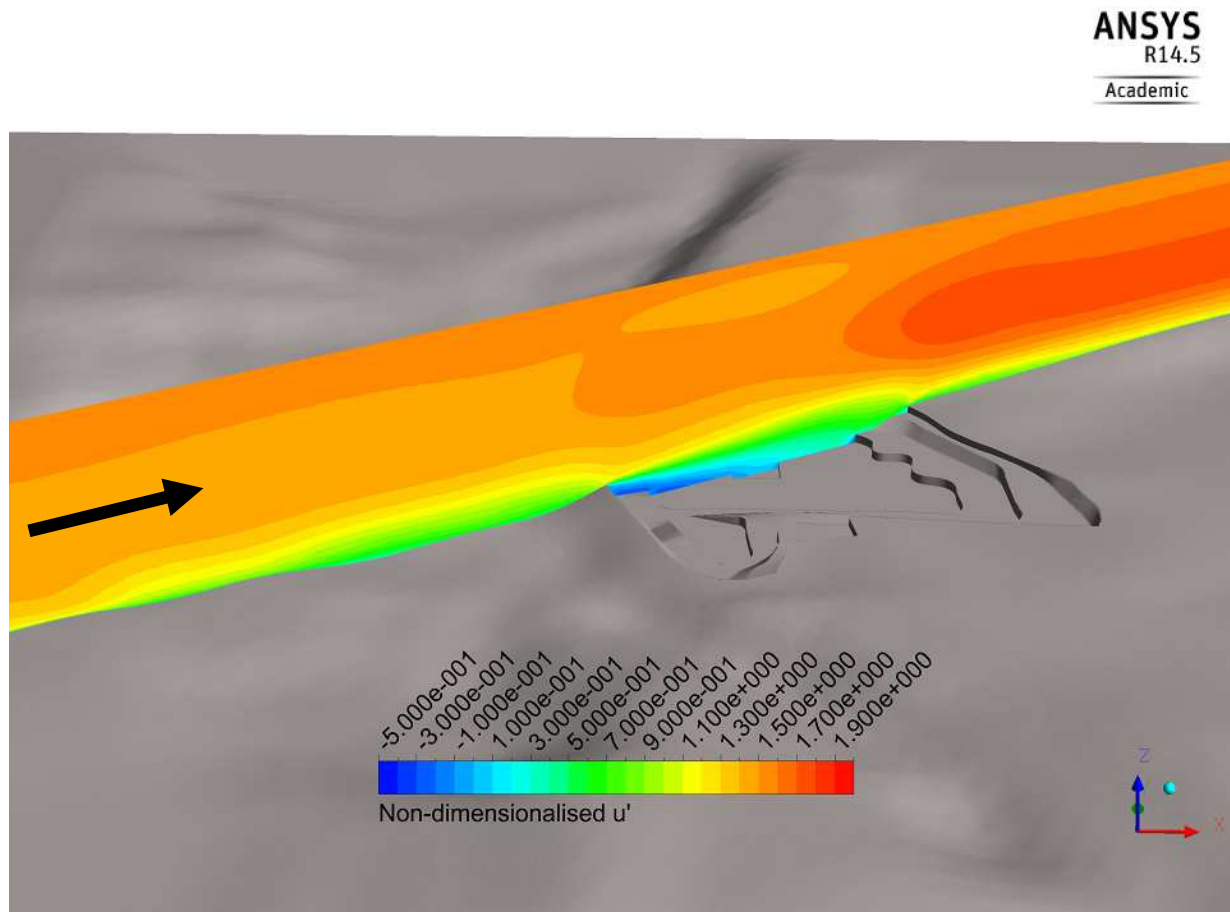


Figure 6.27: non-dimensionalized  $u_\theta$  contour plots for  $\theta = 240.5^\circ$  on 21<sup>st</sup> June.

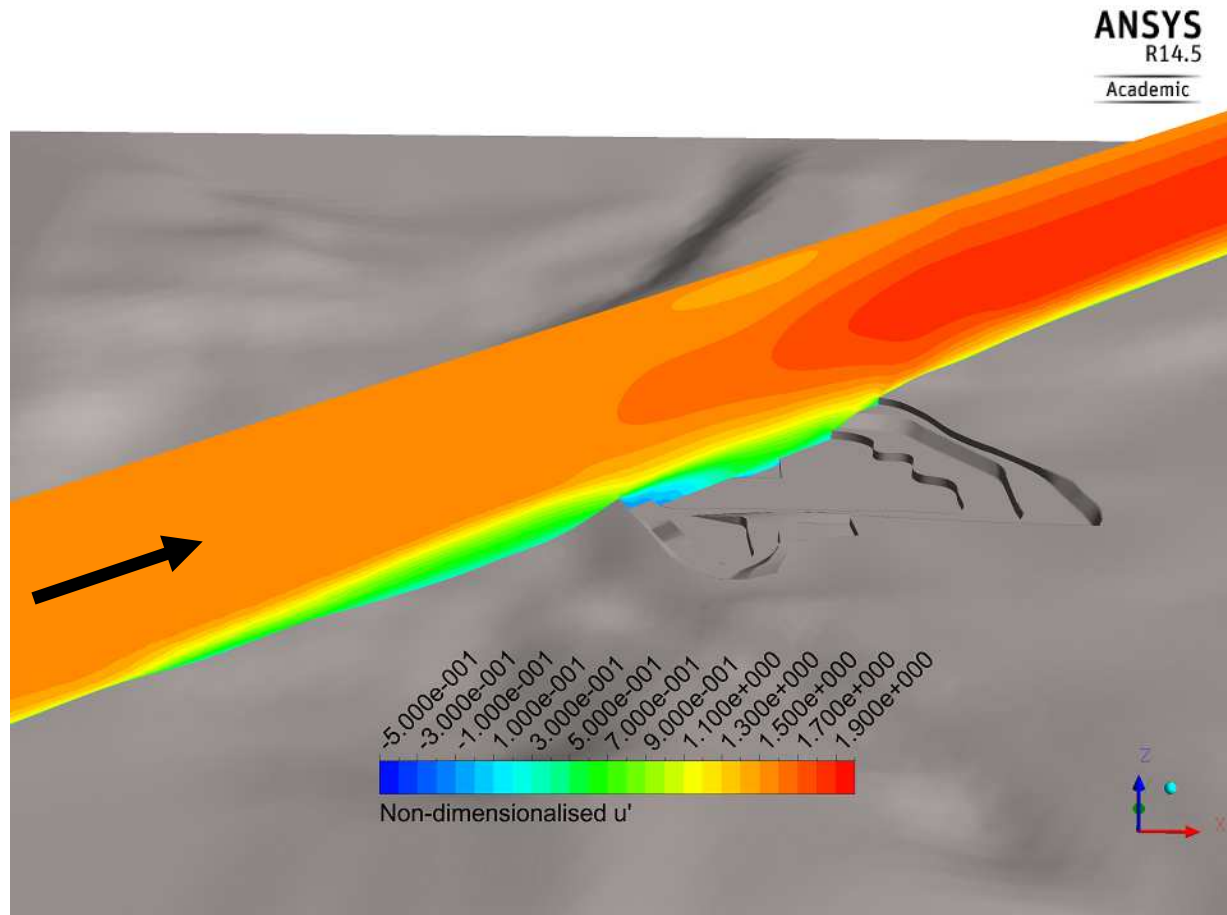


Figure 6.28: non-dimensionalized  $u_\theta$  contour plots for  $\theta = 230.6^\circ$ , on 19<sup>th</sup> June.

### 6.6.2 Evaluating the $k - \varepsilon$ Model Uncertainty

Derwent et al. (2010) noted that it is virtually impossible to replicate the full extent of stochastic atmospheric wind systems in a dispersion model, and as such simplifying assumptions are typically adopted to allow the model to simulate the limited range of atmospheric length scales that are most relevant to the turbulent transport processes influencing the dispersion of air pollutants. Whilst these simplifications reduce model complexity, they contribute to uncertainty and error in model predictions. Additionally, DEFRA (2009) advise that differences between dispersion model predictions and site measurements of pollutant dispersion are bound to arise in dispersion models which rely on the use of emission factor estimates to quantify source activity. Approximations of the site meteorology, which are necessary to supply meteorological input parameters that cannot be directly measured at the site, also limit the accuracy of the model. These approximations are not unique to the modified  $k - \varepsilon$  model proposed in this work and are routinely used in conventional Gaussian models.

It therefore becomes essential to evaluate the uncertainty in dispersion model predictions through the use of statistical performance metrics which assess how well model predictions correlate with field observations. Ultimately, the current work seeks to establish whether quantifiable gains have been realised in the accuracy of dust dispersion predictions from the quarry using the buoyancy modified  $k - \varepsilon$  model. Therefore, evaluation of the  $k - \varepsilon$  model uncertainty is conducted in parallel with that of UK-ADMS, to establish a baseline for evaluating the  $k - \varepsilon$  model performance.

### 6.6.3 Performance Metrics for Dispersion Model Evaluation

Chang and Hanna (2004) have recommended the application of multiple statistical performance metrics for validation of numerical models because individual metrics are not universally applicable to all dispersion conditions and some may be overly skewed by outlying values. Most dispersion model evaluation studies have made use of the Fraction of values within a factor of two of observations, FAC2, which Chang and Hanna (2004); Hanna et al. (2004) describe as the most robust performance metric because it is not overly influenced by outliers. FAC2 is determined from the proportion of the data satisfying,

$$0.5 \leq \frac{X_p}{X_o} \leq 2.0, \quad (6.14)$$

where the subscripts  $p$  and  $o$  denote predicted and observed values respectively, and  $X$ , in the context of this study represents the total mass of deposited dust. Besides FAC2, other statistical performance criteria have been selected for evaluating the reliability of dispersion model predictions in line with recommendations by DEFRA (2009). Metrics such as the Fractional Bias, FB, involve normalization of the mean error between model predictions and actual field measurements and are not skewed to favour models that either over-predict

or under-predict deposition (Hanna, 1988),

$$FB = \frac{\overline{X_o} - \overline{X_p}}{0.5 (\overline{X_o} + \overline{X_p})}. \quad (6.15)$$

Like the FB, the geometric mean bias MG, evaluates the mean error, but on a logarithmic scale. It offers a more balanced treatment of datasets in which individual results vary by several orders of magnitude, however MG is undefined for any zero values which appear in the dataset (Chang and Hanna, 2004),

$$MG = \exp (\overline{\ln X_o} - \overline{\ln X_p}) . \quad (6.16)$$

The preceding metrics are useful insofar as quantification of systematic error is concerned. These errors arise from any inaccuracies in the numerical model or dust deposition measuring apparatus and tend to consistently appear across the entire dataset, leaning towards either over-prediction or under-prediction of deposition values. Consequently, another type of performance metric is required to quantify random errors and ascertain the degree of scatter in the data. The normalized mean square error, NMSE is recommended as one such metric which can be used to evaluate uncertainty arising from a combination of systematic and random errors (Hanna et al., 2004; Chang and Hanna, 2004),

$$NMSE = \frac{\overline{(X_o - X_p)^2}}{\overline{X_o} \overline{X_p}}. \quad (6.17)$$

Chang and Hanna (2004) have derived a relation between NMSE and FB to determine the component of NMSE which is due to systematic errors,

$$NMSE_s = \frac{4FB^2}{4 - FB^2}, \quad (6.18)$$

subsequently the random component of the total NMSE, can be obtained from,

$$NMSE_r = NMSE - NMSE_s. \quad (6.19)$$

In dispersion studies which attempt to analyse the degree of correlation between the observed and predicted data sets, the correlation coefficient  $R^2$  is often computed as a de facto metric for establishing the linear relationship between observed and modelled concentration or deposition. However, Derwent et al. (2010) advise that since  $R^2$  may be significantly influenced by outliers in a dataset, it should not be used with small datasets with less than 20 data pairs, where its value is easily distorted by anomalies manifested in one or two data pairs. Therefore, since the current study contains only 10 deposit gauge readings,  $R^2$  is not employed as a model performance metric. Hanna et al. (2004) have recommended ranges of the performance metrics for which a numerical dispersion model can be considered suitable for research grade experiments. These include an  $FAC2 > 0.5$ , which indicates that over 50% of predictions fall within a factor of 2 of the observations. The mean bias must be within 30% of the mean such that  $-0.3 < FB < 0.3$  and  $0.7 < MG < 1.3$  and a value of  $NMSE_r < 4$  is considered acceptable for the normalized mean square error component due to random scatter.

#### 6.6.4 Using Frisbee Gauge Measurements to Validate the Model

Simulations over the actual quarry terrain included the elevation profile of the surrounding topography and were conducted to predict dust deposition at specific locations in the domain which corresponded to those of the Frisbee gauges stationed at the Old Moor Quarry site. A MIST funded dust monitoring campaign described by Lowndes et al. (2008) was conducted several years prior to this study to deliver dust deposition data for the validation of quarry dust dispersion models. The campaign consisted of the installation of a network of Frisbee gauges at locations outside the south-eastern perimeter of the Old Moor site. The Frisbee gauges each had an effective collection area,  $C_A$ , of  $4.047 \times 10^{-2} \text{ m}^2$ . The collectors were emptied after each monitoring period of roughly one month and gravimetric analyses were performed using a Malvern Mastersizer<sup>TM</sup> to determine the mass of dust retained in each gauge.

The blast logs indicated that bench blasting operations were only conducted on 17 days of the monitoring campaign. The duration of a blast event is generally less than 2 s - from detonation of the explosives to collapse of the bench face and depends on the timing of delay sequences used to detonate the explosive charges. This study is concerned with the dispersion of the dust cloud formed after the blast explosion, thus, the initial state of the particles described in the injection file assumes the energy imparted to the particles by the blast has been dissipated to the surrounding air through viscous drag. Particle injection points were horizontally distributed at 1.67 m intervals throughout the representative plan area of the blast cloud. The injection distribution in the vertical direction along the height of the bench was also 1.67 m. Thus, for the minimum bench height of 13.00 m, a single blast injection was represented using 69120 particles. The simulations were set up to account for the hourly-averaged meteorological conditions at the time of each blast event and continuous dust emission rates were computed to distribute the mass of liberated dust over the meteorological averaging time. The blast logs also recorded some instances of simultaneously blasting at two benches on the same day and accordingly, dust emissions from both bench locations were modelled in the same simulation. The case study simulations characterize the atmospheric conditions at each blast event using the prevailing wind direction and average meteorological parameters corresponding to the PGT classification observed at the time of the blast event. The total accumulated dust  $M_T$  for the monitoring period was calculated using the expression,

$$M_T = \sum_{n=1}^{N_B} \dot{A} \times T_{\text{exposure}} \times C_A, \quad (6.20)$$

where  $T_{\text{exposure}}$  is the time duration of exposure of the gauges to the constant accretion flux  $\dot{A}$  predicted for a blast event.  $N_B$  is the total number of blast events over the monitoring period. Whilst the monitoring period was 41 days, depletion of dust from the ambient air would lead to a reduction in the deposition flux at each receptor location over time. Since the simulations employ a continuous dust emission rate to provide steady-state predictions of the dust accretion, it was deemed necessary to specify an exposure duration over which

the constant deposition flux predicted by the the model would be applicable. Therefore the exposure duration was taken as the meteorological averaging time. The UK-ADMS predictions of dry deposition flux were processed in the same way to ensure consistency in the treatment of both sets of predictions.

Figure 6.29 presents a schematic of the location of Frisbee dust gauges 1 to 10. The Eastings and Northings and  $x, y, z$  coordinates of the Frisbee gauges are listed in Table 6.7 relative to the origin at Eastings 410557, Northings 374269 and  $z$ -coordinate -37.00. The observed dust deposition is equivalent to the mass of dust accumulated on the filtration medium. Table 6.9 contains observed deposition as well as dust deposition predicted by UK-ADMS and the  $k - \varepsilon$  model. The  $k - \varepsilon$  predictions consist of two datasets, one of which incorporates the wind direction variability correction. For each of these datasets, a reduction of the emission factor has been considered resulting in two sub-datasets, *EF100* and *EF50* which correspond to 100% and 50% of the emission factor respectively.

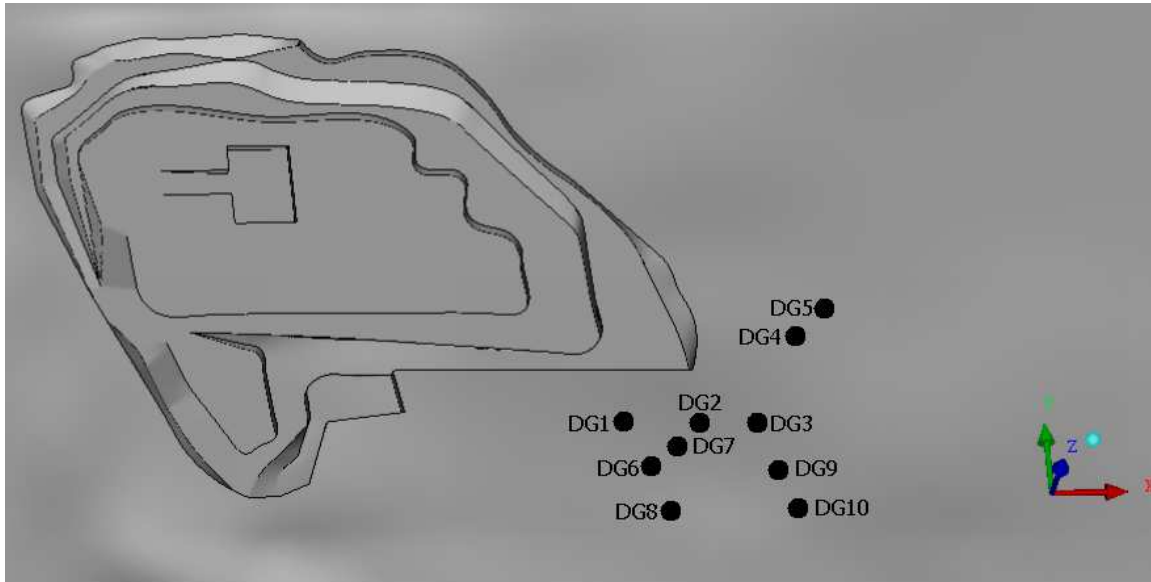


Figure 6.29: Layout of Frisbee dust gauge positions relative to quarry pit. The gauges are indicated by solid black circles labelled DG1 to DG10.

The wind variability post-processing methodology has been applied to obtain weighted summations for the five blast events which contributed most to dust deposition at the gauge locations. Therefore simulations have been carried out in the interval  $\mu_\theta - 3\sigma_\theta$  to  $\mu_\theta + 3\sigma_\theta$ , about the mean wind direction for these blasts. Table 6.8 gives the prevailing wind direction and speed for each of these blast events, since the wind speed was generally above  $5 \text{ ms}^{-1}$ , the minimum  $\sigma_\theta = 5^\circ$  has been applied. The weighted averaging procedure presented in Chapter 4 has been applied to weight each set of predictions according to a Gaussian probability density function. In this way, wind variability averaged accretion rates

Table 6.7: Coordinates of Frisbee Gauges in the domain.

| Gauge ID | Eastings | Northings | $x$ (m) | $y$ (m) | $z$ (m)   |
|----------|----------|-----------|---------|---------|-----------|
| FG1      | 411110   | 373748    | 553     | -522    | 16.18171  |
| FG2      | 411222   | 373750    | 665     | -520    | -14.22400 |
| FG3      | 411320   | 373750    | 763     | -519    | 9.00241   |
| FG4      | 411400   | 373900    | 844     | -370    | -1.44099  |
| FG5      | 411455   | 373936    | 899     | -333    | -2.11196  |
| FG6      | 411150   | 373670    | 593     | -600    | 19.12733  |
| FG7      | 411192   | 373700    | 635     | -570    | 18.22342  |
| FG8      | 411170   | 373600    | 614     | -669    | 18.57594  |
| FG9      | 411348   | 373660    | 792     | -609    | 11.90443  |
| FG10     | 411372   | 373600    | 816     | -669    | 11.19840  |

were determined at each gauge location for the blast event.

Table 6.8: Values of  $u_h$ ,  $\theta$  and  $\sigma_\theta$  for blast events contributing the most to accumulated mass of dust at the gauges.

| Blast<br>date          | 0906  | 1606  | 1906  | 2106  | 2206  |
|------------------------|-------|-------|-------|-------|-------|
| $u_h$ ms <sup>-1</sup> | 5.6   | 4.5   | 6.0   | 7.8   | 9.2   |
| $\theta$ °             | 124.5 | 310.1 | 230.6 | 240.5 | 258.5 |
| $\sigma_{wd}$ °        | 5     | 5     | 5     | 5     | 5     |

The occurrence of zero values in the CFD dataset without wind variability is likely to be indicative of a deficiency in the number of particles used to define the volumetric injection source, since accretion rates at a specific location on the wall boundary are dependent on particles colliding with the wall at that location.

Table 6.9: Predicted dust deposition from CFD and UK-ADMS numerical models compared to site observations of accumulated dust on Frisbee Gauge

| Gauge ID | No wind variability |                   | wind variability  |                   | UK-ADMS | Observations |
|----------|---------------------|-------------------|-------------------|-------------------|---------|--------------|
|          | EF <sub>1.0</sub>   | EF <sub>0.5</sub> | EF <sub>1.0</sub> | EF <sub>0.5</sub> |         |              |
|          | (g)                 | (g)               | (g)               | (g)               | (g)     | (g)          |
| FG1      | 1.64E-1             | 8.20E-2           | 1.68E-1           | 8.40E-2           | 5.07E-1 | 1.36E-1      |
| FG2      | 4.12E-2             | 2.06E-2           | 4.95E-2           | 2.48E-2           | 3.95E-1 | 1.03E-1      |
| FG3      | 1.08E-1             | 5.39E-2           | 5.52E-2           | 2.76E-2           | 1.55E-1 | 1.07E-1      |
| FG4      | 4.17E-1             | 2.08E-1           | 3.01E-1           | 1.50E-1           | 1.91E-2 | 1.10E-1      |
| FG5      | 3.33E-1             | 1.67E-1           | 3.06E-1           | 1.53E-3           | 4.10E-1 | 2.67E-2      |
| FG6      | 0.00E+0             | 0.00E+0           | 4.24E-3           | 2.12E-2           | 3.05E-1 | 6.61E-2      |
| FG7      | 7.50E-2             | 3.75E-2           | 7.73E-2           | 3.87E-2           | 3.10E-1 | 6.38E-2      |
| FG8      | 7.38E-2             | 3.69E-2           | 4.16E-2           | 2.08E-3           | 2.09E-1 | 5.97E-2      |
| FG9      | 4.51E-2             | 2.26E-2           | 1.38E-2           | 6.88E-3           | 8.77E-2 | 5.50E-2      |
| FG10     | 2.73E-2             | 1.37E-2           | 7.62E-3           | 3.63E-3           | 6.40E-2 | 5.00E-2      |

### 6.6.5 Discussion of the $k - \varepsilon$ Model Performance

The  $k - \varepsilon$  model predictions of cumulative dust deposition over the measurement period have been compared to field observations as well as UK-ADMS predictions. The scatter plots in Figures 6.30 to 6.31 illustrate the correlation between predicted and observed deposition. DEFRA (2009) recommends that log values of the data also be compared to determine the correlation between predicted and measured values on a logarithmic scale. Normalization of the data by either the mean observed or mean predicted deposition is recommended in order to offset systematic errors. In the current work these recommendations have been adopted. In addition, 1:2, 2:1 and 1:1 correlation lines have been superimposed on the plots to permit assessment of  $FAC2$  in accordance with the model performance evaluation procedure prescribed by Derwent et al. (2010).

From the scatter plots, it appears that UK-ADMS has a tendency to over predict deposition by a factor of 4. Approximately 60% of the UK-ADMS predictions are greater than 2 times the observed deposition and 30% fall within a factor of 2 of the observations. In contrast, only 20% of  $k - \varepsilon$  model predictions using 100% emission factor are greater than 2 times the observations and 60% fall within a factor of 2 of the observations. Out of the 60% of predictions that were within a factor of 2 of the observations, one was an approximate match. In general, UK-ADMS predictions contain the highest scatter. Application of the wind variability modification reduces the scatter of the CFD predictions compared to UK-ADMS. This method computes a resultant plume using probability-weighted averaging of a number of simulation results according to the methodology presented in Chapter ??, thus it is able to smooth out some of the scatter arising from the random fluctuations in individual simulation results. The linear, logarithmic scale and normalized scatter plots all display corresponding trends with regards to the distribution of the data points in each dataset about the 1:1 correlation line. However, the  $k - \varepsilon$  model predictions are more evenly distributed about the 1:1 line than those of UK-ADMS.

The introduction of wind variability modifications leads to a reduction in the dust deposition predictions of the  $k - \varepsilon$  model. In Chapter 4, wind variability modifications increased lateral plume spread due to the Gaussian probability averaging of the plume over three standard deviations from the mean wind. Over flat terrain, this resulted in a reduction of the peak deposition as well as shortening of the plume length. A similar trend is observed over the quarry in terms of the reduction in the dry deposition predicted by the wind variability modified  $k - \varepsilon$  model. This may ultimately be a closer approximation of the dust deposition arising from the blasts, after the contribution of background dust and dust from other quarry sources is deducted.

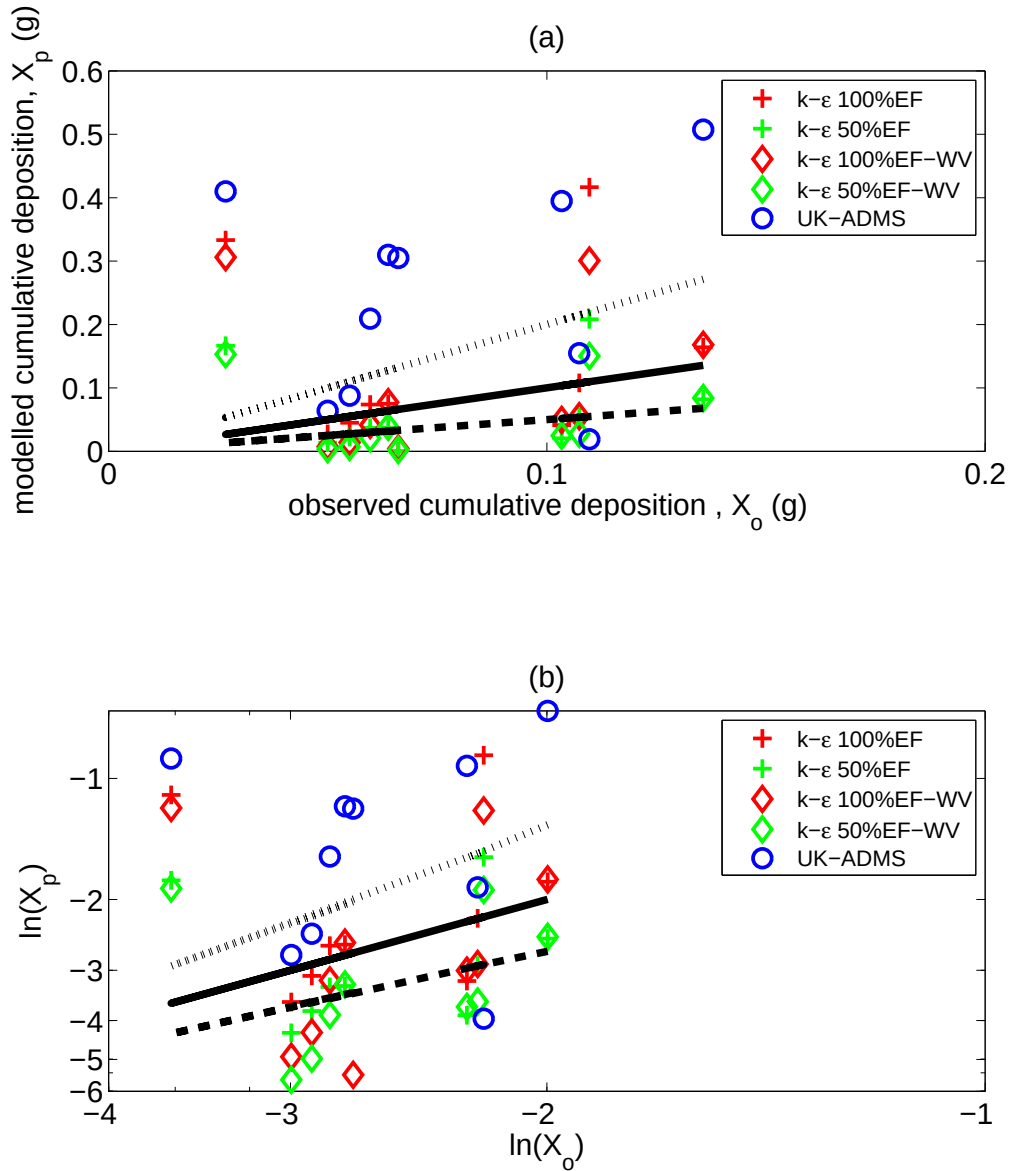


Figure 6.30: Dust deposition observations compared to CFD and ADMS predictions, with and without wind variability correction and emission factor reduction for a) raw data and b) data on a logarithmic scale. The dotted line represents 2:1, solid line represents 1:1 and dashed line represents 1:2

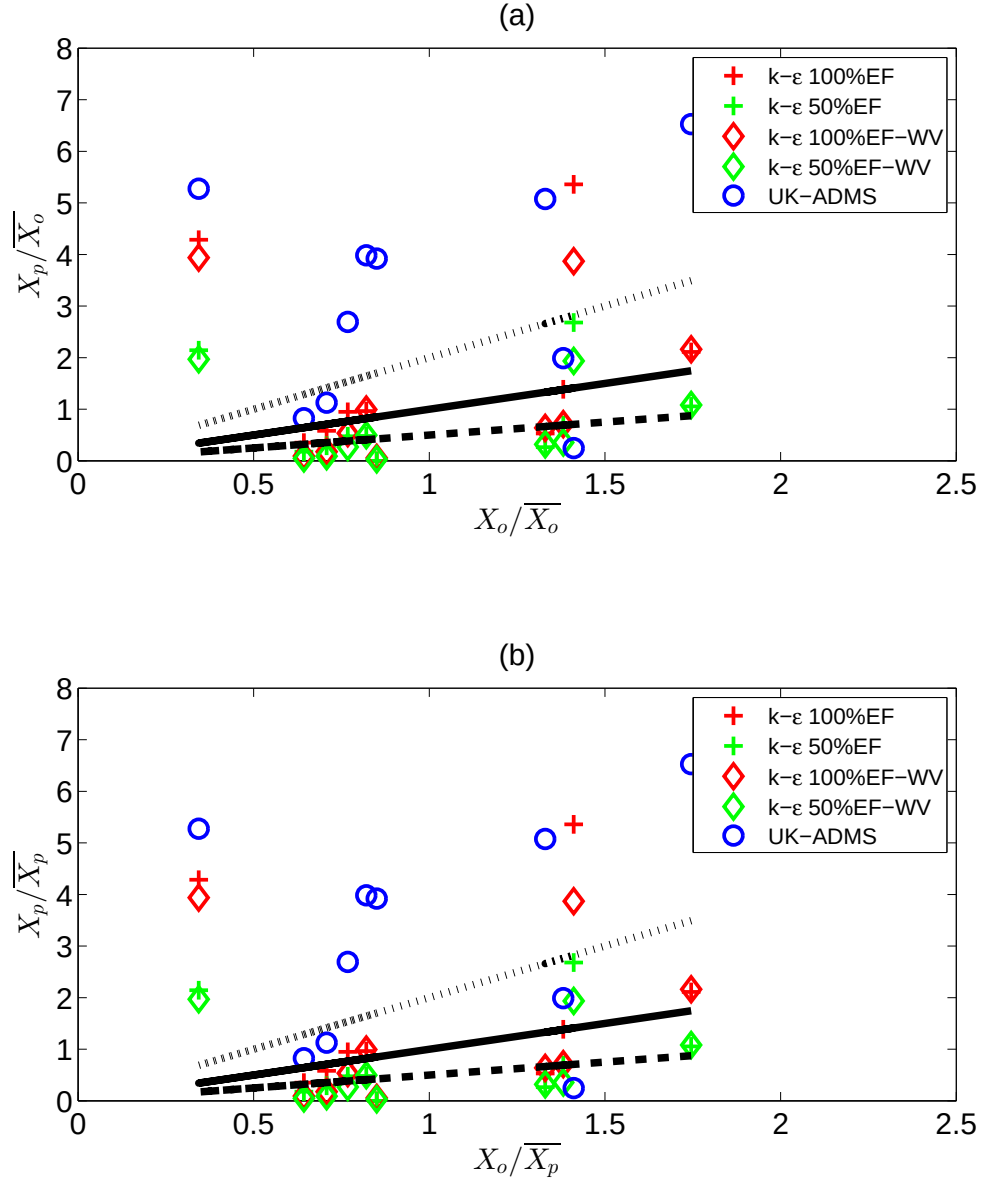


Figure 6.31: Dust deposition observations compared to CFD and ADMS predictions for a) data normalized by the mean observed deposition and b) data normalized by the mean predicted deposition. The dotted line represents 2:1, solid line represents 1:1 and dashed line represents 1:2

Figure 6.32 compares the predicted and observed deposition at each gauge location. According to Barratt (2001), the degree of uncertainty associated with atmospheric dispersion modelling is typically about 50%, however incorrect specification of the input data, such as wind direction and gauge coordinates can produce significant inaccuracies in the model results leading to greater uncertainty, as a result an accuracy up to a factor of two is still considered acceptable for regulatory dispersion models. Error bars have been included in the plot to represent the degree of uncertainty between the predicted and observed data, they range from 0.5 to 2.0 times the observation values.

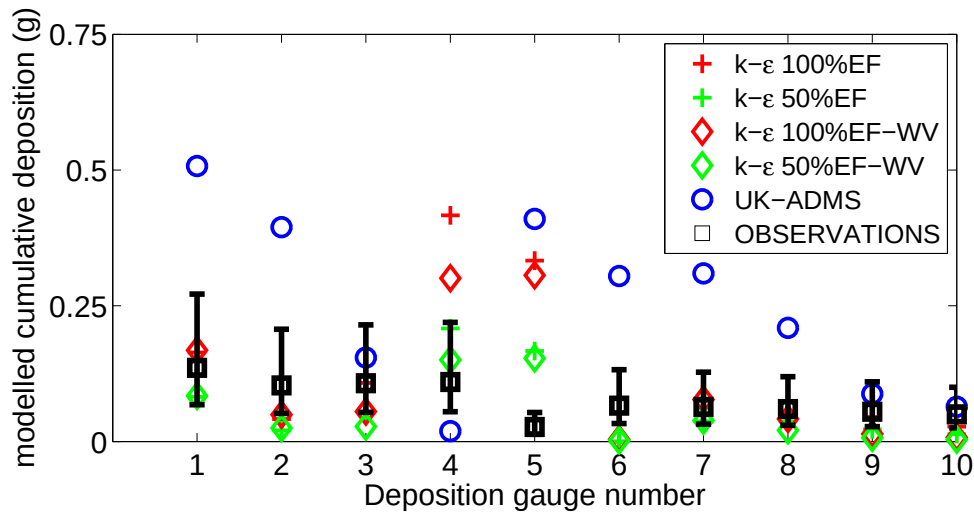


Figure 6.32: Comparison of datasets falling within a factor of 2 of the observed deposition for ADMS and CFD predictions.

Figure 6.32, shows that UK-ADMS grossly over-predicts the deposition at most of the gauges, registering deposition values well above the top range of the error bars. Both the UK-ADMS and the  $k - \varepsilon$  models predict deposition at Gauges 4 and 5, which are very inconsistent with the overall deposition trends. ADMS predicts a near zero value of deposition for gauge 4, whilst the  $k = \varepsilon$  predicts the highest deposition both with and without the inclusion of wind variability modifications. In the case of Gauge 5, the observed deposition is the lowest for the entire measured dataset, however both models predict deposition values at this gauge which are one order of magnitude higher than the

observation, this result appears to suggest a field measurement error. At gauge coordinates further away from the pit boundary, the CFD and UK-ADMS predictions show a greater degree of conformity with the observed deposition.

DEFRA (2009) recommends the use of data conditioning techniques which safeguard against disqualification of otherwise adequate models due to inaccuracies in the input parameters. For short-range model evaluation studies which rely on matching of single data pairs, (DEFRA, 2009) considers a dispersion model to be suitable for regulatory dispersion modelling applications if the model is capable of predicting the maximum short-term ground level pollutant concentrations at any time or place. The data conditioning techniques endorsed by the US EPA 2003 involve either the arc-maximum or quantile-quantile approach. The former technique requires that monitoring stations and the corresponding receptor locations in the modelling domain be configured in a series of concentric arcs at regular distance intervals from the pollutant source. The latter data conditioning technique, was considered more appropriate for the gauge configuration employed in the measurement campaign and involved comparison of the datasets after the data had been sorted in descending order and paired according to size. In this manner, the maximum field observation was compared to the maximum model prediction, as shown in Figure 6.33.

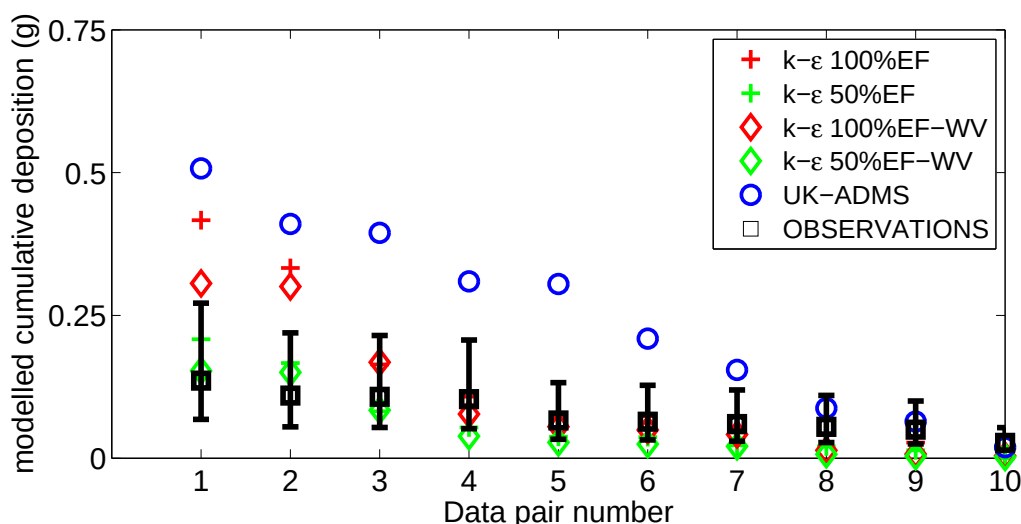


Figure 6.33: Comparison of datasets falling within a factor of 2 of the observed deposition for ADMS and CFD predictions after quantile-quantile data conditioning.

The performance metrics were computed for both the unadjusted and quantile-quantile conditioned datasets in Table 6.10. An  $FAC2$  of 0.6 was achieved for the  $k - \varepsilon$  model predictions without wind variability modifications. The  $FAC2$  improved from 0.6 to 0.7 when the  $k - \varepsilon$  predictions without wind variability were adjusted using the quantile-quantile method. UK-ADMS predictions achieved an  $FAC2$  of 0.4 before data conditioning and 0.3 after, therefore for this study, the  $FAC2$  performance of UK-ADMS was below the recommended minimum of 0.5. The  $FAC2$  performance of the  $k - \varepsilon$  model was marginally better than that of UK-ADMS and within the accepted range, for the simulations with and without wind variability modifications.

Table 6.10: Statistical Performance metrics computed for CFD, with and without wind variability at 100% and 50% of emission factor, and UK-ADMS. Subscript “*cond*” denotes performance metrics computed after quantile-quantile conditioning of datasets

| Performance<br>metric | No wind variability |                   | wind variability  |                   | UK-ADMS |
|-----------------------|---------------------|-------------------|-------------------|-------------------|---------|
|                       | EF <sub>1.0</sub>   | EF <sub>0.5</sub> | EF <sub>1.0</sub> | EF <sub>0.5</sub> |         |
| $FAC2$                | 0.60                | 0.50              | 0.50              | 0.30              | 0.40    |
| $FAC2_{cond}$         | 0.70                | 0.60              | 0.50              | 0.30              | 0.30    |
| $FB$                  | -0.49               | 0.19              | -0.27             | 0.41              | -1.04   |
| $FB_{cond}$           | -0.49               | 0.19              | -0.27             | 0.41              | -1.04   |
| $MG$                  | 0.71                | 1.43              | 1.49              | 2.97              | 0.4     |
| $MG_{cond}$           | 0.71                | 1.43              | 1.49              | 2.97              | 0.4     |
| $NMSE$                | 1.87                | 0.57              | 1.62              | 1.09              | 2.72    |
| $NMSE_{cond}$         | 1.48                | 0.37              | 0.94              | 0.41              | 2.31    |
| $NMSE_s$              | 0.26                | 0.04              | 0.08              | 0.18              | 1.48    |
| $NMSE_{s_{cond}}$     | 0.26                | 0.04              | 0.08              | 0.18              | 1.48    |
| $NMSE_r$              | 1.73                | 0.96              | 1.55              | 0.92              | 1.24    |
| $NMSE_{r_{cond}}$     | 1.23                | 0.34              | 0.86              | 0.23              | 0.83    |

In Table 6.10, the  $FB$  and  $MG$  computations indicate that the  $k - \varepsilon$  model without wind variability modifications over-predicted deposition by a factor of 1.65 when 100% of the emission factor was considered. When the emission factor was reduced by 50%, the model under-predicted by a factor of 1.2. The wind variability modifications improved the correlation of the predictions to the observed deposition as far as the  $FB$  was concerned. When wind variability was included in the CFD model, the over-prediction decreased to 1.3 for 100% of the emission factor. At 50% of the emission factor, the wind variability modified  $k - \varepsilon$  model under-predicted the dust deposition by a factor of 1.5. On the other hand, at 100% of the emission factor, UK-ADMS over-predicted fugitive dust deposition by a factor of 3.2; this over-prediction factor was substantially greater than the corresponding  $k - \varepsilon$  predictions. Therefore the  $k - \varepsilon$  model out-performs UK-ADMS in terms of the  $FB$ . Both models, performed poorly for  $MG$ , and it is likely that the presence of zero values in the

$k - \varepsilon$  predictions without wind variability have affected the reliability of the  $MG$  metric. For  $k - \varepsilon$  predictions without wind variability, the values of relative scatter quantified by  $NMSE$  were 1.87 and 0.57 for 100% and 50% of the emission factor respectively. When the wind variability modifications were included, the  $NMSE$  decreased to 1.62 for the full emission factor. At 50% EF,  $NMSE$  was 1.09. Conditioning of the data using the quantile-quantile approach re-ordered pairing of the data and the total  $NMSE$  improved for all datasets. The component of  $NMSE$  due to systematic errors remains unchanged after data conditioning. The relative scatter of the UK-ADMS predictions was substantially greater than all the  $k - \varepsilon$  predictions, in particular, the component due to systematic error is nearly 5 times greater than that of the 100% EF  $k - \varepsilon$  dataset without wind variability. It may be inferred that such a high systematic error arises due to consistent inadequacies in the resolution of the flow-field by the UK-ADMS model.  $NMSE_r$  was greater for the CFD predictions, as this model employs stochastic tracking, however as mentioned previously the wind variability modifications led to a reduction in the random scatter. A considerable improvement was observed in  $NMSE_r$ , with data conditioning because unlike systematic errors, random errors do not follow any specific trend, nor are they uniformly distributed across the entire data set, hence re-ordering of the data pairs is likely to change the random scatter.

The results indicate that all the models over-predicted deposition when 100% of the emission factor was considered. At 50% of the emission factor, the  $k - \varepsilon$  predictions under-predicted the gauge deposition, suggesting that the emission factor equation put forward by MDEQ (2004) over-predicted the emission rate and should be adjusted using a reduction factor between 0.5 and 1. The  $k - \varepsilon$  model outperformed UK-ADMS for all the metrics, and performed satisfactorily for three out of the four metrics. The mean bias was just outside the range recommended for regulatory models, however the model does not over-predict deposition as severely as UK-ADMS, even without wind variability modifications. The performance metrics show that wind variability corrections appear to improve the model performance. Even with such a small data set, the  $FAC2$  results were promising for the  $k - \varepsilon$  predictions, and showed a definite improvement over UK-ADMS predictions.

#### **6.6.6 $k - \varepsilon$ Model Predictions of In-pit Dust Retention**

The tendency of UK-ADMS to under-predict near source dispersion and over-predict long range transport is exemplified in the accretion plots presented in Figures 6.34 to 6.36. These have been selected for wind directions contributing significantly to dust deposition at the gauges. The  $k - \varepsilon$  model predicts peak accretion rates within the pit up to 2 times that of ADMS peak dry deposition predictions. Whilst the overall accretion rate profile is similar for both models, the  $k - \varepsilon$  accretion plume appears to be more affected by the terrain than that of UK-ADMS and shows evidence of plume deviation and discontinuities in the accretion profile due to the benches. Further downwind, the accretion plumes decay to achieve similar minima to the UK-ADMS dry deposition plumes, supporting the observation that both models show greater conformity with field observations further away from the perturbed flow regime within and immediately around the pit.

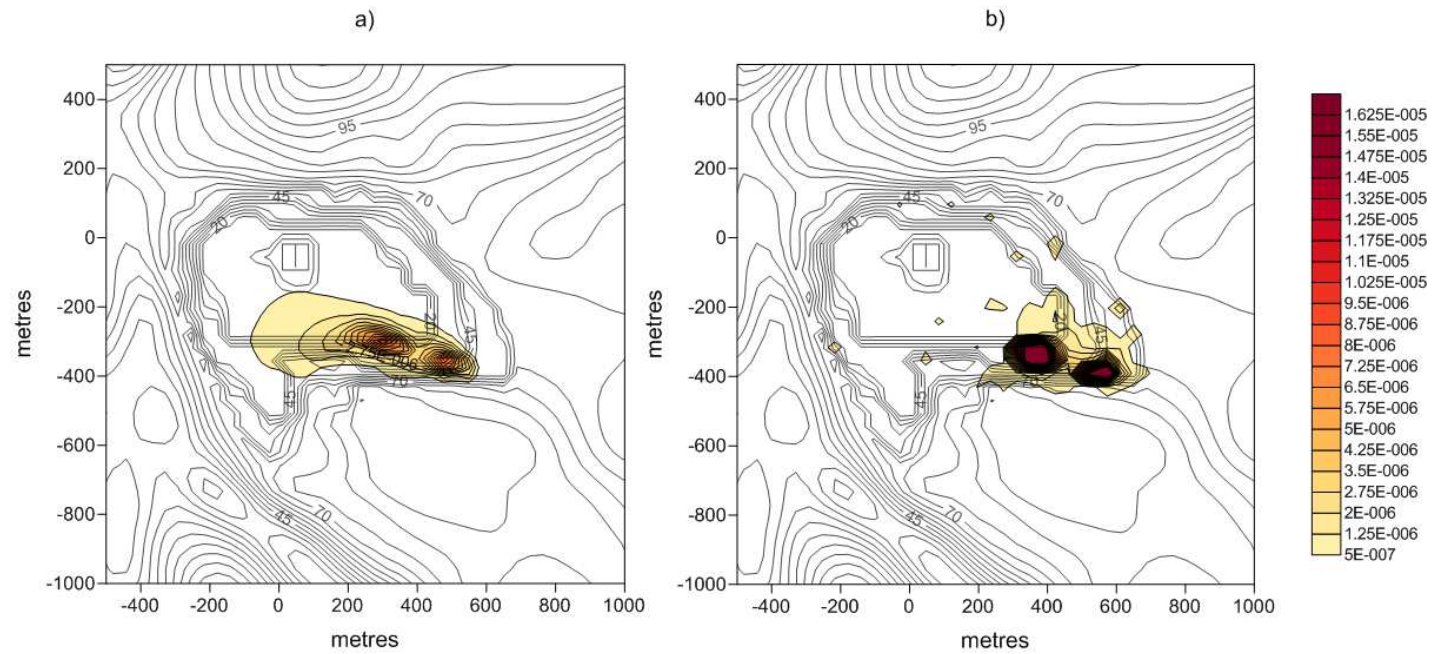


Figure 6.34: a) UK-ADMS contour plot of dry deposition compared to the b) CFD Accretion rate contour for blast event on the 9<sup>th</sup> of June.

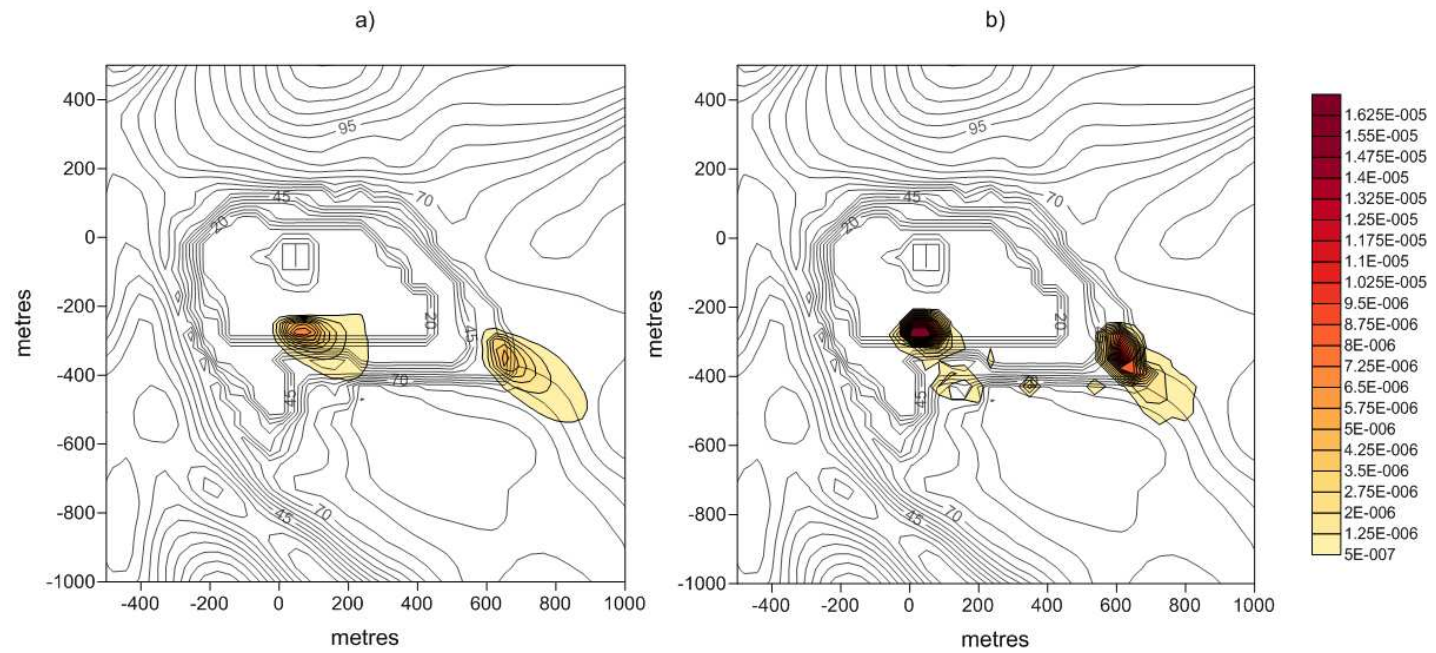


Figure 6.35: a) UK-ADMS contour plot of dry deposition compared to the b) CFD Accretion rate contour for blast event on the 16<sup>th</sup> of June.

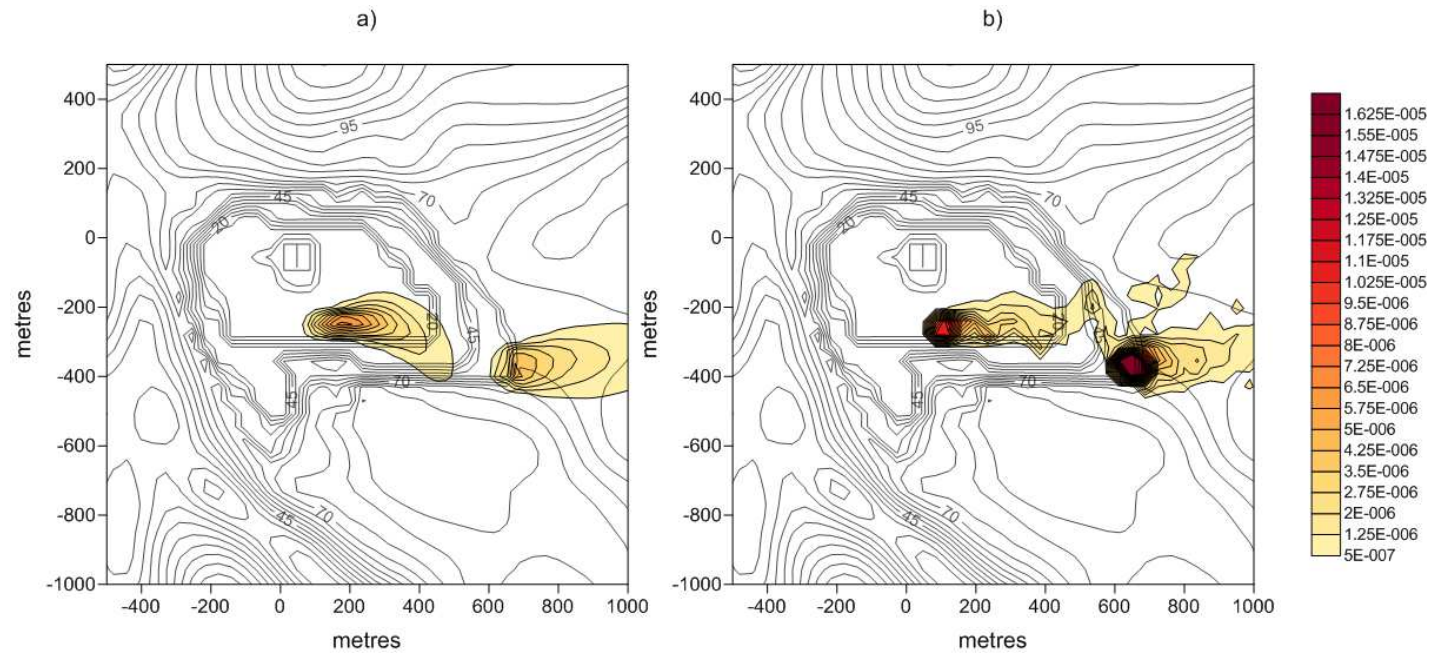


Figure 6.36: a) UK-ADMS contour plot of dry deposition compared to the b) CFD Accretion rate contour for blast event on the 22<sup>nd</sup> of June.

A past study by Silvester et al. (2009) demonstrated that a substantial fraction of the fugitive dust generated within the quarry pit, approximately, 50.06%, is removed near the emission source. Thus, in order to determine whether the CFD model proposed in this work corroborates this finding, in-pit retention percentages have been derived from the CFD simulations and compared to empirical predictions of dust retention computed from pit retention formula proposed by Cole and Fabrick (1984). Pit dust retention for the  $k - \varepsilon$  simulations has been estimated for the blast days in Figure 6.37 by calculating the ratio of trapped particulates which accumulated at the pit wall boundaries to the total number of particulates injected in the domain.

The error bars on Figure 6.37 show that approximately 83% of the  $k - \varepsilon$  model pit retention estimates are within 25% of the empirical predictions, furthermore, as indicated on the Figure, the average pit retention calculated from the  $k - \varepsilon$  simulations is 62.32% compared to 63.34% predicted by the empirical model. This implies good agreement between the average model prediction and the empirical estimate of average pit retention.

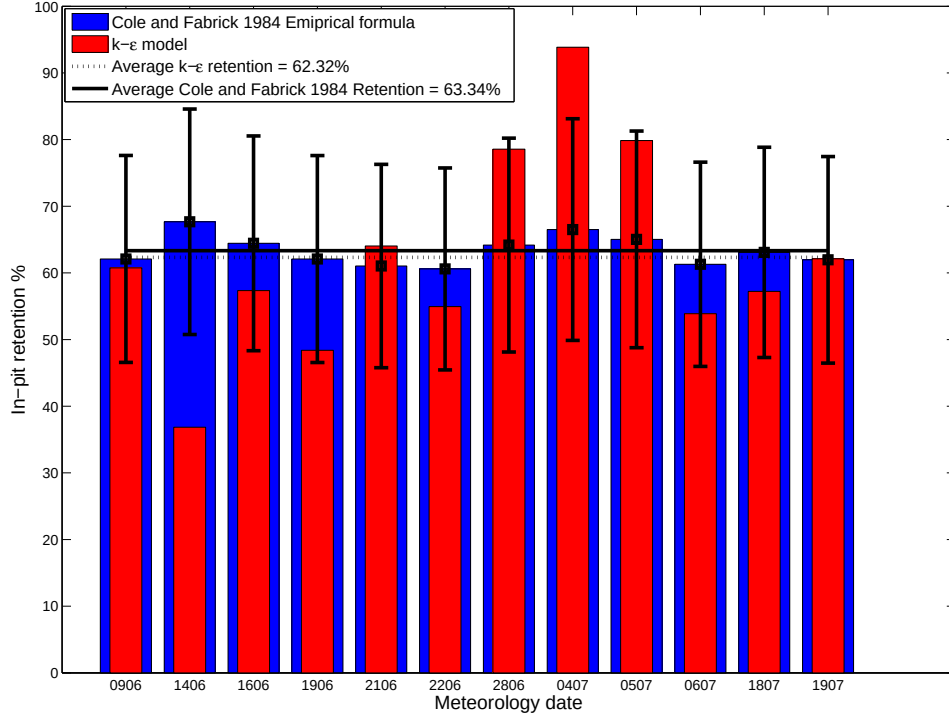


Figure 6.37: Comparison of the  $k - \varepsilon$  model estimates of in-pit retention, to empirical estimates derived from Cole and Fabrick (1984) formula

## 6.7 Summary

The case study commenced with the application of a meteorological pre-processing procedure to derive the requisite model input parameters for Monin-Obukhov scaling of the ABL from routine meteorological data, using the formulations of Holtslag and Van Ulden (1983). Subsequently, average meteorological variables were computed to represent the range of stability regimes observed at the site at the time of blasting. 90% of the meteorological observations were found to fall under the unstable atmospheric classification, which was consistent with the day-time atmospheric conditions expected at the time of blasting.

In the absence of site specific emission data, the USEPA AP-42 Emission factor for bench blasting has been used to estimate fugitive dust emission rates based on the mineral throughput of individual blasts. However, the model performance tests indicate that the emission factor estimates are partially responsible for uncertainty of the predictions, and a reduction factor between 0.5 and 1 is required to compensate for their over-estimation of fugitive dust emissions.

Investigation of the flow structure which developed within the pit revealed that the flow behaviour at the upwind and downwind edges of the pit resembled the flow over backward and forward facing steps respectively. It was seen that external orography had an attenuating effect on the development of recirculation flows within the pit. For instance, when the topography of the Great Rocks Dale valley was included in the computational domain, the backward facing step flow regime did not develop at the entry to the pit for winds perpendicular to the valley axis. Indeed, this appears to suggest that surrounding landforms can potentially disturb the upwind flow and influence the dispersion of dust within and around the quarry.

The model validation exercise formed the crux of the case study, and assessment of the metrics FAC2, FB MG and NMSE revealed that the proposed  $k-\varepsilon$  model outperformed UK-ADMS in terms of the accuracy of its deposition predictions. The model was able to meet the minimum criteria for the FAC2, MG and NMSE for its predictions without wind variability, using 100% of the emission factor. The predictions which included wind variability averaging were able to satisfy the criteria for FAC2, FB and NMSE. In contrast, UK-ADMS was only able to satisfy the NMSE metric, and even so, the component of NMSE due to systematic errors was about five times that of the  $k-\varepsilon$  model without wind variability considerations. Importantly, employing the wind variability post processing methodology reduced the random scatter of the dataset which was likely to be due to the moderating effect of the weighted averaging procedure on random fluctuations of the DPM model.

## Conclusions and Further Work

### 7.1 Conclusions

Indeed, it has been recognized that the quarry sector stands to benefit considerably from improved dust dispersion models that can offer more accurate predictions of the dispersion of fugitive dust over complex topography. This thesis has presented original research which proposes a stepwise methodology, to optimize and test the buoyancy-modified  $k-\varepsilon$  model for quarry dust dispersion modelling. Dust dispersion simulations were performed by coupling the Lagrangian Discrete Phase Model with the Eulerian solution of the flow-field obtained from the  $k-\varepsilon$  model. Thus the robustness of dust dispersion predictions obtained using this coupled approach depended on ensuring that the physics of the atmospheric surface layer were adequately represented in the turbulence model.

Chapters 4 and 5 have described the introduction of two novel techniques to the  $k-\varepsilon$  modelling strategy, namely the incorporation of wind direction variability and the implementation of a wall distance scalar. Both techniques were ultimately combined in the case study simulations, and their overall contributions to the accuracy of the dispersion model predictions were assessed through the statistical evaluation of model performance documented in Chapter 6.

Bench blasting was selected as an ideal static emission source type for model development and the atmospheric boundary layer processes which most greatly influence the dispersion of dust from bench blasting were examined in order to adopt appropriate mathematical equations to consistently represent various turbulent states of the atmosphere. The Atmospheric Boundary Layer (ABL) characterizations explored in the thesis generally pertained to the surface layer and this was justified by the fact that fugitive dust generated by quarrying activity was typically entrained into the lowest 100 m of the ABL. Therefore, it was postulated that the dispersion and transport of fugitive dust emissions generally occurred as a result of particulate interactions with the surface layer flow-field. Monin-Obukhov Similarity theory has been used to successfully characterize the surface layer in a Computational Fluid Dynamics (CFD) study by Alinot and Masson (2005), in which homogeneous profiles

of atmospheric surface layer variables under different stability conditions were produced. The current work has also successfully implemented the Monin-Obukhov Similarity Theory as a mathematical basis for the buoyancy-modified velocity, temperature and turbulence profile equations which were used to characterize the state of the unperturbed boundary layer.

An examination of the length and temporal scales which prevail in the atmospheric surface layer has guided the selection of an appropriate numerical model for the simulation of near-ground flows dominated by small-scale turbulence. The features of various CFD models, namely DNS, LES and DES were examined, and due to the high demand on computational resources imposed by these models, they were found infeasible for the non-academic application considered in this work. It was concluded that RANS CFD models were more suitable for quarry dust dispersion modelling because of their low computational demand, documented stability and the relative ease of deriving input parameters from routine meteorological data. These attributes of the  $k - \varepsilon$  model have made it possible to consider several meteorological conditions and blast locations in the case study simulations of Chapter 6. This research project has further advanced the use of CFD in the modelling of quarry dust emissions by extending the functionality of the ANSYS FLUENT  $k - \varepsilon$  model, based on the findings of Alinot and Masson (2005). Therefore, unlike the predecessor models developed by Silvester et al. (2009) for the adiabatic, neutral atmosphere, the models proposed here were able to also simulate stable and unstable atmospheric conditions. Consequently, they can be used to replicate actual site meteorology, as was evident in the case study.

This project has addressed the occurrence of stream-wise gradients in the undisturbed flow which previous studies by Hargreaves and Wright (2007) and Blocken et al. (2007b), have identified as persistent problems associated with the use of the  $k - \varepsilon$  turbulence model to simulate atmospheric boundary layer flows. The homogeneous profiles obtained by Alinot and Masson (2005) for the undisturbed ABL under characteristic stable, neutral and unstable atmospheric conditions were replicated in Chapter 3. This necessitated selection of appropriate solver settings to optimize the  $k - \varepsilon$  model for simulation of atmospheric flow-fields subject to thermal buoyancy effects. Importantly, the  $k - \varepsilon$  model coefficients were modified and source terms were introduced to the  $k$ ,  $\varepsilon$  and energy equations by means of a User Defined Function. The Boussinesq approximation was also adopted to simplify the effects of density variations in the flow. The former measures ensured that the RANS and  $k - \varepsilon$  closure equations were compatible with Monin-Obukhov Similarity theory and by extension the stability-modified Richards and Hoxey (1993) profile equations imposed at the domain inlet. The later measure improved stability of the models and convergence time of the solutions.

The resultant undisturbed profiles remained homogeneous throughout the length of the empty computational domain, and were found to be in good agreement with Alinot and Masson (2005) and empirical Monin-Obukhov profiles, with an average deviation of less than 2%. For the unstable case, there was a decay of approximately 10% of the turbulent kinetic energy in the top 30 m of the computational domain. This localized inhomogeneity of the unstable kinetic energy profile was confined to the top of the profile and did not appear to

have any effects in the region of interest near the ground. Therefore it was concluded that the buoyancy modifications to the  $k - \varepsilon$  model had succeeded in maintaining a satisfactory degree of homogeneity of the atmospheric profiles.

### 7.1.1 Numerical Model Optimization

Previous work by Mahrt (2010) elucidated the significant contribution of mesoscale wind variability to lateral spreading of a pollutant plume, to the extent that it is likely to be the dominant mechanism of plume dispersion in stable, low-wind conditions. Riddle et al. (2004) strengthened their case for the use of UK-ADMS by demonstrating that the absence of a feature to account for mesoscale wind variability in the CFD models resulted in under-prediction of the lateral spreading of pollutant plume. Thus, this deficiency of the  $k - \varepsilon$  model was addressed in Chapter 4 and a novel post-processing methodology was developed to incorporate wind variability effects in CFD dust dispersion predictions. This involved parametrization of the wind direction variability according to the Moore (1976) generalization, in which wind direction variability is defined as the standard deviation from the mean wind direction,  $\sigma_{wd}$ , and expressed as a function of wind speed and meteorological averaging time. Minimum and maximum limits of  $5^\circ$  and  $30^\circ$ , were imposed on  $\sigma_{wd}$  based on field observations by Mahrt (2010) and empirical formulae by Hanna (1983), Joffre and Laurila (1988) and Davies and Thomson (1999), in order to limit the wind variability to a realistic range.

Since UK-ADMS, employs the Moore (1976) generalization in its plume spread module, its predictions were used as a baseline for evaluating the improvements in lateral plume spread obtained by implementing the proposed CFD modelling methodology. The dispersion of particulates injected into the computational domain from an elevated emission source were simulated using the Discrete Phase model for the three atmospheric stability classes. Thus, the investigation of mesoscale wind variability also provided an opportunity to study the effects of the  $k - \varepsilon$  thermal buoyancy modifications on simulations of particulate dispersion over flat terrain. The expected trends in plume behaviour were predicted by the model, in which stable atmospheric conditions were least dispersive and consequently resulted in the highest deposition near the source. The neutral simulations predicted the lowest near-source deposition due to the dominance of advective transport arising from the high wind speed specified for this case. The deposition near the source was attenuated by a combination of buoyant mixing and mechanical turbulence for the unstable case, consequently the predicted maximum deposition was intermediate to the stable and neutral cases.

The results of the comparative analysis of FLUENT accretion predictions and UK-ADMS dry-deposition predictions indicated that by incorporating wind direction variability through Gaussian probability weighted simulations of wind direction variability in the interval  $\mu_\theta - 3\sigma$  to  $\mu_\theta + 3\sigma$ , FLUENT predictions of lateral spreading of the particulate plume, improved appreciably and were well within 15% of UK-ADMS values. Moreover, unlike previous work by Vervecken et al. (2013), the proposed methodology does not require field measurements of wind direction variability and can be applied to a broad range of meteorological conditions, because the standard deviation of wind direction is calculated from the empirically-derived

Moore (1976) generalization.

The role of the Lagrangian Integral time scale constant,  $c_L$  as a means to moderate the influence of turbulent fluctuations on the particle trajectories was explored. The default value of  $c_L = 0.15$  was modified by factors of 2 and 0.25 respectively. In this way, the constant was calibrated to alter the dispersive characteristics of the FLUENT plume, so that better agreement of FLUENT and UK-ADMS predictions was obtained in terms of the location and magnitude of peak deposition values. These parametric tests have confirmed that  $c_L$  is analogous to the turbulent Schmidt number employed in the advection-diffusion equation for scalar transport of a pollutant, as discussed in work by Gorlé et al. (2009). Modifications to the values of  $c_L$  altered plume dispersion in all three dimensions due to the isotropic nature of the turbulence model. This implied that  $c_L$  could not be relied upon as the sole means of improving lateral plume spread predictions, and the wind variability methodology was more appropriate for incorporating the effects of mesoscale wind variability in the FLUENT predictions.

A significant outcome of the study of flow over idealized cosine depressions of varying aspect ratio in Chapter 5, was the introduction of a wall distance scalar in the form of a Poisson transport equation with a Dirichlet boundary condition of 0 imposed at the wall. This allowed the  $k - \varepsilon$  turbulence model to produce atmospheric profiles which conformed to the shape and elevation of the wall, thereby adapting the model for flow simulations over variable terrain. The experimental profiles of the  $u$  velocity component and Reynolds stress component,  $\sigma_u$ , obtained by Ishihara et al. (1999) in a wind tunnel investigation of flow over a cosine hill have been used to validate the idealized terrain flow-field computed by the  $k - \varepsilon$  model. Upwind of the hill crest, the profiles simulated by the numerical model agreed well with the wind tunnel results. Subsequently, there was divergence between the simulated and measured profiles in the recirculation region on the leeward side of the hill, where the peak  $\sigma_u$  predicted by the  $k - \varepsilon$  model was two thirds of the wind tunnel measurement. Whilst this discrepancy was expected to be primarily due to the  $k - \varepsilon$  turbulence isotropy assumption, it is worth noting that the friction Reynolds number of the wind tunnel flow was less than the critical value of 2.5 required to ensure Reynold number independence; therefore non-similarity of the experimental flow was also likely to contribute to the discrepancy between the measured and simulated flow-fields. This validation exercise demonstrated the limitations of the RANS assumption of turbulence isotropy. Nevertheless, even with this loss of accuracy in the  $k$  predictions, the  $k - \varepsilon$  complex terrain capabilities far surpass those of UK-ADMS and the results of the idealized terrain simulations provided conclusive evidence that UK-ADMS is unsuitable for aspect ratios below 3.

The idealized terrain simulations indicated that flow reversal were likely to occur nearer the leading edge of the depression with increasing depth. As the depression deepened, recirculation flows became well established and particulates entrained in the recirculation zone were swept upwind of the source and remained trapped within the valley for the 2.67 and 2 aspect ratio cases. It was seen that flow separation and the development of recirculation zones depended on the magnitude of the mean wind velocity and reversed flow was more likely to occur in deep depressions under stable atmospheric conditions. Conversely,

the high wind conditions associated with the neutral atmosphere favoured ventilating flow regimes in the depressions.

The  $k - \varepsilon$  model predicted that the presence of a depression produced a spike in turbulence near the ground as a consequence of increased shear generation as the flow was displaced downward. This near-ground spike in turbulence was not observed in the UK-ADMS results. The results indicated that thermal buoyancy dictated how the spike in turbulence was propagated through the domain and atmospheric instability favoured quicker recovery of the ABL from the turbulent perturbations induced by the depression, owing to the fact that the increase in turbulence could be distributed upwards since vertical mixing is not suppressed in the unstable atmosphere. This study briefly examined the critical Froude number,  $Fr$ , as an indicator of boundary layer detachment, and the strong recirculation regime observed for the 2 aspect ratio valley was correctly matched by a Froude number below the critical value of 1.3. The FLUENT models predicted enhancement of stable atmospheric conditions in the deep depression in terms of a strengthening of the near-ground temperature inversion. The findings of this study echoed the findings of earlier research by Snyder et al. (1991) which investigated flow within valleys and provided evidence that the flow-fields over complex terrain were best captured using CFD.

#### **7.1.2 Validation of the buoyancy modified $k - \varepsilon$ dispersion model**

The evaluation of model uncertainty was an essential component of model development. Frisbee gauge dust deposition measurements obtained during a monitoring campaign at the Old Moor quarry between June 9th and July 19th 2006 were used to validate the buoyancy-modified  $k - \varepsilon$  model developed in this work. The atmospheric variables required for parametrizing the surface boundary layer were derived from a meteorological pre-processing routine based on the equations of Holtslag and Van Ulden (1983). This permitted calculation of the Monin-Obukhov length scale, surface sensible heat flux and the friction velocity from routine meteorological data recorded at the quarry over the duration of the monitoring campaign. Average meteorology representative of each of the Pasquill-Guifford-Turner (PGT) stability classes was computed for the monitoring period based on the frequency distribution of the various stability regimes.

The effect of the in-pit terrain on the atmospheric flow-field was examined in isolation by excluding the surrounding landforms from the computational domain. This enabled identification of the dominant flow structures over the upwind and downwind benches, which were found to resemble those commonly identified over backward and forward facing steps respectively. Flow separation zones were predicted at the entrance and exit of the pit, as well as over the deepest bench. Separation of the flow from the overhead ABL was especially prominent for the strongly unstable case, justifying the inclusion of thermal buoyancy effects in the model. The Artificial Terrain simulations of dust dispersion revealed that the model was responsive to overall changes in the stability regime as opposed to small changes in meteorological variables and, on this basis, the averaged meteorology was used in the Actual Terrain simulations.

Statistical evaluation of the performance of the buoyancy modified  $k - \varepsilon$  model demonstrated

that the model was able to produce better fugitive dust deposition predictions than UK-ADMS. Specifically, the model predictions met the minimum performance specifications for FAC2, MG and NMSE for simulations without wind variability effects. When wind variability averaging was applied to the predictions, the NMSE performance showed marked improvement, in particular there was a decrease in the random component of NMSE, which implied that the wind variability averaging procedure was able to smooth out some of the random fluctuations of the stochastic model which contributed towards uncertainty of the predictions. In contrast, UK-ADMS dust deposition predictions were unsatisfactory for 3 of the 4 metrics, with only the NMSE falling within the acceptable range. Even after Quantile-Quantile conditioning of the datasets, the  $k - \varepsilon$  model outperformed UK-ADMS for all the metrics and emerged as the more accurate predictor of quarry dust deposition. The fact that the  $k - \varepsilon$  model was able to satisfy 3 out of 4 performance criteria and also out-perform the current regulatory model lends compelling support to the hypothesis that CFD methods are required to accurately simulate quarry dust dispersion.

Estimates of the average in-pit retention corroborated the findings of Silvester et al. (2009). There was a high degree of variance between the overall in-pit retention over the duration of the monitoring period and the in-pit retention for individual blasts due to the fact that blast location and the prevailing meteorology greatly influenced particle residence time. As a result, greater in-pit retention was predicted for blasts situated deeper within the quarry or at the upwind edge of the pit relative to the prevailing wind direction.

### 7.1.3 Limitations of the Model

The modelling methodology proposed in this thesis has used Monin-Obukhov Similarity scaling to characterize the surface atmospheric boundary layer, consequently the flow solver is valid within the asymptotic limits of Monin-Obukhov similarity scaling, that is  $z \leq |L_{MO}|$ . Therefore, the model is not applicable to very convective conditions where  $L_{MO} < 50$  m and the surface layer occupies a thin layer near the ground, because in these cases, it is unable to reliably compute the flow-field beyond 50 m. Additionally, under strongly convective conditions, especially combined with deeper pit cavities, where the flow is dominated by large-scale anisotropic eddies, the isotropic, steady-state turbulence model proposed in this work is only applicable to the near-wall region and as such LES and DES methods would be more appropriate for resolving detached regions of the flow.

## 7.2 Further Work

This research project has developed an improved fugitive dust dispersion modelling methodology which has been adapted for the actual meteorology and complex topography of surface quarries. It is envisioned that these improved dust dispersion models can ultimately guide the targeted application of dust abatement strategies and the optimization of mineral extraction sequences. Moreover, they can enable quarry operators to fully adopt the recommendations of the UK Minerals Policy contained in the Technical Guidance to the National Planning and Policy Framework, in which they are advised to utilize knowledge of the site meteorology and surrounding topography to mitigate fugitive dust emissions. The various strategies involved in model development have exposed both the strengths and limitations of the proposed model. At this stage, it is useful to look towards avenues for future development of the model to circumvent some of these limitations.

### 7.2.1 Application to other source types

The results of the model performance evaluation confirmed that the buoyancy modified  $k - \varepsilon$  model is a viable prototype for a CFD-based quarry dust dispersion modelling strategy for bench blast emissions. In Chapter 2, the primary sources of fugitive dust at a typical surface quarry operation were identified. In particular, haul road transport, material stockpiles, loading and unloading of haul trucks and comminution circuits were listed as major contributors to the overall quarry fugitive dust inventory. Whilst the modelling methods proposed for the Eulerian solution of the background wind field would be applicable to any source type, the particulate injection file and the DPM solver must be customized for each source type such that the initial state of the particulate injection and the terms in the particle force balance equation are consistent with the dust liberation mechanisms associated with the fugitive dust emission source. For instance, whilst material stockpiles may be treated as static, areal dust emission sources, the dynamic nature of moving sources such as haul trucks would warrant special consideration. Therefore it is recommended that future development of the modelling methodology should involve accurate characterization of all quarry dust sources in addition to an extension of the model evaluation exercise to include validation of the model fugitive dust dispersion predictions for other source categories.

### 7.2.2 Improving boundary layer characterization

The turbulence model has been developed to exclusively simulate the surface ABL, however to make allowances for modelling particulate dispersion in the very unstable atmosphere characterized by  $|L_{MO}| < 50$  m, where the surface layer is confined to a shallow region near the ground, future work should explore the possibility of extending the functionality of the model to include consideration of the convective mixed layer. This may be achieved by including logical statements in the UDF which permit switching from Monin-Obukhov scaling of the boundary layer to convective mixed layer scaling in regions of the flow where the asymptotic limits of Monin-Obukhov length scale and the corresponding Businger-Dyer

similarity functions have been reached. This would serve to make the model applicable to a more comprehensive range of atmospheric stability conditions.

### 7.2.3 Emission factors

The accuracy of the  $k - \varepsilon$  quarry dust dispersion predictions obtained for the case study quarry was dependent on the robustness of the US-EPA AP-42 Emissions Factor estimates employed to quantify dust emissions. This is invariably true of any dust dispersion model which relies on the use of these emission factor equations. It became apparent in the case study simulations that a high degree of uncertainty is associated with the use of US-EPA AP-42 emission factor estimates. They were found to consistently over-predicted the fugitive dust emissions generated by bench blasting, therefore a precise reduction factor should be applied to the emission estimates obtained from the current emission factor equations to allow more accurate quantification of the dust liberated from quarry sources. Suffice to say, additional parametric tests would be required to arrive at an appropriate value for this reduction factor. Alternatively, future model development may choose to entirely forgo the US-EPA AP-42 emission factors and aim towards the formulation of new emission factor equations which are optimized for the quarry sector. Such an endeavour would require extensive field measurements at potentially significant costs, but would deliver emission factor equations that are fit for purpose.

### 7.2.4 Improved validation techniques

The prototype  $k - \varepsilon$  dust dispersion model should be subjected to more extensive validation, inclusive of evaluation of its predictions of long-term and short-term dust deposition and air-borne concentration. Further evaluation of the model would require a denser network of Frisbee gauges, to provide better coverage of the selected dispersion site and more importantly to produce a sufficiently large dataset to allow regression analysis and calculation of the confidence intervals of the model predictions. It would be particularly useful if future monitoring campaigns involved strategic positioning of deposition gauges and sampling of dust laden air in pre-defined locations which map out a series of concentric arcs so that the arc-maximum data conditioning approach could be also employed in evaluation of the model performance.

### 7.2.5 Automating the simulations

Wind direction variability was incorporated in the simulation results using a probability-weighted averaging strategy which required 13 sets of simulations to obtain a resultant plume for each wind direction. This technique was an important component of the proposed  $k - \varepsilon$  modelling methodology, which allowed the model to produce lateral plume spread predictions which were comparably to those of UK-ADMS, as demonstrated in Chapter 4. However, the proposed method presently requires the user to manually change the wind variation angle for each of the 13 simulations, export the field results once the simulations

are concluded and calculate the resultant plume using a MATLAB script. Such a high degree of user intervention makes the method susceptible to error. It is proposed that future work should consider the formulation of scripts for the automation of the wind variability simulations and the Gaussian averaging procedure. One possible approach involves writing of Linux shell scripts which would oversee the creation of individual case files for each wind variation angle and the running of the simulations on a parallel computing cluster. The script could also execute post-processing commands to extract the field results and perform the probability-weighted averaging to determine the resultant plume. This would eliminate the need for the user to handle a large number of datasets and would also improve the feasibility of using the model in the quarry sector.



## UDF to Introduce Inlet Profiles and Buoyancy Modifications to FLUENT $k - \varepsilon$ Model

```
#include "udf.h"

/* Define some constants */
#define VON_K 0.42
#define GRAV 9.81 /* Acceleration due to gravity */
#define RHO 1.225
#define CP 1006.43
#define C_MU 0.0333
#define RT_C_MU 0.182
#define BETA 0.003356 /* Thermal expansion coefficient (1/K) */
#define C_EPS_1 1.176 /* Epsilon 1 model coefficient */
#define C_EPS_2 1.92 /* Epsilon 2 model coefficient */
#define SIGMAT 1.0 /* Turb. Prandtl number (Fluent default value) */

/* Declare static variables - these are modified in the Scheme panel */
static real uRef; /* Reference wind speed (m/s) */
static real theta; /* Wind angle (degrees) */
static real zRef; /* Reference height (m) */
static real z0; /* Roughness height (m) */
static real lMo; /* Monin-Obukhov length (m) */
static real tWall; /* Ground temperature (K) */
static real qWall; /* Ground heat flux (W/m2) */

/* Define which user-defined scalars to use */
enum
{
    MU_T, PHI, N_REQUIRED_UDS
};
```

```

/* ...and the user-defined memory */
enum
{
    GRADMUT, GRADT, BUOY, CEPS3, GRADPHI, ZPRIME, N_REQUIRED_UDM
};

/*****
/* Function to update user-defined scheme variables */
*****/
void updateScheme()
{
    #if !RP_NODE
        uRef = RP_Get_Real("abl/u-ref");
        theta = RP_Get_Real("abl/theta");
        zRef = RP_Get_Real("abl/z-ref");
        z0 = RP_Get_Real("abl/z0");
        lMo = RP_Get_Real("abl/l-mo");
        tWall = RP_Get_Real("abl/t-wall");
        qWall = RP_Get_Real("abl/q-wall");
    #endif

    /* This function does nothing in serial */
    host_to_node_real_7(uRef,theta,zRef,z0,lMo,tWall,qWall);
}

/* This function calculates phi_m(z/L), Eqn (13) in A&M */
real phiM(real monin, real z)
{
    real phi;

    if ( monin < 0 )
        phi = pow(1.0-16.0*(z/monin),-0.25);
    else
        phi = 1.0 + 5.0*(z/monin);

    return(phi);
}

/* This function calculates phi_epsilon(z/L), Eqn (19) in A&M */
real phiEpsilon(real monin, real z)
{
    real phi;

    if ( monin < 0 )
        phi = 1.0-(z/monin);
    else

```

```
    phi = phiM(monin,z)-(z/monin);

    return(phi);
}

/* This function calculates stability dependent epsilon 3 coeff.*/
real C_EPS3(real monin, real z)
{
    int i;
    real ceps3;
    real a[6]={0.0,1.0,2.0,3.0,4.0,5.0};
    real p[6]={0.0,1.0,2.0,3.0,4.0,5.0};

    if(monin > 0)
    {
        if ( z/monin < 0.33)
        {
            a[0]=4.181; a[1]=33.994; a[2]=-442.398;
            a[3]=2368.12; a[4]=-6043.544; a[5]=5970.776;
        }
        else
        {
            a[0]=5.225; a[1]=-5.269; a[2]=5.115;
            a[3]=-2.406; a[4]=0.435; a[5]=0.000;
        }
    }
    else
    {
        if( fabs(z/monin) < 0.25)
        {
            a[0]=-0.0609; a[1]=-33.672; a[2]=-546.880;
            a[3]=-3234.06; a[4]=-9490.792; a[5]=-11163.202;
        }
        else
        {
            a[0]=1.765; a[1]=17.1346; a[2]=19.165;
            a[3]=11.912; a[4]=3.821; a[5]=0.492;
        }
    }

    ceps3 = 0.0;
    for (i=0;i<6;i++)
        ceps3 += a[i]*pow((z/monin),p[i]);

    return(ceps3);
}
```

```
DEFINE_PROFILE(u_profile,ft,i)
{
    real phi_m,u_star;
    face_t f;

    /* Calculate phi_m at the reference height */
    phi_m = phiM(lMo,zRef);

    /* Calculate u_star using the reference height */
    if(lMo < 0)
        u_star = uRef*VON_K/(log(zRef/z0)+log(8.0*pow(phi_m,4.0)
        / (pow(phi_m+1.0,2.0)*(pow(phi_m,2.0)+1.0))))
        - (M_PI/2.0)+(2.0*atan(1.0/phi_m)));
    else
        u_star = uRef*VON_K/(log(zRef/z0)+phi_m-1.0);

    /* Loop through the faces, calculating the u profile from
       Eqn (16) in A&M */
    begin_f_loop(f,ft)
    {
        real z;
        real f_cen[ND_ND];

        F_CENTROID(f_cen,f,ft);
        /*z = f_cen[2];*/
        z = C_UDMI(F_C0(f,ft),ft->t0,ZPRIME);

        /* Calculate phi_m at the face centroid, z */
        phi_m = phiM(lMo,z);

        if(lMo < 0)
            F_PROFILE(f,ft,i) = (u_star/VON_K)*sin(theta*M_PI/180.0)
            *(log(z/z0)+log(8.0*pow(phi_m,4.0)
            / (pow(phi_m+1.0,2.0)*(pow(phi_m,2.0)+1.0))))
            - (M_PI/2.0)+(2.0*atan(1.0/phi_m)));
        else
            F_PROFILE(f,ft,i) = (u_star/VON_K)*sin(theta*M_PI/180.0)
            *(log(z/z0)+phi_m-1.0);

    }
    end_f_loop(f,ft);
}

DEFINE_PROFILE(v_profile,ft,i)
{
    real phi_m,u_star;
    face_t f;
```

```
/* Calculate phi_m at the reference height */
phi_m = phiM(lMo,zRef);

/* Calculate u_star using the reference height */
if(lMo < 0)
    u_star = uRef*VON_K/(log(zRef/z0)+log(8.0*pow(phi_m,4.0)
    / (pow(phi_m+1.0,2.0)*(pow(phi_m,2.0)+1.0)))
    - (M_PI/2.0)+(2.0*atan(1.0/phi_m)));
else
    u_star = uRef*VON_K/(log(zRef/z0)+phi_m-1.0);

/* Loop through the faces, calculating the u profile from
   Eqn (16) in A&M */
begin_f_loop(f,ft)
{
    real z;
    real f_cen[ND_ND];
    F_CENTROID(f_cen,f,ft);
    /*z = f_cen[2];*/
    z = C_UDMI(F_CO(f,ft),ft->t0,ZPRIME);

    /* Calculate phi_m at the face centroid, z */
    phi_m = phiM(lMo,z);

    if(lMo < 0)
        F_PROFILE(f,ft,i) = (u_star/VON_K)*cos(theta*M_PI/180.0)
        *(log(z/z0)+log(8.0*pow(phi_m,4.0)
        / (pow(phi_m+1.0,2.0)*(pow(phi_m,2.0)+1.0)))
        - (M_PI/2.0)+(2.0*atan(1.0/phi_m)));
    else
        F_PROFILE(f,ft,i) = (u_star/VON_K)*cos(theta*M_PI/180.0)
        *(log(z/z0)+phi_m-1.0);

    end_f_loop(f,ft);
}
}

DEFINE_PROFILE(temp_profile,ft,i)
{
    real phi_m, u_star, t_star;
    face_t f;

    /* Calculate phi_m at the reference height */
    phi_m = phiM(lMo,zRef);
```

```

/* Calculate u_star using the reference height */
if(lMo < 0)
    u_star = uRef*VON_K/(log(zRef/z0)+log(8.0*pow(phi_m,4.0)
    / (pow(phi_m+1.0,2.0)*(pow(phi_m,2.0)+1.0))))
    - (M_PI/2.0)+(2.0*atan(1.0/phi_m)));
else
    u_star = uRef*VON_K/(log(zRef/z0)+phi_m-1.0);

/* Calculate t_star from Eqn (15) in A&M */

begin_f_loop(f,ft)
{
    real z;
    real f_cen[ND_ND];
    F_CENTROID(f_cen,f,ft);
    /*z = f_cen[2]*/;
    z = C_UDMI(F_C0(f,ft),ft->t0,ZPRIME);

    t_star = -qWall/(F_R(f,ft)*CP*fabs(u_star));

    /* Calculate phi_m at the face centroid, z */
    phi_m = phiM(lMo,z);

    /* Calculate the temperature profile from Eqn (17) in A&M */
    if(lMo < 0)
        F_PROFILE(f,ft,i) = ((t_star/VON_K)*(log(z/z0)
        - (2.0*log(0.5*(1.0+pow(phi_m,-2.0))))))
        - (GRAV*(z-z0)/CP)+tWall;
    else
        F_PROFILE(f,ft,i) = ((t_star/VON_K)*(log(z/z0)+phi_m-1.0))
        - (GRAV*(z-z0)/CP)+tWall;
}
end_f_loop(f,ft);
}

DEFINE_PROFILE(k_profile,ft,i)
{
    real phi_m, phi_epsilon, u_star, u_star2;
    face_t f;

    /* Calculate phi_m at the reference height */
    phi_m = phiM(lMo,zRef);

    /* Calculate u_star using the reference height */
    if(lMo < 0)
        u_star = uRef*VON_K/(log(zRef/z0)+log(8.0*pow(phi_m,4.0)

```

```
    / (pow(phi_m+1.0,2.0)*(pow(phi_m,2.0)+1.0)))
    - (M_PI/2.0)+(2.0*atan(1.0/phi_m)));
else
    u_star = uRef*VON_K/(log(zRef/z0)+phi_m-1.0);

    u_star2 = u_star*u_star;

/* Calculate the k profile from Eqn (20) in A&M */
begin_f_loop(f,ft)
{
    real z;
    real f_cen[ND_ND];
    F_CENTROID(f_cen,f,ft);
    /*z = f_cen[2];*/
    z = C_UDMI(F_C0(f,ft),ft->t0,ZPRIME);

    /* Calculate phi_m at the face centroid, z */
    phi_m = phiM(lMo,z);

    /* Calculate phi_epsilon at the face centroid, z */
    phi_epsilon = phiEpsilon(lMo,z);

    F_PROFILE(f,ft,i) = 5.48*u_star2*sqrt(phi_epsilon/phi_m);
}
end_f_loop(f,ft);
}

DEFINE_PROFILE(eps_profile,ft,i)
{
    real phi_m, phi_epsilon, u_star, u_star3;
    face_t f;

    /* Calculate phi_m at the reference height */
    phi_m = phiM(lMo,zRef);

    /* Calculate u_star using the reference height */
    if(lMo < 0)
        u_star = uRef*VON_K/(log(zRef/z0)+log(8.0*pow(phi_m,4.0)
        / (pow(phi_m+1.0,2.0)*(pow(phi_m,2.0)+1.0)))
        - (M_PI/2.0)+(2.0*atan(1.0/phi_m)));
    else
        u_star = uRef*VON_K/(log(zRef/z0)+phi_m-1.0);

    u_star3 = fabs(u_star*u_star*u_star);

    /* Calculate the k profile from Eqn (20) in A&M */
```

```
begin_f_loop(f,ft)
{
    real z;
    real f_cen[ND_ND];
    F_CENTROID(f_cen,f,ft);
    /*z = f_cen[2];*/
    z = C_UDMI(F_CO(f,ft),ft->t0,ZPRIME);

    /* Calculate phi_epsilon at the face centroid, z */
    phi_epsilon = phiEpsilon(lMo,z);

    F_PROFILE(f,ft,i) = (u_star3/(VON_K*z))*phi_epsilon;
}
end_f_loop(f,ft);

}

DEFINE_PROFILE(uds1_profile,ft,i)
{
    face_t f;

    /*inlet profile for uds-1*/
    begin_f_loop(f,ft)
    {
        F_PROFILE(f,ft,i)=C_UDSI(F_CO(f,ft),ft->t0,PHI);
    }
    end_f_loop(f,ft);
}

DEFINE_INIT(initialise_flow,domain)
{
    Thread *ct;
    cell_t c;
    real phi_m, phi_epsilon, u_star, u_star2, u_star3, t_star;

    /* Update the Scheme variables */
    updateScheme();

    /* Calculate phi_m at the reference height */
    phi_m = phiM(lMo,zRef);

    /* Calculate u_star at the reference height */
    if(lMo < 0)
        u_star = uRef*VON_K/(log(zRef/z0)+log(8.0*pow(phi_m,4.0)
        / (pow(phi_m+1.0,2.0)*(pow(phi_m,2.0)+1.0))))
        - (M_PI/2.0)+(2.0*atan(1.0/phi_m)));
    else
        u_star = uRef*VON_K/(log(zRef/z0)+phi_m-1.0);
```

```
u_star2 = u_star*u_star;
u_star3 = fabs(u_star*u_star*u_star);

/* Looping over all cell threads in the domain */
thread_loop_c(ct,domain)
{
    begin_c_loop(c,ct)
{
    real z;
    real c_cen[ND_ND];
    C_CENTROID(c_cen,c,ct);
    z = c_cen[2];

    t_star = -qWall/(C_R(c,ct)*CP*fabs(u_star));

    /* Calculate phi_m and phi_epsilon at the cell centroid, z */
    phi_epsilon = phiEpsilon(lMo,z);
    phi_m = phiM(lMo,z);

    /*initialising calculations for flow variables at cell centroid from
    Eqns 16, 17, 18, 20 in A&M */
    if(lMo < 0)
    {
        C_U(c,ct) = (u_star/VON_K)*cos(theta*M_PI/180.0)*(log(z/z0)
            +log(8.0*pow(phi_m,4.0)
            / (pow(phi_m+1.0,2.0)*(pow(phi_m,2.0)+1.0)))
            - (M_PI/2.0)+(2.0*atan(1.0/phi_m)));
        C_V(c,ct) = (u_star/VON_K)*sin(theta*M_PI/180.0)*(log(z/z0)
            +log(8.0*pow(phi_m,4.0)
            / (pow(phi_m+1.0,2.0)*(pow(phi_m,2.0)+1.0)))
            - (M_PI/2.0)+(2.0*atan(1.0/phi_m)));
        C_T(c,ct) = ((t_star/VON_K)*(log(z/z0)
            - (2.0*log(0.5*(1.0+pow(phi_m,-2.0)))))
            - (GRAV*(z-z0)/CP)+tWall;
    }
    else
    {
        C_U(c,ct) = (u_star/VON_K)*cos(theta*M_PI/180.0)*(log(z/z0)+phi_m-1.0);
        C_V(c,ct) = (u_star/VON_K)*sin(theta*M_PI/180.0)*(log(z/z0)+phi_m-1.0);
        C_T(c,ct) = ((t_star/VON_K)*(log(z/z0)+phi_m-1.0))
            - (GRAV*(z-z0)/CP)+tWall;
    }

    C_K(c,ct) = 5.48*u_star2*sqrt(phi_epsilon/phi_m);
    C_D(c,ct) = (u_star3/(VON_K*z))*phi_epsilon;
```

```

}

end_c_loop(c,ct);
}
}

DEFINE_ADJUST(adjust, d)
{
  Thread *ct, *ft;
  cell_t c;
  face_t f;
  real gradt, phi, gradPhi;

  /* Update the Scheme variables */
  updateScheme();

  if(n_uds < N_REQUIRED_UDS)
    Internal_Error("not enough UDS allocated");
  thread_loop_c(ct,d)
  {
    if(NULL != THREAD_STORAGE(ct, SV_UDS_I(MU_T)))
  {
    begin_c_loop(c,ct)
    {
      C_UDSI(c,ct,MU_T)= C_MU_T(c,ct);
    }
    end_c_loop(c,ct);
  }

    thread_loop_c(ct,d)
    {
      if(NULL != THREAD_STORAGE(ct, SV_T_G) &&
        NULL != T_STORAGE_R_NV(ct, SV_T_G) )
  {
    begin_c_loop(c,ct)
    {
      gradt = C_T_G(c,ct)[2];
      C_UDMI(c,ct,GRADT) = gradt;
    }
    end_c_loop(c,ct);
  }

    thread_loop_c(ct,d)
    {

```

```
        if(NULL != THREAD_STORAGE(ct, SV_UDS_I(MU_T)) &&
NULL != T_STORAGE_R_NV(ct, SV_UDSI_G(MU_T)))
{
    begin_c_loop(c,ct)
    {
        C_UDMI(c,ct,GRADMUT) = NV_MAG(C_UDSI_G(c,ct,MU_T));
    }
    end_c_loop(c,ct);
}

}

thread_loop_c(ct,d)
{
    if(NULL != THREAD_STORAGE(ct, SV_UDS_I(PHI)) &&
NULL != T_STORAGE_R_NV(ct, SV_UDSI_G(PHI)))
{
    begin_c_loop(c,ct)
    {
        C_UDMI(c,ct,GRADPHI) = NV_MAG(C_UDSI_G(c,ct,PHI));
    }
    end_c_loop(c,ct);
}

}

thread_loop_c(ct,d)
{
    if(NNULLP(THREAD_STORAGE(ct,SV_UDM_I)))
        begin_c_loop(c,ct)
{
    phi = C_UDSI(c,ct,PHI);
    gradPhi = C_UDMI(c,ct,GRADPHI);
    C_UDMI(c,ct,ZPRIME) = -fabs(gradPhi)+sqrt(pow(fabs(gradPhi),2.0)
        +(2.0*phi));
}
    end_c_loop(c,ct);
}

thread_loop_f(ft,d)
{
    if(NNULLP(THREAD_STORAGE(ft,SV_UDM_I)))
begin_f_loop(f,ft)
{
    F_UDMI(f,ft,ZPRIME) = C_UDMI(F_CO(f,ft),ft->t0,ZPRIME);
}
    end_f_loop(f,ft);
}
```

```
}
```

```
DEFINE_SOURCE(k_source, c, ct, dS, eqn)
{
    real turbVisc, buoy, source;

    turbVisc = C_UDSI(c,ct,MU_T);

    buoy = -BETA*GRAV*(turbVisc/SIGMAT)*(C_UDMI(c,ct,GRADT)+(GRAV/CP));

    C_UDMI(c,ct, BUOY)= buoy;

    if(fabs(lMo) < 1.0e5)
        source = -BETA*GRAV*(turbVisc/SIGMAT)*(GRAV/CP);
    else
        source = C_UDMI(c,ct,BUOY);

    dS[eqn] = 0.0;

    return source;
}
```

```
DEFINE_SOURCE(eps_source, c, ct, dS, eqn)
{
    real z, k, eps, c_eps3, source;

    z = C_UDMI(c,ct,ZPRIME);

    k = C_K(c,ct);
    eps = C_D(c,ct);
    c_eps3 = C_EPS3(lMo,z);

    C_UDMI(c,ct,CEPS3) = c_eps3;

    source = C_EPS_1*eps*(1.0-c_eps3)*C_UDMI(c,ct,BUOY)/k;

    dS[eqn] = C_EPS_1*(1.0-c_eps3)*C_UDMI(c,ct,BUOY)/k;

    return source;
}
```

```
DEFINE_SOURCE(energy_source, c, ct, dS, eqn)
{
    real source = C_UDMI(c,ct,GRADMUT)*GRAV/SIGMAT;
```

```
    dS[eqn] = 0.0;  
    return source;  
}
```



## Cuboid Source Particle Injection File Code

```
#include <stdio.h>
#include <math.h>
/* Define minimum and maximum dimensions in x,y,z directions */
#define XMIN    50.0
#define XMAX    55.0
#define YMIN    97.5
#define YMAX    102.5
#define ZMIN    10.0
#define ZMAX    15.0

#define NX      25
#define NY      25
#define NZ      25

#define NMF      4

#define MASSFLOW 0.568
#define INJTEMP  288.0

static double massFraction[NMF] = { 0.05, 0.45, 0.2, 0.3 };
static double diameter[NMF] = { 2.5E-06, 1.0E-05, 3.0E-05, 7.5E-5 };

int main()
{
    int i, j, k;
    int n;
    int num;

    double lx, ly, lz;

    lx = XMAX-XMIN;
```

```

ly = YMAX-YMIN;
lz = ZMAX-ZMIN;
num = NX*NY*NZ;

for (n=0; n<NMF; n++)
{
    for (i=0; i<NX; i++)
{
    for (j=0; j<NY; j++)
    {
        for (k=0; k<NZ; k++)
        {
            printf("( (%12.3e%12.3e%12.3e%12.3e%12.3e%12.3e",
XMIN+(double)i*lx/(double)(NX-1),
YMIN+(double)j*ly/(double)(NY-1),
ZMIN+(double)k*lz/(double)(NZ-1),
0.0, 0.0, 0.0);
            printf("%12.3e%12.3e%12.3e))\n",
diameter[n], INJTEMP, massFraction[n]*MASSFLOW/num);
        }
    }
}

return 0;
}

```



## MATLAB Wind Variability Averaging Script

```
%Gaussian curve of wind direction fluctuations
mu = 0;
sigma = 6;
deltax = 3;
x = -18:deltax:18;
y=(1/(sigma*sqrt(2*pi)))*exp(-((x-mu).^2)/(2*sigma*sigma));
f = @(x)(1/(sigma*sqrt(2*pi)))*exp(-((x-mu).^2)/(2*sigma*sigma));
plot(x,y,'+');
xlabel('wind direction variation (\theta^o)');
ylabel('probability');
title('Gaussian Distribution Curve of Wind direction variations');
for i=1:numel(x)
    sprintf('%d, %d\n',x(i),y(i));
end

%Importing Neutral DPM data from all ASCII files
xrange = 'B2..B3466';
yrange = 'C2..C3466';
dpmrange = 'E2..E3466';
delimiter = ',';
files = {'AMStable-18', 'AMStable-15', 'AMStable-12'...
        'AMStable-09', 'AMStable-06', 'AMStable-03', 'AMStable00'...
        'AMStable03', 'AMStable06', 'AMStable09', 'AMStable12'...
        'AMStable15', 'AMStable18'};
for i=1:numel(files)
    A(:,i)= dlmread(files{i}, delimiter, dpmrange);
end
xcoor = dlmread(files{1}, delimiter, xrange);
ycoor = dlmread(files{1}, delimiter, yrange);

%Weighting DPM Accretion rates based on probabilities of wind direction
for i=1:numel(files)
```

```

        B(:,i)= (quad(f,(x(i)-(deltax/2)),(x(i)+(deltax/2))))*A(:,i);
    end
    C=sum(B,2)/trapz(x,y);

    %Writing ASCII file
    D = [xcoor,ycoor,C];
    dlmwrite('Stable_final2',D, delimiter);

    %Sort output file and extract x= 200m and y = 100m values
    E = sortrows(D,1);
    F = sortrows(D,2);

    %Reading ADMS numerical file
    xlrage = 'E2:I3527';
    G = xlsread('ADMS_All',xlrage);
    H = sortrows(G,1);
    I = sortrows(G,2);

    J = dlmread('Stable_final', delimiter);
    K = sortrows(J,1);
    L = sortrows(J,2);

    dlmwrite('ADMS_stab1',H,delimiter);
    dlmwrite('ADMS_stab2',I,delimiter);
    dlmwrite('DPM_stab1',E,delimiter);
    dlmwrite('DPM_stab2',F,delimiter);
    dlmwrite('DPM_stab1a',K,delimiter);
    dlmwrite('DPM_stab2a',L,delimiter);

    %Ploting DPM Accretion rates at centrelines
    subplot(2,1,1);
    plot(E(1093:1113,2),E(1093:1113,3),'.');
    hold on;
    plot(K(1093:1113,2),K(1093:1113,3),'+');
    plot(H(1108:1148,2),H(1108:1148,5));hold off;
    xlabel('y distance (m)');
    ylabel('Accretion/ Dry deposition rate (kgm-2s-1)');
    axis([0 200 0 1e-4]);
    title('DPM Accretion and Dry Deposition rates at x=135m','FontWeight','bold');
    legend('DPM Accretion Cl=0.0375','DPM Accretion Cl=0.15', 'ADMS Dry Deposition');

    subplot(2,1,2);
    plot(F(1651:1815,1),F(1651:1815,3),'.');
    hold on;
    plot(L(1651:1815,1),L(1651:1815,3),'+');
    plot(I(1721:1806,1),I(1721:1806,5));
    xlabel('x distance (m)');
    ylabel('Accretion/ Dry deposition (kgm-2s-1)');

```

```
axis([0 425 0 1e-4]);  
title('DPM Accretion and Dry Deposition rates at y=100m','FontWeight','bold');  
legend('DPM Accretion Cl=0.0375','DPM Accretion cl=0.15', 'ADMS Dry Deposition');
```

## Bibliography

- AEA Technology plc. Management, mitigations and monitoring of nuisance dust and PM10 emissions arising from the extractive industries: an overview. Technical report, The Mineral Industry Research Organisation (MIRO), 2011.
- E. Agency. Technical Guidance Note (Monitoring) M17, Monitoring Particulate Matter in Ambient Air around Waste Facilities, 2013.
- C. Alinot. *Analyse aerodynamique des parcs eoliens immerges dans une couche limite terrestre ayant differentes conditions de stabilite thermiques*. PhD thesis, L'Ecole de Technologie Superieure, Universite du Quebec, 2003.
- C. Alinot and C. Masson.  $k - \varepsilon$  model for the atmospheric boundary layer under various thermal stratification. *Journal of Solar Energy Engineering*, 127:438–443, 2005.
- R. Allington, D. Jarvis, I. Brown, S. Reed, T. Horward, and F. Sharman. A quarry design handbook. Technical report, Department for Communities and Local Government, 2007.
- J. Anderson Jr. *Computational Fluid Dynamics, The Basics with Applications*. McGraw-Hill Series in Mechanical Engineering. McGraw-Hill Inc., Singapore, 1995.
- D. Anfossi, D. Oetl, G. Degrazia, and A. Goulart. An analysis of sonic anemometer observations in low wind speed conditions. *Boundary-Layer Meteorology*, 114(1):179–203, 2005.
- ANSYS. FLUENT 12.0 User's Guide. *Copyright 2009 ANSYS, Inc.*, 2009a.
- ANSYS. FLUENT 12.0 Theory Guide. *Copyright 2009 ANSYS, Inc.*, 2009b.
- T. J. Appleton, S. W. Kingman, I. S. Lowndes, and S. A. Silvester. The development of a modelling strategy for the simulation of fugitive dust emissions from in-pit quarrying activities: a UK case study. *International Journal of Mining, Reclamation and Environment*, 20(1):57–82, 2006.
- D. D. Apsley and I. P. Castro. Flow and dispersion over hills: Comparison between numerical predictions and experimental data. *Journal of Wind Engineering and Industrial Aerodynamics*, 6768(0):375–386, 1997.
- P. Arya. *Introduction to Micrometeorology*, volume 42 of *International Geophysics Series*. Academic Press Inc., San Diego, California, 1988.
- N. Ashgriz and J. Mostaghimi. *An Introduction to Computational Fluid Dynamics*, chapter 24. McGraw-Hill Handbooks. McGraw-Hill, New York; London, 2002.
- K. Ashrafi and G. A. Hoshyaripour. A model to determine atmospheric stability and its correlation with CO concentration. *Proceedings of World Academy of Science: Engineering & Technology*,

- 46:186–191, 2008.
- D. D. Aspley and CERC. Modelling dry deposition, 2012.
- J. S. Baggett. On the feasibility of merging LES with RANS for the near wall region of attached turbulent flows. *Annual Briefs 1998, Stanford University, Center for Turbulence Research*, pages 267–277, 1998.
- G. I. Barenblatt. *Similarity, Self Similarity and Intermediate Asymptotics*. Consultants Bureau, Plenum Publishing Corporation, 1979.
- R. Barratt. *Atmospheric dispersion modelling: an introduction to practical applications*. Business and the Environment: Practitioner Series. Earthscan Taylor & Francis Group, London, UK, 2001.
- R. J. Barthelmie. The effects of atmospheric stability on coastal wind climates. *Meteorological Applications*, 6(1):39–47, 1999.
- R. Bell and R. O. R. Y. Thompson. Valley ventilation by cross winds. *Journal of Fluid Mechanics*, 96(04):757–767, 1980.
- R. Berkowicz and L. P. Prahm. Generalization of K theory for turbulent diffusion. part i: Spectral turbulent diffusivity concept. *Journal of Applied Meteorology*, 18(3):266–272, 1979.
- BGS. Minerals UK, Centre for sustainable mineral development, 2014.
- T. Bide, T. Brown, S. Hobbs, and N. Idoine. United Kingdom Minerals Yearbook 2013. Technical report, British Geological Survey, Natural Environment Research Council, 2013.
- R. Biswas and R. C. Strawn. Tetrahedral and hexahedral mesh adaptation for CFD problems. *Applied Numerical Mathematics*, 26(12):135–151, 1998.
- B. Blocken, J. Carmeliet, and T. Stathopoulos. CFD evaluation of wind speed conditions in passages between parallel buildings-effect of wall-function roughness modifications for the atmospheric boundary layer flow. *Journal of Wind Engineering and Industrial Aerodynamics*, 95(9-11):941–962, 2007a.
- B. Blocken, T. Stathopoulos, and J. Carmeliet. CFD simulation of the atmospheric boundary layer: wall function problems. *Atmospheric Environment*, 41(2):238–252, 2007b.
- B. Blocken, T. Stathopoulos, P. Saathoff, and X. Wang. Numerical evaluation of pollutant dispersion in the built environment: comparisons between models and experiments. *Journal of Wind Engineering and Industrial Aerodynamics*, 96(1011):1817–1831, 2008.
- B. Boersma, M. Kooper, F. T. M. Nieuwstadt, and P. Wesseling. Local grid refinement in large-eddy simulations. *Journal of Engineering Mathematics*, 32:161–175, 1997.
- M. Bottema. Urban roughness modelling in relation to pollutant dispersion. *Atmospheric Environment*, 31(18):3059–3075, 1997.
- BSI. Workplace atmospheres - size fraction definitions for measurement of airborne particles, 1993.
- M. Burger, G. Klose, G. Rottenkolber, R. Schmehl, D. Giebert, O. Schafer, R. Koch, and S. Wittig. A combined Eulerian and Lagrangian method for prediction of evaporating sprays. *Journal of Engineering for Gas Turbines and Power*, 124(3):481–488, 2002.
- J. A. Businger, J. C. Wyngaard, Y. Izumi, and E. F. Bradley. Flux-profile relationships in the atmospheric surface layer. *Journal of the Atmospheric Sciences*, 28(2):181–189, 1971.
- X. Cai, D. G. Steyn, and I. S. Gartshore. Resolved-scale turbulence in the atmospheric surface layer from a large eddy simulation. *Boundary-Layer Meteorology*, 75(3):301–314, 1995.
- B. Cantrell, S. Stein, H. Patashnick, and D. Hassel. Status of a Tapered Element Oscillation Microbalance-based continuous respirable coal mine dust monitor. *Applied Occupational and Environmental Hygiene*, 11(7):624–629, 1996.
- S. Cao and T. Tamura. Effects of roughness blocks on atmospheric boundary layer flow over a two-dimensional low hill with/without sudden roughness change. *Journal of Wind Engineering and Industrial Aerodynamics*, 95(8):679–695, 2007.
- S. Cao, T. Wang, Y. Ge, and Y. Tamura. Numerical study on turbulent boundary layers over

- two-dimensional hills effects of surface roughness and slope. *Journal of Wind Engineering and Industrial Aerodynamics*, 104-106, 2012.
- D. Carruthers, C. McHugh, A. Robins, B. Davies, D. Thompson, and M. Montgomery. The UK Atmospheric Dispersion Modelling System: comparisons with Kinkaid, Lillestom and Copenhagen. *Journal of Wind Engineering and Industrial Aerodynamics*, 52:139–153, 1994.
- D. Carruthers, H. Edmunds, K. Ellis, C. McHugh, B. Davies, and D. Thompson. The atmospheric dispersion modelling system (ADMS): comparisons with data from the Kinkaid experiments. *International Journal of Environment and Pollution*, 5:111–120, 1995.
- D. Carruthers, S. Dyster, and C. McHugh. Contrasting methods for validating ADMS using the indianapolis dataset. *Proceedings 5<sup>th</sup> International Conference on Harmonisation within Dispersion modelling for Regulatory Purposes*, pages 104–110, 1998.
- D. J. Carruthers, C. McHugh, E. Vanyyve, M. Seaton, and E. Solazzo. Comparison of ADMS and AERMOD meteorological preprocessor and dispersion algorithms, 2009.
- D. J. Carruthers, M. D. Seaton, C. A. McHugh, X. Sheng, E. Solazzo, and E. Vanvyve. Comparison of the complex terrain algorithms incorporated into two commonly used local-scale air pollution dispersion models (ADMS and AERMOD) using a hybrid model. *Journal of the Air & Waste Management Association*, 61(11):1227–1235, 2011.
- I. P. Castro and D. D. Apsley. Flow and dispersion over topography: A comparison between numerical and laboratory data for two-dimensional flows. *Atmospheric Environment*, 31(6):839–850, 1997.
- S. J. Caughey and S. G. Palmer. Some aspects of turbulence structure through the depth of the convective boundary layer. *Quarterly Journal of the Royal Meteorological Society*, 105(446):811–827, 1979.
- CERC. FLOWSTAR complex terrain module. *UK-ADMS 5 Technical Specification Documents, Cambridge Environmental Research Consultants*, (P14/01Q/13), 2013.
- CERC Ltd. FLOWSTAR, modelling flow over complex terrain, user guide, 2011.
- H. Cevizci and H. T. Ozkahraman. The effect of blast hole stemming length to rockpile fragmentation at limestone quarries. *International Journal of Rock Mechanics and Mining Sciences*, 53:32–35, 2012.
- A. Chan. Atmospheric turbulent boundary layer development due to a change in surface roughness. *International Journal of Engineering Science*, 39(17):2001–2014, 2001.
- J. C. Chang and S. R. Hanna. Air quality model performance evaluation. *Meteorology and Atmospheric Physics*, 87(1-3):167–196, 2004.
- A. Chatzipanagiotidis and D. Olivari. Pollutant dispersal downstream of a hill in different wind conditions. *Journal of Wind Engineering and Industrial Aerodynamics*, 64(23):233–248, 1996.
- M. Chavez, B. Hajra, T. Stathopoulos, and A. Bahloul. Near-field pollutant dispersion in the built environment by CFD and wind tunnel simulations. *Journal of Wind Engineering and Industrial Aerodynamics*, 99(4):330–339, 2011.
- M. Chavez, B. Hajra, T. Stathopoulos, and A. Bahloul. Assessment of near-field pollutant dispersion: Effect of upstream buildings. *Journal of Wind Engineering and Industrial Aerodynamics*, 104106(0):509–515, 2012.
- S. Chen, Y. Shi, Z. Xiao, Z. Xia, and J. Wang. *Constrained Large eddy Simulation of Wall-Bounded Turbulent Flows*, volume 117 of *Notes on Numerical Fluid Mechanics and Multidisciplinary Design*, chapter 10, pages 121–130. Springer Berlin Heidelberg, 2012.
- S. Chinthala and M. Khare. *Particle Dispersion Within a Deep Open Cast Coal Mine*, chapter 6. 2011.
- C. Claiborn, A. Mitra, G. Adams, L. Bamesberger, G. Allwine, R. Kantamaneni, B. Lamb, and H. Westberg. Evaluation of PM10 emission rates from paved and unpaved roads using tracer

- techniques. *Atmospheric Environment*, 29(10):1075–1089, 1995.
- Cleaner Quarries. Cleaner quarries: Optimising environmental performance. Technical report, University of Nottingham, 2004.
- C. Cole and A. J. Fabrick. Surface mine pit retention. *Journal of the Air Pollution Control Association*, 34(6):674–675, 1984.
- G. Coleman and R. Sandberg. A primer on direct numerical simulation of turbulence - methods, procedures and guidelines. Technical report, Aerodynamics and Flight Mechanics Research Group, School of Engineering Sciences, University of Southampton, 2010.
- M. Coulson. *The History of Mining. The Events, Technology and People Involved in the Industry that Forged the Modern World*. Harriman House Ltd., Hampshire, Great Britain, 2012.
- R. Countess. Methodology for estimating fugitive windblown and mechanically resuspended road dust emissions applicable for regional scale air quality modeling. Technical report, Western Governors Association, Countess Environmental, 2001.
- Countess Environmental. WRAP fugitive dust handbook. Technical report, Western Regional Air Partnerships Dust Emissions Joint Forum, 2006.
- T. Craft, S. Gant, H. Iacovides, and B. E. Launder. A new wall function approach for complex turbulent flows. *Numerical Heat Transfer, Part B*, 45:301–318, 2004.
- A. Crespo and J. Hernandez. Turbulence characteristics in wind-turbine wakes. *Journal of Wind Engineering and Industrial Aerodynamics*, 61(1):71–85, 1996.
- H. Datson and M. Fowler. A method for the characterisation of ambient dust: geochemical analyses of directional sticky pad dust samples. *WIT Transactions on Ecology and the Environment*, 101: 413–429, 2007.
- B. M. Davies and D. J. Thomson. Comparisons of some parametrizations of wind direction variability with observations. *Atmospheric Environment*, 33(29):4909–4917, 1999.
- DCLG. Minerals policy statement 2: Controlling and mitigating the environmental effects of mineral extraction in england, 2005.
- DCLG. Technical Guidance to the National Planning and Policy Framework, 2012.
- P. E. B. de Mello and J. I. Yanagihara. Numerical prediction of gas concentrations and fluctuations above a triangular hill within a turbulent boundary layer. *Journal of Wind Engineering and Industrial Aerodynamics*, 98(2):113–119, 2010.
- D. M. Deaves and I. G. Lines. The nature and frequency of low wind speed conditions. *Journal of Wind Engineering and Industrial Aerodynamics*, 73(1):1–29, 1998.
- DEFRA. Process Guidance Notes 3/8 (04): Secretary of State’s guidance for quarry processes, 2004.
- DEFRA. Part IV of the Environmental Act 1995, Environment (Northern Ireland) Order 2002 Part III Local Air Quality Management Technical Guidance LAQM.TG(09), 2009.
- G. Degrazia and D. Anfossi. Estimation of the Kolmogorov Constant  $C_o$  from classical statistical diffusion theory. *Atmospheric Environment*, 32(20):3611–3614, 1998.
- A. Dehbi. A CFD model for particle dispersion in turbulent boundary layer flows. *Nuclear Engineering and Design*, 238(3):707–715, 2008.
- D. Derwent, A. Fraser, J. Abbott, M. Jenkins, P. Willis, and T. Murrells. Evaluating the Performance of Air Quality Models. Technical Report Issue 3, DEFRA, [www.defra.gov.uk](http://www.defra.gov.uk), 2010.
- S. Di Sabatino, R. Buccolieri, B. Pulvirenti, and R. Britter. Simulations of pollutant dispersion within idealised urban-type geometries with CFD and integral models. *Atmospheric Environment*, 41(37):8316–8329, 2007.
- M. Diebold, C. Higgins, J. Fang, A. Bechmann, and M. Parlange. Flow over hills: A Large-Eddy Simulation of the Bolund Case. *Boundary-Layer Meteorology*, 148(1):177–194, 2013.
- N. Djordjevic. Origin of blast-induced fines. *Mining Technology*, 111(2):143–146, 2002.
- S. Du, B. Sawford, J. Wilson, and D. Wilson. Estimation of the Kolmogorov Constant ( $C_o$ ) for

- the Lagrangian structure function using a second-order Lagrangian model of grid turbulence. *Physics of Fluids*, 7(12):3083–3090, 1995.
- S. Duranti, G. Pezzuto, and F. Pittaluga. Numerical prediction of neutral atmospheric boundary layers (RUSHIL experiment). *Journal of Wind Engineering and Industrial Aerodynamics*, 7476: 263–272, 1998.
- G. Eggenspieler. Turbulence modeling. *ANSYS, Inc.*, page 36, 2011.
- M. El-Fadel, L. Abi-Esber, and T. Ayash. Managing emissions from highly industrialized areas: Regulatory compliance under uncertainty. *Atmospheric Environment*, 43(32):5015–5026, 2009.
- J. Ferziger and M. Peric. *Computational Methods for Fluid Dynamics*. Springer-Verlag, 3rd edition, 2002.
- J. H. Ferziger and M. Peric. Further discussion of numerical errors in CFD. *International Journal for Numerical Methods in Fluids*, 23(12):1263–1274, 1996.
- S. Finardi, M. Morselli, and P. Jeannet. Wind flow models over complex terrain for dispersion calculations. Technical report, European Cooperation in Science and Technology, 1997.
- A. L. Flint and S. W. Childs. Use of the Priestley-Taylor evaporation equation for soil water limited conditions in a small forest clearcut. *Agricultural and Forest Meteorology*, 56(34):247–260, 1991.
- F. Flores, R. Garreaud, and R. C. Muoz. OpenFOAM applied to the CFD simulation of turbulent buoyant atmospheric flows and pollutant dispersion inside large open pit mines under intense insolation. *Computers & Fluids*, 90:72–87, 2014.
- T. Foken. 50 years of the MoninObukhov Similarity Theory. *Boundary-Layer Meteorology*, 119(3): 431–447, 2006.
- A. Folz and J. M. Wallace. Near-surface turbulence in the atmospheric boundary layer. *Physica D: Nonlinear Phenomena*, 239(14):1305–1317, 2010.
- J. Franke, A. Hellsten, H. Schlunzen, and B. Carissimo. Best practice guidelines for CFD simulation of flows in the urban environment. Technical report, 2007.
- R. Fransen, E. Collado Morata, F. Duchaine, N. Gourdain, L. Gicquel, L. Vial, and G. Boneau. Comparison of RANS and LES in high pressure turbines, 17-18 November 2011.
- J. R. Garratt. Review: the atmospheric boundary layer. *Earth-Science Reviews*, 37(12):89–134, 1994.
- B. Garvey, I. Castro, G. Wiggs, and J. Bullard. Measurements of flows over isolated valleys. *Boundary-Layer Meteorology*, 117(3):417–446, 2005.
- M. K. Ghose and S. R. Majee. Air pollution caused by opencast mining and its abatement measures in India. *Journal of Environmental Management*, 63(2):193–202, 2001.
- C. Górlé, J. van Beeck, P. Rambaud, and G. Van Tendeloo. CFD modelling of small particle dispersion: The influence of the turbulence kinetic energy in the atmospheric boundary layer. *Atmospheric Environment*, 43(3):673–681, 2009.
- P. Gousseau, B. Blocken, and G. J. F. van Heijst. CFD simulation of pollutant dispersion around isolated buildings: On the role of convective and turbulent mass fluxes in the prediction accuracy. *Journal of Hazardous Materials*, 194:422–434, 2011.
- C. Grainger and R. Meroney. Dispersion in an open-cut coal mine in stably stratified flow. *Boundary-Layer Meteorology*, 63(1-2):117–140, 1993.
- C. Greenfield and G. Quarini. A Lagrangian simulation of particle deposition in a turbulent boundary layer in the presence of thermophoresis. *Applied Mathematical Modelling*, 22(10):759–771, 1998.
- C. Gromke, R. Buccolieri, S. Di Sabatino, and B. Ruck. Dispersion study in a street canyon with tree planting by means of wind tunnel and numerical investigations evaluation of cfd data with experimental data. *Atmospheric Environment*, 42(37):8640–8650, 2008.
- G. Gualtieri and S. Secci. Comparing methods to calculate atmospheric stability-dependent wind speed profiles: A case study on coastal location. *Renewable Energy*, 36(8):2189–2204, 2011.

- D. Hall, A. Spanton, F. Dunkerley, M. Bennett, and R. Griffiths. A review of dispersion model intercomparison studies using ISC, R91, AERMOD and ADMS. Technical report, Environmental Technology Centre, Dept. of Chemical Engineering UMIST, 2000.
- D. J. Hall, S. L. Upton, and G. W. Marsland. Designs for a deposition gauge and a flux gauge for monitoring ambient dust. *Atmospheric Environment*, 28(18):2963–2979, 1994.
- S. R. Hanna. Lagrangian and Eulerian time-scale relations in the daytime boundary layer. *Journal of Applied Meteorology*, 20(3):242–249, 1981.
- S. R. Hanna. Lateral turbulence intensity and plume meandering during stable conditions. *Journal of Climate and Applied Meteorology*, 22(8):1424–1430, 1983.
- S. R. Hanna. Air quality model evaluation and uncertainty. *JAPCA*, 38(4):406–412, 1988.
- S. R. Hanna, O. R. Hansen, and S. Dharmavaram. FLACS CFD air quality model performance evaluation with Kit Fox, MUST, Prairie Grass, and EMU observations. *Atmospheric Environment*, 38(28):4675–4687, 2004.
- D. M. Hargreaves and N. G. Wright. On the use of the  $k\epsilon$  model in commercial CFD software to model the neutral atmospheric boundary layer. *Journal of Wind Engineering and Industrial Aerodynamics*, 95(5):355–369, 2007.
- P. Hem. Pits and Quarries. *InfoMine Inc.*, 2012.
- D. Highley, G. Chapman, and B. K.A. The economic importance of minerals to the uk. Technical report, British Geological Survey, Natural Environment Research Council, 2004.
- R. Hill, E. Lutman, and A. Arnot. Atmospheric dispersion modelling in complex terrain. Technical report, A report prepared for UK Atmospheric Dispersion Modelling Liaison Committee (ADM-LC), Westlakes Scientific Consulting, 2005.
- N. S. Holmes and L. Morawska. A review of dispersion modelling and its application to the dispersion of particles: An overview of different dispersion models available. *Atmospheric Environment*, 40(30):5902–5928, 2006.
- A. A. M. Holtslag and F. T. M. Nieuwstadt. Scaling the atmospheric boundary layer. *Boundary-Layer Meteorology*, 36(1-2):201–209, 1986.
- A. A. M. Holtslag and A. P. Van Ulden. A simple scheme for daytime estimates of the surface fluxes from routine weather data. *Journal of Climate and Applied Meteorology*, 22(4):517–529, 1983.
- S. Hong, I. Lee, H. Hwang, I. Seo, J. Bitog, K. Kwon, J. Song, O. Moon, K. Kim, H. Ko, and S. Chung. CFD modelling of livestock odour dispersion over complex terrain, part ii: Dispersion modelling. *Biosystems Engineering*, 108(3):265–279, 2011.
- A. Huber, W. Tang, A. Flowe, B. Bell, K. Kuehlert, and W. Schwarz. Development and applications of CFD simulations in support of air quality studies involving buildings, August 23-27 2004.
- J. C. R. Hunt and W. H. Snyder. Experiments on stably and neutrally stratified flow over a three-dimensional hill. *Journal of Fluid Mechanics*, 96:671–704, 1980.
- I. S. A. Isaksen, C. Granier, G. Myhre, T. K. Berntsen, S. B. Dalsren, M. Gauss, Z. Klimont, R. Benestad, P. Bousquet, W. Collins, T. Cox, V. Eyring, D. Fowler, S. Fuzzi, P. Jckel, P. Laj, U. Lohmann, M. Maione, P. Monks, A. S. H. Prevot, F. Raes, A. Richter, B. Rognerud, M. Schulz, D. Shindell, D. S. Stevenson, T. Storelvmo, W. C. Wang, M. van Weele, M. Wild, and D. Wuebbles. Atmospheric composition change: Climatechemistry interactions. *Atmospheric Environment*, 43(33):5138–5192, 2009.
- T. Ishihara, K. Hibi, and S. Oikawa. A wind tunnel study of turbulent flow over a three-dimensional steep hill. *Journal of Wind Engineering and Industrial Aerodynamics*, 83:95–107, 1999.
- P. S. Jackson and J. C. R. Hunt. Turbulent wind flow over a low hill. *Quarterly Journal of the Royal Meteorological Society*, 101(430):929–955, 1975.
- M. Z. Jacobson. Fundamentals of atmospheric modelling, 1999.
- A. Jimenez, M. Van Tongeren, and J. Cherrie. A review of monitoring methods for inhalable hard-

- wood dust. Technical report, World Health Organisation Collaborating Centre for Occupational Health, 2011.
- S. M. Joffe and T. Laurila. Standard deviations of wind speed and direction from observations over a smooth surface. *Journal of Applied Meteorology*, 27(5):550–561, 1988.
- J. Kaimal and J. Finnigan. *Atmospheric boundary layer flows, their structure and measurement*. Oxford University Press, New York, USA, 1994.
- G. Kallio and M. Reeks. A numerical simulation of particle deposition in turbulent boundary layers. *International Journal of Multiphase Flow*, 15(3):433–446, 1989.
- S. Kawai and J. Larsson. Wall-modeling in large eddy simulation: Length scales, grid resolution, and accuracy. *Physics of Fluids (1994-present)*, 24(1):39–46, 2012.
- A. Kelany, M. Negem, A. Ishani, and T. Heldal. Granite quarry survey in the Aswan region, Egypt: Shedding new light on ancient quarrying. *Geological Survey of Norway, Special Publication*, 12, 2009.
- L. H. Khurshudyan, W. H. Snyder, and I. V. Nekrasov. Flow and dispersion of pollutants over two-dimensional hills. Technical report, US EPA, 1981.
- S. W. Kingman, I. S. Lowndes, E. Petavratzi, and D. Whittles. An investigation into the mechanisms of dust generation in a tumbling mill. *Journal of rock mechanics and tunnelling technology*, 14(2), 2009.
- F. Kissell. Handbook for dust control in mining, 2003.
- H. Kose, C. Aksoy, A. Gonnen, M. Kun, and T. Malli. Economic evaluation of optimum bench height in quarries. *The Journal of The South African Institute of Mining and Metallurgy*, pages 127–135, 2005.
- P. H. S. W. Kulatilake, W. Qiong, T. Hudaverdi, and C. Kuzu. Mean particle size prediction in rock blast fragmentation using neural networks. *Engineering Geology*, 114(34):298–311, 2010.
- J. Labovsk and L. Jelemensk. Verification of CFD pollution dispersion modelling based on experimental data. *Journal of Loss Prevention in the Process Industries*, 24(2):166–177, 2011.
- J. Larsson and S. Kawai. Wall-modelling in large eddy simulation: length scales, grid resolution and accuracy. *Annual Research Briefs, Center for Turbulence Research, Stanford University*, 2010.
- B. E. Launder, N. Sandham, and (eds.). Closure strategies for turbulent and transitional flows, 2002.
- G. F. Lawler and V. Limic. *Random Walk: A Modern Introduction*, volume 123 of *Cambridge Studies in Advanced Mathematics*. Cambridge University Press, 2010.
- D. Lenschow, J. C. Wyngaard, and W. Pennell. Mean-field and second-moment budgets in a baroclinic, convective boundary layer. *Journal of the Atmospheric Sciences*, 37:1313–1326, 1980.
- L. S. Leo, M. Y. Thompson, S. Di Sabatino, and H. J. S. Fernando. Stratified flow past a hill: Dividing streamline concept revisited. *Boundary-Layer Meteorology*, pages 1–24, 2015.
- X. Li, C. Liu, D. Y. C. Leung, and K. M. Lam. Recent progress in CFD modelling of wind field and pollutant transport in street canyons. *Atmospheric Environment*, 40(29):5640–5658, 2006.
- P. Libby. *Introduction to Turbulence*. Combustion: An International Series. Taylor & Francis, New York, 1996.
- W. Ling, J. Chung, T. Troutt, and C. Crowe. Direct numerical simulation of a three dimensional temporal mixing layer with particle dispersion. *Journal of Fluid Mechanics*, 358:61–85, 1998.
- I. S. Lowndes, S. A. Silvester, S. W. Kingman, and D. M. Hargreaves. The application of an improved multi-scale computational modelling techniques to predict fugitive dust dispersion and deposition within and from surface mining operations, 2008.
- J. MacCarthy, Y. Pang, T. Murrells, N. Passant, C. Martinez, J. Thomas, G. Thistlethwaite, and T. Misselbrook. Air Quality Pollutant Inventories for England, Scotland, Wales and Northern Ireland: 1990-2009. Technical report, Department for Environment, Food and Rural Affairs, 2011.

- P. B. MacCready. The inertial subrange of atmospheric turbulence. *Journal of Geophysical Research*, 67(3):1051–1059, 1962.
- L. Mahrt. Weak-wind mesoscale meandering in the nocturnal boundary layer. *Environmental Fluid Mechanics*, 7(4):331–347, 2007.
- L. Mahrt. Surface wind direction variability. *Journal of Applied Meteorology and Climatology*, 50(1):144–152, 2010.
- G. Matheson and B. Duthie. The design of quarry faces and slopes, 2010.
- A. Maurizi. Numerical simulation of turbulent flows over 2-D valleys using three versions of the  $k\varepsilon$  closure model. *Journal of Wind Engineering and Industrial Aerodynamics*, 85(1):59–73, 2000.
- J. McAlpine and M. Ruby. *Using CFD to Study Air Quality in Urban Microenvironments*, chapter 1. The EnviroComp Institute, 2004.
- MDEQ. Calculating air emissions for the Michigan air emissions reporting system (MAERS). Technical report, Clean Air Assistance Program, Environmental Science and Services Division, Michigan Department of Environmental Quality, 2004.
- MDEQ. Managing fugitive dust, a guide for compliance with the air regulatory requirements for particulate matter generation. Technical report, Michigan Department of Environmental Quality, 2014.
- C. Mitchell. Quarry fines and waste, 2009.
- M. Mohan and T. A. Siddiqui. Analysis of various schemes for the estimation of atmospheric stability classification. *Atmospheric Environment*, 32(21):3775–3781, 1998.
- A. Monin and A. Obukhov. Basic laws of turbulent mixing in the surface layer of the atmosphere. *Tr.Akad. Nauk SSSR Geophys. Inst.*, 24(151):163–187, 1954.
- D. J. Moore. Calculation of ground level concentrations for different sampling periods and source locations(from power plant smokestack). *Atmospheric pollution*, pages 51–60, 1976.
- S. Morsi and A. Alexander. An investigation of particle trajectories in two-phase flow systems. *Journal of Fluid Mechanics*, 55(2), 1972.
- D. Neff and R. N. Meroney. Reynolds number independence of the wind-tunnel simulation of transport and dispersion about buildings. Technical report, Sponsored by the U.S. National Science Foundation through NSF Cooperative Grant No. BCS-882142, 1996.
- F. T. M. Nieuwstadt and P. G. Duynkerke. Turbulence in the atmospheric boundary layer. *Atmospheric Research*, 40(24):111–142, 1996.
- N. V. Nikitin, F. Nicoud, B. Wasistho, K. D. Squires, and P. R. Spalart. An approach to wall modeling in large-eddy simulations. *Physics of Fluids (1994-present)*, 12(7):1629–1632, 2000.
- NIOSH. Criteria for a recommended standard: occupational exposure to crystalline silica. Technical report, National Institute for Occupational Safety and Health, U.S. Department of Health, Education, and Welfare, Public Health Service, Center for Disease Control, 1974.
- Office for National Statistics. Mineral Extraction in Great Britain 2012. Technical report, Department of Communities and Local Government, 2014.
- I. Onederra. Breakage and fragmentation modelling for underground production blasting applications, 2004.
- J. M. L. M. Palma, F. A. Castro, L. F. Ribeiro, A. H. Rodrigues, and A. P. Pinto. Linear and nonlinear models in wind resource assessment and wind turbine micro-siting in complex terrain. *Journal of Wind Engineering and Industrial Aerodynamics*, 96(12):2308–2326, 2008.
- S. V. Patankar. *Numerical Heat Transfer and Fluid Flow*. Hemisphere Publishing Corporation, New York, 1980.
- H. Patashnick and R. Rupprecht. Continuous PM10 measurements using the Tapered Element Oscillating Microbalance. *Journal of the Air & Waste Management Association*, 41:1079–1083, 1991.

- R. Petersen. Applications of wind tunnel modeling for assessing odor impacts. In *Proceedings of the 2008 WEF & AWMA Odor Speciality Conference*, 2008.
- T. Phillips and C. Roy. Evaluation of extrapolation0based discretization error and uncertainty estimators, 4-7 January 2011.
- U. Piomelli, E. Balaras, H. Pasinato, K. D. Squires, and P. R. Spalart. The innerouter layer interface in large-eddy simulations with wall-layer models. *International Journal of Heat and Fluid Flow*, 24(4):538–550, 2003.
- T. Poinso, S. Candel, and A. Trouv. Applications of direct numerical simulation to premixed turbulent combustion. *Progress in Energy and Combustion Science*, 21(6):531–576, 1995.
- M. Pontiggia, M. Derudi, V. Busini, and R. Rota. Hazardous gas dispersion: A CFD model accounting for atmospheric stability classes. *Journal of Hazardous Materials*, 171(13):739–747, 2009.
- M. Pontiggia, G. Landucci, V. Busini, M. Derudi, M. Alba, M. Scaioni, S. Bonvicini, V. Cozzani, and R. Rota. CFD model simulation of LPG dispersion in urban areas. *Atmospheric Environment*, 45(24):3913–3923, 2011.
- S. Pope. *Turbulent Flows*. Cambridge University Press, Cambridge, 2000.
- S. Pope. Ten questions concerning the large eddy simulation of turbulent flows. *New Journal of Physics*, 6(35):1–24, 2004.
- A. D. Quinn, M. Wilson, A. M. Reynolds, S. B. Couling, and R. P. Hoxey. Modelling the dispersion of aerial pollutants from agricultural buildings an evaluation of computational fluid dynamics (CFD). *Computers and Electronics in Agriculture*, 30(13):219–235, 2001.
- P. Richards and R. Hoxey. Appropriate boundary conditions for computational wind engineering models using the  $k - \epsilon$  turbulence model. *Journal of Wind Engineering and Industrial Aerodynamics*, 46-47:145–153, 1993.
- A. Riddle, D. Carruthers, A. Sharpe, C. McHugh, and J. Stocker. Comparisons between FLUENT and ADMS for atmospheric dispersion modelling. *Atmospheric Environment*, 38(7):1029–1038, 2004.
- U. Rizza, G. A. Degrazia, C. Mangia, and E. P. M. Filho. Estimation of the Kolmogorov constant for the Lagrangian velocity spectrum and structure function under different PBL stability regimes generated by LES. *Physica A: Statistical Mechanics and its Applications*, 389(19):4009–4017, 2010.
- P. J. Roache. Quantification of uncertainty in computational fluid dynamics. *Annual Review of Fluid Mechanics*, 29(1):123–160, 1997.
- W. Ryan and B. Lamb. Determination of dividing streamline heights and Froude numbers for predicting plume transport in complex terrain. *Journal of the Air Pollution Control Association*, 34(2):152–155, 1984.
- S. Sabatino, R. Buccolieri, B. Pulvirenti, and R. Britter. Flow and pollutant dispersion in street canyons using FLUENT and ADMS-Urban. *Environmental Modeling and Assessment*, 13(3):369–381, 2008.
- M. Saeedi, P. P. LePoudre, and B. Wang. Direct numerical simulation of turbulent wake behind a surface-mounted square cylinder. *Journal of Fluids and Structures*, 51, 2014 (In Press, Corrected Proof).
- P. Sagaut. *Large Eddy Simulation for Incompressible Flows*. Springer-Verlag Berlin Heidelberg, Germany, 2 edition, 1998.
- J. M. Santos, N. C. Reis Jr, E. V. Goulart, and I. Mavroidis. Numerical simulation of flow and dispersion around an isolated cubical building: The effect of the atmospheric stratification. *Atmospheric Environment*, 43(34):5484–5492, 2009.
- F. Scargiali, E. Di Rienzo, M. Ciofalo, F. Grisafi, and A. Brucato. Heavy gas dispersion modelling over a topographically complex mesoscale: A CFD based approach. *Process Safety and*

- Environmental Protection*, 83(3):242–256, 2005.
- H. Schlichting and K. Gersten. *Boundary Layer Theory*. Springer-Verlag, Berlin, Germany, 8 edition, 2000.
- M. Segal. Atmospheric thermal stratification and the position of mechanical ventilation air intakes. *Building and Environment*, 24(3):239–243, 1989.
- G. A. Sehmel. Particle deposition from turbulent air flow. *Journal of Geophysical Research*, 75(9):1766–1781, 1970.
- N. Sharma, K. Chaudhry, and C. Chalapati Rao. Review - air pollution dispersion studies through environmental wind tunnel (*ewt*) investigations: A review. *Journal of scientific and industrial research : JSIR*, 64(8):549–559, 2005.
- R. H. Shaw and A. R. Pereira. Aerodynamic roughness of a plant canopy: A numerical experiment. *Agricultural Meteorology*, 26(1):51–65, 1982.
- P. Sheppard. Airflow over mountains. *Quarterly Journal of the Royal Meteorological Society*, 75:41–56, 1956.
- S. A. Silvester, I. S. Lowndes, J. Docx, and S. W. Kingman. The application of fluid dynamics to the improved prediction of dust emission from surface quarry operations. In *Fifth international conference on CFD in the process industries*. CSIRO, 2006.
- S. A. Silvester, I. S. Lowndes, and D. M. Hargreaves. A computational study of particulate emissions from an open pit quarry under neutral atmospheric conditions. *Atmospheric Environment*, 43(40):6415–6424, 2009.
- G. Simangunsong, K. Matsui, H. Shimada, B. Sulistiano, I. Arif, and S. Kramadibrata. *Analysis of ground vibration and fragmentation by blasting: case study at limestone and shale-stone quarries of PT Indocement Tungal Prakarsa, West Java, Indonesia*, pages 309–315. Taylor and Francis Group, London, 2004.
- R. J. Smith. A gaussian model for estimating odour emissions from area sources. *Mathematical and Computer Modelling*, 21(9):23–29, 1995.
- W. H. Snyder. Some observations of the influence of stratification on diffusion in building wakes. In *Presentation at the Inst. of Math. & Its Applications Meeting on Stably Stratified flows*, 1992.
- W. H. Snyder, R. S. Thompson, R. E. Eskridge, R. E. Lawson, I. P. Castro, J. T. Lee, J. C. R. Hunt, and Y. Ogawa. The structure of strongly stratified flow over hills: dividing-streamline concept. *Journal of Fluid Mechanics*, 152:249–288, 1985.
- W. H. Snyder, L. H. Khurshudyan, I. V. Nekrasov, R. E. Lawson Jr, and R. S. Thompson. Flow and dispersion of pollutants within two-dimensional valleys. *Atmospheric Environment. Part A. General Topics*, 25(7):1347–1375, 1991.
- P. R. Spalart. Strategies for turbulence modelling and simulations. *International Journal of Heat and Fluid Flow*, 21(3):252–263, 2000.
- E. Spiegel and G. Veronis. On the Boussinesq approximation for a compressible fluid. *Astrophysical Journal*, 131:442, 1960.
- K. D. Squires and J. Eaton. Measurements of particle dispersion obtained from direct numerical simulations of isotropic turbulence. *Journal of Fluids Engineering*, 226:1–35, 1991.
- M. K. Srivastava and P. P. Sarthi. Turbulent kinetic energy in the atmospheric surface layer during the summer monsoon. *Meteorological Applications*, 9(2):239–246, 2002.
- Z. Su. The surface energy balance system (SEBS) for estimation of turbulent heat fluxes. *Hydrol. Earth Syst. Sci.*, 6(1):85–100, 1999.
- H. Sundqvist, E. Berge, and J. E. Kristjansson. Condensation and cloud parameterization studies with a mesoscale numerical weather prediction model. *Monthly Weather Review*, 117(8):1641–1657, 1989.
- O. Sutton. *Micrometeorology, A study of physical processes in the lowest layers of the Earth's*

- atmosphere*. Magraw-Hill Book Company, Inc., 1953.
- W. C. Swinbank. Long-wave radiation from clear skies. *Quarterly Journal of the Royal Meteorological Society*, 89(381):339–348, 1963.
- L. Tarmac. Tunstead and Old Moor Quarries, Buxton. Application for determination of conditions under the Review of Mineral Permission Provisions of the Environmental Act 1995 and the Environmental Impact Assessment Regulations 2008 and 2011. *Environmental Statement Non-technical Summary*, 6:35, 2013.
- H. Tennekes and J. Lumley. *A First Course in Turbulence*. Massachusetts Institute of Technology, 16 edition, 1972.
- R. Thompson and A. Visser. Selection, performance and economic evaluation of dust palliatives on surface mine haul roads. *The Journal of The South African Institute of Mining and Metallurgy*, 107(450):435–450, 2007.
- D. J. Thomson. Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *Journal of Fluid Mechanics*, 180:529–556, 1987.
- Z. F. Tian, J. Y. Tu, G. H. Yeoh, and R. K. K. Yuen. On the numerical study of contaminant particle concentration in indoor airflow. *Building and Environment*, 41(11):1504–1514, 2006.
- Y. Tominaga and T. Stathopoulos. Numerical simulation of dispersion around an isolated cubic building: Comparison of various types of  $k\varepsilon$  models. *Atmospheric Environment*, 43(20):3200–3210, 2009.
- Y. Tominaga and T. Stathopoulos. CFD modeling of pollution dispersion in building array: Evaluation of turbulent scalar flux modeling in RANS model using LES results. *Journal of Wind Engineering and Industrial Aerodynamics*, 104106:484–491, 2012.
- A. M. Tompkins. Impact of temperature and humidity variability on cloud cover assessed using aircraft data. *Quarterly Journal of the Royal Meteorological Society*, 129(592):2151–2170, 2003.
- N. Tripcevich and K. Vaughn. *Mining and Quarrying in the Ancient Andes: Sociopolitical, Economic and Symbolic Dimensions*. Springer, New York, 2013.
- P. G. Tucker. Assessment of geometric multilevel convergence robustness and a wall distance method for flows with multiple internal boundaries. *Applied Mathematical Modelling*, 22(45):293–311, 1998.
- USEPA. AP 42, Fifth Edition, Volume I Chapter 13: Miscellaneous sources: Explosives detonation. Technical report, U.S. Environmental Protection Agency, 1980.
- USEPA. AP 42, Fifth Edition, Volume 1 Chapter 11: Mineral products industry. Technical report, U.S. Environmental Protection Agency, 1998.
- USEPA. Appendix A: Surface characteristics tables ,aersurface user’s guide. Technical report, U. S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Air Quality Assessment Division, Air Quality Modeling Group, 2008a.
- USEPA. Quality assurance handbook for air pollution measurement systems, 2008b.
- H. W. Vallack. A field evaluation of Frisbee-type dust deposit gauges. *Atmospheric Environment*, 29(12):1465–1469, 1995.
- A. Venkatram. A critique of empirical emission factor models: a case study of the AP-42 model for estimating PM10 emissions from paved roads. *Atmospheric Environment*, 34(1):1–11, 2000.
- J. M. Veranth, E. R. Pardyjak, and G. Seshadri. Vehicle-generated fugitive dust transport: analytic models and field study. *Atmospheric Environment*, 37(16):2295–2303, 2003.
- H. Versteeg and W. Malalasekera. *An introduction to computational fluid dynamics. The finite volume method*. Addison Wesley Longman Ltd, Malaysia, 1995.
- L. Vervecken, J. Camps, and J. Meyers. Accounting for wind-direction fluctuations in reynolds-averaged simulation of near-range atmospheric dispersion. *Atmospheric Environment*, 72:142–150, 2013.

- D. Vickers, L. Mahrt, and D. Belui. Particle simulations of dispersion using observed meandering and turbulence. *Acta Geophysica*, 56(1):234–256, 2008.
- C. J. Walcek. Cloud cover and its relationship to relative humidity during a springtime midlatitude cyclone. *Monthly Weather Review*, 122(6):1021–1035, 1994.
- J. Watson and J. Chow. Reconciling fugitive dust emissions inventory and ambient source contribution estimates: Summary of current knowledge and needed research. Technical report, Desert Research Institute, Energy and Environmental Engineering Centre, 2000.
- J. Watson, J. Chow, and T. Pace. *Fugitive dust emissions*. Air pollution engineering manual. Van Nostrand Reinhold, New York, USA, 2000.
- WHO. Air quality guidelines for Europe. Technical report, World Health Organization Regional Office for Europe, 2000.
- G. Wiggs, J. Bullard, B. Garvey, and I. Castro. Interactions between airflow and valley topography with implications for aeolian sediment transport. *Physical Geography*, 23(5):366–380, 2002.
- J. L. Woodward. *Appendix A: Atmospheric Stability Classification Schemes*, pages 209–212. John Wiley & Sons, Inc., 1999.
- J. Xu, C. Yan, and J. Fan. Computations of wall distances by solving a transport equation. *Applied Mathematics and Mechanics*, 32(2):141–150, 2011.
- L. Yee, M. Yusoff, and N. Shuaib. Tetrahedral mesh generator for CFD simulation of complex geometry. In *3rd International Conference on Energy and Environment ICEE*, pages 330–336. IEEE, 2009.
- P. K. Yeung. Lagrangian investigations of turbulence. *Annual Review of Fluid Mechanics*, 34(1):115–142, 2002.
- P. Zanetti. *Air Pollution Modelling, Theories, Computational Methods and Available Software*. Van Nostrand Reinhold, Southampton, Boston, 1990.
- O. Zikanov. *Essential computational fluid dynamics*. John Wiley & Sons, 2010.