

Simulating air pollution in the urban microclimate

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All the work presented in this thesis is that of the author. Any work or contribution made by others is referenced appropriately.

Tom Grylls
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Abstract

Simulating air pollution in the urban microclimate

Tom Grylls

Under the supervision of Dr Maarten van Reeuwijk

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With continuing urbanisation and business-as-usual emission regulation policies, mortalities due to urban air quality will continue to rise in the period up to 2050. Poor urban air quality has significant impacts across the three capitals of sustainability (environmental, economic and social effects). Our understanding of and ability to model air pollution in urban areas is integral towards the development of both short- and long-term solutions to this problem. This thesis covers the development of the model capabilities required to study urban air pollution at the microclimate scale; with a focus on five key elements: 1) morphology, 2) emissions, 3) chemistry, 4) atmospheric stability and 5) trees. Following the conceptual methodology outlined in this thesis, these elements are systematically investigated within the context of the inherently multi-scale and heterogeneous nature of urban environments.

Large-eddy simulation (LES) models are capable of resolving the energetic turbulent scales of the unsteady urban flow field up to the highest possible resolutions ($O(1\text{ m}, 0.1\text{ s})$), which is integral to accurately capturing the dispersion of pollutants within the urban canopy layer (UCL). The application of the urban LES model, uDALES, to study pollution dispersion within realistic urban morphologies is validated against wind tunnel data. uDALES is coupled to a traffic microsimulation model to capture realistic vehicular emissions and the LES model is further extended to resolve the chemical reactions of the null cycle.

In terms of atmospheric stability, the incorporation of thermal effects into urban LES results in slow transients and significant changes in the modelled boundary layer dynamics. A comprehensive study is therefore conducted to formulate best practice guidelines for the modelling of non-neutral urban boundary layers in statistical steady states. A novel method is devised in which a developing convective or stable boundary layer can be ‘frozen’ in time.

Trees are an integral part of the urban form and their presence within the UCL affects the transfer of momentum, radiation, temperature, moisture and pollutants. A minimal model for trees is presented that captures all of these processes whilst minimising the number of additional free parameters introduced to the problem. A bulk parametric study is used to investigate the sensitivities of the resulting energy balance system, with a focus

on the attribution between tree’s transpirational and shading cooling effects. Trees are shown to have both positive and negative effects on urban air quality depending on the incorporation of thermal effects and the roadside-background concentration ratio of the considered pollutant (a reduction in PM_{2.5} of 40% under neutral conditions and an 8% increase in NO_x under convective conditions are found). In the vicinity of high emissions, the drag imposed by the tree canopies (as well as the elevated buoyancy sink and reduced surface heat flux) are shown to lead to degradations in air quality. However for pollutants that exist more homogeneously within the urban environment, the deposition of pollutants onto the tree canopy can lead to local reductions in pollutant concentrations.

The discussed model developments are showcased through a comprehensive case study over South Kensington, London, UK. Incorporating all of the five elements of urban air quality into one investigation presents a significant contribution towards realistically modelling and fully resolving air pollution in the urban microclimate. LES results are systematically compared to gain a fundamental insight into the change in air quality due to the switch between e.g. neutral and convective conditions (16% reduction in pedestrian-averaged NO_x concentrations) and with and without trees (maximum increase in pedestrian-averaged NO_x concentrations of 87.9% and maximum decrease of 15.4%).

Comparable simulations are also run over the case study region using the operational air quality model SIRANE. This enables an evaluation of the assumptions, simplifications and parametrisations used in operational models and makes use of the high resolution capabilities and numerical control of uDALES. SIRANE is generally shown to provide a good prediction of canyon-averaged NO_x concentrations over a range of different conditions. The assumption of photostationarity is shown to lead to over- (average fractional bias, FB = -0.20) and under-predictions (FB = 0.11) of reactive NO and O₃ respectively. It is also found that the use of canyon-average concentrations in SIRANE results in a systematic under-prediction of pedestrian-level exposure.

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Contents

Abstract	iii
Acknowledgements	v
Table of contents	vi
List of figures	xi
List of tables	xv
Nomenclature	xvi
1 Introduction	1
1.1 Urban heterogeneity	4
1.2 Urban flow field	6
1.3 Urban microclimate	7
1.4 Methodology	8
1.5 Urban air pollution	9
1.5.1 Emissions	10
1.5.2 Dispersion	12
1.5.3 Chemical reactions	16
1.5.4 Removal	19
1.6 Scope	20
1.7 Structure of this thesis	21
2 Modelling	23
2.1 Introduction	23
2.2 SIRANE	25
2.3 uDALES	27
2.3.1 Governing equations	27

2.3.2	Numerical discretisation	30
2.3.3	Lateral and top boundary conditions	31
2.3.4	Immersed boundary method	32
2.3.5	Wall functions	32
2.3.6	Statistics	34
2.4	Validation	35
2.4.1	The DAPPLE project	36
2.4.2	Simulation set-up	36
2.4.3	Results	39
2.4.4	Discussion	43
2.5	A note on LES set-ups	44
3	Simulating air pollution in the urban microclimate I: morphology, traffic and chemistry	47
3.1	Introduction	47
3.2	Models	50
3.2.1	SIRANE	50
3.2.2	uDALES	51
3.3	Case study	52
3.3.1	Morphology	52
3.3.2	Traffic and emissions	56
3.3.3	Meteorological conditions	57
3.3.4	Boundary conditions	58
3.4	Results	59
3.4.1	Inert case	60
3.4.2	Reactive case	67
3.5	Conclusion	71
4	Steady-state large-eddy simulations of convective and stable urban boundary layers	73
4.1	Introduction	73
4.2	How to create steady-state UBLs	76
4.2.1	Integral description of the UBL	77
4.2.2	Steady-state methods	78
4.3	Large-eddy simulation set-up	85
4.4	Results	88
4.4.1	Transient non-neutral UBLs	88

4.4.2	Steady-state convective UBLs	90
4.4.3	Steady-state stable UBLs	95
4.5	Steady-state uncapped non-neutral UBLs	98
4.5.1	Fixed-point solution method	99
4.5.2	Frozen transient method	99
4.6	Conclusion	103
5	A minimal model for trees in urban large-eddy simulations	107
5.1	Introduction	107
5.2	Minimal tree model	110
5.2.1	Drag	112
5.2.2	Deposition	113
5.2.3	Canopy energy balance	113
5.2.4	Urban surface energy balance	119
5.3	Bulk parametric study	119
5.4	Verification	124
5.4.1	Full-canopy	125
5.4.2	Full- and half-canopy comparison	126
5.4.3	Single row of trees	130
5.5	Trees in infinite canyons	133
5.5.1	Simulation set-up	133
5.5.2	Results	137
5.6	Future work	147
5.7	Conclusion	149
6	Simulating air pollution in the urban microclimate II: atmospheric stability and trees	151
6.1	Introduction	151
6.2	Case study	153
6.2.1	Atmospheric stability	154
6.2.2	Trees	156
6.3	Results	161
6.3.1	uDALES-uDALES comparison	162
6.3.2	uDALES-SIRANE comparison	171
6.4	Conclusion	175

7	Conclusion and future work	179
7.1	Overview	179
7.2	Contributions	181
7.3	Role of large-eddy simulations	187
7.4	Future work	188
A	Appendices	209
A.1	Net radiation parametrisation	209
A.2	Null cycle chemical scheme implementation	210
A.3	Chemistry validation	211
A.4	A note on the tree canopy radiation budget	211
A.5	Tree canopy Penman-Monteith derivation	215

List of Figures

1.1	Aerial photograph of Paris, highlighting the heterogeneity of urban environments.	4
1.2	Street canyons across global urban environments.	5
1.3	Schematic of the the urban boundary layer, roughness sublayer and the urban canopy layer flows.	6
1.4	Schematic of flow structure and simplified control volume analysis for an infinite canyon.	12
1.5	Schematic of relevant VOC-NO _x -O ₃ chemical reactions.	17
2.1	Diagrammatic representation of the varying scales of pollution dispersion models.	25
2.2	Diagrammatic view of the street-network representation in the model SIRANE	26
2.3	Arakawa C-grid as applied in uDALES.	29
2.4	Diagrammatic view of the lateral boundary conditions used in urban large-eddy simulations.	32
2.5	Diagrammatic view of the urban morphologies used in the uDALES validation cases.	37
2.6	Vertical profiles of the precursor simulation used in the uDALES validation case.	39
2.7	Vertical profiles at position R for the uDALES validation cases (compared to wind tunnel data).	41
2.8	Quiver plots for uDALES validation cases (compared to wind tunnel data).	42
2.9	Scalar concentrations and variances for the uDALES validation (compared to wind tunnel results).	43
2.10	x - y plane of scalar concentrations for the uDALES validation cases.	44
3.1	Aerial view of the case study area in South Kensington, London, UK.	53

3.2	Diagram of the urban morphology, street-network and emissions used in the case study.	55
3.3	NO _x concentrations from uDALES and SIRANE under neutral conditions. .	61
3.4	Scatter and box plots evaluating SIRANE's predictive performance on NO _x concentrations and along-canyon velocities under neutral conditions.	62
3.5	Scatter and box plots investigating in-canyon variability of NO _x and the applicability of a correction factor.	64
3.6	Scatter and box plots evaluating SIRANE's predictive performance on reactive pollutant concentrations under neutral conditions.	67
3.7	Instantaneous and time averaged photostationary steady-state defects in uDALES under neutral conditions.	68
3.8	Box plots illustrating the in-canyon variability of reactive pollutant concentrations in uDALES under neutral conditions.	69
4.1	Diagrammatic view of the diurnal cycle of the planetary boundary layer. . .	77
4.2	Diagram of the staggered cubic array used to study non-neutral urban boundary layers.	85
4.3	Developing mean and turbulent vertical profiles of convective and stable urban boundary layers.	89
4.4	Mean and turbulent profiles of steady-state convective urban boundary layers I.	91
4.5	Mean and turbulent profiles of steady-state convective urban boundary layers II.	93
4.6	Time series of bulk wind speed for steady-state stable urban boundary layers showing intermittency.	96
4.7	Mean and turbulent profiles of steady-state stable urban boundary layers. .	97
4.8	Profiles of the forcings used in the novel 'frozen-transient' method.	100
5.1	Diagrammatic representation of the different scales of tree modelling.	111
5.2	Diagrams and example profiles illustrating the one-dimensional radiative budget applied in the minimal tree model.	115
5.3	Diagram of the idealised set up of a single row of trees in a crossflow used to conduct the bulk parametric study.	120
5.4	Analysing the sensitivity of the minimal tree model to the leaf area index. .	122
5.5	Analysing the sensitivity of the minimal tree model to the net radiation. . .	124
5.6	Domain and tree canopy set-ups for the tree verification cases.	125

LIST OF FIGURES

5.7	Mean and turbulent vertical profiles of the full-canopy simulation in uDALES compared to previous studies.	126
5.8	Mean profiles of velocity, potential temperature and water vapour specific humidity for the half-canopy simulation.	128
5.9	Plots of the instantaneous, mean and root-mean-square wind speeds, potential temperatures and water vapour specific humidities for the single-row-of-trees simulation.	131
5.10	Radiative, sensible and latent heat fluxes at the leaf surface for the single row of trees simulation, compared to a previous study.	132
5.11	Domain and canopy set-up applied for the simulations of trees in infinite urban canyons.	134
5.12	Quiver plots of the flow fields for the four trees in infinite canyons cases. . .	138
5.13	Streamline plots of the flow fields for the four trees in infinite canyons cases.	139
5.14	Plots of the potential temperature for the four trees in infinite canyons cases.	140
5.15	Plots of the volumetric sources and sink terms of the tree canopy under convective conditions.	142
5.16	Plots of the streamwise development of the emitted scalar field in two of the trees in infinite canyon cases.	143
5.17	Plots of the ‘effective’ NO_x concentrations for the four trees in infinite canyons cases.	145
5.18	Plots of the ‘effective’ $\text{PM}_{2.5}$ concentrations for the four trees in infinite canyons cases.	146
6.1	Images indicating the processing of LIDAR data to form a representation of tree canopies within urban large-eddy simulations.	158
6.2	Diagrammatic representation of the domain and tree canopies for the case study uDALES simulation under convective conditions with trees.	160
6.3	Comparison of the NO_x concentrations over the case study region under neutral and convective conditions.	163
6.4	Mean and turbulent vertical profiles of the neutral, convective and convective with trees uDALES simulations.	164
6.5	Comparison of the velocity fields within the urban canopy layer over the case study region under neutral and convective conditions.	165
6.6	Comparison of the reactive pollutant concentrations over the case study region under neutral and convective conditions.	166
6.7	Photostationary steady-state deficits over the case study region under neutral, convective and convective with trees conditions.	166

6.8	Comparison of the NO_x concentrations over the case study region under convective and convective with trees conditions.	168
6.9	Comparison of the pedestrian-level NO_x concentrations over the case study region under convective and convective with trees conditions.	169
6.10	Scatter and box plots comparing the NO_x concentrations and along-canyon velocities under convective and convective with trees conditions.	170
6.11	Scatter and box plots comparing the reactive pollutant concentrations under convective and convective with trees conditions.	171
6.12	Scatter and box plots evaluating SIRANE's predictive performance on NO_x concentrations and along-canyon velocities under convective and convective with trees conditions.	173
6.13	Scatter and box plots evaluating SIRANE's predictive performance on reactive pollutant concentrations under convective and convective with trees conditions.	174
A.1	Vertical profiles of the spanwise- and time averaged NO_x for the chemistry validation.	212
A.2	Comparison of the net radiative flux through a tree canopy using different radiation schemes.	213

List of Tables

1.1	Table showing the five elements of urban air quality identified for study in this thesis.	11
2.1	Simulation set-ups for uDALES validation case.	38
3.1	Case study properties of SIRANE and uDALES.	54
3.2	Statistical indices used to evaluate SIRANE for south-westerly and westerly wind directions under neutral conditions.	60
3.3	Correction factors, m , for the linear regressions of DA-p against DA-s for westerly and south-westerly wind directions and under neutral conditions. .	65
4.1	A summary of the thermal forcings and boundary conditions used to produce steady-state non-neutral urban boundary layers in the literature and as defined in this study.	79
4.2	A summary of the flow forcings (F_u and F_v) used in this study.	81
4.3	Details on the set of convective and stable simulations used to analyse different steady-state methods.	87
4.4	Summary of the main challenges, results and guidelines regarding the modelling of steady-state non-neutral urban boundary layers.	104
5.1	Bulk environmental and tree parameters used in the parametric study. . . .	121
5.2	Environmental and tree parameters used in the four simulations of the trees in infinite canyons study.	135
6.1	Statistical indices used to evaluate SIRANE for convective conditions and with trees.	172
6.2	Correction factors, m , for the linear regressions of DA-p against DA-s under convective conditions and with trees.	175

Nomenclature

Abbreviations

CBL	Convective boundary layer
CFD	Computational fluid dynamics
CFL	Courant-Friedrichs-Lewy
CSA	Comprehensive spatial averaging
FAC2	Fraction in a factor of 2
FB	Fractional bias
IBM	Immersed boundary method
ISA	Intrinsic spatial averaging
LES	Large-eddy simulation
NMSE	Normalised mean square error
PM	Particulate matter
PSS	Photostationary steady-state
RANS	Reynolds-averaged Navier-Stokes
RSL	Roughness sub-layer
SBL	Stable boundary layer
SGS	Sub-grid scale
TKE	Turbulent kinetic energy
UBL	Urban boundary layer

UCL	Urban canopy layer
UHI	Urban heat island
VOC	Volatile organic compound

Constants

κ	von Kármán constant,	0.41
c_d	Heat capacity of dry air,	1004 J kg ⁻¹ K ⁻¹
g	Gravitational acceleration of Earth,	9.81 m s ⁻²
L_v	Latent heat of vaporisation,	2.26×10 ⁶ J kg ⁻¹
Pr	Prandtl number of air,	0.71
R_d	Gas constant for dry air,	287.04 J kg ⁻¹ K ⁻¹
R_v	Gas constant for water vapour,	461.5 J kg ⁻¹ K ⁻¹

Symbols

α	Extinction coefficient	[-]
β	Wind angle	[°]
δ_{ps}	Photostationary steady-state deficit	[%]
Γ	Lapse rate	[K m ⁻¹]
γ	Psychometric constant	[Pa K ⁻¹]
Λ	Longwave radiation	[W m ⁻²]
λ_l	Canopy volume fraction	[-]
Ω	Decoupling factor	[-]
ω	Weighting factor	[-]
ϕ, ϕ_θ	Potential temperature flux	[Km s ⁻¹]
ϕ_q	Water vapour specific humidity flux	[kgm kg ⁻¹ s ⁻¹]
ψ	Scalar quantity	[various]

LIST OF TABLES

ρ	Density of air	[kg m ⁻³]
σ	Standard deviation of velocity	[m s ⁻¹]
Θ	Latitude	[°]
θ	Potential temperature	[K]
θ_v	Liquid water virtual potential temperature	[K]
ε	Vapour pressure	[Pa]
φ	Pollutant scalar concentration	[various]
A	Albedo	[-]
a	Leaf area density	[m ² m ⁻³]
c	Heat capacity	[J kg ⁻¹ K ⁻¹]
Cld	Cloud coverage index	[Octas]
D	Vapour pressure deficit	[Pa]
d	Leaf area index	[-]
E	Emissivity	[-]
e	Turbulent kinetic energy	[m ² s ⁻²]
H	Building/ canopy height	[m]
h	Boundary layer height	[m]
J	Photolysis rate	[s ⁻¹]
K	Shortwave radiation	[W m ⁻²]
k	Reaction rate	[m ³ mole ⁻¹ s ⁻¹]
L	Obukhov length	[m]
l	Leaf size	[m]
l_z	Domain height	[m]
p	Atmospheric pressure	[Pa]

Q^*	Net radiation	$[\text{W m}^{-2}]$
Q_E	Latent heat flux	$[\text{W m}^{-2}]$
Q_H	Sensible heat flux	$[\text{W m}^{-2}]$
Q_S	Storage heat flux	$[\text{W m}^{-2}]$
q_v	Water vapour specific humidity	$[\text{kg kg}^{-1}]$
R	Volumetric source/ sink of potential temperature	$[\text{K s}^{-1}]$
r	Resistance	$[\text{s m}^{-1}]$
s	Slope of the curve relating saturation pressure to temperature	$[\text{Pa K}^{-1}]$
T	Temperature	$[\text{K}]$
t	Time	$[\text{s}]$
U	Along-canyon velocity	$[\text{m s}^{-1}]$
u_d	Deposition velocity	$[\text{m s}^{-1}]$
u_e	Exchange velocity	$[\text{m s}^{-1}]$
u_i	Velocity component (u , v or w)	$[\text{m s}^{-1}]$
u_*	Friction velocity	$[\text{m s}^{-1}]$
w_s	Stabilising velocity	$[\text{m s}^{-1}]$
x_i	Coordinate in Euclidian space (x , y or z)	$[\text{m}]$
z_0	Aerodynamic roughness length	$[\text{m}]$

Chapter 1

Introduction

More than half of the global population now lives in urban areas and this proportion is expected to continue to increase in the future (United Nations, 2014). As cities grow and become more dense, the interaction between the urban population, built environment and climate is increasingly important in terms of the sustainability of urban life. The concept of urban metabolism (Newman, 1999) provides a useful framework through which to consider these interactions, analogising the behaviour of an urban system to a living organism; consuming material and energy resources and producing waste (e.g. the emission of heat and pollutants). The anthropogenic forms and processes that drive this system culminate in urban environments that deviate further and further away from their rural counterparts. The resulting climate of a city (air quality, temperature, humidity etc.), particularly conditions within the urban canopy, has impacts across the three capitals of sustainability: 1) environmental, 2) economic and 3) social (Keeble, 1988; Basiago, 1998; Hasna et al., 2007; Hasna, 2010).

The ‘metabolic’ consumption of energy and materials results in the emission of a range of primary pollutants into the urban atmosphere (e.g. nitrogen oxides (NO_x) from the combustion of fuel in a petrol engine and volatile organic compounds (VOCs) due to their evaporation from paint). Alongside the ambient air pollution of the regional climate, the life cycle (emission, dispersion, reaction and removal) of these pollutants within the urban environment determines air quality at street-, neighbourhood- and city-scales.

Heightened concentrations of these by-products of urban metabolism pose environmental and health risks over a large range of spatial and temporal scales (traces of New York’s urban plume have even been detected in Europe) and present the most prevalent challenge to life in the urban climate. The effect of poor air quality on public health has been highlighted as the largest single environmental health risk by the World Health Organisation (WHO); estimated to cause 4.2 million deaths a year (7.6% of all deaths in 2016) with 91%

of the global population living in areas that exceed WHO guideline limits (World Health Organization, 2016). The cost to European economies from air pollution was quantified to US\$1.6 trillion in 2014 (almost 10% of the region’s total GDP), a result of premature deaths, losses in productivity and health care costs (Salvi and Brickman, 2015). London exceeded EU annual pollution limits of NO_2 within the first week of 2017 and a YouGov poll has indicated that Londoners perceive air pollution to be the greatest health threat facing the city (Cecil, 2016). Conditions are worse in many low- to middle-income countries. In megacities such as Beijing and Delhi understanding, controlling and alleviating air quality issues is one of the most significant challenges facing the local governments.

The key to long-term improvements in urban air quality is through reduced emissions, e.g. the electrification of heating, cooling and transport (alongside renewable local power generation, decarbonised national generation and energy storage). However, 1) emission control and regulation is an incremental process and requires large-scale, long-term infrastructural and behavioural change (as well as significant economic investment) and 2) recent studies increasingly illustrate the complexity and global variability of source contributions and in particular the prevalence and importance of non-combustible emission sources (e.g. particulate matter from brakeware; Lelieveld et al., 2015). For these reasons, pollution levels will remain a challenge to the urban environment for the coming decades. Lelieveld et al. (2015) suggest that with continuing urbanisation and business-as-usual emission regulation policies, mortalities due to urban air quality will continue to rise in the period up to 2050. Hence, more immediate and flexible solutions to these challenges are necessary as well as feasible long-term pathways towards clean urban air.

The formation of sustainable air quality management strategies is reliant on our understanding of and ability to identify the challenges of urban air quality. The interaction between the heterogeneous urban environment and mesoscale meteorological conditions results in highly unsteady and turbulent pollutant concentration fields over cities that are determined by processes at a wide range of scales. Urban planners and public authorities rely on a combination of observational data and operational pollution dispersion models to resolve these fields and use this data to develop both short- and long-term solutions. Networks of stationary and mobile sensors are integral to understanding and identifying local challenges in air quality, whilst operational models provide information on the spatial and temporal evolution of pollutants over a city. The main limitation of these tools is the resolution and accuracy at which the concentration of pollutants can be resolved. The turbulent urban flow field is computationally demanding to resolve. An inherent trade-off therefore arises in numerical models between the given resolution and accuracy and the cost and speed of computation. Operational models parametrise either the bulk disper-

sive processes and exchanges or the role of turbulence in the urban flow field in order to minimise these computational costs. The level of abstraction taken in such operational models inhibits their physical verisimilitude; in particular it is challenging for these models to accurately capture smaller scale dynamics, thermal effects and details of the urban environment (e.g. trees).

Operational models are therefore used to study urban pollution dispersion at large spatial and temporal scales. They have been instrumental in the implementation and analysis of city-scale solutions such as temporary limitations on transport and sustainable urban planning (Borge et al., 2018). However more accurate and higher resolution modelling of pollution dispersion at a neighbourhood- and street-scale is imperative both towards developing our fundamental understanding of urban air quality (particularly pedestrian-level exposure) and developing solutions at this microclimate scale, e.g. sustainable urban design (optimising city ‘breathability’ and the use of green infrastructure; Llaguno-Munitxa and Bou-Zeid, 2018) and technological innovations (outdoor air purification, photocatalytic pavements etc.; Sikkema et al., 2015).

Large-eddy simulation (LES) models provide the capability to simulate pollution dispersion at the required scales by resolving the urban flow field at the highest possible resolutions ($O(1\text{ m}, 0.1\text{ s})$; Letzel et al., 2008; Salim et al., 2011b; Tominaga and Stathopoulos, 2013). This thesis presents a systematic study into air pollution in the urban microclimate utilising high-resolution urban LES. Five elements of urban air quality are identified that are both key determinants in the life cycle of urban air pollutants and have scope for developing our fundamental understanding of the research area: morphology, emissions, chemistry, atmospheric stability and trees. This thesis presents the studies conducted and the methodologies created during the development of an urban LES model to resolve these five elements. Both isolated studies and a comprehensive case study are used to draw conclusions on the modelling of these elements and their importance in determining pedestrian-level exposure to harmful pollutants. The case study is also used to compare against and evaluate the performance of an operational air quality model. This comparison helps to contextualise the role of LES in this research area and also provides suggestions and solutions for improving the performance of operational air quality modelling. The remainder of the chapter introduces the key concepts and outlines the methodology used in this thesis.



Figure 1.1: Aerial photograph of Paris, highlighting the heterogeneity of urban environments. From: <https://pixabay.com> with Pixabay License.

1.1 Urban heterogeneity

The urban form is inherently heterogeneous; composed of buildings, trees, green spaces and bodies of water that combine to form complex morphologies comprised of a variety of materials. Human behaviour (e.g. transport, heating and cooling) results in similarly complex networks of anthropogenic emissions which vary both spatially throughout the city but also temporally over diurnal, weekly and annual time scales. Alongside the natural variability in meso- and larger-scale meteorological conditions, these heterogeneous properties amalgamate to form highly complex and diverse urban environments over a large range of scales. This complexity is depicted by the aerial photograph of Paris in Figure 1.1, which captures the inherent variability and multi-scale nature of a real urban environment; as well as its relationship with the wider environment in terms of the ambient meteorology and the incoming solar radiation. For these reasons, when modelling the urban microclimate, one is faced by a large parameter space and numerous degrees of freedom.

Studies into the urban microclimate (field, experimental and numerical) generally account for this heterogeneity by utilising appropriate assumptions and simplifications; often

1.1 URBAN HETEROGENEITY



Figure 1.2: Street canyons across global urban environments. All from <https://pixabay.com> with Pixabay Licenses.

aiming to isolate particular phenomena or processes of interest in order to produce meaningful results. A classical example is the street canyon, which forms the basis of a vast body of research into the urban microclimate (Oke, 1988). Figure 1.2 illustrates six examples of different street canyons globally, highlighting that despite the apparent heterogeneity in terms of form, composition and environment, a consistent structure is evident in these urban morphologies. Research into these idealised infinite canyons has been fundamental to developing our understanding of complex urban environments and is a prime example of a simplification that acts to clarify urban heterogeneity.

Broadening the study of urban climates to e.g. more realistic urban morphologies or non-neutral conditions causes the relevant parameter space to grow very quickly in light of this heterogeneity. As such, with increasing complexity it becomes increasingly challenging to conduct systematic investigations and to produce generalised results. Heterogeneity is a key factor that is implicit in the life cycle of urban air pollutants and in all five of the defined elements of urban air quality.

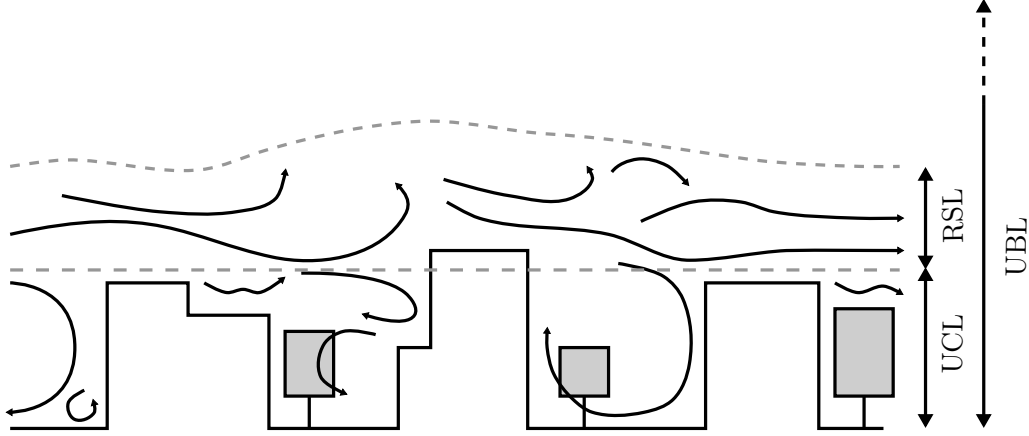


Figure 1.3: Schematic representation of the urban boundary layer (UBL), the roughness sublayer (RSL) and the urban canopy layer (UCL).

1.2 Urban flow field

The movement of air within and above the city acts to transport and mix air pollution. Highly turbulent and unsteady flows arise within and above urban areas due to the interaction of the planetary boundary layer (PBL) with the large scale roughness imposed by buildings and trees as well as the thermal properties and anthropogenic activities of a city. As shown diagrammatically in Figure 1.3, an urban boundary layer (UBL) forms with two additional sublayers: the urban canopy layer (UCL) which resides below the average building height and the roughness sublayer (RSL) which rises up above this to the height at which the effect of individual roughness elements affect the local flow dynamics (Barlow, 2014). Flow in the UCL exhibits strong spatial variability, which is imposed due to its general composition of two dichotomous elements: buildings (bluff and opaque bodies with high thermal inertia) and trees (permeable bodies that impose drag, produce shade and evapotranspire; Oke, 1989). It is the heterogeneity of these urban forms that results in the RSL above the UCL where the flow remains spatially dependant on the turbulent footprint of the downwind morphology.

The inherently unsteady and spatially variant nature of the urban flow field means that averaging is required to obtain statistically stable data from which the characteristics of these flows can be better understood. Averaging (denoted by $\bar{\cdot}$) the components of the velocity vector, u_i , or any scalar variable e.g. a passive pollutant concentration, φ , gives (Reynolds decomposition)

$$u_i = \bar{u}_i + u'_i \quad (1.1)$$

$$\varphi = \bar{\varphi} + \varphi' \quad (1.2)$$

where the first terms on the righthand sides are mean values and the second terms represent deviations away from this mean (fluctuations). The product of these two terms provides the flux of the scalar field φ in the direction of u_i . Applying the same averaging procedure to this term and simplifying yields

$$\overline{u_i \varphi} = \overline{u_i} \overline{\varphi} + \overline{u'_i \varphi'}. \quad (1.3)$$

The average flux of a scalar within a turbulent flow field is therefore composed of both mean and turbulent flux components.

These mean and turbulent quantities act to define the transport and mixing of pollutants in a city. Therefore obtaining converged statistics is imperative towards fully capturing the dispersion of urban air pollutants. It is often not feasible to apply ensemble averaging in urban studies. The ergodic hypothesis (Monin and Yaglom, 2013; Ghannam et al., 2015) stipulates that if a flow is statistically stationary it can be averaged temporally and if it is horizontally homogeneous it can be averaged in any homogeneous spatial direction in an analogous manner to ensemble averaging (Pope, 2000). The production of statistically steady-state urban flow fields is therefore key to obtaining a coherent understanding of the dispersion of pollutants over urban areas.

More detail on specific urban flow structures and the dominant processes and phenomena determining pollution dispersion within the UCL is provided in Section 1.5.2. The multi-scale nature of the urban climate, as discussed in Section 1.1, alongside the demands of resolving small-scale turbulence and producing converged statistics results in a computationally intensive modelling problem. LES is capable of resolving the inherent unsteadiness of the urban flow field whilst other pollution dispersion models typically parametrise its effects (see Chapter 2).

1.3 Urban microclimate

The urban microclimate refers to the temperature, moisture, pollutant and velocity fields at a street- (10 m) or neighbourhood- (100-1000 m) scale within a city. Microclimatic conditions form as a result of complex interactions between physical, radiative, thermodynamic and chemical processes that act over a range of spatial and temporal scales. The most important larger-scale effect, which acts beyond the bounds of a defined urban microclimate, is mesoscale meteorology. Ambient meteorological conditions act to ‘drive’ a microclimatic system; determining e.g. the pressure gradient that drives the UBL flow above the urban area and the incoming fluxes of short- and longwave radiative energy that drive the warming or cooling of urban surfaces. At the microclimate scale, mesoscale

processes therefore determine extrinsic properties of the system. In turn, the intrinsic properties of the urban microclimate (the forms of buildings, positions of trees, timings of traffic lights etc.) combine with these extrinsic properties to determine the local climatic conditions. Both these extrinsic and intrinsic properties can be inherently variable and transient, which highlights the prevalence of heterogeneity at the microclimate scale.

Intrinsic heterogeneity at the microclimate scale is used to make classifications of urban areas at the city-scale (e.g. Local Climate Zones; Stewart and Oke, 2012). These classifications use similarities in e.g. urban form and land use to homogenise these heterogeneous characteristics and to categorise the nature of different urban microclimates. When studying the urban microclimate it is important to note these variabilities and to determine the case of interest. The focus on air quality in this thesis means that central urban areas with relatively high emissions are predominantly of interest. Significant variability exists within this broad microclimate classification and within such urban areas it is important to note that locations other than busy roads exist (e.g. pedestrianised areas and parks).

1.4 Methodology

A methodology is required in order to conduct systematic and targeted investigations into what has been shown to be a multi-scale problem with a large corresponding parameter space. Oke et al. (2017) stipulates that successful studies of urban climates must identify 1) the properties or processes of interest, 2) the physical extent of the system of interest and 3) a strategy for accounting for the horizontal, vertical and temporal variation within this system. The first two points have been addressed above, leaving the requirement to devise a method to account for the system's variability, which relates directly back to the discussed heterogeneity of the urban microclimate.

The applied methodology is driven primarily by the focus on modelling at the microclimate scale. By construction, in urban LES it is necessary to sufficiently resolve the turbulent urban flow field ($O(1 \text{ m}, 0.1 \text{ s})$) but also to capture the larger-scale system forcings ($O(100 \text{ m})$) and to obtain converged statistics ($O(1 \text{ hour})$). Variability across these scales must be dealt with in different ways:

- $<O(1 \text{ m}, 0.1 \text{ s})$: the lower limit of model resolution essentially acts as a low pass filter and variability and processes occurring at smaller scales must be parametrised, e.g. wall roughness and subgrid fluxes.
- $O(1 \text{ m}, 0.1 \text{ s}) - O(100 \text{ m}, 1 \text{ hour})$: examples of intrinsic variability at a microclimate scale, e.g. traffic, the presence of trees, street aspect ratios. These processes or

phenomena can be 1) neglected completely, 2) simplified via some idealisation or assumption (e.g. infinite canyon assumption; see Section 1.1) and therefore dealt with as extrinsic variability and studied across numerous simulations or 3) explicitly resolved within a given simulation and therefore possible to analyse over a single simulation. For the latter option it is advantageous to capture sufficient variability such that meaningful results can be obtained.

- $>O(100 \text{ m}, 1 \text{ hour})$: examples of extrinsic system variability at a microclimate scale, e.g. city-scale morphological differences and diurnal changes in the mesoscale meteorology. Capturing extrinsic variability within a single simulation typically results in transients or developing flows that, if not the main point of interest in a study, act to increase the associated degrees of freedom and complexity of the problem. Computational modelling provides the numerical control to limit these forms of variability. Through the application of appropriate simplifications and the use of boundary conditions and forcings, extrinsic variability can be controlled such that statistical steady states are achieved in a given simulation. These forms of variability must then be investigated through a carefully specified set of steady-state simulations.

The next step is to then identify to what level of abstraction these effects must be considered and how many free parameters they introduce to a given simulation. This approach permits systematic simulations to be run with two main aims: 1) to minimise the degrees of freedom of a given problem and 2) to produce statistical steady states over which converged statistics can be obtained. The elements of urban air quality that have been identified for investigation in this thesis consist of both intrinsic and extrinsic properties of the urban microclimate. Following this methodology, these elements can be investigated through a combination of isolated, idealised studies (where model developments are tested and analysed) and more extensive, realistic case studies (where different elements are modelled together and the interplay between them can be explored). The application of this methodology to the identified elements of urban air quality is discussed throughout the following section.

1.5 Urban air pollution

The life-cycle of air pollutants within the urban microclimate determines local air quality and therefore human exposure to harmful pollutants. This cycle encompasses their 1) emission into the urban atmosphere, 2) dispersion through the urban flow field, 3) chemical reaction resulting in transformation and formation and 4) removal from the urban atmosphere. Each stage of this cycle is reviewed in the remainder of this section, providing

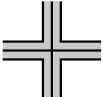
a platform from which to highlight the role of the elements of urban air quality in this thesis: morphology, emissions, chemistry, atmospheric stability and trees. These elements, which both play an integral role in determining the nature of this life-cycle and require further work in terms of developing our understanding of this role, are discussed within the following text and are summarised in Table 4.3.

1.5.1 Emissions

A wide range of pollutants with different physical and chemical properties and health and environmental effects are emitted into the urban atmosphere. Here we are interested in pollutants that are risks to public health within the city, such as carbon monoxide (CO), nitrogen oxides (NO_x), volatile organic compounds (VOCs), ozone (O₃) and particulate matter (PM). Each of these pollutants is emitted from a range of sources. Contributions can be broken down by sector (e.g. road, buildings, industry etc.; UK National Atmospheric Emission Inventory, 2018). The level of abstraction to take in modelling these emissions sources is dependant on each source's spatial and temporal variability within the urban microclimate as well as its percentage contribution to the pollutants of interest.

Emissions due to road transport are often a focus of studies into urban pollution dispersion due to their strong spatial and temporal variability, location within street canyons and at pedestrian level, ubiquity within urban environments and high percentage contributions (51% and 44% for NO_x and PM emissions respectively; UK National Atmospheric Emission Inventory, 2018). Both idealised line and point sources of pollutants and more realistic emissions modelled using a traffic microsimulation model (where the intrinsic spatial variability is therefore captured) are used in this thesis (see Chapter 3). Emission sources that exist more homogeneously at the scale of interest (e.g. 54% of VOC emissions arising due to evaporative emissions from solvents; UK National Atmospheric Emission Inventory, 2018) can be captured through the assigned background concentration levels at the microclimate scale (applying the extrinsic approach as outlined in Section 1.4). Localised releases, typically from industrial and commercial sources, can be important to capture the pollution levels in specific locations, however their lower percentage contribution (e.g. 12% of NO_x emissions attributed to 'point' sources; UK National Atmospheric Emission Inventory, 2018) and their general positioning above street-level means that these are neglected in the following study. The far field contribution of these kind of sources can also be expected to be captured through the specified background concentrations.

Table 1.1: Table showing the five elements of urban air quality identified for study in this thesis. Their interaction with the pollutant life-cycle is indicated, ● and ○ denote processes that are captured and that are neglected in this study respectively.

Element	Options	Description	Emissions	Dispersion	Reaction	Removal
Morphology	 Idealised  Realistic	The form of buildings acts to define the flow structures and subsequent dispersion within the UCL. Studies of idealised morphologies have resulted in a fundamental and well-established understanding of generalised flow structures (e.g. canyon vortices, recirculation zones and channelling). There is now scope for studies to investigate more complex, realistic morphologies in order to assess how well these idealised flow structures translate to such heterogeneity and what other important flow characteristics arise from this additional complexity.	●			
Emissions	 Idealised  Realistic	Road traffic is the largest contributor to both NO _x and PM emissions. Emissions are often represented as idealised area or line sources. The spatial and temporal variability of emissions can be important in terms of e.g. the formation of pollutant hotspots. It is possible to model realistic traffic flows using traffic microsimulation models (PTV AG, 2017b). The movement of vehicles also acts to produce small scale turbulence (this effect is not investigated in the following study).	●	○		
Chemistry	 Inert  Reactive	Pollutants reacting at a similar timescale to their dispersion significantly alters their spatial and temporal evolution at the microclimate scale. This phenomena is particularly important in accurately capturing NO ₂ and O ₃ concentrations. By time-resolving these reactions within urban LES a greater insight can be gained into the affect these have on e.g. pedestrian-level exposure.			●	
Atmospheric stability	 Neutral  Convective  Stable	The stability of the atmosphere alters both the vertical exchange of pollutants out of the urban canopy layer and the mixing of pollutants over the boundary layer depth. Thermal effects introduce an additional degree of freedom to the problem that makes forming steady-state conditions more challenging. By reviewing existing and forming new methodologies to enforce steady-state conditions, simulations can be carried out that realistically capture the mean and turbulent state of the non-neutral UBL.	●			
Trees	 No trees  Trees	Trees fundamentally alter their local environment; the drag imposed on the urban flow field and change to the surrounding energy balance significantly affect the local dispersion of pollutants. The increased surface area of the tree canopy also results in enhanced deposition of pollutants. By including all of these affects in a tree model for urban LES, an insight can be gained into the effect of trees on urban air quality. Trees also emit VOCs (this effect is not considered in the following study).	○	●		●

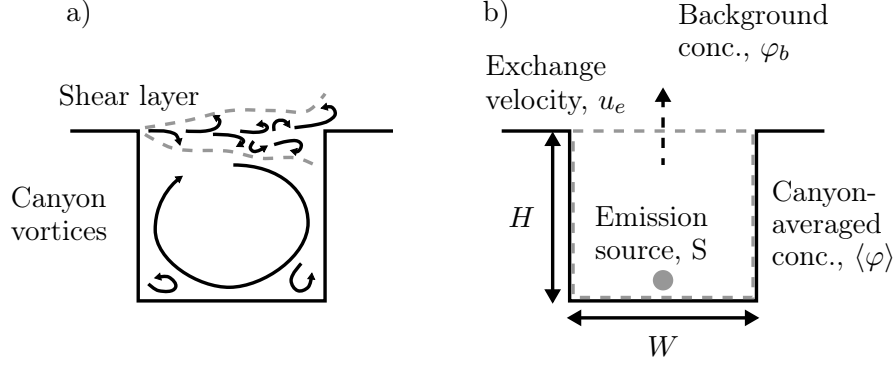


Figure 1.4: Schematic representation of a) the formation of a shear layer and vortex under the skimming regime for an infinite canyon and b) the control volume and bulk parameters used to produce a simplified representation of pollution dispersion in the UCL and above.

1.5.2 Dispersion

The dispersion of pollutants in the urban microclimate is a result of the transport and mixing induced by the urban flow field. The unsteady, heterogeneous and turbulent dynamics of the urban flow field were introduced in Section 1.2. The presence of buildings and trees in urban areas imposes significant drag on the PBL flow. The form of the urban fabric results in flow structures (reduced wind speeds and recirculations) within the UCL that cause pollutants to be dispersed more slowly into the UBL aloft and away from pedestrians.

As discussed in Section 1.1, research into the urban microclimate and pollution dispersion has relied upon the study of idealised morphologies to provide a fundamental understanding of the physics and processes of the UCL and RSL. Studies into infinite canyons provide an initial insight into the importance of these flow dynamics on urban air quality. The same idealised set up is used in this section to introduce the topic of pollution dispersion and how the elements of urban air quality interact with it. Oke (1988) identified three flow regimes dependant on the aspect ratio (H/W) of the canyon. For aspect ratios $H/W > 0.65$ a skimming flow occurs, resulting in the formation of an intermittent shear layer at the canyon top and of vortices within the street canyon as depicted in Figure 1.4b. Integrating over the control volume illustrated in Figure 1.4c, a simple prognostic equation can be obtained for the canyon-averaged concentration in a street canyon of length, $\mathcal{L}$,

$$\frac{d\langle \varphi \rangle}{dt} = \frac{S}{WH\mathcal{L}} - \frac{u_e}{H} (\langle \varphi \rangle - \varphi_b) \quad (1.4)$$

where u_e is the pollutant exchange velocity (Kubilay et al., 2017)

$$u_e = \frac{\iint \bar{w} \bar{\varphi} + \overline{w'\varphi'} dx dy}{W\mathcal{L}(\langle \bar{\varphi} \rangle - \varphi_b)}. \quad (1.5)$$

The canyon-averaged concentration can then be defined as $\langle \bar{\varphi} \rangle = \varphi_b + S/(u_e W \mathcal{L})$ assuming steady-state conditions. The strength of the emissions source and the magnitude of the exchange velocity are therefore integral to the air quality in an idealised street canyon.

The exchange velocity is determined by the net flux of pollutants out of the street canyon. The highly turbulent and intermittent nature of the shear layer results in complex dynamics that define this street-atmosphere interaction. Numerous studies have been conducted to better understand this process and to form parametrisations of the exchange velocity for use in operational models. The exchange velocity is a function of both the UBL flow that drives it and the local turbulence within the canyon and across the shear layer (Rotach, 1999; Soulhac and Perkins, 2000; Caton et al., 2003). Salizzoni et al. (2009) illustrated that the dynamics of both the shear layer and canyon vortex are highly dependant upon the fluxes of mean and turbulent kinetic energy from the UBL above and that the dominant scaling for the exchange velocity is the standard deviation of the vertical velocity in the PBL. This simple example therefore highlights that when modelling pollution dispersion in the urban microclimate it is necessary to accurately model both the mean (e.g. wind speed and direction) and turbulent (e.g. Reynolds stresses and turbulent kinetic energy) characteristics of the UBL flow (considered as extrinsic properties of the urban microclimate as defined in Section 1.4).

The turbulent intensity of the UBL arises due to the relationship between the mechanical production and buoyant production/ dissipation of turbulence. The Obukhov length, L , quantifies this relationship within the PBL's surface layer

$$L = -\frac{u_*^3 \theta_v}{\kappa g \phi_{0,v}} \quad (1.6)$$

where u_* is the friction velocity (a velocity scale that is representative of the surface shear stress and therefore the mechanical generation of turbulence), θ_v is the virtual potential temperature, κ is the von Kármán constant (classically $\kappa \approx 0.4$), g is the gravitational acceleration and $\phi_{0,v}$ is the surface virtual potential temperature flux (either a source or sink of buoyancy depending on its sign; Obukhov, 1971). Negative values of the Obukhov length indicate convective conditions where buoyancy acts as a source of turbulence in the surface layer and leads to the transportation of turbulent kinetic energy over the height of the convective boundary layer (CBL). The CBL is characterised by large-scale thermals, large boundary layer heights (h ; 1000-2000 m), a convective mixed layer and an entrainment zone that interacts with quiescent free atmosphere aloft. Mixed-layer similarity theory has been applied to convective UBLs with good agreement (Wood et al., 2010). Positive values of the Obukhov length are indicative of stable conditions where buoyancy conversely acts to

inhibit vertical motion. Under stable conditions, the state of the boundary layer is defined by the local balance between the mechanical generation of and buoyant suppression of turbulence. The stable boundary layer (SBL) has been shown to be harder to classify in the literature (both generally and over urban areas; Mahrt, 1999; Barlow, 2014). If present over urban areas, weakly stable conditions are most prevalent with boundary layer heights of 100-200 m, continuous turbulence, an elevated inversion and local scaling of turbulence above the RSL (Uno et al., 1988). UBLs are typically less stable and deeper than their rural counterpart (Roth, 2000; Barlow, 2014).

The majority of urban LES studies have simplified the problem via the assumption of neutral conditions (L becomes infinite since $\phi_{0,v} = 0$). However, boundary layer flows over cities are generally not neutral. Recent studies have highlighted the importance of thermal effects in urban flows (Boppana et al., 2014; Tomas et al., 2015) and the stability of the atmosphere directly affects the magnitude of the exchange velocity in the case of an infinite canyon (the divergence of the heat flux acts as an effective source/ sink of turbulence kinetic energy and affects the turbulent intensity of the modelled flow; CERC, 2001). Mixed convection where the buoyancy force is dominant but wind shear phenomena are also important is the most common case for UBL flows ($|L| \ll h$; Fedorovich and Conzemius, 2008). For this reason, atmospheric stability is a key point of interest in this thesis. A key challenge in applying the methodology outlined in Section 1.4 to non-neutral conditions is the formation of realistic steady-state conditions (see Chapter 4).

Continuing with the simplified example of an infinite street canyon, the concentration field is typically not uniform within the canyon as assumed in Figure 1.4c. The main canyon vortex disperses traffic emissions initially towards the leeward side of the canyon before pollutant is mixed with the cleaner air in the UBL aloft via intermittent turbulent fluctuations over the shear layer (e.g. sweeps and ejections; typically studied through quadrant analysis; Li et al., 2015). This process can lead to asymmetry between the windward and leeward sides of the canyon, depending on the efficiency of mixing and the residence time of pollutants within the canyon. Pollutants are also mixed between the inner and outer regions of the canyon vortex during this process. Salizzoni et al. (2009) highlighted that this process introduces an additional, longer timescale when studying the flushing of pollutants out of urban canyons. These processes leads to in-canyon variability of a passive pollutant concentration field. The highest concentrations are typically found at pedestrian-level in the centre and leeward sides of the canyon (Yazid et al., 2014).

Objects within an urban canyon can act to either increase or decrease this in-canyon variability by changing the flow structure or enhancing the mixing respectively. Trees impose drag on the surrounding flow field that, when situated within an urban canyon

(e.g. in Figure 1.4b and c), fundamentally alters the dynamics of the canyon vortices and reduces the vertical exchange. This effect has been investigated under neutral conditions in both wind tunnel and numerical studies and has been shown to result in significant increases of in-canyon concentrations (Salim et al., 2011b; Gromke and Ruck, 2012; Moonen et al., 2013). Trees also remove pollutants from the urban atmosphere via the process of deposition (see Section 1.5.4). The balance between these two processes (drag and deposition; dispersion and removal) characterises their combined effect on the life-cycle of pollutants (Janhäll, 2015). Yet relatively few studies (field, experimental or numerical) have considered both their depositional and aerodynamic effects simultaneously (Buccolieri et al., 2018). Even under highly idealised conditions (the infinite canyon assumption), the studies that have considered both effects exhibit disagreements on the fundamental question of if trees have a net positive or negative effect on urban air quality (Vos et al., 2013; Santiago et al., 2017; Jeanjean et al., 2017). The ambiguity illustrates the complexity of tree's interaction with urban air pollutants. The growing consensus in recent review papers is that this problem is inherently case specific and that on average they lead to a deterioration in air quality ($\approx 20\text{-}96\%$ increase in local concentrations; Abhijith et al., 2017). This question remains a key area of research and is highly relevant to potential air quality mitigation strategies and to urban design. A factor that hitherto has rarely been considered is the thermal effects of trees and how these further alter trees' effects on the surrounding flow field. Developing a tool to model the integrated role of trees (inclusive of their thermal effects and minimising the number of additional parameters) is therefore a key area of interest in this thesis (Chapters 5 and 6).

The idealised set-up used in the above discussions considered an infinite canyon with a specific aspect ratio and a perpendicular wind angle of incidence. Small changes to this idealised urban configuration result in more complex flow structures and therefore pollution dispersion mechanisms. For example, changing the wind angle of incidence results in helical flows or channelling along the canyon and larger aspect ratios lead to multiple stacked vortices (Soulhac et al., 2008; Oke et al., 2017). Studies have investigated other dominant urban flow structures by studying more complex urban morphologies, e.g. different roof types (Yassin, 2011) and isolated tall buildings (Fuka et al., 2018; Aristodemou et al., 2018). Moving away from assumed spanwise homogeneity in the urban morphology results in the formation of secondary flows and recirculation zones (Castro et al., 2017). Street intersections are also characterised by the interactions between different along-canyon flow structures and can lead to advective fluxes of pollutants out of the UCL and 'conveyor belt' flows (Zajic et al., 2011; Oke et al., 2017). Intersections may also exhibit more complex unsteady behaviour such as bi-modal structures (Hertwig et al., 2012; Michioka et al.,

2014). Differing heights of buildings affect both the UCL and RSL flows. Xie et al. (2008) highlights the complexity and non-uniformity of flow behaviour in the presence of random building heights. Studies have also modelled realistic urban morphologies (Xie and Castro, 2009; Jeanjean et al., 2017; Kurppa et al., 2018; Grylls et al., 2019). The dominance of the turbulent flux component in the exchange out of an infinite canyon is then affected by the presence of coherent flow structures resulting in advective fluxes in and out of the UCL. Defining simple exchange velocities over realistic urban morphologies is more challenging (Panagiotou et al., 2013).

Generally, as the complexity of the urban morphology increases, the application of idealised flow structures and simplified parametrisations becomes more challenging to capture the dispersion of pollutants. Real urban morphologies vary hugely between different microclimate classifications and are subsequently also challenging to generalise. There is scope to study such realistic morphologies in order to gain an understanding of how this complexity affects the dispersion of pollutants and if bulk, generalised relations can be obtained. The case study presented in thesis therefore models the urban morphology of a real case study region. In modelling a real urban area with a range of e.g. street aspect ratios and orientations, aspects of this morphological heterogeneity and complexity can be analysed as intrinsic properties within a given simulation (see Chapters 3 and 6).

1.5.3 Chemical reactions

A huge range of chemical reactions occur between different urban air pollutants across a wide range of time scales. Many of these reactions are photochemical meaning that they are initiated by the absorption of energy in the form of light. The network of relevant reactions and chemical species to urban air pollution is very large (thousands of reactions across thousands of species), particularly when considering the complex arrays of different compounds that combine to form pollutant groups such as VOCs or particulate matter (Seinfeld and Pandis, 2016).

As with other aspects of urban modelling it is therefore necessary to isolate the most important phenomena and to apply relevant simplifications such that these can be feasibly modelled. At the microclimate scale it is important to resolve the reactions that occur at a similar timescale to the dispersion of pollutants within the UCL (a few minutes; intrinsic variability) and therefore e.g. alter the spatial distribution of pollutants within an infinite canyon. The modelling of vehicular emissions in this thesis also leads to a corresponding focus upon the reactions affecting the resulting primary and secondary pollutants (Section 1.5.1).

Chemical mechanism reduction schemes exist that work quantitatively under the same

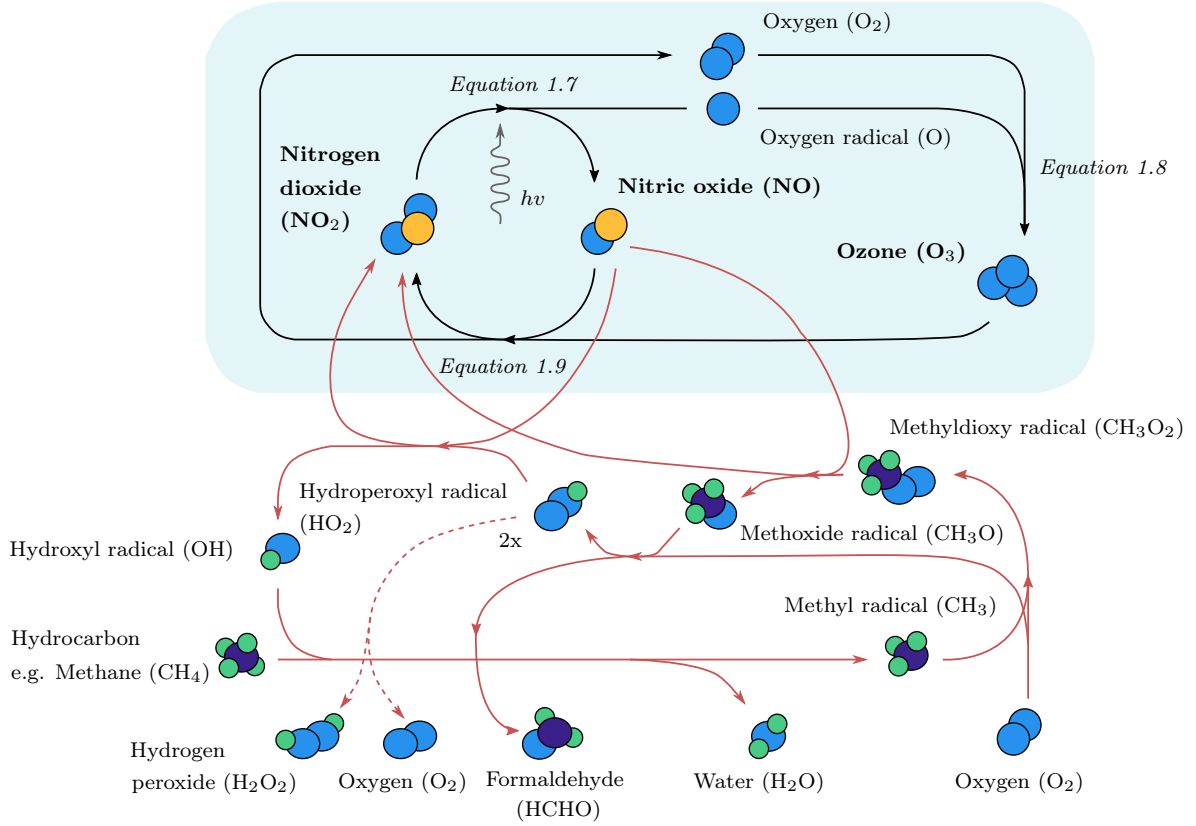


Figure 1.5: Selected chemical reactions that affect the spatial and temporal distribution of pollutants in the urban microclimate. An example is used of the methyl radical (CH_3) but similar catalytic cycles occur for other hydrocarbon radicals. The reactions of the null cycle are highlighted in the blue shaded area (adapted from Oke et al., 2017).

methodology to reduce the complexity of chemical systems whilst maintaining the accuracy of the provided solution. The relevant system of reactions can be converted into a system of ordinary differential equations via a stoichiometric matrix (Cardelli, 2008). The quasi-steady-state approximation calculates the resulting Jacobian matrix of the system of ordinary differential equations to determine the relaxation speed and lifetime of each of the chemical species (Heard et al., 1998; Lowe and Tomlin, 2000). Considering the timescales of interest to the problem, fast species with fast relaxations speeds can be assumed to be in equilibrium and species with long lifetimes can be assumed to be chemically inert (Zhong et al., 2017). One can also identify redundant species or parameters that have little effect on the chemical species of interest (e.g. Oxygen molecules in the air for which any change in concentration is negligible against the background level). One of the main challenges of implementing these schemes within pollution dispersion models is that pollutants are often out of equilibrium due to transport and these schemes apply analysis around the chemical

equilibrium condition.

The most important reactions of pollutants for this work are the photochemical reactions between NO_x , O_3 and VOCs. This set of reactions also acts to define the formation of photochemical smog (Oke et al., 2017). The relevant reactions are shown in Figure 1.5. The chemistry of the null cycle, which has no net chemical effect (meaning that NO_x and O_x are conserved), is highlighted in blue in Figure 1.5 (Crutzen, 1979). This null cycle follows



where J_{NO_2} is the photolysis rate for NO_2 , k_1 is the $\text{O}^\bullet + \text{O}_2$ reaction rate and k_2 is the $\text{NO} + \text{O}_3$ reaction rate (Wallace and Hobbs, 2006).

The reaction between the oxygen radical and molecular oxygen occurs very fast (k_1 is very large), meaning that this reaction can be assumed to occur instantaneously ($d[\text{O}]/dt = 0$). As discussed above, oxygen is redundant in this system of equations as it is abundant in the atmosphere and can therefore be assigned a constant value. Following from these assertions, the cyclic set of reactions can be simplified and defined only using J_{NO_2} (proportional to the intensity of ultra-violet radiation) and k_2 (which scales with the ambient air temperature). A photostationary steady-state (PSS) is achieved when (Leighton, 2012)

$$k_2 [\text{O}_3] [\text{NO}] = J_{\text{NO}_2} [\text{NO}_2]. \quad (1.10)$$

Baker et al. (2004) introduced the chemistry of the null cycle into LES studies of infinite urban canyons. The reactions of the pollutants resulted in significant in-canyon variability in terms of the concentrations of NO , NO_2 and O_3 . The PSS defect

$$\delta_{ps} = 100 \left(\frac{k_2 [\text{NO}] [\text{O}_3]}{J_{\text{NO}_2} [\text{NO}_2]} - 1 \right), \quad (1.11)$$

which represents the local deviation from the chemical equilibrium, was found to be a good indicator of the chemical imbalance in different locations within the canyon.

The system of reactions associated with VOCs complicate the chemistry of the null cycle by providing a pathway through which NO can be converted to NO_2 without depleting O_3 . The reactions associated with this process follow the catalytic cycle that is shown outside of the highlighted region in Figure 1.5 (methane is used as an example hydrocarbon in this case; Oke et al., 2017). It is important to note the role of VOCs for this reason (they play an integral role in the formation of photochemical smog). However, even following

stringent mechanism reduction schemes, capturing the role of VOCs requires modelling a total of ≈ 51 species (Bright et al., 2013).

In order to minimise the computational expense of the simulations conducted in this thesis, the reactions of the null cycle are focused upon. To the author’s knowledge reactive scalars have not been modelled within realistic urban morphologies using LES.

1.5.4 Removal

Pollutants are removed from the atmosphere through dry deposition, gravitational settling and wet deposition. Dry deposition is a process through which gases and particles are transported to surfaces via turbulent mixing (Sehmel, 1980). This process occurs at small scales and therefore must be parametrised within pollution dispersion models. Classically a deposition velocity, u_d , is defined that acts as a conductance term to define the flux of pollutant between the air and the surface, ϕ_φ ,

$$\phi_\varphi = -u_d\varphi. \quad (1.12)$$

The conductance is a function of the aerodynamic, laminar boundary layer and surface resistances ($u_d = (r_a + r_{la} + r_{su})^{-1}$; Oke et al., 2017).

Gravitational settling is a similar process but with the additional effect that the mass of particulates acts to settle them down towards urban surfaces. Heavier particulates (e.g. PM10) settle at relatively fast rates. But the settling of fine particulates is impeded by the urban flow field and these can remain airborne for weeks or months. Wet deposition is the process through which pollutants are removed by incorporation into cloud droplets and rain droplets (Oke et al., 2017).

All three of these processes occur relatively homogeneously over urban areas and can therefore already be reasonably captured within operational models. These processes are not incorporated into the following LES study for that reason. However, the large surface areas of trees within the UCL result in an enhanced, spatially variable and potentially advantageous form of deposition, this effect is incorporated alongside the thermal and drag effects of trees as discussed in Section 1.5.2. Removal from the urban atmosphere also occurs via advection out of the city in the urban plume. As urban microclimates are studied here this effect is neglected. The assigned boundary conditions in each simulation determines the flux of pollutants in and out of the modelled domain.

Urban LES also presents a good opportunity to develop our understanding of the use of sustainable innovations, e.g. outdoor air purifiers and photocatalytic pavements. The model developments and simulation capabilities developed in this thesis provide a platform from which these could be investigated in realistic urban conditions.

1.6 Scope

The main aim of this thesis is the development of model capabilities to systematically study air pollution in the urban microclimate in order to aid solutions to the challenges of urbanisation, in particular urban air quality. A comprehensive study, using both urban LES and operational models, is conducted; probing the main elements that amalgamate to define local air quality at the microclimate scale. As introduced in Section 1.5, five main elements of urban air quality are identified for study in this thesis (selected due to their importance in defining the life-cycle of urban air pollutants and their respective scope for developments in the research area using LES): morphology, emissions, chemistry, atmospheric stability and trees. The following objectives have been formulated:

- Develop the model capabilities to study the five elements of urban air quality using LES, this includes:
 - Processing of LIDAR data to capture realistic urban forms (both trees and buildings) in LES.
 - Coupling an LES model with a traffic microsimulation model to enable the input of realistic traffic emissions.
 - Incorporating the chemistry of the null cycle into an LES model.
 - Investigating the best practice for and devising new methods towards producing statistically steady-state non-neutral UBLs in LES.
 - Developing a minimal model to capture the integrated (drag, thermal and depositional) effects of trees whilst minimising the number of additional free parameters.
- Conduct an extensive case study using LES where all five of the elements of urban air quality are investigated in a real urban microclimate.
- Evaluate the performance of an operational air quality model using LES.

Two types of studies are used to achieve these objectives. The first type consists of targeted LES investigations in which the degrees of freedom are minimised and a chosen element is isolated (applied to both atmospheric stability and trees). In terms of atmospheric stability, introducing thermal effects significantly alters the dynamics of the UBL and also makes the process of forming steady states more challenging. A study is therefore carried out on identifying the best practice for simulating non-neutral conditions in urban LES. As discussed in Section 1.5.2, trees interact with the urban environment in a complex

manner. An integrated, minimal tree model is therefore devised and a study is conducted on the impact of trees within idealised, infinite canyons.

The second study type involves a comprehensive case study in which the role of all of the elements are analysed as well as the interplay between them. Incorporating all of these key elements of urban air quality into one investigation presents a significant contribution towards realistically modelling and fully resolving air pollution in the urban microclimate. Further insight is obtained by conducting comparable simulations over the case study area using an operational model. This process allows for the typical operational assumptions, simplifications and parametrisations to be evaluated using LES.

Conclusions are therefore drawn from the research that have applications towards both microclimate- and city-scale modelling. The LES model developments will enable future studies to systematically incorporate complex processes and phenomena that are integral to understanding urban air quality. The application of these studies can then be targeted towards formulating solutions to the challenges of urban air quality.

1.7 Structure of this thesis

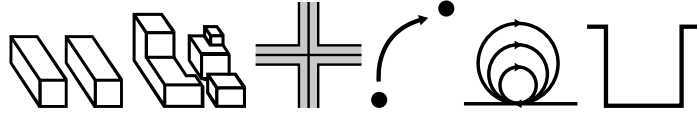
The thesis is structured as follows. The background of air pollution in the urban microclimate and the methodology were introduced in this chapter. In Chapter 2, the two numerical models that are used in this thesis are introduced and the urban LES model is validated against wind tunnel data. A comprehensive case study is introduced in Chapter 3 where the capabilities to capture realistic urban morphologies and emissions in LES are presented and the coupling of the urban LES model with a null cycle chemical scheme is outlined. Equivalent simulations are run over the case study region using both the LES and operational air quality model. These facilitate an evaluation of the predictive performance of the operational model. Chapter 4 presents a targeted study into the best practice for modelling non-neutral UBLs in LES. Guidelines are provided for future studies and a novel method is devised through which the state of a transient boundary layer can be ‘frozen’ in time. A minimal tree model for LES (inclusive of drag, thermal and depositional effects) is then presented in Chapter 5. The model is verified, applied in a bulk parametric study and then used in a targeted LES study on the role of trees in infinite canyons. Based upon the conclusions drawn and model capabilities gained from Chapters 4 and 5, the case study introduced in Chapter 3 is expanded upon by introducing non-neutral conditions and the presence of trees in Chapter 6. The results presented in this chapter showcase the model capabilities developed as part of the work on this thesis and also provide a further evaluation of the operational model. Finally the contributions of this work are stated,

conclusions are drawn and recommendations are made for future studies in Chapter 7. The option symbols for the five elements of urban air quality, which are introduced in Table 4.3, are displayed at the start of each chapter as an indication of the elements that are investigated within that study. This culminates in Chapter 6 where all five of these elements are explored over a realistic urban microclimate.

Chapter 2

Modelling

The two models used in this thesis span the gap between high-resolution, computationally intensive and highly parametrised, operational modelling of urban pollution dispersion. Both the operational model, SIRANE, and the large-eddy simulation model, uDALES, are introduced in this chapter. The two models have been validated extensively in previous studies. A further validation is conducted for the application of uDALES to model air pollution within realistic urban morphologies.



2.1 Introduction

There are a range of models that consider the problem of urban pollution dispersion with different levels of abstraction, modelling approaches and spatial and temporal scales (e.g. Gaussian, semi-empirical, box, Eulerian and Lagrangian models). An inherent trade off exists between the provided resolution and accuracy of a given model against its costs and speed of computation.

At the microclimate scale, the most computationally demanding aspect of this problem is resolving the unsteady, heterogeneous and turbulent flows that occur within and above the urban canopy. Operational models (e.g. box models) typically parametrise the dominant dispersive exchanges and flows of the urban environment to produce a bulk approximation of this complex flow field (Baklanov et al., 2009). This simplified flow representation ($O(100\text{ m})$) is combined with detailed data (e.g. traffic flows, background

concentrations, meteorological conditions and street morphologies) and physico-chemical schemes (e.g. chemistry and deposition) to provide estimates of pollution levels at a city or neighbourhood scale over days or longer time periods with limited computational cost. Computational fluid dynamics (CFD) models present alternative tools through which the flow field and subsequent dispersion is resolved (Di Sabatino et al., 2007; Blocken, 2015). Operational CFD models parametrise the role of turbulence resulting in (quasi-)steady solutions (e.g. Reynolds-averaged Navier-Stokes (RANS) models). LES models are computationally more expensive such that they cannot currently feasibly be used as operational tools. However they are capable of modelling the unsteady three-dimensional flow field to the highest possible resolutions ($O(1\text{ m}, 0.1\text{ s})$; Letzel et al., 2008; Tominaga and Stathopoulos, 2013; Salim et al., 2011b). Extensive research has been conducted into the relative advantages and disadvantages of the use of RANS and LES models for urban studies (Blocken, 2018). LES models are capable of capturing more complex, unsteady dynamics and higher order statistics and generally provide increased accuracy. On the other hand, the computational requirements of LES are significantly higher, subgrid schemes can lead to inaccuracies where the grid is too coarse and there is a paucity of best practice guidelines (Blocken, 2015).

The range of scales that a particular pollution dispersion model is able to resolve determines the processes and properties that 1) must be parametrised, 2) are intrinsically variable within a given simulation and 3) are extrinsic to the modelled system (see Section 1.4). Typically, LES models have been used in intensive, generalised studies to formulate the parametrisations that define many operational models (Soulhac et al., 2011). In such studies, intrinsic properties of the urban microclimate, which LES is able to resolve, are neglected or simplified so that generalised results can be obtained to be applied within coarser models (a process depicted by the dark blue lines in Figure 2.1).

However increasing computational capabilities mean that it is now possible to produce realistic urban LES at a comparable scale to operational models (the crossover point between these models is at the microclimate (neighbourhood-) scale over time periods of hours). Figure 2.1 provides a diagrammatic representation of the role of operational and LES models in this research area. It highlights how the level of abstraction taken in a model propagates to the other key simulation inputs (examples used here are the emissions and morphology) such that this resolution defines the amount of information utilised by these models. Conducting comparable simulations between these two models, without simplifying intrinsic properties within the LES, provides a novel method through which to evaluate the operational model and better understand the results obtained via LES.

Both an urban LES and operational model are therefore used in this thesis, spanning

2.2 SIRANE

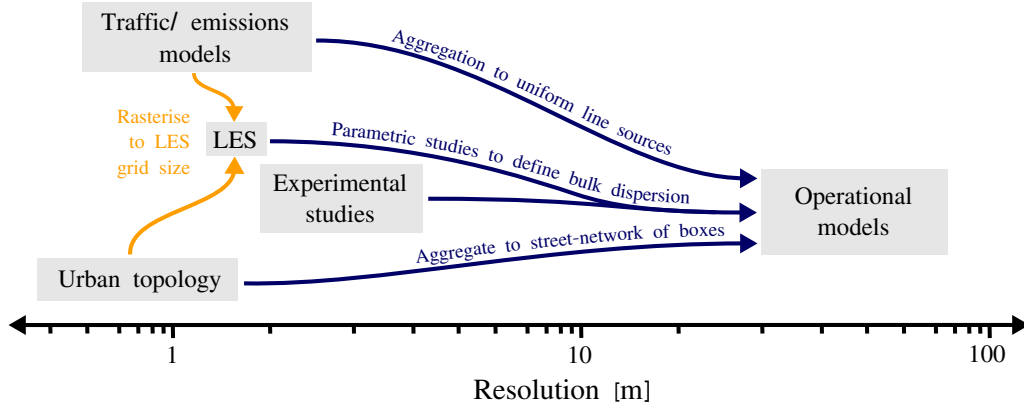


Figure 2.1: A diagrammatic representation of the models and example data inputs for pollution dispersion studies, indicating the required preprocessing for operational (blue) and LES (orange) models.

the gap between computationally intensive, time-resolving simulations and the city-scale operational modelling that is used by practitioners. The operational street-network model, SIRANE, and a modified version of the Dutch Atmospheric Large-Eddy Simulation model (uDALES) are used to this end. Details of the two models are provided in the following sections and a validation is presented for the use of uDALES in studying pollution dispersion with realistic urban morphologies at the neighbourhood scale.

2.2 SIRANE

SIRANE is an operational pollution dispersion model, which allows users to model urban air quality at a city-scale at low computational costs. The model is described comprehensively in Soulhac et al. (2011) so the discussion here is limited to a brief overview of its main characteristics.

The domain is divided into two sub-domains: the urban canopy and the external atmosphere. The urban canopy is represented by street canyons (spaces between the buildings) which are modelled as a series of connected boxes (a street network). The pollutant concentration in each box is assumed to be uniform and is computed as a mass balance which includes the advective transfer along the street, turbulent transfer at roof level, chemical transformations occurring inside the canyon and dispersion at intersections (Soulhac et al., 2009). These processes are modelled through parametrisations (often derived from intensive experimental or LES studies) over hourly time-steps. For example, the street-atmosphere exchange is captured through the exchange velocity of an infinite street-canyon as introduced in Equations 1.4 and 1.5. However, as the pollutant fluxes are not resolved,

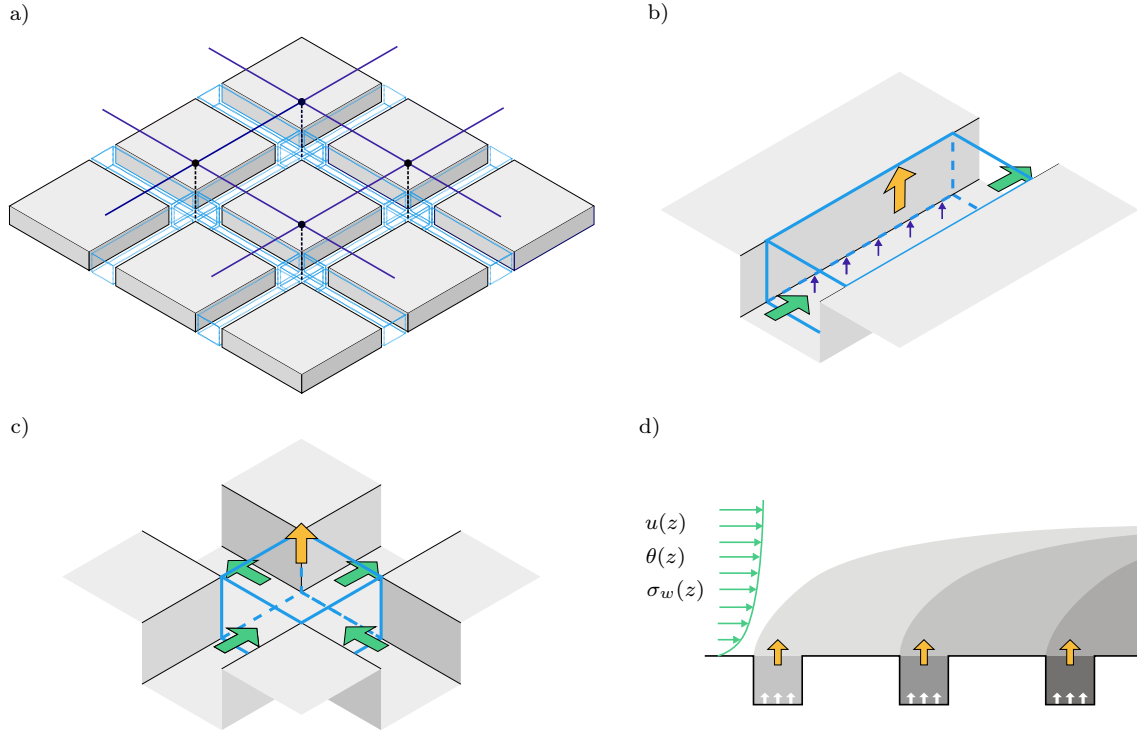


Figure 2.2: Diagrammatic view of the street-network representation in the model SIRANE showing a) the street-network, b) the box model for each street, c) the fluxes at a street intersection and d) the modified Gaussian model for the external flow. Adapted from Soulhac et al. (2011).

this term is parametrised as

$$u_e = \frac{\sigma_w}{\sqrt{2\pi}} \quad (2.1)$$

where σ_w is the standard deviation of the vertical velocity in the lower UBL which captures the intensity of turbulent fluctuations just above the UCL. This term is defined as a function of the friction velocity (under neutral and stable atmospheric conditions) or the friction velocity and convective velocity scale (under convective atmospheric conditions; CERC, 2001).

A Gaussian plume model is used to model pollution dispersion above the street network. The spread of the plumes are determined by the level of atmospheric stratification, represented by either the Pasquill Gifford stability classes or a continuous parametrisation (Salizzoni et al., 2009). A diagrammatic view of SIRANE's methodology is provided in Figure 2.2.

The chemical equilibrium between NO , NO_2 and O_3 is assumed to follow the null cycle. SIRANE accounts for these reactions by first simulating the passive dispersion of NO_x through and above the street network and then uses the resulting NO_x concentration

field and the background concentrations of NO, NO₂ and O₃ to solve the resulting system of equations by satisfying the Leighton relationship (Equation 1.10). This methodology therefore follows the assumption that the pollutants reach a photostationary steady-state (PSS) within each canyon over SIRANE’s hourly time steps.

The mesoscale meteorological properties (boundary layer height, friction velocity, surface heat flux etc.) are calculated through parametrisations based upon observational data such as wind speed, wind direction, cloud cover, precipitation and surface albedo (Holtslag and Van Ulden, 1983; Fisher et al., 2001; CERC, 2001). The empirical parametrisation of the net radiation above the modelled urban area is provided in Appendix A.1. SIRANE has been validated extensively against wind tunnel experiments and real measurements in Lyon, France (Soulhac et al., 2012, 2017; Carpentieri et al., 2012b; Salem et al., 2015).

2.3 uDALES

uDALES is a high-resolution, flow-resolving atmospheric LES model (Heus et al., 2010; Tomas et al., 2015, 2016a) that solves the equations of motion at the energetically dominant scales of turbulent motion. The dynamic core, DALES, has been used to study atmospheric processes for over 30 years (Nieuwstadt and Brost, 1986; Heus et al., 2010). Tomas et al. (2015) introduced the ability to model obstacles using the immersed boundary method (IBM) and Suter (2018) extended the model through the application of a three-dimensional energy balance model, wall functions and the reintroduction of wet thermodynamics. An outline of the numerics and functionalities of uDALES is provided below. Further additions to the model are introduced throughout the remainder of this thesis.

2.3.1 Governing equations

The governing equations of uDALES are based upon the constitutive equations for the conservation of mass, momentum and energy. These equations are filtered implicitly using the grid as a low-pass filter (filtering is denoted by $\tilde{\cdot}$ in this section). The Boussinesq approximation is applied such that variations in fluid properties are neglected other than density variation terms that are multiplied by gravitational acceleration (inertial effects are negligible but buoyancy effects are significant; Turner, 1979). This approximation is applied widely in numerical models of atmospheric flows.

Given that density variations are neglected, the continuity equation reads

$$\frac{\partial \tilde{u}_i}{\partial x_i} = 0, \quad (2.2)$$

where the Einstein summation notation is used, u_i is the velocity vector along the base

vector x_i and t denotes time. Filtering and applying the Boussinesq approximation to the conservation of momentum gives

$$\frac{\partial \tilde{u}_i}{\partial t} = -\frac{\partial}{\partial x_j} (\tilde{u}_j \tilde{u}_i) - \frac{1}{\rho_0} \frac{\partial \Pi}{\partial x_i} + \frac{g}{\theta_0} \tilde{\theta}_v \delta_{i3} - \frac{\partial \tau_{ij}}{\partial x_j} + \mathcal{F}_i \quad (2.3)$$

where ρ_0 is a reference value of the density of air, Π is the modified pressure, g is the gravitational acceleration, θ_v is the virtual potential temperature, θ_0 is a reference value of virtual potential temperature, δ_{i3} is the Kroenecker delta, τ is the deviatoric component of the subgrid-scale (SGS) momentum flux (the normal components are resolved within Π) and $\mathcal{F}_i$ represents other forces on the flow. The transport equation for scalar field variables is

$$\frac{\partial \tilde{\psi}}{\partial t} = -\frac{\partial}{\partial x_j} (\tilde{u}_j \tilde{\psi}) - \frac{\partial \mathcal{R}_{\psi,j}}{\partial x_j} + S_\psi \quad (2.4)$$

where ψ is a scalar field that represents the potential temperature (θ), specific humidity (q) or pollutant fields (φ ; chemical species or particulates). $\mathcal{R}_{\psi,j}$ is the SGS scalar flux vector and S_ψ represents additional volumetric source/ sink terms. The modified pressure term is

$$\Pi = \frac{\tilde{p}}{\rho_0} + \frac{2}{3} e_{sgs} \quad (2.5)$$

where p is pressure, ρ is the density of air and e_{sgs} is the SGS turbulent kinetic energy (the normal component of the subgrid momentum flux). The virtual potential temperature, θ_v , is approximated following Emanuel (1994)

$$\theta_v = \theta \left(1 - \left(1 - \frac{R_v}{R_d} \right) (q_v + q_l) - \frac{R_v}{R_d} q_l \right) \quad (2.6)$$

where θ is the potential temperature, q_v is the water vapour specific humidity, q_l is the liquid water specific humidity, R_v and R_d are the gas constants for water vapour and dry air respectively. For the applications of uDALES conducted in this thesis, liquid water is not present such that $q_l = 0$. The filtering operation results in unknown subgrid flux terms which are modelled following the gradient diffusion hypothesis (treating these terms in a similar way to viscous stresses)

$$\tau_{ij} = -K_m \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \quad (2.7)$$

$$\mathcal{R}_{\psi,j} = -K_h \frac{\partial \tilde{\psi}}{\partial x_j} \quad (2.8)$$

where K_m is the subgrid viscosity and K_h is the eddy diffusivity. The Vreman subgrid model is used to define the eddy viscosity throughout this study (Vreman, 2004). This subgrid model is of similar complexity to the widely used Smagorinsky model (Smagorinsky,

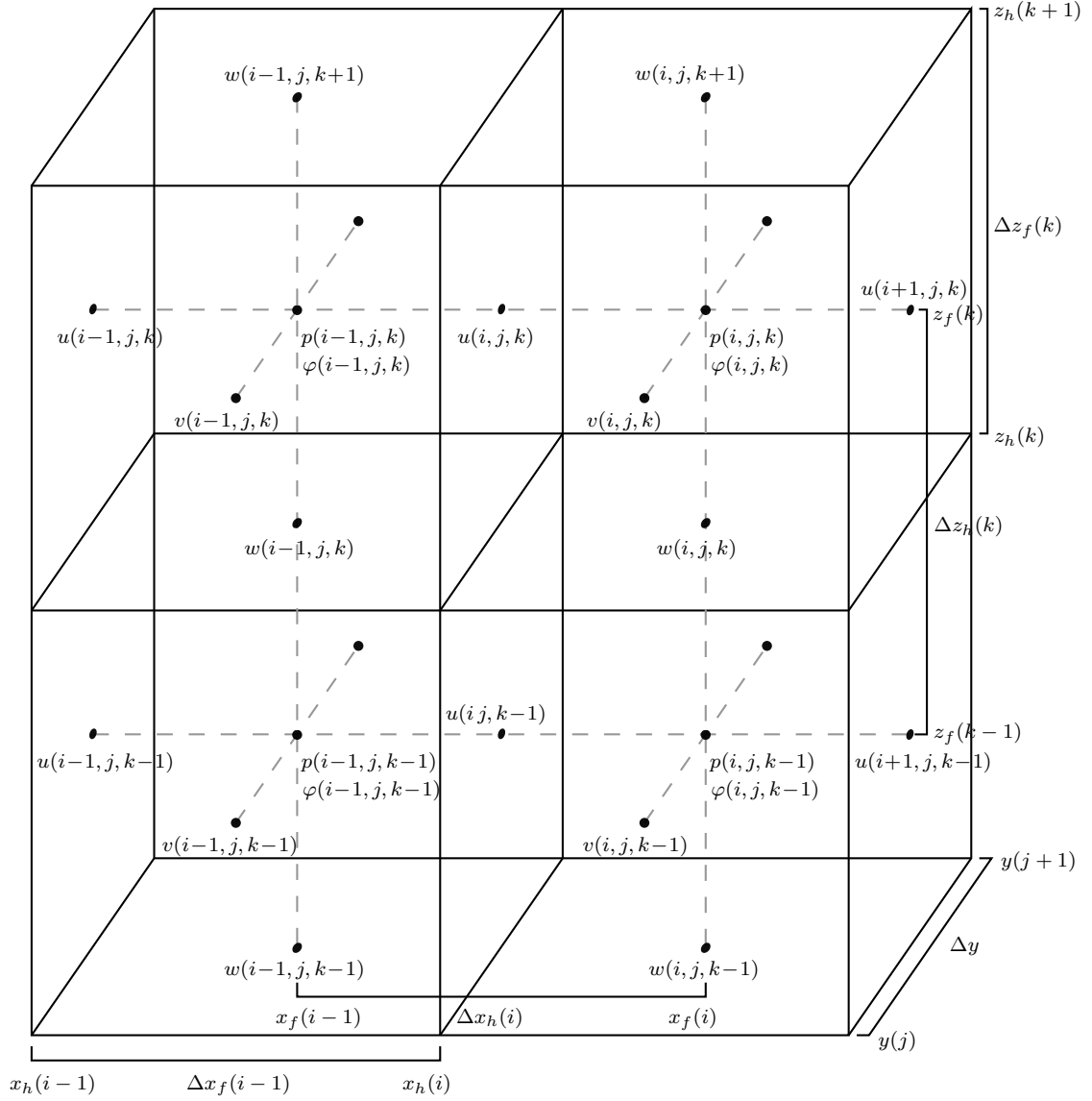


Figure 2.3: Arakawa C-grid as applied in uDALES. Pressure and scalar variables (p , ψ) are defined at the cell centres and the three velocity components (u , v , w) are defined on the west, south and bottom side of the cell respectively. The grid can be stretched in the x - and z -directions in which case Δx_f , Δx_h , Δz_f , Δz_h vary along x and z respectively. The grid is invariant in the y -direction and as such Δy is equal along y and across the cell centre and face.

1963) with the advantage that it behaves better in near-wall regions (Vreman, 2004; Tomas, 2016). The eddy diffusivity is calculated from the eddy viscosity using the turbulent Prandtl number, Pr_T , which is set to 0.71 throughout this thesis. The filtering notation is omitted from the rest of the thesis for clarity.

2.3.2 Numerical discretisation

Equations 2.2, 2.3 and 2.4 are solved numerically in space and time. uDALES applies the finite difference method. The field variables are spatially discretised using the Arakawa C-grid, where the scalar fields (ψ) and pressure (p) are defined at the cell centres and the three velocity components (u , v and w) are defined at the cell faces. The grid is therefore structured and follows a Cartesian coordinate system (Figure 2.3).

The advection terms in Equations 2.3 and 2.4 are discretised using the ‘staggered’ nature of the grid, e.g. in the x -direction as

$$\frac{\partial}{\partial x} (u_i \Psi_i) \approx \frac{F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}}{\Delta x} \quad (2.9)$$

where Ψ represents the prognostic field variables (u , v , w and ψ) and $F_{i-\frac{1}{2}}$ represents the advective flux of that variable through the $i - \frac{1}{2}$ plane. For all of these field variables except pollutant concentrations, a second-order central differencing scheme is applied

$$F_{i-\frac{1}{2}}^{2nd} = u_{i-\frac{1}{2}} \frac{\Psi_i + \Psi_{i-1}}{2}. \quad (2.10)$$

In the case of pollutant concentrations where monotonicity is required (e.g. for chemically reacting species), a κ -advection scheme in which a flux-limiter ensures positivity is used to determine the advective flux (Hundsdofer et al., 1995)

$$F_{i-\frac{1}{2}}^{\kappa} = u_{i-\frac{1}{2}} \left[\Psi_{i-1} + \frac{1}{2} \kappa_{i-\frac{1}{2}} (\Psi_{i-1} - \Psi_{i-2}) \right] \quad (2.11)$$

when $u > 0$. $\kappa_{i-\frac{1}{2}}$ serves as a switch between third order and first order upwind in case of strong upwind gradients of Ψ . This scheme ensures monotonicity but can be more dissipative particularly in the presence of strong gradients (Heus et al., 2010).

An explicit third-order Runge-Kutta scheme is applied for time integration following Wicker and Skamarock (2002). The prognostic field at a time step $n + 1$ at time $t + \Delta t$ is calculated as

$$\Psi^* = \Psi^n + \frac{\Delta t}{3} \frac{\partial \Psi^n}{\partial t}, \quad (2.12)$$

$$\Psi^{**} = \Psi^n + \frac{\Delta t}{2} \frac{\partial \Psi^*}{\partial t}, \quad (2.13)$$

$$\Psi^{n+1} = \Psi^n + \Delta t \frac{\partial \Psi^{**}}{\partial t}, \quad (2.14)$$

where $*$ denotes intermediate time steps and the temporal derivatives are equal to the right hand sides of Equations 2.3 and 2.4.

The updated velocity fields must satisfy both the continuity equation (Equation 2.2) and the conservation of momentum (Equation 2.3). To achieve this within the discussed

time integration scheme, the ‘pressure correction’ method is followed. At each intermediate time step, $\partial u_i / \partial t$ is first calculated using the known pressure and velocity field before a correction is applied to the pressure field such that mass conservation is satisfied. This process requires solving the Poisson equation which is achieved via a discrete Fourier transform in the y -direction (Van Loan, 1992) and a cyclic reduction scheme in the x - and z -directions. (see Tomas (2016); Sweet, 1974). This discretisation allows for the grid to be stretched in the x - and z -directions.

The time step Δt is defined adaptively such that the numerical scheme remains stable. The stability criteria are the Courant-Friedrichs-Lewy (*CFL*) number and the diffusion number d (Courant et al., 1928; Wesseling, 1996):

$$CFL = \max \left(\left| \frac{\tilde{u}_i}{\Delta t} \right| \Delta x_i \right) \quad (2.15)$$

$$d = \max \sum_{i=1}^3 \frac{K_m \Delta t}{\Delta x_i^2} \quad (2.16)$$

CFL must be less than 1.5 in the absence of any pollutant scalar fields or 1.1 in simulations where the κ -advection scheme is applied and d must be less than 0.25.

The code is written in Fortran and parallelised using MPI. The Poisson equation solver is contained in the ‘FISH-PACK’ library. Parallelisation is achieved by slicing the domain in the y -direction.

2.3.3 Lateral and top boundary conditions

The lateral boundary conditions can be set as periodic or ‘inflow-outflow’ (using either Neumann and Dirichlet conditions). For an inflow-outflow simulation set-up, the inflow condition can be defined by either 1) running a precursor simulation from which outlet planes are used to ‘drive’ a later simulation or 2) following the cell perturbation method (Kong et al., 2000; Tomas et al., 2015). A diagrammatic view of these three simulation configurations is shown in Figure 2.4. The lateral boundary conditions are important in determining the boundary layer flow that is modelled in uDALES. In this thesis, both periodic and driver set-ups are used. The applicability of these boundary conditions towards satisfying the methodology outlined in Section 1.4 is discussed in more detail in Section 2.4. The top boundary condition for momentum is free slip. For the scalar fields, both Neumann and Dirichlet conditions can be applied at the boundary layer top as required.

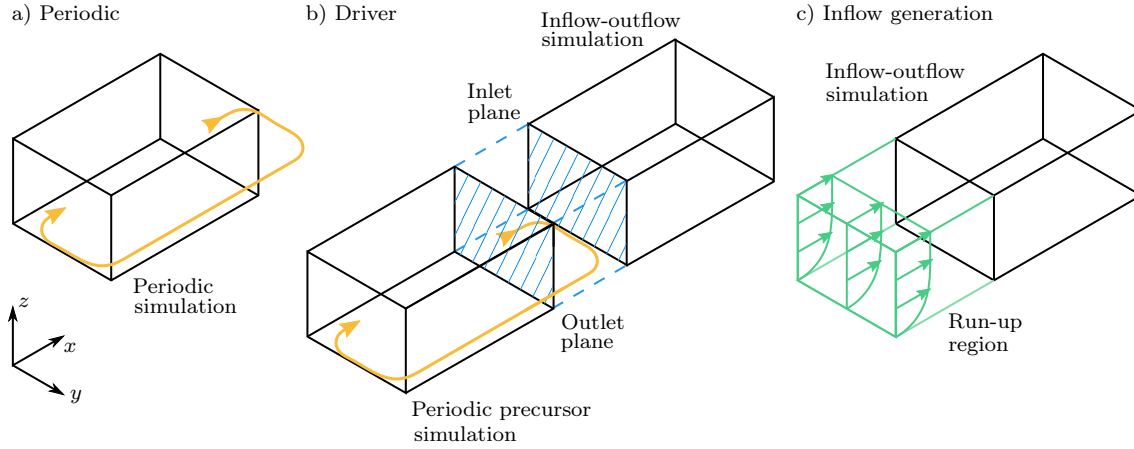


Figure 2.4: Diagrammatic view of the lateral boundary conditions available in uDALES. a) Periodic simulation set-up, b) driver simulation set-up (composed of a periodic precursor simulation and an inflow-outflow main simulation) and c) inflow generation set-up (turbulent profiles generated numerically at the inlet and a run-up region in the streamwise direction to allow the flow to develop).

2.3.4 Immersed boundary method

The solid-fluid boundary between the air and the urban form is defined through the IBM and wall functions (the latter is discussed in Section 2.3.5). The IBM allows for obstacles to be placed inside the fluid domain. It works on the principle that solid boundaries can be modelled by adapting the body force terms in Equations 2.3 and 2.4 in the cells that are adjacent to the defined boundaries (Mittal and Iaccarino, 2005). This technique is in contrast to other methods where the computational grid is defined such that it conforms to the solid-fluid boundary. The advantages of using the IBM are that the grid is relatively simple to generate and that the pressure field can be solved directly via a fast Fourier-based transform method.

The IBM introduced into uDALES by Tomas et al. (2015) is defined such that the obstacles must conform to the defined Cartesian grid (Pourquie et al., 2009). Boundaries are defined at the cell faces such that the normal component of the velocity can be set to zero (and therefore to ensure that there is no advective flux through the wall by construction). The SGS flux terms acting across this plane are also nullified in the cells adjacent to the boundary. This version of the IBM is second-order accurate but limits the obstacles modelled in the domain to be rectangular and grid-conforming.

2.3.5 Wall functions

Wall functions are necessary to capture interactions between the air and the boundary itself (e.g. SGS roughness, heat and moisture transfer). Most urban surfaces are aerodynamically

rough meaning that their surface roughness elements (e.g. window sills and shutters) are larger than the corresponding thickness of the viscous sublayer. This roughness results in complex turbulent flow interactions between the air and urban surfaces that occurs at scales smaller than the defined grid. Wall functions provide a method to predict the momentum, temperature and moisture fluxes at the urban surface based on known parameters.

Updated wall functions were recently introduced into uDALES that are discussed extensively and validated in Suter (2018) and Suter et al. (2020). The log-law wall functions follow the approach of Uno et al. (1988) and Cai (2012) in applying Monin-Obukhov similarity theory to both horizontal and vertical walls. A relationship is obtained for the surface fluxes of momentum and heat using the tangential flow velocity adjacent to the wall, the change in temperature between the wall and the adjacent cell and parametrically defined momentum and heat transfer coefficients (Louis, 1979). The challenge in this regard is that the roughness lengths for momentum and other scalar variables are not equal (there is no equivalent to the pressure difference caused by form drag on the scalar fields meaning that momentum roughness lengths are typically larger). The temperature is therefore not known at the momentum roughness length. The system of equations is solved following the one-step iterative approach of Uno et al. (1988) which is computationally inexpensive. This approach first calculates the bulk Richardson's number using the surface temperature, then uses this to calculate stability functions that allow a second estimate of the bulk Richardson's number to be made between the adjacent cell and the momentum roughness length. Finally the stability functions are estimated again using the updated bulk Richardson's number.

In cases where a constant temperature flux condition is applied over an urban surface (as is specified throughout this thesis), the stability (thermal) effects of the wall function are neglected. The wall temperature is not resolved under these idealised boundary conditions. Therefore the drag imposed by the wall function is simplified by following Monin-Obukhov similarity theory under neutral conditions. The wall shear stress at the adjacent cell, τ_w , is then defined by

$$\tau_w = \frac{u_T^2 \kappa^2}{\ln\left(\frac{z'}{z_0}\right)^2} \quad (2.17)$$

where u_T is a tangential component of velocity adjacent to the wall, z' is the perpendicular distance from the wall to the cell centre and z_0 is the wall roughness length for momentum.

The use of wall functions in uDALES negates the requirement to refine the resolution of the model close to solid boundaries. However as a result of using wall functions, the wall shear stress must be estimated following the methodology outlined above.

2.3.6 Statistics

As part of the work conducted in this thesis, a statistical routine was developed within uDALES. As introduced in Section 1.2, the turbulent nature of the UBL and UCL flows mean that averaging is required to produce statistically stable data for analysis. The devised statistical routine enables averaging of any field in any combination of time, x - and y -directions. Mean quantities are produced alongside advective, dispersive, turbulent and subgrid fluxes and variance terms (as applicable).

Time averaging a field variable, Ψ , over an averaging period, Δt , gives

$$\overline{\Psi}(x, y, z) = \frac{1}{\Delta t} \int_{\Delta t} \Psi(x, y, z, t) dt \quad (2.18)$$

from which, following the Reynolds decomposition, one obtains $\Psi(x, y, z, t) = \overline{\Psi}(x, y, z) + \Psi'(x, y, z, t)$ where $\overline{\Psi'} = 0$. If applying temporal averaging alone, covariance and variance turbulent statistics follow the derivation outlined in Section 1.2; i.e. rearranging Equation 1.3 for $\overline{u'_i \psi'} = \overline{u_i \psi} - \overline{u_i} \overline{\psi}$ (the Reynolds average).

Spatial averaging is complicated by 1) the position of buildings within the fluid domain in uDALES and 2) the resulting heterogeneity of the flow field within the UCL and RSL. Two averaging methods exist to account for the presence of buildings; intrinsic (ISA) and comprehensive spatial averaging (CSA; Xie and Fuka, 2018). A mask function, M , is defined that is equal to 0 in the position of the buildings and 1 everywhere else. The spatial averaging procedure then differs for ISA and CSA. For example, averaging field Ψ in both the x - and y -direction gives

$$\text{ISA} : \langle \Psi \rangle(z, t) = \frac{\int_A M(x, y, z) \Psi(x, y, z, t) dA}{\int_A M(x, y, z) dA} \quad (2.19)$$

$$\text{CSA} : \langle \Psi \rangle(z, t) = \frac{\int_A M(x, y, z) \Psi(x, y, z, t) dA}{\int_A dA} \quad (2.20)$$

where the integration domain A is the horizontal extent of the modelled domain. The two spatial averaging methods therefore differ in the area that is averaged over when buildings are present in the direction of averaging. ISA results in step changes in the averaging area that change the values of e.g. turbulent fluxes. CSA averages over an area of a greater extent than the considered variables, which fundamentally alters the mean statistics. The statistics routine in uDALES permits both ISA and CSA. Throughout the remainder of the thesis, ISA is applied.

A different notation is defined for the spatial decomposition. Following the slab-averaging in Equation 2.19, an instantaneous field can be defined as $\Psi(x, y, z, t) = \langle \Psi \rangle(z, t) + \Psi''(x, y, z, t)$. The flow is, by construction, not horizontally homogeneous if buildings exist

in the spatial averaging direction and therefore, under these conditions, the fluctuation term Ψ'' encompasses both spatial and temporal deviations from $\langle \Psi \rangle$. The corresponding flux $\langle u_i'' \Psi'' \rangle = \langle u_i \Psi \rangle - \langle u_i \rangle \langle \Psi \rangle$ therefore also encapsulates both a turbulent and dispersive flux component where the flow is not horizontally homogeneous (within the UCL and RSL). The horizontal domain sizes in urban LES are generally insufficiently large to produce converged statistics from spatial averaging alone. However spatially averaged statistics can be useful to track the progress of a simulation during runtime.

It is advantageous to be able to average in both space and time that, in the presence of spatial inhomogeneity, results in a triple decomposition. For example, averaging in both spanwise directions and also in time (the averaging procedures are commutative for the targeted statistics) gives $\Psi(x, y, z, t) = \langle \bar{\Psi} \rangle(z) + \tilde{\Psi}(x, y, z) + \Psi'(x, y, z, t)$. The second term in this decomposition represents the spatial variations of the time average $\tilde{\Psi} = \bar{\Psi}'' = \bar{\Psi}(x, y, z) - \langle \bar{\Psi} \rangle(z)$ and therefore captures spatial heterogeneity of the flow in the directions of spatial averaging. Averaging over spatially heterogeneous urban morphologies means that this term is significant when considering urban flows. Applying both spatial and temporal averaging to the term introduced in Equation 1.3 and simplifying gives

$$\langle \overline{u_i \Psi} \rangle = \langle \overline{u_i} \rangle \langle \bar{\Psi} \rangle + \langle \tilde{u_i} \tilde{\Psi} \rangle + \langle \overline{u_i' \Psi'} \rangle. \quad (2.21)$$

where $\langle \tilde{u_i} \tilde{\Psi} \rangle = \langle \overline{u_i \Psi} \rangle - \langle \overline{u_i} \rangle \langle \bar{\Psi} \rangle$ and $\langle \overline{u_i' \Psi'} \rangle = \langle \overline{u_i \Psi} - \overline{u_i} \bar{\Psi} \rangle$. The slab- and time averaged flux of Ψ is therefore composed of advective, dispersive and turbulent terms. The dispersive flux term arises directly as a result of spatial heterogeneity and can be used to e.g. calculate the height of the RSL.

Each of these terms is calculated within the statistical routine for any prognostic field. The commutativity of the averaging procedures ($\langle \bar{\Psi} \rangle = \overline{\langle \Psi \rangle}$) and rules such as $\langle \bar{w} \rangle = 0$ are applied to calculate the statistics in a computationally efficient manner. The staggered nature of the grid in uDALES means that fields must be interpolated to produce product based statistics. Interpolation is conducted preferentially towards the cell face as opposed to the cell centres so that values on or within the immersed boundaries are neglected and set to arbitrary values within the statistics routine.

2.4 Validation

The dynamic core of uDALES (DALES) has been validated extensively and used as part of several atmospheric intercomparison studies (Heus et al., 2010). The adapted version of the code with the IBM implemented has been validated against both wind and water tunnel data for idealised geometries (Tomas et al., 2016a; Tomas, 2016) and more recent

introductions into the code (e.g. wall functions) have also been verified (Suter, 2018). In this section, a further validation is presented for its application to realistic urban morphologies and passive scalar dispersion. As discussed in Section 2.2, SIRANE has been validated extensively against wind-tunnel and field data and a further validation is not presented here.

2.4.1 The DAPPLE project

Wind-tunnel data from the Dispersion of Air Pollution and its Penetration into the Local Environment (DAPPLE) project is used to validate the application of uDALES to realistic urban morphologies. DAPPLE was a large, multi-disciplinary study of both urban meteorology and pollution dispersion that consisted of field measurements, wind tunnel modelling and computational simulations (Arnold et al., 2004). The case study area was the region surrounding the junction of Marylebone Road and Gloucester Place in Central London, UK.

Wind tunnel experiments were conducted over the case study region as part of this project (alongside passive scalar releases in the field; Carpentieri et al., 2009, 2012a). The wind tunnel model was set-up at a 200:1 scale, the freestream velocity was 2.5 m s^{-1} , the wind direction was south-westerly and a turbulent neutral boundary layer was developed upstream of the urban geometry using Irwin spires and 2-D roughness elements. Xie and Castro (2009) conducted an LES study that reproduced these wind-tunnel results with good agreement. SIRANE has previously been validated over the same case study region and wind tunnel dataset (Carpentieri et al., 2012b).

2.4.2 Simulation set-up

Two set-ups were investigated to simulate the wind tunnel measurements in order to 1) perform a fundamental validation of uDALES and 2) to investigate the applicability of different lateral boundary conditions as outlined in Section 2.3.3. Simulation D uses inflow-outflow boundary conditions in the streamwise direction and is driven through the precursor simulation, pre-D. Simulation P uses periodic lateral boundary conditions for momentum and inflow-outflow conditions for scalar fields. Details of the three simulations are provided in Table 2.1.

Diagrammatic views of the modelled urban morphologies are shown in Figure 2.5 (reproducing the model used in the wind tunnel experiment at full scale; some details have been approximated due to a lack of available data). The case study morphology of simulation D is rotated such that the south-westerly direction is aligned with the x_D -axis. The morphology of simulation P is rotated so that the majority of buildings are aligned

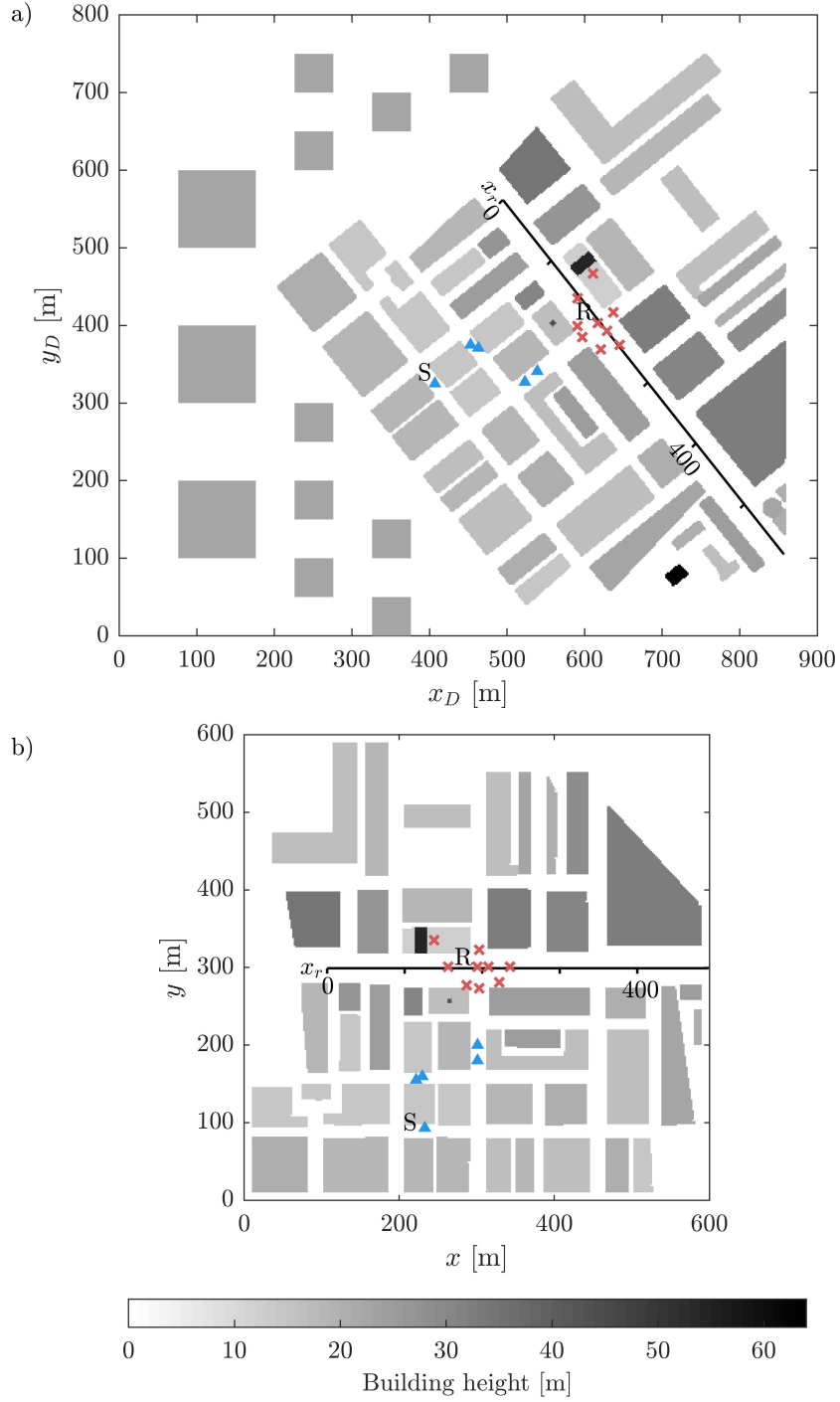


Figure 2.5: Diagrammatic view of the urban morphologies used in simulations a) D and b) P. The positions of the measuring points around the main intersection are denoted by red crosses (point R used in this validation) and the position of the scalar releases are denoted by blue triangles (release point S discussed here). An additional horizontal axis, x_r , is shown on both plots that is used to plot a profile of the spanwise pollutant concentration along the Marylebone Road.

Table 2.1: Simulation set-up details for simulations pre-D, D and P used in the uDALES validation. Boundary conditions (BC) defined for the x - and y -directions. $\hat{u}$ and $\hat{v}$ signify domain averaged velocities and an assigned constant volume flow rate forcing.

	Simulation		
	pre-D	D	P
Domain size [m]	$400 \times 800 \times 200$	$900 \times 800 \times 200$	$600 \times 600 \times 200$
Grid size	$200 \times 400 \times 100$	$450 \times 400 \times 100$	$300 \times 300 \times 100$
x momentum BCs	Periodic	Inflow-outflow	Periodic
y momentum BCs	Periodic	Periodic	Periodic
x scalars BCs	-	Inflow-Outflow	Inflow-Outflow
y scalar BCs	-	Inflow-Outflow	Inflow-Outflow
Flow forcing	$\mathcal{F}_u = 0.000125 \text{ m s}^{-2}$	Inlet from pre-D	$\hat{u} = 1.13 \text{ m s}^{-1}$ & $\hat{v} = 1.41 \text{ m s}^{-1}$
Run-up time [s]	50,400	-	100,800
Averaging period [s]	-	25,200	25,200

to the Cartesian grid of uDALES (therefore minimising the ‘saw-tooth’ effect associated with oblique building angles and the number of individual blocks that must be modelled). The mean building height, h_m , is 22 m and the reference velocity, u_{ref} , is 2.5 m s^{-1} . The scaling of the validation case is possible because, at high ‘effective’ Reynolds numbers, such a dependency becomes negligible (Xie and Castro, 2006).

The two set-ups present fundamentally different approaches to capturing the dynamics of the boundary layer flow above the modelled urban morphology. The use of a precursor simulation for simulation D allows for the incoming boundary layer to be defined independently of the main simulation (which can be particularly useful when reproducing wind tunnel experiments or studying transitional flows). On the other hand, the boundary layer flow in simulation P develops in time over the modelled urban morphology and its mean and turbulent state are therefore directly dependant upon e.g. the roughness imposed within the simulation itself.

Simulation pre-D is set up to reproduce the boundary layer dynamics obtained upwind of the wind tunnel morphology in the experiment of Cheng and Robins (2004). Using the friction velocity and estimations of the displacement height (extracted from the mean velocity profile using the log-law relationship), the relationship defined by Macdonald et al. (1998) is used to obtain the building height (4 m) and packing density (0.25) necessary to reproduce the same mean wind profile. A staggered cubic array was therefore used

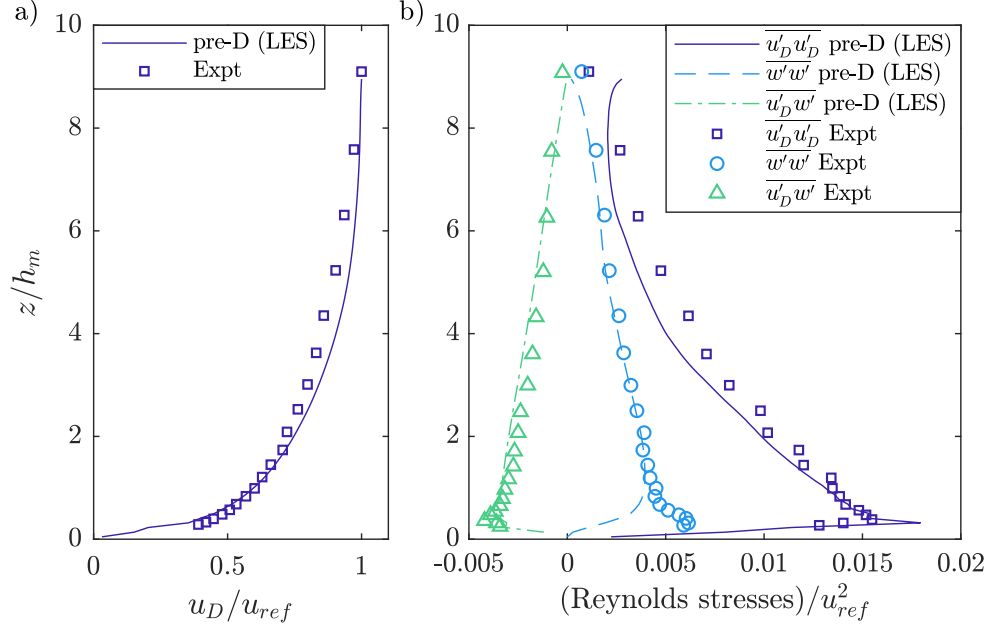


Figure 2.6: a) Mean and b) turbulent profiles of the precursor simulation, pre-D, and the boundary layer developed before the urban area in the wind tunnel experiments of the DAPPLE project. Note the use of subscript D to denote alignment with the axes x_D and y_D (see Figure 2.5).

in simulation pre-D with a building height of 4 m. Figure 2.6 compares the mean and turbulent statistics produced in simulation pre-D against the incoming profiles from the wind tunnel. A reasonable agreement is shown indicating that the inlet to simulation D closely matches that of the wind tunnel data. Both simulations pre-D and P had to be ‘run-up’ to reach a statistical steady state prior to obtaining converged statistics (run-up times and averaging periods are given in Table 2.1).

2.4.3 Results

Mean and turbulent flow and scalar statistics obtained in uDALES are compared to those of the wind tunnel experiments. Figure 2.7 compares the mean and turbulent vertical profiles obtained at position R (note all variables are rotated for alignment with the axes x and y ; refer to Figure 2.5). Position R is situated within a large intersection and directly downwind of an elevated spire. Simulation D illustrates a good agreement between all three mean velocity profiles. The higher order statistics are also shown to generally provide a good agreement, with the most significant discrepancy shown to be the relatively larger peaks in the Reynolds stress profiles at $z = 2h_m$. These peaks are related to the wake of the upwind spire. Capturing the form of this spire is challenging in simulation D due to its

oblique angle upon the Cartesian grid (refer to Figure 2.5) and as such both its frontal area and vertical form may lead to the relatively larger fluxes over this region (the dimensions of the spire also had to be approximated due to a lack of available data).

Simulation P systematically underestimates the mean horizontal velocities for $z > h_m$ and underestimates the root mean square velocities for $z > 2h_m$. These discrepancies relate to the properties of the boundary layer flow that is produced when using periodic boundary conditions. The boundary layer is fully developed in this simulation, but in contrast to the relatively small roughness elements used to emulate the wind tunnel in simulation pre-D, the roughness elements in P are that of the case study morphology (resulting in a significantly larger roughness length). As such, for a simulation with the same freestream velocity, the friction velocity of simulation P is also larger. The boundary layer flow is therefore more turbulent and exhibits a different logarithmic wind profile due to these key length and velocity scales. Despite these differences in the modelled boundary layer, both the mean and turbulent statistics show a better agreement than simulation D within the UCL. In particular, there is no overestimation of Reynolds stresses in the wake of the spire. This finding illustrates the importance of the local morphology on the flow statistics within and just above the UCL. Similar agreement was obtained over 8 other positions within the modelled domains in both simulations D and P (the red crosses in Figure 2.5).

Figure 2.8 compares quiver plots obtained over the Marylebone Road and Gloucester Place junction for the wind tunnel data and both simulations D and P. All of the dominant trends are shown to qualitatively agree well with the wind tunnel data for both simulations. For example, two prominent separation bubbles are predicted and shown to be of similar size and the cross-canyon flow induced by the relatively taller building on the north-east side of the canyon is evident (Xie and Castro (2009) indicated that a RANS model was incapable of capturing these flow structures for the same case study). A difference between the flow fields of the two simulations is the magnitude of the flow reversal within the south-east separation bubble in simulation P in comparison to simulation D. This difference relates to the defined urban morphologies. In simulation D the side of the buildings exhibit a ‘saw-tooth’ effect as the building edges are at oblique angles to the grid. These buildings are therefore relatively more rough than the ‘smooth’ facades modelled in simulation P.

Validating the model against a point source release of a passive scalar acts to validate the integrative effects of the modelled flow field (both within and above the UCL) and the treatment of scalars in the model (in particular the κ -advection scheme).

Figure 2.9 displays the normalised pollutant concentration and variance along the axis x_r (as defined in Figure 2.5). Simulation D is shown to provide a very close agreement to the results obtained in the wind tunnel experiment both in terms of the mean concentration

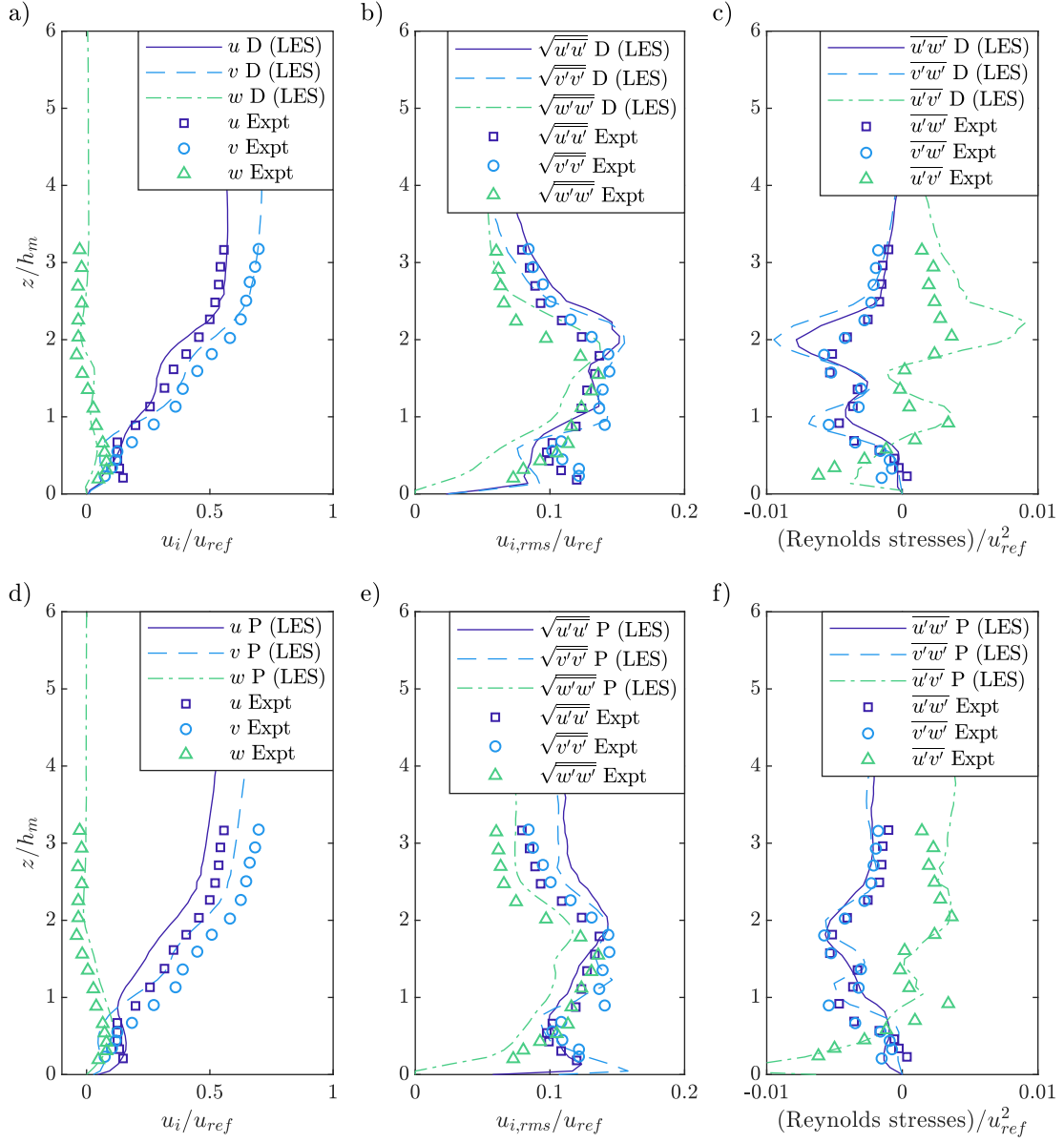


Figure 2.7: Vertical profiles of the mean velocities, root-mean-square velocities and Reynolds stresses at position R from simulation D (a, b and c) and simulation P (d, e and f). Plotted against the wind tunnel experiment results of the DAPPLE project.

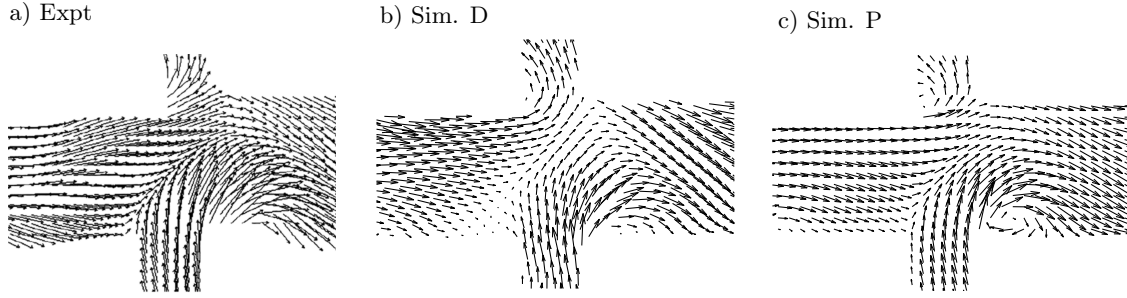


Figure 2.8: Quiver plots of the flow field at the horizontal plane $z = 0.235h_m$ for a) the wind tunnel experiments of DAPPLE, b) simulation D and c) simulation P.

and the normalised root mean square concentration. This finding validates the application of uDALES to model pollution dispersion within realistic urban morphologies. The results of simulation P do not exhibit as good an agreement. The same peak of concentrations is obtained at $x_r = 200$ m but lower concentrations are found along the rest of the Marylebone Road.

The difference between the time-averaged concentrations of simulations D and P occur due to two main factors. As discussed above, the use of periodic boundary conditions results in different mean and turbulent properties of the boundary layer in simulation P. The boundary layer profile is representative of the roughness of the case study region as opposed to the smaller scale roughness positioned upwind in the wind tunnel experiment. As such the differences between P and D point to the importance of capturing the characteristic heterogeneity of the (upwind) simulation region. Figure 2.10 displays the pollutant concentrations at $z = 1$ m for simulations D and P, which indicates that a significant proportion of the scalar field is being dispersed above the UCL to downstream positions. The increased capacity for mixing in the UBL of simulation P therefore results in greater mixing above the UCL and subsequently lower detrainment downstream. There is also a small difference in the near-field dispersion of the pollutants in these two simulations. This phenomenon may occur due to the differences in upwind morphology close to the release point. Simulation D has a roughness element placed close to the upwind edge of the urban morphology whereas simulation P effectively has the real urban morphology at the corresponding downstream edge of the domain.

The significance of the SGS flux components in these LES can be investigated by their percentage contribution to the total spanwise and time averaged vertical momentum flux (turbulent, dispersive and subgrid components). In simulation P the SGS component is 13.7% in the lowest cell of the domain but no greater than 3.2% everywhere else (average

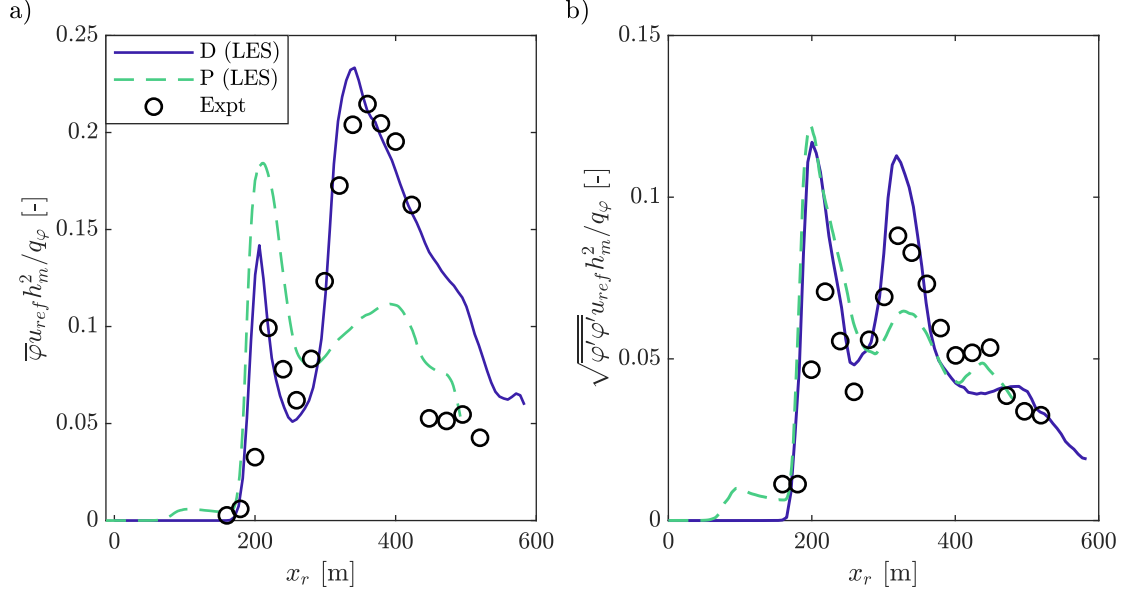


Figure 2.9: Comparison of the a) normalised scalar concentrations φ and b) root-mean-square concentrations of the wind tunnel experiments of DAPPLE and simulations D and P along the axis x_r for a point source scalar release at position S.

of 1.4%). In simulation D the subgrid component is 30.1% in the lowest cell (owing to the more numerous corners on the urban morphology) but no more than 4.5% elsewhere (average of 1.8%). These results indicate that the use of a uniform grid and resolutions of ≈ 2 m are sufficient to resolve the majority of the energetic turbulent scales of the urban flow field. But also that the fluxes close to the urban surface have a tendency to require a greater SGS flux component and that the application of the wall function at the urban surface is imperative to accurately capturing dynamics in these regions.

2.4.4 Discussion

The above validation illustrates the ability of uDALES to predict urban pollution dispersion in realistic urban morphologies. This finding is particularly evident from the results of simulation D where the inflow condition was matched closely to that of the targeted wind tunnel experiments. Simulation D is shown to accurately reproduce the downwind dispersion of a passive scalar field.

The two simulation set-ups highlight key differences in the applied modelling approaches. Simulation P uses periodic lateral boundary conditions and therefore assumes upwind morphological similarity which is not the case for the wind tunnel experiment. However although this condition is not as well suited to the above validation case, this

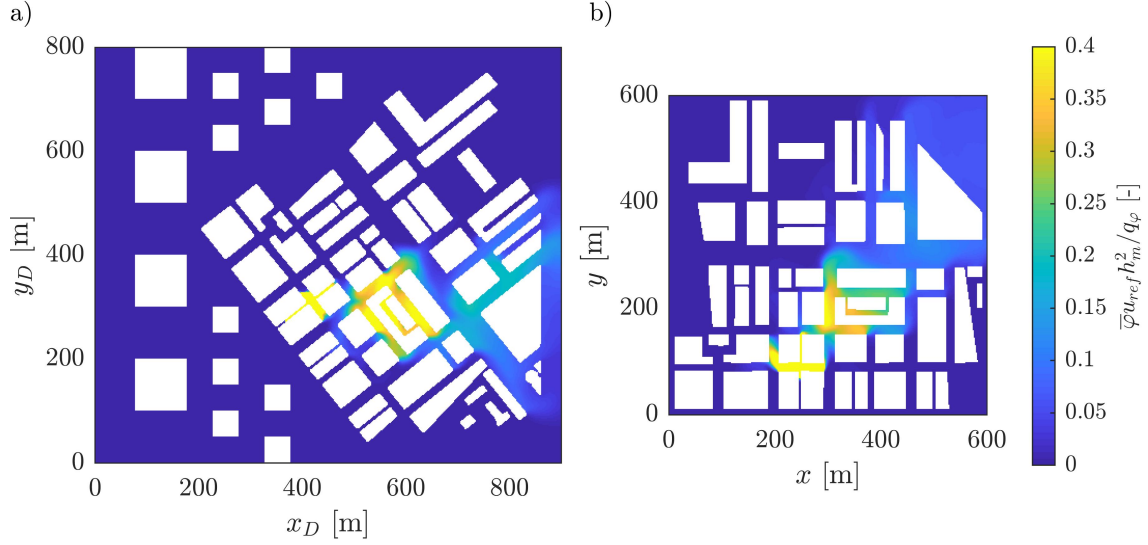


Figure 2.10: Normalised scalar concentrations φ at the horizontal plane $z = 1$ m for simulations a) D and b) P for a point source release at S (with mass flux q_φ).

finding does not mean that this simulation set-up is generally inferior. It highlights that the lateral boundary conditions are important in correctly modelling the boundary layer flow above the UCL and that both are applicable given the nature of the relevant study and with the understanding of their effects. The difference in the near-field dispersion of the modelled scalar release highlights that the treatment of the local morphology at the upwind side of the domain is challenging under both simulation set-ups. Neither method is able to reproduce the real urban morphology upwind of the area of interest. Therefore consideration is required of the flow field close to the upwind edge of the urban morphology when reproducing ‘realistic’ as opposed to wind tunnel conditions. An advantage of the periodic simulation set-up is that the morphology can be rotated such that the ‘saw-tooth’ effect and number of individual blocks modelled within uDALES are minimised. A note is provided on the use of these simulation set-ups in the following section.

2.5 A note on LES set-ups

Figure 2.4 illustrates the lateral boundary conditions that can be applied to the prognostic variables in uDALES. In Section 2.4 it was shown that both inflow-outflow and periodic boundary conditions can be applied to the problem of urban pollution dispersion and that their application effects the flow structure of the modelled boundary layer and treatment of the upwind morphology.

The principle difference between these two set-ups is that the boundary layer flow is

either predefined independently of the urban area of interest (inflow-outflow) or developed over this area meaning that the flow structure is a function of the e.g. morphology of the study region (periodic). The properties of these two set-ups directly relate to the thesis methodology defined for accounting for urban heterogeneity in Section 1.1 (the aims of reducing the degrees of freedom and producing statistical steady states).

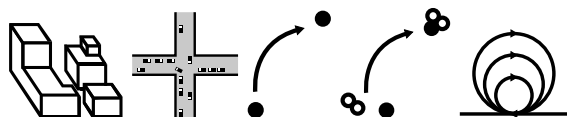
Inflow-outflow simulations are statistically stationary once developed but exhibit horizontal inhomogeneity as the flow continues to develop over the streamwise length of the domain (Muñoz-Esparza and Kosović, 2018). The properties of these simulations are advantageous for modelling developing or transitional flows or for coupling the LES with mesoscale models (Nakayama et al., 2012). However, the streamwise inhomogeneity limits the applicability of the ergodic principle to spanwise and temporal averaging and either a proportion of the domain upwind of the region of interest is required to allow the flow to develop (inflow generation) or it is necessary to run a precursor simulation prior to the simulation of interest (driver). Conversely, periodic simulations develop both spatially and temporally but have the capability to become both statistically stationary and horizontally homogeneous (above the roughness sublayer) under the right conditions, e.g. for a fully developed neutral boundary layer as discussed above. Run-up time is required to allow the flow field to initially develop and upwind morphological similarity is assumed, but if an equilibrium condition is reached then the bulk flow properties are equivalent across the domain and converged statistics can be obtained over long time-periods. A periodic simulation set-up therefore allows the UBL flow properties to be reduced to vertical profiles and represented by bulk flow properties, which is advantageous to producing simplified representations of the flow and conducting targeted simulations.

In terms of reducing the degrees of freedom of the problem, periodic simulations therefore provide a tool through which to do this. In real urban areas the boundary layer is constantly evolving as a function of changes in e.g. the roughness, emissions, heat and moisture fluxes. There is value in capturing all of these transitional internal boundary layers however the nature of these variabilities is highly case-specific and a combination between just these four changes results in a very large parameter space for investigation. For microclimate modelling of urban air pollution, a methodology is therefore followed in this thesis where the aim is to produce statistically stationary flows over which the e.g. friction velocity and Richardsons number is constant. The prognostic field that can then be varied within these ‘control’ variables is the pollutant concentration scalar fields of interest.

Chapter 3

Simulating air pollution in the urban microclimate I: morphology, traffic and chemistry

The model capabilities to capture 1) realistic urban morphologies from LIDAR data, 2) realistic emissions via a coupling with a traffic microsimulation model and 3) the chemistry of the null cycle in urban large-eddy simulations are introduced. A case study is conducted over a real urban microclimate to showcase these model developments. The results of this case study are used to systematically evaluate the performance of an operational air quality model. This chapter interpolates material from a publication by the author (Grylls et al., 2019), coauthored with Cl  mence M. A. Le Cornec, Pietro Salizzoni, Lionel Soulhac, Marc E. J. Stettler and Maarten van Reeuwijk.



3.1 Introduction

Air quality is the largest single environmental health risk globally (World Health Organization, 2016). Nitrogen oxides (NO_x ; nitric oxide (NO) and nitrogen dioxide (NO_2)) emissions lead to degradations in air quality, with adverse short- and long-term health and environmental effects (EEA, 2017). Exposure to NO_2 is related to cardiovascular diseases, decreased lung functionality, aggravated asthma, low birth weights and premature

deaths (Andersen et al., 2012; Vineis et al., 2006). NO_2 and ozone (O_3) are precursors of acid rain, particulate matter and are partially responsible for the eutrophication and acidification of soil and water. Despite stringent regulations on both emissions and air quality, NO_2 concentrations in many European cities exceed regulations (see Chapter 1; EEA, 2017). The problems associated with urban air quality are generally more severe in low- to middle-income countries.

There are numerous sources of NO_x into the atmosphere (Wallace and Hobbs, 2006), but harmful concentrations in cities are principally a result of fossil fuel combustion (see Section 1.5.1; Palmgren et al., 1996; UK National Atmospheric Emission Inventory, 2018). The chemistry associated with tropospheric NO_x is complex, however considering that the timescale at which pollutant dispersion occurs in the urban canopy is typically a few minutes (Soulhac et al., 2011), it is often simplified to the reactions of the null cycle (Crutzen, 1979). NO_x emissions primarily consist of NO that, during the day, is oxidized by O_3 to NO_2 . NO then rapidly establishes an equilibrium with NO_2 as a result of photodissociation (Wallace and Hobbs, 2006). The reactions of the null cycle are introduced in Section 1.5.3.

Urban pollution dispersion models are able to provide information on the temporal and spatial evolution of e.g. NO , NO_2 and O_3 in and above the urban canopy layer (UCL). They are thus an integral tool for researchers, urban planners and public authorities to understand, estimate and subsequently combat the challenges associated with outdoor air quality. A range of dispersion models exist that consider this problem at different levels of abstraction, with an inherent trade off between the provided resolution and accuracy against the costs and speed of computation.

The most computationally demanding aspect of this problem is resolving the unsteady, heterogeneous and turbulent flows that occur within and above the urban canopy. As discussed in Chapter 2, a range of different assumptions, simplifications and parametrisations are applied in order to provide a representation of the urban flow field at the scale of interest of the respective model. Ranging from operational models that typically apply parametrisations to obtain a bulk representation of this flow field ($\text{O}(100 \text{ m}, 1 \text{ hr})$; Baklanov et al., 2009) to large-eddy simulation (LES) models that resolve the unsteady turbulent three-dimensional flow field to the highest possible resolutions ($\text{O}(1 \text{ m}, 0.1 \text{ s})$; Letzel et al., 2008; Tominaga and Stathopoulos, 2013; Salim et al., 2011b). These flow representations are combined with detailed data (e.g. traffic flows, background concentrations, meteorological conditions and street morphologies) and physico-chemical schemes (e.g. chemistry and deposition) to provide estimates of pollution levels at street, neighbourhood or city scales over hours, weeks or longer time periods. The level of abstraction taken by a model to capture the urban flow field propagates to define the resolution at which these other

effects are generally resolved (discussed further in Section 2.1).

LES models have typically been used in intensive, generalised studies to formulate the parametrisations that define operational models. However, increasing computational capabilities mean that it is now possible to produce realistic urban LES at a comparable scale to operational models (the crossover point between these models is at the microclimate (neighbourhood) scale over time periods of hours). Conducting comparable simulations between operational and LES models, without simplifying intrinsic properties within the LES, provides a novel method through which to evaluate an operational model and contextualises the results obtained via LES.

Operational dispersion models have been validated extensively against both experimental and field data (Soulhac et al., 2012, 2017) and comparative studies between operational and Reynolds-Averaged Navier-Stokes (RANS) models exist (Di Sabatino et al., 2007), but to the authors' knowledge this study presents the first evaluation of an operational model using LES. The use of LES in this analysis has the advantage of simulating real-time urban pollution dispersion (as would be captured in field or experimental studies) but with the computational advantages of 1) high-resolution mean and turbulent statistics over the entire domain and study period, 2) the numerical control to conduct systematic, targeted simulations (e.g. with or without chemistry/ buoyancy effects) and 3) capturing the same fundamental simulation conditions as the operational model and therefore vastly reducing the associated uncertainty (e.g. carefully matching the modelled morphology, emissions and meteorology but at a hugely enhanced resolution; Chang and Hanna, 2004). This methodology does not present a further validation of an operational model (due to the associated modelling and numerical uncertainty; Stern et al., 2001), but it does therefore provide the opportunity to systematically analyse the assumptions, simplifications and parametrisations used by operational models against an 'ideal' dataset.

In this chapter, a comparison is conducted between the operational air quality model SIRANE (Soulhac et al., 2011), and the LES code uDALES (Heus et al., 2010; Tomas et al., 2015, 2016a). Comparable simulations are run using a case study area of South Kensington, London, UK with a focus on the concentrations of inert NO_x and reactive NO , NO_2 and O_3 . The case study showcases LES model capabilities that have been developed as part of the work conducted in this thesis (specifically the modelling of the urban morphology, emissions and chemistry) and facilitates an evaluation of SIRANE. The evaluation objective is to assess the predictive skill of SIRANE over its quasi-steady hourly time steps and to systematically analyse the applicability of SIRANE's parametrisations and assumptions using the high-resolution capabilities of uDALES.

A brief overview of the two models is provided in Sections 3.2.1 and 3.2.2 including the

introduction of a chemistry scheme into uDALES (more detailed outlines of the two models are provided in Sections 2.2 and 2.3). The set-up of the case study is described in Section 3.3, detailing how the morphology, emissions and meteorology of the case study region were systematically matched for both SIRANE and uDALES. The processing of LIDAR data to capture the urban morphology of the case study region is discussed in Section 3.3.1 and the coupling of both models with the traffic microsimulation model VISSIM is presented in Section 3.3.2. The results for inert and reactive pollutants alongside the sensitivity to wind direction are discussed in Sections 3.4.1 and 3.4.2 respectively. In order to assess the validity of SIRANE’s uniform in-canyon concentration assumption, the pedestrian, leeward and windward concentrations from uDALES are analysed. The role of intersections within the case study area and other impacts of resolving the heterogeneity of real urban morphology are discussed. Finally conclusions are drawn upon the strengths and shortcomings of SIRANE.

3.2 Models

SIRANE and uDALES are both physically-based numerical models that differ in the scale at which they resolve the flow. SIRANE operates at street scale, and therefore relies on flow and turbulence parametrisations to estimate the dispersion of pollutants through a defined street network, whereas uDALES operates at metre-scale, and thus resolves the turbulent and unsteady 3-D flow field around buildings and the subsequent dispersion of emissions within and above the urban canopy. A brief description of the models’ relevant properties are provided below (further details are presented in Sections 2.2 and 2.3). The implementation of the null cycle within uDALES is also outlined.

3.2.1 SIRANE

SIRANE is an operational urban dispersion model (Soulhac et al., 2011). The domain is divided into two sub-domains: the urban canopy and the external atmosphere. The urban canopy is represented by street canyons (spaces between the buildings) which are modelled as a series of connected boxes (a street network). The pollutant concentration in each box is assumed to be uniform and is computed as a mass balance which includes the advective transfer along the street, turbulent transfer at roof level, chemical transformations occurring inside the canyon and dispersion at intersections (Soulhac et al., 2009). The pollutant dispersion above the canopy is represented by a Gaussian model. The mesoscale meteorological properties (boundary layer height, friction velocity, surface heat flux etc.) are calculated through parametrisations based upon observational data such as wind speed,

wind direction, cloud cover, precipitation and surface albedo (Soulhac et al., 2008, 2013).

The chemical equilibrium between NO, NO₂ and O₃ is assumed to follow the null cycle. SIRANE accounts for these reactions by first simulating the passive dispersion of NO_x through and above the street network and then uses the resulting NO_x concentration field and the background concentrations of NO, NO₂ and O₃ to solve the resulting system of equations by satisfying the Leighton relationship (see Section 1.5.3; Leighton, 2012):

$$\frac{J_{\text{NO}_2}}{k_2} = \frac{[\text{NO}] [\text{O}_3]}{[\text{NO}_2]}, \quad (3.1)$$

where J_{NO_2} is the photolysis rate for NO₂ and k_2 is the NO + O₃ reaction rate. This methodology therefore follows the assumption that the pollutants reach a photostationary steady-state (PSS) within each canyon over SIRANE’s hourly time steps. SIRANE has been validated against wind tunnel experiments and real measurements in Lyon, France (Soulhac et al., 2012, 2017; Carpentieri et al., 2012b; Salem et al., 2015).

3.2.2 uDALES

uDALES is a high-resolution, flow-resolving atmospheric LES model (Heus et al., 2010; Tomas et al., 2015, 2016a) that solves the equations of motion at the energetically dominant scales of turbulent motion. The three-dimensional flow field is modelled at resolutions of O(1m) and O(0.1s), satisfying the filtered Navier-Stokes equations throughout the domain. The Vreman subgrid model is used to parametrise the dynamics at the subgrid scale (SGS; Vreman, 2004). The pollutant scalar fields, φ , are modelled following the governing equation

$$\frac{\partial \tilde{\varphi}}{\partial t} = -\frac{\partial}{\partial x_j} (\tilde{u}_j \tilde{\varphi}) - \frac{\partial \mathcal{R}_{\varphi,j}}{\partial x_j} + S_\varphi + \epsilon_\varphi \quad (3.2)$$

where $\tilde{\cdot}$ denotes the filtered part, $\mathcal{R}_{\varphi,j}$ is the SGS scalar flux vector, S_φ is a source term for volumetric emissions and ϵ_φ is an additional term from Equation 2.4 that performs chemical transformations.

The numerical scheme consists of a spatial discretisation on an Arakawa C-grid, utilising a second-order central-differencing scheme for all field variables except for the pollution concentration, which employs a κ scheme to ensure positivity. A third-order Runge-Kutta time integration scheme is applied. An immersed boundary method (IBM) has been incorporated into uDALES in order to provide the capability to place objects in the domain (Tomas et al., 2015). The SGS roughness of the buildings and dynamics close to the wall are modelled by log-law wall functions (Uno et al., 1995; Suter, 2018). uDALES has been validated against wind and water tunnel data (Tomas et al., 2016a; Tomas, 2016) and

the dynamic core, DALES, has been validated extensively and has been part of several atmospheric intercomparison studies (Heus et al., 2010).

The chemical processes of the null cycle were added into uDALES for the purposes of this study. The relatively high reactivity of $\text{O}\bullet$ permits a simplification of the null cycle leading to the following prognostic relationships (Zhong et al., 2015):

$$\epsilon_{\text{NO}} = J_{\text{NO}_2} [\text{NO}_2] - k_2 [\text{NO}] [\text{O}_3] \quad (3.3)$$

$$\epsilon_{\text{NO}_2} = -J_{\text{NO}_2} [\text{NO}_2] + k_2 [\text{NO}] [\text{O}_3] \quad (3.4)$$

$$\epsilon_{\text{O}_3} = J_{\text{NO}_2} [\text{NO}_2] - k_2 [\text{NO}] [\text{O}_3]. \quad (3.5)$$

The chemistry is implemented following a fully implicit time-integration scheme, details of which are provided in Appendix A.2. A validation of the chemical scheme is also provided in Appendix A.3.

3.3 Case study

The case study region is situated in South Kensington, a district that is located centrally within London, UK. The study area spans 672x1344 m and contains a range of morphological features (street lengths, building heights, open spaces etc.) and street types (pedestrianised, high streets, a-roads etc.). There are also numerous trees that enable later analysis in Chapter 6. An aerial image of the case study area is shown in Figure 3.1. High resolution emissions data was available through the augmentation of traffic counts with the traffic microsimulation model VISSIM (PTV AG, 2017a).

SIRANE and uDALES operate at different scales and are based on fundamentally different numerical representations of the urban environment. These differences mean that consideration is required in terms of matching the simulation properties; e.g. the morphology, emissions, meteorological conditions (wind, chemistry) and boundary conditions. A detailed description of the methodology used in producing consistent simulation properties is given below. An outline of the case study properties of both models is provided in Table 3.1.

3.3.1 Morphology

The representation of the urban morphology in both uDALES and SIRANE was obtained using one metre resolution LIDAR data with an applied building mask (Environmental Agency, 2017). Following a similar pre-processing routine as that discussed in Suter (2018), the LIDAR data is first manipulated using geographic information systems (GIS;



Figure 3.1: Aerial view of the case study area highlighting the main roads and points of interest. Image obtained from Google Earth Pro 7.3.2.5776 (4th Sep. 2018). South Kensington, London. 51°29 N 0°10 W. Eye alt 2.3 km.

specifically SAGA GIS and QGIS). The coordinates are altered to a projected system and the data is cropped over the case study area. The data is rasterised to the desired resolution of the targeted LES and the mean building heights are represented through a single grayscale image. A MATLAB routine has been developed that automates further image processing by altering the resulting set of buildings to work optimally with the implemented IBM. Morphological details that result in small gaps along building walls are filled, isolated protruding cells are removed and enclosed features (e.g. courtyards) below a threshold area ($<100 \text{ m}^2$) are filled. These alterations avoid small spatial features where the number of cells can be insufficient to effectively resolve the fluid flow. A representation of the resultant buildings as processed for uDALES over the case study area is shown in Figure 3.2a. The applied pre-processing routine leads to flat roofs and therefore details

Table 3.1: Case study properties of SIRANE (SI) and uDALES (DA) for the south-westerly simulation.

Property	Units	Value	SI	DA
Date	d/m/y	7/7/2017	○	
Time	hr	12:00	○	
Domain				
Domain size, l_x	m	672	○	○
Grid resolution, Δx	m	1.75	○	○
Domain size, l_y	m	1344	○	○
Grid resolution, Δy	m	1.75	○	○
Domain size, l_z	m	412.6		○
Grid resolution, Δz	m	2.15		○
Latitude, Θ	°	51.49	○	
Meteorology				
Wind direction	-	SW	○	○
Friction velocity, u_*	m/s	0.33	○	○
Boundary layer height, h	m	412.6	○	○
Stability	-	Neutral	○	○
Cloud cover	octas	6	○	
Precipitation	mm/h	0	○	
Site parameters				
Aerodynamic roughness length	m	1.0	○	
Building roughness length	m	0.05	○	
Displacement height	m	13.3	○	
Emissivity	-	0.88	○	
Albedo	-	1.0	○	
Priestley-Taylor coefficient	-	0.5	○	
Chemistry				
Photolysis rate, J_{NO_2}	1/s	0.0063	○	○
NO+O ₃ reaction rate, k_2	m ³ /mol s	10042	○	○
[NO] _b	μg/m ³	6.85	○	○
[NO ₂] _b	μg/m ³	18.09	○	○
[O ₃] _b	μg/m ³	51.88	○	○
[NO _x] _b	μg/m ³	28.59	○	○

of the heterogeneity on the building tops are not captured. A newer version of the pre-processing routine has been developed as part of the work conducted in this thesis that permits uneven, adjacent building heights (it is also consistent with the rules defined for the implemented three-dimensional radiative transfer model; Suter, 2018). By using point cloud LIDAR data in the future it will be possible to therefore resolve super-grid-scale roughness on building roofs. More stringent rules have also been developed to further satisfy the guidelines of Blocken (2015). Morphological operations, such as image erosion and dilation with a carefully specified structural element, enable building and canyon sizes to be more precisely controlled (the form and size of the structural element can be defined to satisfy best practice guidelines e.g. a threshold of 10 cells per cubic root of the build-

3.3 CASE STUDY

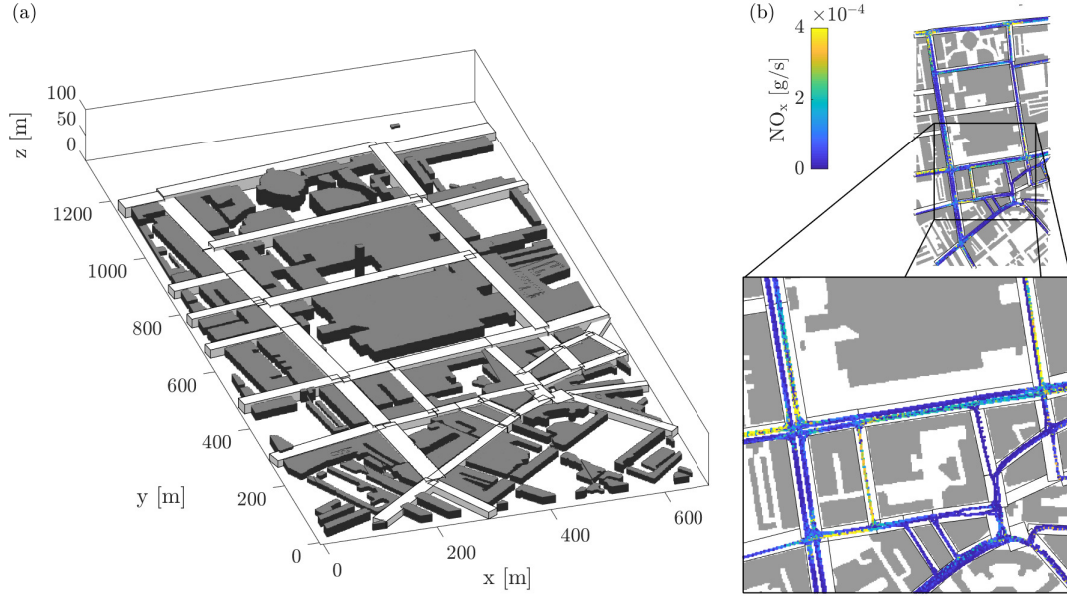


Figure 3.2: (a) Diagram of the representation of buildings in uDALES (grey) and the subsequent network of boxes used in SIRANE (white) and (b) plan view with zoom of the point source emissions used in uDALES overlaid by SIRANE's box outlines and the uDALES blocks.

ing volume; Blocken, 2015). The pre-processing routine remains in active development to optimise the modelling of realistic urban morphologies for the grid-conforming IBM and structured grid used in uDALES.

Contrary to uDALES, SIRANE does not explicitly model the buildings within the domain. Streets are instead represented as boxes which are positioned within the urban canopy (see Figure 2.2). By overlaying the street network of the case study area (Ordnance Survey, 2017) onto the buildings processed for use within uDALES, the network of SIRANE's boxes could be defined. First, street canyons are assumed to be straight, with their beginning and end points at the centre point of the connecting intersections. Second, the average heights and widths on either side of the box centre line are calculated from the mean height of and respective distance to the surrounding buildings. Rules are defined for the maximum horizontal distance to an adjacent building and the proportion of the street segment that exceeds this distance before the street segment is assumed to be adjacent to an open space. This process has also been developed as a pre-processing routine that uses both GIS and MATLAB. The construction of the network follows the guidelines outlined by Soulhac et al. (2011) and results in the street network shown in Figure 3.2a.

3.3.2 Traffic and emissions

High quality traffic and emissions data is imperative to obtaining useful results from pollution dispersion models. In this study, high-resolution emissions data was obtained through the coupling of the traffic microsimulation and emissions models outlined below. The resulting second-by-second emissions data over the case study area was then processed for use within both SIRANE and uDALES. As discussed in Section 1.5.1, only emissions due to road transport are considered in this study.

A representation of the traffic flow in South Kensington is first necessary to estimate the vehicular emissions. The traffic flow characteristics were obtained using a VISSIM traffic microsimulation. VISSIM (version 9.00-12 is used here) is a traffic, time step and behaviour microsimulation model (Bloomberg and Dale, 2000), based on both traffic flow and light signal control models (PTV AG, 2017a). The traffic flow model is derived from a psycho-physical approach which states that the behaviour of each driver can be classified into four different modes (free driving, approaching, following and braking), responding to the perceived relative speed and distance to the preceding vehicle (Gomes et al., 2004). The software also accounts for driving styles via a distribution of speed and distance behaviour (PTV AG, 2017a). Fixed traffic lights were implemented throughout the network and manual traffic count records of the local rush hour were used to calibrate the model. The simulation was run for one hour in order to match SIRANE’s time step; instantaneous data of location, speed and acceleration was given for every vehicle in the network on a second-by-second basis.

An appropriate emissions model is essential to transform the instantaneous data into estimations of NO_x for use within SIRANE and uDALES. Average-speed models (e.g. COP-ERT) are known to systematically underestimate NO_x and overestimate CO_2 emissions (Achour et al., 2011), meaning that an instantaneous emissions model was required. These instantaneous models, which are usually based on various parameters (e.g. instantaneous speed and acceleration, road grade, etc.), were developed following the observation that exhaust emissions are directly related to instantaneous driving behaviour (smooth versus aggressive; Tzirakis et al., 2007) and environmental conditions. Existing studies (Abou-Senna et al., 2013; Song et al., 2012) use various emission models and fleet compositions to compute instantaneous emissions from their VISSIM simulations (the Comprehensive Modal Emission Model, MOVES, look-up table etc.). In this study, a fully diesel vehicle fleet was assumed and a general regression model developed by Luc Int Panis (2006) was used. The assumption of a diesel fleet provided a worse case scenario regarding NO_x (O’Driscoll et al., 2018). It should be noted that, as the primary aim of this work is to compare two dispersion models and not to provide the most realistic representation of the

real world, this assumption does not limit the validity of the evaluation.

The resultant second-by-second emissions data was processed for use within both uDALES and SIRANE. In uDALES the data was time averaged and rasterised to the defined grid size, resulting in a network of point sources which capture the spatial variability of emissions to a high resolution (shown in Figure 3.2b). These emissions were then spatially averaged over the boxes defined in SIRANE to produce uniform emissions within each box. An NO_2/NO_x emissions ratio of 0.2 was assigned to the emissions in both models (Carslaw et al., 2016; O’Driscoll et al., 2016; UK National Atmospheric Emission Inventory, 2018).

3.3.3 Meteorological conditions

As an operational model, simulations within SIRANE are set up to utilise field data of the designated study area. For this reason, typical meteorological conditions of South Kensington, London were applied within SIRANE: a summer’s day (July, 1 pm) with neutral stability (enforced by setting an albedo of 1), partial cloud cover, no precipitation, a wind speed of 2.5 m/s at 30 m and a south-westerly wind direction. The predominant wind direction is south-westerly and the mean wind speed is approximately 4.6 m/s (data from Heathrow Airport; Windfinder, 2017)

SIRANE utilises parametrisations to produce a boundary layer height ($h = 412.6$ m) and friction velocity ($u_* = 0.33$ m/s) from the assigned conditions. These were matched in uDALES by setting the domain height, l_z , equal to h and enforcing constant uniform pressure gradients, $\rho^{-1}\partial p/\partial x = \rho^{-1}\partial p/\partial y = u_*^2/(\sqrt{2}h) = 0.000187$ m/s² (for the south-westerly wind direction). Neutral conditions were produced within uDALES by neglecting buoyancy, moisture and thermal forcings.

The photolysis rate ($J_{\text{NO}_2} = 0.0063$ s⁻¹) and $\text{NO} + \text{O}_3$ reaction rate ($k_2 = 10041.8$ m³/mole s) were also automatically assigned through parametrisations within SIRANE, as a function of the solar elevation and cloud cover and air temperature respectively (Kasten and Czeplak, 1980; Soulhac et al., 2011; Seinfeld and Pandis, 2016). Background concentrations were obtained from the hourly data available from the Greater London Authority (King’s College London, 2017). The background concentrations were averaged over the specified date and time across a 10 year data set. The resulting concentrations were relatively close to satisfying the photostationary steady-state (PSS) condition with the defined reaction rates. In order to enforce photostationarity, the concentrations were equilibrated to the corresponding PSS. The final background concentrations were $\text{NO}_b = 6.85$ $\mu\text{g}/\text{m}^3$, $\text{NO}_{2,b} = 18.09$ $\mu\text{g}/\text{m}^3$, $\text{O}_{3,b} = 51.88$ $\mu\text{g}/\text{m}^3$ and $\text{NO}_{x,b} = 28.59$ $\mu\text{g}/\text{m}^3$ (Baukal and Eleazer, 1998).

3.3.4 Boundary conditions

The differences between the two models also required consideration when defining the boundary conditions. SIRANE applies the background concentrations at the upwind sides of the domain, with the Gaussian model capturing the downwind dispersion of pollutants across the domain. It also assumes that the form of the boundary layer is spatially and temporally steady over each time step.

These boundary conditions satisfy the thesis methodology by negating the spatial and temporal variability of the boundary layer flow and thus treating the mean and turbulent state of the boundary layer as an extrinsic property of the simulation (therefore assuming upwind morphological similarity, which holds for the case study area). The prognostic fields of interest (the pollutant fields), on the other hand, develop in the streamwise direction through the domain and are therefore intrinsically variant. The homogeneity of the boundary flow (above the roughness sublayer) means that the pollution dispersion characteristics are representative of a single boundary layer state. These boundary conditions also assume that the background concentrations are sufficiently representative of combined emissions from the upwind urban area (see Section 1.5.1).

These flow characteristics were reproduced in uDALES by applying periodic horizontal boundary conditions and a free slip condition at the top of the domain for velocity (a periodic set-up as introduced in Section 2.3.3). The simulation was run up until a steady-state, fully developed boundary layer had developed matching the friction velocity and boundary layer height discussed in Section 3.3.3. The upwind scalar concentration profiles were set to background levels and outflow conditions were set for the scalars at the downstream boundaries. In order to avoid direct interaction between morphological features on the upwind and downwind edges of the domain (due to the periodic horizontal boundary conditions for velocity) and to ensure that the scalar boundary conditions do not have a direct impact on the concentration field in the canopy layer, a 12 m buffer region was defined at the domain's edge where neither emissions nor buildings were modelled.

The case study comparison is conducted for a single hourly time step within SIRANE. In order to produce converged statistics from uDALES the simulation was run for 10800 s ($\approx 8.5h/u_*$, where h is the boundary layer height and u_* is the friction velocity) with a sampling time of 5 s. Criteria for the convergence of the obtained statistics was satisfied through analysis of the time and horizontally-averaged momentum flux profiles. The dispersive momentum fluxes reduced to negligible values and the turbulent momentum fluxes exhibited a linear profile above the roughness sublayer (Coceal et al., 2006; Vinuesa et al., 2016). The computational requirements for the simulations were 35 hours on 192 cores for uDALES and 1 s on 16 cores for SIRANE.

3.4 Results

In order to isolate the dispersive performance of the models from their respective chemistry schemes, a comparison is first conducted between inert simulations where NO_x emissions are dispersed passively with no chemical reactions. The comparison is then broadened by switching on the respective chemistry schemes of the two models. The sensitivity of the results to wind direction is discussed by comparing the findings of the south-westerly case study to an equivalent study with a defined westerly wind. Altering the wind angle by 45° produces significantly different angles of incidence over the canyons, with many more streets either perpendicular or parallel to the wind for the westerly case. The results for the westerly case are shown alongside those of the south-westerly case where they have been discussed in detail within the text.

The evaluation of SIRANE is conducted with two main points of focus. Firstly, the predictive skill of SIRANE in modelling canyon-averaged properties is analysed by temporally and spatially averaging uDALES's three-dimensional dataset to produce directly comparable results (denoted by DA-s). Secondly, the high-resolution mean and turbulent statistics of uDALES are used to directly analyse the strengths and shortcomings of SIRANE's parametrisations. For example, the in-canyon variability is assessed to understand the impact of the uniform concentration assumption and the fluxes at the canyon tops within uDALES are discussed to assess the parametrisation of vertical exchange within SIRANE.

Box and scatter plots are used as tools to analyse both the bulk and street-by-street properties of the resulting datasets. Quantitative analysis of SIRANE's predictive skill is provided using the normalised mean square error (NMSE, a metric quantifying the overall deviation or scatter between the two sets of results), fractional bias (FB, a metric quantifying mean bias and therefore identifying potential sources of systematic error) and the fraction in a factor of two (FAC2, a more robust metric of model performance as it is not overly influenced by outliers; Chang and Hanna, 2004). These statistical indices are displayed in Table 3.2. The same metrics have been applied to previous experimental and field validations of SIRANE (Soulhac et al., 2012, 2017) alongside the criteria for «good» model performance ($|\text{FB}| \leq 0.3$, $\text{NMSE} \leq 4$ and $\text{FAC2} \geq 0.5$; Chang and Hanna, 2004; Hanna and Chang, 2012). These criteria are not directly applicable to this study because of the reduction in uncertainty associated with the use of LES as opposed to field or experimental measurements. The limits for «good» model performance must be redefined for application to evaluations of this form; however, as this study is the first to utilise LES for this purpose, there are no other benchmarks with which to refine these limits (Chang and Hanna, 2004). The statistical indices are therefore interpreted in the context of the

Table 3.2: Overview of the statistical indices used to quantify the performance of SIRANE’s canyon-averaged predictions against the results of uDALES for a south-westerly (SW) and westerly (W) wind direction.

Index	Wind direction	Along-canyon velocity, U	Inert NO_x	Reactive		
				NO	NO_2	O_3
FB ¹	SW	-0.18	-0.08	0.03	-0.18	0.14
	W	-0.02	-0.11	-0.03	-0.20	0.15
NMSE ²	SW	0.11	0.08	0.12	0.08	0.03
	W	0.26	0.09	0.11	0.10	0.04
FAC2 ³	SW	0.94	1.00	0.96	1.00	1.00
	W	0.68	1.00	0.98	1.00	1.00

¹ Fractional bias, $\text{FB} = (\overline{X_{DA}} - \overline{X_{SI}}) / 0.5(\overline{X_{DA}} + \overline{X_{SI}})$

² Normalised mean squared error, $\text{NMSE} = (\overline{X_{DA}} - \overline{X_{SI}})^2 / \overline{X_{DA}} \overline{X_{SI}}$

³ Fraction in a factor of 2, $\text{FAC2} = 0.5 \leq \overline{X_{SI}} / \overline{X_{DA}} \leq 2$ where X_{DA} and X_{SI} are the canyon-averaged results of uDALES and SIRANE respectively.

original limits with the understanding that more stringent criteria are necessary. Following future similar evaluations, redefined limits can be developed to indicate the requirements for «good» model performance in this context.

There is a monitoring station situated on the junction of Cromwell Rd and Queen’s Gate in the case study region (Air Quality England, 2019). The obtained concentrations of inert NO_x and reactive NO and NO_2 in this study (both from SIRANE and uDALES) are within the observed ranges of the corresponding hourly means measured at this site. Whilst the aim of the study is not to reproduce measured concentrations in the field, this finding indicates that the modelled emissions, background concentrations and reaction rates are realistic.

3.4.1 Inert case

Figure 3.3 shows three NO_x concentration fields, providing a visual comparison between the nature of the data produced by SIRANE and uDALES. An instantaneous field of NO_x at pedestrian level (1.8 m above ground) from uDALES (Figure 3.3a) is presented illustrating the turbulent and spatially heterogeneous nature of pollution dispersion within the urban canopy. This concentration field contrasts with the coarser results of SIRANE (SI; Figure 3.3b) that display the canyon-averaged concentrations over the street network and the external concentrations elsewhere for the hourly time step. A qualitative comparison can

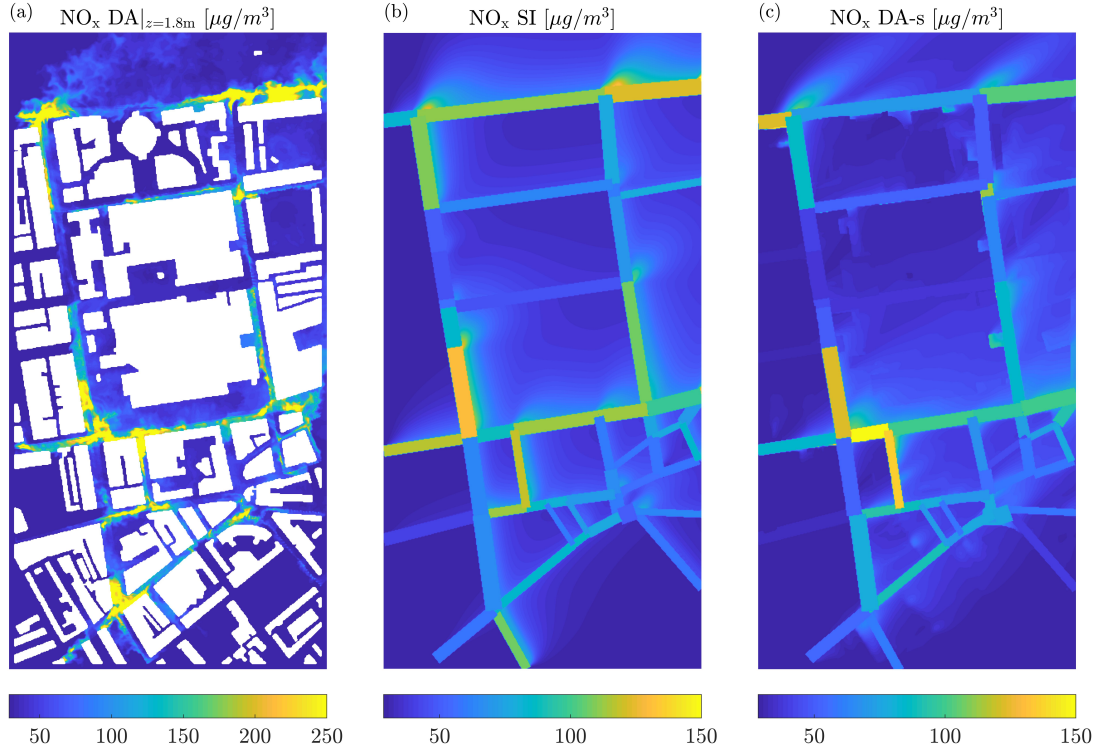


Figure 3.3: (a) Instantaneous pedestrian level concentrations from uDALES, (b) data from SIRANE (SI) and (c) data from uDALES processed to match the form of SI (DA-s) for a south-westerly wind direction.

be drawn between this field and the processed results of uDALES (DA-s; Figure 3.3c). DA-s was calculated by temporally and spatially averaging the data of uDALES to form a 2-D field that is comparable to the results of SIRANE. In the positions of SIRANE's boxes, the canyon-averaged concentration is taken and elsewhere the external concentrations were taken at a height of 20 m (as defined within SIRANE; if the building height exceeded 20 m then the first cell above the building was used in DA-s). Qualitatively it can be seen that both the canyon-averaged and external concentrations of SIRANE and uDALES are in reasonably good agreement. In particular, the vertical exchange at the intersection and subsequent downwind dispersion looks to have been captured effectively.

The predictive skill of SIRANE is assessed in Figure 3.4a through the comparison of the canyon-averaged concentrations of both models. The box plot for canyon-averaged NO_x indicates that the bulk statistics of SI and DA-s are matched well with a very similar median and upper quartile. This performance is confirmed by the statistical indices shown in Table 3.2 for both wind directions. The scatter plot presents a more detailed analysis in which the performance can be broken down into a range of street types. The parametrisations defined for the boxes in SIRANE are based upon studies of idealised infinite canyons. Three

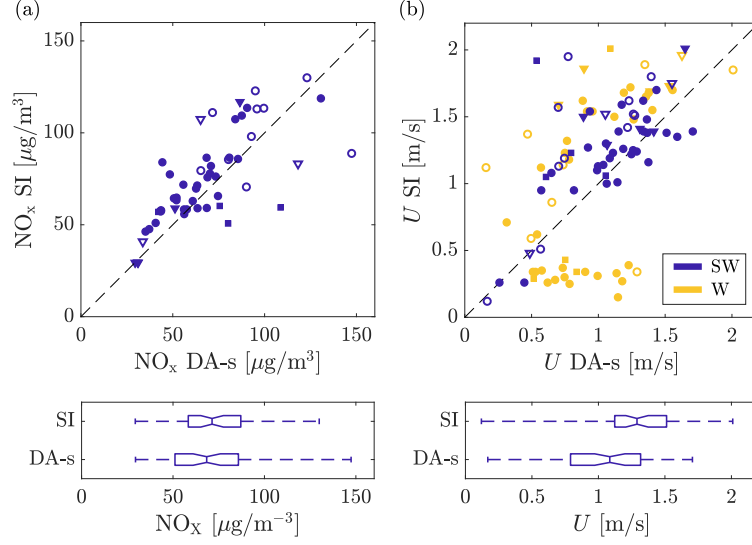


Figure 3.4: Scatter and box plots of canyon-averaged (a) NO_x concentrations and (b) along-canyon velocities, U , for SIRANE (SI) and uDALES (DA-s). The colour signifies the wind direction, dark blue for south-westerly (SW) and orange for westerly (W). Triangles represent streets that are connected to the upwind side of the domain, squares represent short streets (length $\approx$ width) and circles are typical street canyons that are not in the two previous categorisations. Empty markers denote streets adjacent to an open space.

street types were identified that deviate from these simplified conditions:

- Short streets, $\mathcal{L} \approx W$ (square markers). Short streets are dominated by secondary flows at intersections and other heterogeneity that SIRANE does not account for.
- Streets adjacent to open spaces (unfilled markers). These streets will not exhibit the classical canyon vortex, channelling or shear layer of an infinite canyon. The short-coming of dealing with open spaces has been identified within SIRANE’s literature (Soulhac et al., 2011).
- Upwind streets (triangular markers). The boundary conditions as defined in both SIRANE and uDALES do not model the region upwind of the domain. Conditions are matched through the assignment of background concentrations upwind, but the representations of the incoming flow fields have localised limitations.

The scatter plot in Figure 3.4a indicates that the most erroneous concentrations can be attributed to these street types. This finding illustrates the challenge in representing highly heterogeneous real urban morphologies through idealised parametrisations. The predictive skill of SIRANE was shown to be robust against the range of angles of incidence and street aspect ratios across the case study region. On the whole, the findings for canyon-averaged

inert NO_x indicate that the operational model has successfully captured the dominant processes of pollution dispersion through its parametrisations, as can be seen by the low NMSE values (0.08 and 0.09 for south-westerly and westerly wind respectively).

The flow within the street network can be analysed by comparing the canyon-averaged velocity along the street axis, U , in both models. The along-canyon velocity is a key variable in defining the exchange that occurs at SIRANE's intersections. It is parametrised as a function of the entrainment into the canyon from the external flow and the drag induced by the building walls (Soulhac et al., 2008). Figure 3.4b compares the values of U for both models, indicating that SIRANE overpredicts the along-canyon velocities for the south-westerly case. The corresponding fractional bias ($\text{FB} = -0.18$) indicates a source of systematic bias within SIRANE. The overestimation can also be attributed to the assumption in SIRANE that all streets are infinite canyons with a defined surface roughness. The parametrisation for U neglects the role of secondary flows at intersections (which are captured within uDALES) that act to reduce along-canyon velocities. The fractional bias for the westerly wind case ($\text{FB} = -0.02$) does not indicate the same tendency for systematic overestimation. However the corresponding fraction in a factor of 2 is significantly lower ($\text{FAC2} = 0.68$). It can be seen from Figure 3.4b that this discrepancy occurs due to the set of streets that are underestimated with low along-canyon velocities in SIRANE. The other streets in the westerly dataset illustrate the same systematic overestimation as in the south-westerly case. The selection of streets which exhibit an underprediction all have angles of incidence exceeding 77° . Analysis of the time averaged flow field within the UCL from uDALES illustrates that in these high-angle-of-incidence streets, the exchanges at the corresponding intersections can induce along-canyon flow (both through imposed pressure gradients and the presence of morphological features such as changing road widths at these intersections). SIRANE therefore has a tendency to overestimate U in streets with angles of incidence lower than 77° and potentially underestimate those with angles that exceed this threshold value. Despite this, the results for canyon-averaged NO_x indicate that the flow within the street network is captured sufficiently well to predict the canyon-averaged concentrations.

Coupling SIRANE with a detailed street canyon model has been discussed as future work within the literature as a method to account for the in-canyon variability of the concentration field and potentially increase the complexity of other parametrisations (e.g. additional scaling of the exchange velocity with the canyon aspect ratio; Soulhac et al., 2011). The high-resolution mean and turbulent statistics of uDALES were used to analyse 1) the importance of accounting for the spatial variation of pollutants within the canyons (pedestrian level concentrations and asymmetry) and 2) the nature of vertical exchange

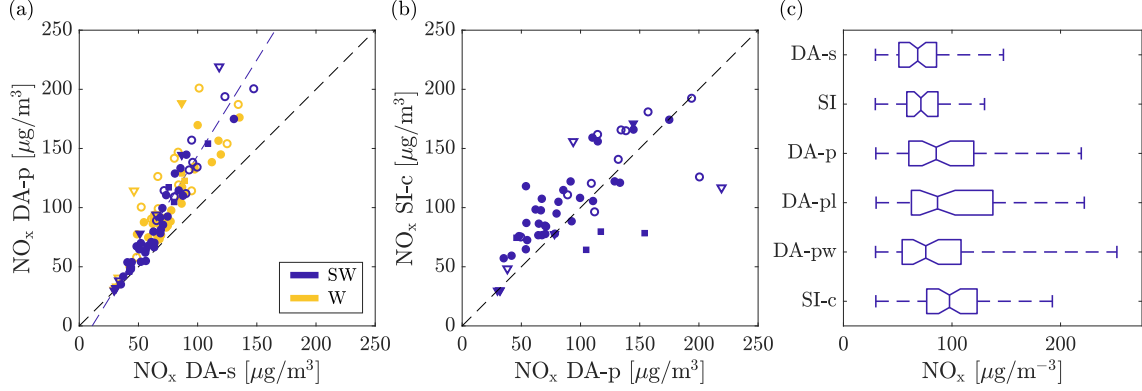


Figure 3.5: (a) Scatter plot comparing canyon- (DA-s) and pedestrian-averaged (DA-p) NO_x concentrations from uDALES, (b) scatter plot comparing the corrected NO_x concentrations of SIRANE (SI-c) and the pedestrian-averaged NO_x concentration of uDALES and (c) box plot indicating the variability of canyon- (DA-s and SI), pedestrian- (DA-p), corrected (SI-c), leeward- (DA-pl) and windward- (DA-pw) averaged concentrations. The colour signifies the wind direction, dark blue for south-westerly (SW) and orange for westerly (W). The markers are consistent with Figure 3.4.

occurring at the canyon tops.

The NO_x concentration fields of uDALES are spatially averaged over each box's horizontal extent at a height of 1.8 m and time averaged over the simulation period to provide pedestrian-averaged concentrations (DA-p). This data is analysed against DA-s in Figure 3.5a to study the relationship between canyon- and pedestrian-averaged concentrations. The scatter plot displays a strong quasi-linear relationship indicating that the pedestrian-averaged concentrations are proportionally larger than the canyon-averaged values, a result of both the proximity to the emissions source and the mixing induced by the canyon vortex. The increased magnitude of concentrations at pedestrian level is also evident in the box plots in Figure 3.5c where the data for DA-p is comparatively skewed towards higher concentrations. Whilst this relationship between pedestrian- and canyon-averaged concentrations may be self-evident, it highlights a fundamental shortcoming in that the use of SIRANE's canyon-averaged concentrations to assess pedestrian level exposure will lead to significant underestimations of inert NO_x . The linearity of this relationship suggests that despite the range of e.g. emissions, angles of incidence, aspect ratios and street types, the spatial distribution of the pollutant concentrations in this study can be reasonably represented through the application of a simple correction factor. Applying a linear least-squares regression that intercepts the background concentration ($\varphi_{\text{DA-p}} = \varphi_b + m(\varphi_{\text{DA-s}} - \varphi_b)$ where m is a correction factor and φ_b is the background concentration) permits the formation of a formula that therefore describes a simplified relationship between pedestrian- and canyon-averaged concentrations. Table 3.3 displays the resulting correction factors and cor-

3.4 RESULTS

Table 3.3: Overview of the correction factors, m , and corresponding R^2 values for the linear regressions of DA-p against DA-s for each pollutant. All linear regressions were defined to intercept the background concentration following $\varphi_{\text{DA-p}} = \varphi_b + m(\varphi_{\text{DA-s}} - \varphi_b)$.

Pollutant		Wind direction	m	R^2
Inert	NO_x	SW	1.62	0.92
		W	1.57	0.75
Reactive	NO	SW	1.75	0.93
		W	1.70	0.75
	NO_2	SW	1.39	0.93
		W	1.36	0.78
	O_3	SW	1.16	0.94
		W	1.19	0.90

responding R-squared values. The linear relationship as calculated for the south-westerly wind direction ($m = 1.62$) is overlaid onto Figure 3.5a. Considering the complexity and variability of the dispersion processes that are being captured through this linear regression, the corresponding R-squared value ($R^2 = 0.92$) is remarkably high and indicates a strong correlation. The westerly case exhibits a similar correction factor ($m = 1.57$) with a lower R-squared value ($R^2 = 0.75$), the increased spread can be seen in Figure 3.5a and is a result of the the greater range of angles of incidence.

A corrected dataset (SI-c) is calculated by applying this relationship to SIRANE's canyon-averaged concentrations ($\varphi_{\text{SI-c}} = \varphi_b + m(\varphi_{\text{SI}} - \varphi_b)$). This dataset is compared to the pedestrian-averaged concentrations of uDALES in Figure 3.5b. The agreement between SI-c and DA-p illustrates that the application of the correction factor has achieved a similar level of performance in predicting pedestrian-averaged quantities as was provided by the canyon-averaged quantities in Figure 3.4a. The applied correction factor is evidently a simplified solution. Substantial further work would be necessary to fully assess its sensitivity to what is a large parameter space (e.g. different atmospheric stabilities and wind speeds). However, it is clear that such a correction (or a more comprehensive coupling with a street canyon model) is necessary when considering using SIRANE to evaluate pedestrian level exposure and that, in this case study, a simple linear regression provides an effective tool to account for this correction. This finding also agrees with results from the field study of Xie et al. (2003) where similar vertical gradients were observed in the daily NO (and NO_x) and CO concentration profiles within a street canyon.

The results of Xie et al. (2003) also indicate the role of asymmetry within the street canyon, the effect where concentrations on the leeward side of the canyon are greater than

the windward side due to the dispersion induced by the canyon vortex. Other operational models have utilised parametrisations to account for this difference in concentrations. The Operational Street Pollution Model (OSPM) splits the street canyon into lee and windward receptors, using the assumption of a helical structure within the canyon (accounting for the wind direction) to differentiate between the fluxes of pollutant received in opposing sides of the canyon (Berkowicz, 2000). The advection of the emissions towards the leeward side of the canyon is evident in the pedestrian level instantaneous concentration field in Figure 3.3a. The NO_x concentration fields of uDALES were processed to calculate pedestrian-averaged concentrations on the lee- (DA-pl) and windward (DA-pw) sides of each box in order to assess the prevalence of asymmetry over the case study area. These results are included in the box plot in Figure 3.5c. The quartiles illustrate a bulk trend of higher leeward concentrations, although there are street segments where the asymmetry effect was not exhibited and the magnitude of the difference between DA-pl and DA-pw scales in comparison to the difference between DA-s and DA-p. The asymmetry effect is less pronounced because the exchanges at intersections complicate the idealised helical flow representation, producing recirculation zones and drawing in fluxes of cleaner or more polluted air into the canyon. The asymmetry effect is therefore most dominant downwind from intersections. No dominant scaling was found between the asymmetry ratio ($\varphi_{\text{DA-pl}}/\varphi_{\text{DA-pw}}$) over the street network for factors such as angle of incidence or aspect ratio.

SIRANE utilises the friction velocity of the external flow to define a uniform exchange velocity across the street network and therefore the vertical flux of pollutants at the top face of each box (Salizzoni et al., 2009). The vertical fluxes of NO_x from uDALES, spatially averaged over the top face of each box and time averaged over the simulation time, were analysed to investigate how this idealised parametrisation compares to the exchange occurring within a realistic urban morphology. The predominant finding was that the heterogeneity of the morphology over the case study area challenges the typical shear layer as defined in idealised studies. Uneven building heights and secondary flows at intersections induce flow structures that cause advective as opposed to turbulent flux components to dominate. The heterogeneity of the urban morphology means that the tops of the defined boxes reside in the roughness sublayer where the flow is highly three-dimensional and the turbulent footprint is an amalgamation of the upwind microclimatic features. Applying the same averaging process to the vertical velocities in uDALES illustrated that there was an effective bulk transport in and out of the canopy in different locations. Typical values of exchange velocity were therefore challenging to extract from the 3-D roughness sublayer, however the overall vertical exchange from the canopy layer (canyons and intersections)

3.4 RESULTS

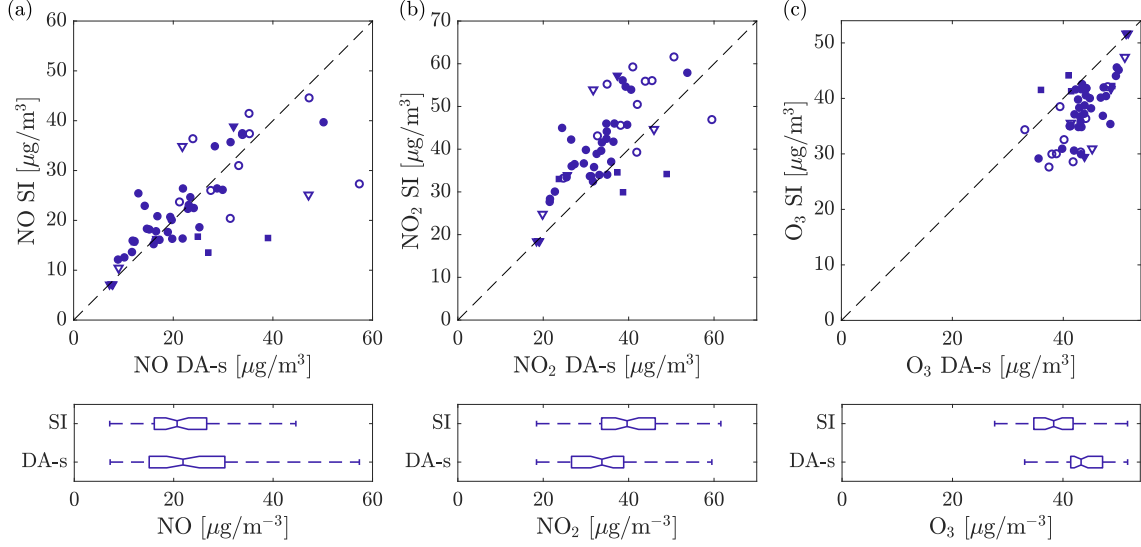


Figure 3.6: Scatter and box plots of canyon-averaged (a) NO, (b) NO₂ and (c) O₃ concentrations for SIRANE (SI) and uDALES (DA-s) for a south-westerly wind direction. The markers are consistent with Figure 3.4.

must be captured well within SIRANE in order for there to be little fractional bias in the canyon-averaged NO_x concentrations. As the friction velocity and boundary layer height were matched within uDALES this bulk parametrisation is shown to provide a good approximation of the bulk exchange out of the defined street network. These findings were reproduced within the westerly simulations.

3.4.2 Reactive case

In this section both models are run under the same conditions but with the respective chemistry schemes active. As previously discussed, the reactions of the null cycle act to equilibrate the concentrations of NO, NO₂ and O₃ towards a photostationary steady-state (PSS) at a timescale of minutes during the day. The NO_x emissions result in a local chemical imbalance from the background PSS state which SIRANE solves by calculating an in-canyon equilibrium and which uDALES resolves in real-time alongside the dispersion of the emissions through the domain.

Figure 3.6 provides a comparison between the canyon-averaged NO, NO₂ and O₃ concentrations from SIRANE and uDALES. The results for NO exhibit a similar trend to that of inert NO_x in Section 3.4.1. The clear shift between the quartiles of SI and DA-s in the box plots of Figure 3.6b and c indicate that there is a significant over- (FB = -0.18) and underprediction (FB = 0.14) of NO₂ and O₃ respectively by SIRANE. The reason for this source of systematic bias is the assumption of a PSS in SIRANE. Whilst the assumption

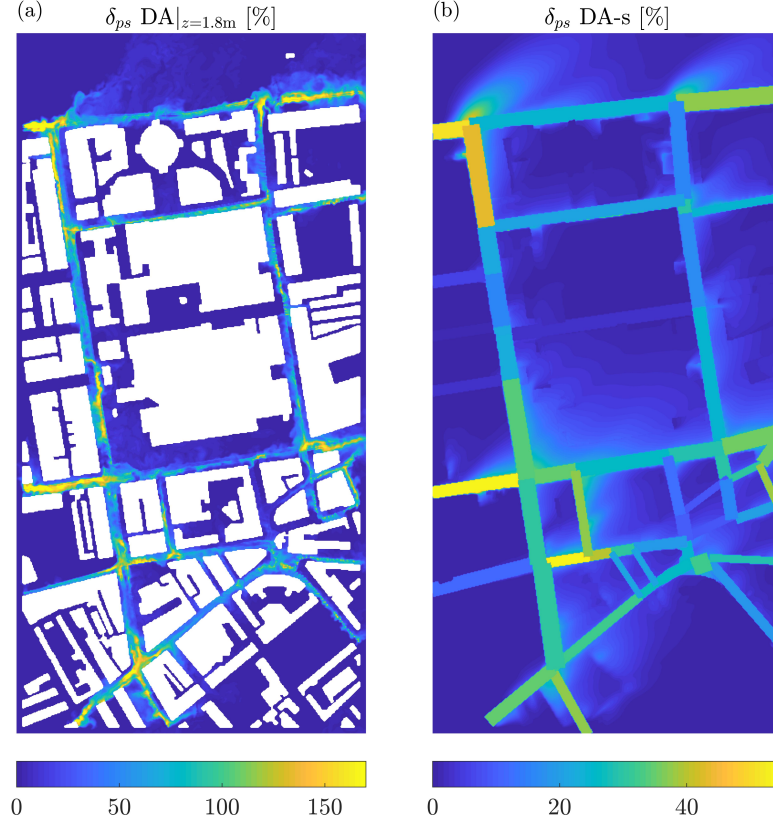


Figure 3.7: (a) Instantaneous pedestrian level and (b) canyon-averaged (DA-s) PSS defects processed from uDALES for a south-westerly wind direction.

of a quasi-steady chemical state over the hourly time period holds due to the timescale over which the null cycle acts, it is not assured that photostationarity would be achieved throughout the urban canyon. Vehicular NO_x emissions are NO rich and cause a local deviation from the PSS. The timescale at which an equilibrium is reached is of similar order of magnitude to the local dispersion meaning that, in the proximity of emission sources, a deviation from the PSS is expected. The chemical imbalance can be quantified by the PSS defect, δ_{ps} , given by (Equation 1.11):

$$\delta_{ps} = 100 \left(\frac{k_2[\text{NO}][\text{O}_3]}{J_{\text{NO}_2}[\text{NO}_2]} - 1 \right). \quad (3.6)$$

Figure 3.7 displays the instantaneous pedestrian level and canyon-averaged (DA-s) PSS defects. Values greater than zero indicate that a chemical imbalance exists ($k_2[\text{NO}][\text{O}_3] > J_{\text{NO}_2}[\text{NO}_2]$). In these locations the net effect of the null cycle is to deplete the concentrations of NO and O_3 and produce NO_2 . In uDALES these reactions are modelled in real time as the pollutants are dispersed. SIRANE's PSS assumption considers that the

3.4 RESULTS

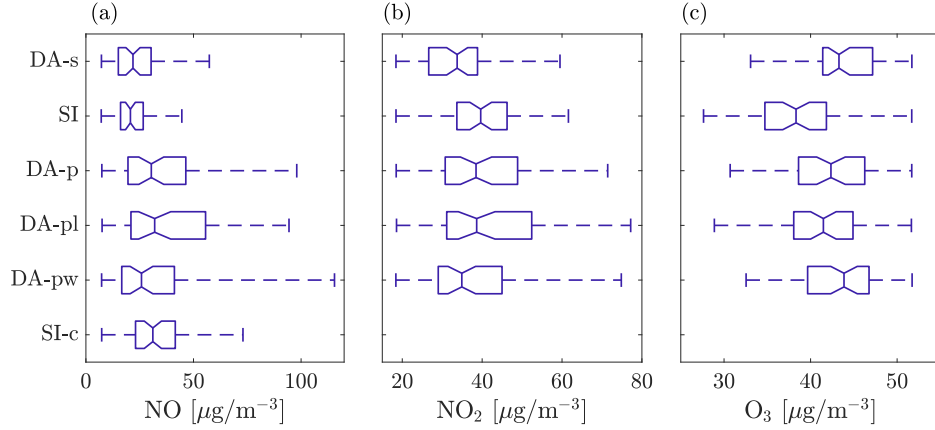


Figure 3.8: Box plots of the canyon- (DA-s and SI), pedestrian- (DA-p), corrected (SI-c), leeward- (DA-pl) and windward- (DA-pw) averaged concentrations for (a) NO, (b) NO₂ and (c) O₃ concentrations for a south-westerly wind direction.

concentrations equilibrate throughout the defined domain but the PSS defects in Figure 3.7b illustrate that this is not the case. The PSS defects calculated here concur with magnitudes found in the literature (100-200% near busy roads; Tong and Leung, 2012; Chate et al., 2014; Zhong et al., 2016). The trends exhibited in Figure 3.6 indicate that the concentration of O₃ is the limiting factor in terms of the production of NO₂ in this case study. This state is a result of the background concentrations, reaction rates, magnitude of the emissions and NO₂/NO_x emissions ratio but is consistent with other research findings (Palmgren et al., 1996). The similarities between the results for reactive NO and inert NO_x indicate that the emission of NO into the canyon is dominating over its depletion due to the chemical cycle. PSS defects in the westerly case exhibit the same trends.

The PSS defect also scales approximately with the residence time of the pollutant within the canyon. This effect has been captured in street canyon models where the emissions, exchange rate and chemical reactions can be solved analytically under an assumed steady-state (Palmgren et al., 1996). Whilst this can be implemented relatively simply for a single infinite canyon, the chemistry scheme in SIRANE would have to be directly coupled to the dispersion model to account for the exchange of pollutants throughout the street network and above (Soulhac et al., 2011).

The in-canyon variability of the concentration fields as defined in Section 3.4.1 is further complicated by the non-linear interaction between the simultaneous reaction and dispersion of the pollutants. The null cycle acts to produce and deplete the pollutants temporally and spatially throughout the domain as a function of the local chemical imbalance. Figure 3.8 provides box plots comparing the bulk statistics of canyon- and pedestrian-averaged concentrations and Table 3.3 presents the linear regression analysis for the reac-

tive pollutants (following the same process as in Section 3.4.1). Fig 3.8a reiterates that the canyon-averaged NO concentrations follow a similar trend to that of inert NO_x. The role of chemistry is evident however in the increased correction factor calculated for NO ($m = 1.75$). The correction factor for NO was applied to produce the improved estimation of pedestrian level concentrations SI-c in Figure 3.8a. The difference between pedestrian and canyon-averaged concentrations for NO₂ and O₃ is less pronounced ($m = 1.39$ and 1.16 respectively), which can be expected as secondary pollutants exist more spatially homogeneously (Breuer and Bower, 1999). This finding once again agrees with the field study of Xie et al. (2003) where the vertical distributions of NO₂ and O₃ exhibit an increase and decrease respectively but to a lesser extent than the primary pollutants (NO and CO). The correction factors were not applied to NO₂ SI and O₃ SI as the systematic error introduced to these by the assumption of photostationarity outweighs the corresponding improvement. The linear regression analysis for the reactive pollutants indicates again that a simple linear model is capable of accounting for pedestrian level concentrations for the conditions investigated in this case study. Figure 3.8 also presents the lee- and windward-averaged concentrations at pedestrian level. The same general trend of higher concentrations (lower for O₃) on the leeward side of the street canyon is exhibited. In a domain with longer streets the role of asymmetry is likely to be of greater importance, particularly in terms of the variability of the secondary pollutants.

The results presented in this section are consistent with field studies (Palmgren et al., 1996; Derwent et al., 1995; Chate et al., 2014) and a monitoring station that is present in the case study region (Air Quality England, 2019). However it is important to note the sensitivity of these results to the chemical state of the system (emissions ratio and magnitude, background concentrations and reaction rates). The magnitude and spatial distribution of the PSS defect captures the relationship between the dispersion and chemical transformation of pollutants within the street canyon. An understanding of the sensitivity of these results can be obtained by considering the expected change in this term. For example, a decrease in the magnitude of emissions would result in lower PSS defects and therefore a reduction in the error caused by the assumption of photostationarity in SIRANE. The emissions used in this study were relatively high and therefore SIRANE would be expected to perform better under lower emissions scenarios. The emissions ratio has been highlighted as a sensitive variable in the study of reactive dispersion models (Vardoulakis et al., 2007). One would expect that a reduction in the emissions ratio would result in larger PSS defects, particularly close to the emissions sources. The bias caused by the PSS assumption would therefore be more pronounced and e.g. the correction factor for NO₂ would be decreased (as a result of the reduced role of the primary emissions of NO₂

and increased role of secondary formation). Further work is required to quantify these sensitivities.

3.5 Conclusion

Simulations were conducted over a case study region in South Kensington, London, UK under neutral conditions using both the LES model uDALES and the operational model SIRANE. Model capabilities developed as part of the work on this thesis were showcased: 1) capturing realistic urban morphologies from LIDAR data, 2) capturing realistic emissions via a coupling with the traffic microsimulation model VISSIM and 3) the integration of a null cycle chemical scheme within urban LES.

The case study was systematically set up to produce comparable results between the two models and therefore facilitate an evaluation of SIRANE. The use of LES as a tool to perform this evaluation provided an element of numerical control (e.g. with or without chemistry), thereby negating typical sources of uncertainty, and facilitated analysis against an "ideal" dataset. This methodology enabled a targeted analysis of SIRANE's simplifications, assumptions and parametrisations over a realistic urban morphology. The study outlines a novel approach to the evaluation of operational pollution dispersion models that can be used alongside necessary validations against field and experimental data.

Considering the differences in resolution and computational cost, SIRANE was shown to qualitatively and quantitatively capture the dominant trends in canyon-averaged and above-canyon concentrations and velocities. Streets segments that deviated away from idealised, infinite canyons (short streets and streets next to open spaces) were shown to result in the most erroneous predictions by SIRANE across the evaluation. The most significant source of systematic bias resulted from the assumption of photostationarity in SIRANE. PSS defects as high as 170% were exhibited by uDALES close to busy roads. The PSS assumption was shown to lead to over- ($FB = -0.18$) and underpredictions ($FB = 0.14$) of NO_2 and O_3 respectively. SIRANE was shown to have a general tendency to overpredict ($FB = -0.18$) along-canyon velocities because it does not capture the inhibiting role of secondary flows at intersections. Although an underprediction was exhibited in streets with high angles of incidence ($> 77^\circ$) where along-canyon flow was induced in uDALES due to morphological details within the street network.

The high-resolution capabilities of uDALES were used to investigate the applicability of SIRANE's uniform in-canyon concentration assumption. The use of canyon-averaged concentrations to assess pedestrian level exposure was shown to result in a significant underestimation. It was shown that a linear correction factor was capable of accounting for

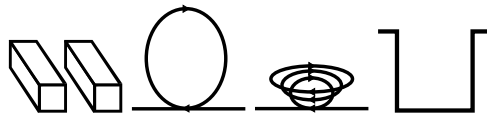
the difference between pedestrian- and canyon-averaged concentrations. The application of this correction factor to inert NO_x ($m = 1.62$) and reactive NO ($m = 1.75$) was shown to significantly improve SIRANE's capability to predict pedestrian level exposure. The high corresponding R-squared values indicated that the linear trend was robust to the range of e.g. angles of incidence, wind directions, aspect ratios and emissions present in this study. The sensitivity of these correction factors to other meteorological, morphological and chemical conditions was not investigated, however this finding highlights the need to conduct such a study or to couple SIRANE with a more detailed street canyon model in the future. Analysis of the vertical exchange out of the UCL highlighted the significant differences between the shear layers present over realistic heterogeneous urban morphologies and over classical infinite canyons. Despite these differences the bulk exchange out of the street network in SIRANE was proven to be captured with a reasonable agreement.

The explicit definition of street canyons within the LES domain allowed for a direct comparison with SIRANE, but more importantly served to reduce the inherent complexity of the flows within the streets to its essential features (mean concentrations, pedestrian exposure, wind effects, exchange with the atmosphere). This approach could be of benefit more generally for urban pollution dispersion studies of realistic morphologies, as additional sophistication (e.g. by introducing separate control volumes at the intersections and higher order statistics) can be incorporated straightforwardly.

Chapter 4

Steady-state large-eddy simulations of convective and stable urban boundary layers

A comprehensive investigation is carried out to establish best practice guidelines for the modelling of statistically steady-state non-neutral urban boundary layers (UBL) in large-eddy simulation studies (thus to satisfy the thesis methodology of accounting for the spatial and temporal variability of the UBL). A novel method that is able to ‘freeze’ the flow state in transient simulations (including entrainment at the boundary layer top) is shown to work well for both stable and convective conditions. This chapter interpolates material from an under review publication by the author (Grylls et al., 2020), coauthored with Ivo Suter and Maarten van Reeuwijk.



4.1 Introduction

As cities continue to grow and become more dense, it becomes increasingly important to understand the urban climate, particularly in regard to the sustainability of urban life and global challenges such as urban air quality and the urban heat island effect. The ability to model urban environments is integral to developing this understanding. The urban fabric and the anthropogenic processes occurring within it interact with the planetary boundary layer (PBL) to produce a complex modelling problem over a large range of

spatial and temporal scales (discussed further in Chapter 1). High-resolution modelling of the urban canopy layer (UCL) is imperative to resolving the unsteady and heterogeneous urban flow field, rendering large-eddy simulations (LES) a key modelling tool (Tominaga and Stathopoulos, 2013; Barlow, 2014; Lateb et al., 2016).

Considering both the state of the of the urban boundary layer (UBL) and urban form (morphology, trees etc.) results in a large parameter space with multiple degrees of freedom and high associated computational costs. As defined in the thesis methodology, studies must therefore be conducted with the aims of 1) isolating particular phenomena or processes of interest and 2) accounting for horizontal, vertical and temporal variability (Oke et al., 2017). The production of statistical steady states is integral to satisfying these aims. Enforcing steady-state conditions in urban LES allows for converged statistics to be obtained and for targeted studies to be conducted (both directly with periodic boundary conditions and when used as a pre-cursor driver simulation; see Section 2.3.3 and Figure 2.4; Tomas et al., 2015). For a steady-state, fully developed boundary layer in a periodic simulation, the state of the boundary layer becomes an extrinsic variable of the modelled urban microclimate and its effects can be systematically investigated across multiple simulations.

In terms of simulating air pollution in the urban microclimate, this condition has the advantage that the interaction of the modelled boundary layer with the roughness sublayer (RSL) and UCL flows is consistent throughout the modelled domain and over all time steps. The resulting pollutant dispersion characteristics throughout the domain can therefore be characterised by a single boundary layer profile. If the UBL is developing in the streamwise direction then there is an additional, redundant degree of freedom to the problem (for studies that are not focussed on such transitional flows).

Aligned with these aims, extensive research has been carried out in order to understand the fundamental physics and processes of the urban flow field under neutral conditions (a steady-state neutral UBL was also used in Chapter 3; Walton and Cheng, 2002; Belcher, 2005; Letzel et al., 2008; Xie and Castro, 2009). As our understanding progresses, additional levels of complexity have been incorporated into urban LES investigations under the same framework. Much of this work has involved modelling thermal effects (e.g. atmospheric stability (Xie et al., 2013; Boppana et al., 2014), radiative models (Resler et al., 2017) and trees (Li and Wang, 2018; Matsuda et al., 2018); see Section 1.5.2). Recent studies have moved to combine all of these additional effects to utilise LES to study realistic integrated urban environments (Kurppa et al., 2018). Hanna (1989) highlighted the likelihood of degrading modelling performance with additional complexity. Blocken (2015) used this assertion to indicate the need for more extensive best practice guidelines

for urban LES and this is particularly prevalent in the case of non-neutral conditions.

The fundamental physics of the UBL are altered by the role of buoyancy and an additional degree of freedom is introduced into the modelling problem as a result of the slow transients associated with convective (CBL) and stable boundary layer (SBL) dynamics. Mesoscale meteorological conditions, radiative transfer, anthropogenic heat sources etc. combine to produce a complex urban surface energy balance, which drives a diurnal cycle in the UBL. The development of the CBL and SBL during the day and night respectively and the transitions between them result in time-dependent boundary-layer heights and stabilities driven by turbulent entrainment at their top and temperature changes at the surface (see Figure 4.1). UBLs tend to be less stable and deeper than their rural counterparts (Roth, 2000; Barlow, 2014). The form of the UBL can be characterised by three key length scales: the boundary layer height, h , the Obukhov length, L , and the average building height, H . A range of stability regimes exist under both the convective and stable classifications. The UBL is generally non-neutral and sheared convective conditions are typically the most prevalent regimes (Kotthaus and Grimmond, 2018). In terms of the SBL, weak stability with continuous turbulence is the dominant regime over urban areas (Uno et al., 1988; Barlow, 2014).

Field, experimental and numerical investigations have indicated the importance of the UBL height and stability on the urban climate. Numerical studies have illustrated the effects upon e.g. the urban heat island effect (Schrijvers et al., 2015), the form of the RSL (Barlow, 2014) and the dispersion of pollutants (Caton et al., 2003; Salizzoni et al., 2009; Li et al., 2016). Wind tunnel experiments have shown the effect of local stability on the turbulent structure within the UCL (Uehara et al., 2000; Kanda and Yamao, 2016). Numerous field studies have identified atmospheric stability as the prevailing meteorological factor in determining urban air quality (Mayer, 1999; Sánchez-Ccoyllo and De Fátima Andrade, 2002; Hien et al., 2002; Perrino et al., 2008). Developing the ability to model non-neutral conditions is therefore fundamental to understanding the urban environment and facing the challenges it presents. A prevalent example is the modelling of pollutant dispersion under convective and stable conditions (poor air quality often occurs as a result of stable stratifications and low-level inversions above urban areas however these have rarely been studied using urban LES).

A key challenge in this regard is the formation of statistically steady-state non-neutral boundary layers. LES investigations have taken different levels of abstraction in modelling the heat fluxes of the urban surface, from idealised isothermal boundary conditions (Boppana et al., 2014) to full three-dimensional radiative transfer models (Resler et al., 2017). A wide range of forcings and boundary conditions have similarly been applied to

enforce steady states on the resulting unstable and stable conditions (summarised in Table 4.1 and discussed in detail in Section 4.2). Many of the simplifications that are used for neutral conditions have been applied to the non-neutral case with little consideration of their effects on the flow statistics. The use of these different forcings, boundary conditions and domain heights fundamentally alters the resulting mean and turbulent characteristics of the boundary layer. Studies citing the same bulk Richardson’s numbers or Obukhov lengths can exhibit different turbulent structures as a result of the applied steady-state methodologies. The aim of this study is to outline the best practice for producing statistically steady-state and physically realistic CBL and SBLs in urban LES (employing periodic boundary conditions). Much of the presented results and analysis is equally applicable to generic (non-urban) boundary layers and the findings can be applied as such. The urban context is implicit within the approach taken in this thesis and in the formation of the devised guidelines (e.g. the aim of simplifying the problem and the requirement to have sufficient resolution to capture flows within the UCL; Blocken, 2015).

This chapter is structured as follows. Section 4.2 introduces the prognostic equations of the UBL and provides a comprehensive review on what forcings and boundary conditions can be applied to create statistical steady states in non-neutral conditions. A description of the LES model and the suite of simulations carried out as part of this study is provided in Section 4.3. Two transient simulations of the developing CBL and SBL are discussed in Section 4.4.1. Sets of steady-state simulations that aim to reproduce the conditions of the transient CBL and SBL after 10 hours using different steady-state methodologies are displayed in Sections 4.4.2 and 4.4.3. The shortcomings of particular methodologies and best practice for conducting non-neutral urban LES investigations are outlined from this analysis. Section 4.5 discusses a novel methodology in which transient simulations can be ‘frozen’ in a specific state without modifying their statistical properties. Finally, the best practice guidelines are summarised and conclusions are drawn in Section 4.6.

4.2 How to create steady-state UBLs

Real UBLs exhibit horizontal, vertical and temporal variation over a range of scales, driven by e.g. meteorological and morphological changes. A steady-state UBL is defined hereafter as a flow that satisfies statistical stationarity and horizontal homogeneity (neglecting local scale heterogeneity in the RSL). By definition, the mean and turbulent properties of the boundary layer must therefore be temporally and horizontally invariant given sufficiently long sampling (Pope, 2000). The criterion for horizontal homogeneity is satisfied by the focus on LES with periodic boundary conditions in this study.

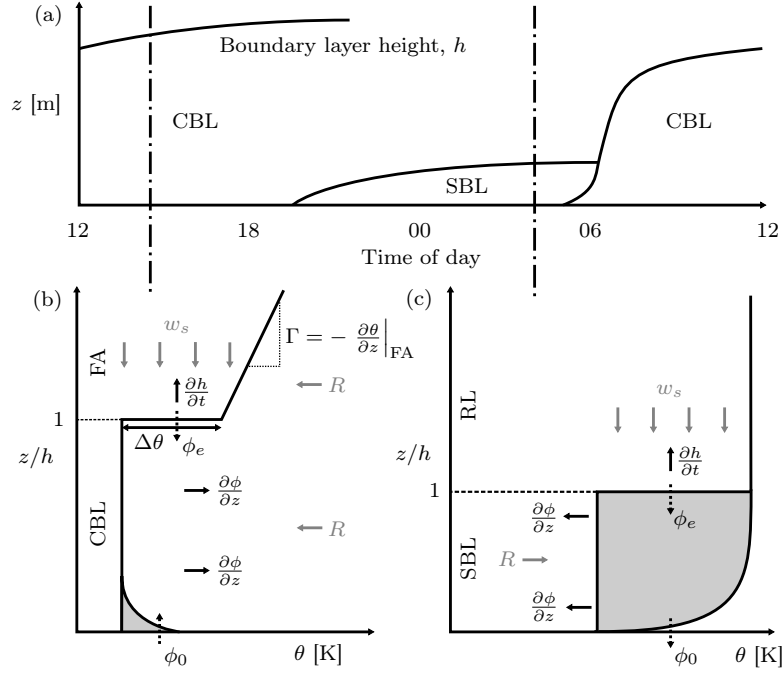


Figure 4.1: Diagrammatic view of (a) the diurnal cycle of the PBL, (b) a canonical CBL potential temperature profile (and the free atmosphere (FA) aloft) and (c) a canonical range of SBL potential temperature profiles (with the residual layer (RL) aloft). Black solid arrows indicate temporal development of the potential temperature profiles, dotted lines denote fluxes of potential temperature into or out of the boundary layer and grey arrows are possible volumetric thermal forcing terms (discussed in more detail in Table 4.1 and Section 4.5).

4.2.1 Integral description of the UBL

The prognostic boundary layer equations illustrate the inherent transiency of the problem and allow us to understand how statistical steady states can be achieved in urban LES. Defining the horizontal averaging operator $\langle \cdot \rangle$ and assuming horizontally homogeneous conditions, the equations for the horizontal velocity and potential temperature in the UBL are given by

$$\frac{\partial \langle u \rangle}{\partial t} = \langle F_u \rangle - \frac{\partial \langle \tau_x \rangle}{\partial z} \quad (4.1)$$

$$\frac{\partial \langle v \rangle}{\partial t} = \langle F_v \rangle - \frac{\partial \langle \tau_y \rangle}{\partial z} \quad (4.2)$$

$$\frac{\partial \langle \theta \rangle}{\partial t} = \langle F_\theta \rangle - \frac{\partial \langle \phi \rangle}{\partial z} \quad (4.3)$$

where F_u and F_v are forcing terms applied to model the mesoscale flow forcing, τ_x and τ_y are the shear stresses in the two horizontal directions, F_θ denotes a thermal forcing term and ϕ is the total vertical heat flux. Under normal circumstances, F_θ is very small compared to the other terms in Equation 4.3 in the UBL. The role of the heterogeneous

urban canopy (form drag) and other meteorological forcings (e.g. subsidence, divergence of radiative flux, moisture etc.) have not been included here but can be added without loss of generality (Raupach and Thom, 1981; Xie and Fuka, 2018).

In Equations 4.1 and 4.2 it is evident that the time derivative/ storage term will reduce to zero under the conditions that the magnitude of the local flow forcing balances the divergence of the local shear stress. However, there is generally no equivalent forcing term for potential temperature (since $F_\theta \approx 0$ in normal circumstances) meaning that the storage term is directly determined by the local divergence of the vertical heat flux, which can therefore only reach a steady-state in the limit of a uniform heat flux, $\partial\langle\phi\rangle/\partial z = 0$. This assertion indicates that in the presence of a non-zero local divergence in vertical heat flux, which is expected across the majority of typical CBL and SBLs, the mean potential temperature will be inherently transient.

Further insight can be obtained by integrating Equations 4.1-4.3 over the boundary-layer height, $h(t)$, which results in

$$h \frac{d\hat{u}}{dt} + (\hat{u} - \langle u \rangle_h) \frac{dh}{dt} = \hat{F}_u + \langle \tau_x \rangle_0 - \langle \tau_x \rangle_h \quad (4.4)$$

$$h \frac{d\hat{v}}{dt} + (\hat{v} - \langle v \rangle_h) \frac{dh}{dt} = \hat{F}_v + \langle \tau_y \rangle_0 - \langle \tau_y \rangle_h \quad (4.5)$$

$$h \frac{d\hat{\theta}}{dt} + (\hat{\theta} - \langle \theta \rangle_h) \frac{dh}{dt} = \hat{F}_\theta + \langle \phi \rangle_0 - \langle \phi \rangle_h \quad (4.6)$$

where the Leibniz integration rule has been used. The hat symbol $\hat{\cdot}$ denotes an integral property of the boundary layer and subscripts h and 0 denote the value at the boundary layer top (hereafter defined as the top of the inversion) and urban surface respectively. The terms on the left hand side of Equations 4.4-4.6 demonstrate two distinct ways in which the UBL can be transient: 1) via the bulk change in the boundary layer's integral properties (e.g. bulk cooling or heating) and 2) via the vertical growth of the boundary layer due to entrainment/encroachment (also diagrammatically shown for both the CBL and SBL in Figure 4.1). The presence of two time derivatives here illustrates the challenges associated with the variable depth boundary layer equations. All steady-state methodologies must therefore tackle both mechanisms as well as the local balance determined by the divergence of vertical flux terms.

4.2.2 Steady-state methods

Investigations into non-neutral UBLs face the same challenges as the neutral case but are complicated by the inherent imbalance exhibited by Equations 4.3 and 4.6 and the fundamental differences in the turbulent structure and boundary-layer heights of the modelled

4.2 HOW TO CREATE STEADY-STATE UBLs

Table 4.1: A summary of the thermal forcings and boundary conditions used to produce steady-state non-neutral UBLs in the literature and as defined in this study. Indices are repeated for methods with equivalent time averaged effects. Periodic lateral boundary conditions are assumed and any bottom boundary condition is possible given that some statistically steady $\langle \phi_0 \rangle$ exists. The volumetric source/sink term, R , and the stabilising velocity, w_s , are shown diagrammatically in Figure 4.1.

Form (name)	Comments	Ind.
$F_\theta = 0, \phi_{l_z} = 0$ (Unforced)	Flow is capped by zero flux condition at the top of the domain. The mean temperature profile develops in time but the turbulent heat flux reaches a steady state assuming self-similar behaviour (Li and Wang, 2018).	(i)
Boundary conditions		
$\langle \phi_0 \rangle = \phi_{l_z} = \text{const.}$ (Constant flux)	Boundary layer capped by heat flux at the top of the domain (equal to flux from urban surface). Results in uniform heat flux profile over domain height (Boppana et al., 2014).	(ii)
$\theta_{l_z} = \text{const.}$ (Isothermal)	Boundary layer capped by an isothermal top boundary condition. Equivalent to steady state constant flux condition (Li et al., 2010, 2016; Chan and Liu, 2013).	(ii)
Vol. source/ sink		
$F_\theta = R = \frac{\phi_{l_z} - \langle \phi_0 \rangle}{l_z}$ (Uniform)	Volumetric term applied to balance the bulk heating/ cooling of the boundary layer. Results in a linear turbulent heat flux profile up to top of the domain (Boppana et al., 2014; Shen et al., 2017).	(iii)
$F_\theta(t) = R = -\frac{\hat{\theta} - \theta_i}{t_N}$ (Uniform, time dependent)	As above, except R is redefined at each time step by ‘nudging’ towards a predefined bulk temperature. Consideration required on the relaxation timescale, t_N .	(iii)
$F_\theta(z) = R$ (e.g. $= \frac{\Delta \langle \bar{\theta} \rangle}{\Delta t}$) (Non-uniform)	Volumetric term that permits non-linear turbulent heat flux profiles. Must satisfy $\hat{F}_\theta = \langle \phi_{l_z} \rangle - \langle \phi_0 \rangle$. Can be calculated from a transient simulation or set <i>a priori</i> to produce a predefined heat flux profile.	(iv)
$F_\theta(z, t) = R = -\frac{\langle \bar{\theta} \rangle - \theta_i}{t_N}$ (Non-uniform, time-dependent)	Volumetric term defined by nudging towards predefined temperature profile, θ_i . Consideration required for the magnitude of t_N and translation of temperature profile that arises. If applied in top cells, uniform heat flux below the nudged layer (Matsuda et al., 2018).	(v)
Vol. source/ sink and stabilising velocity		
$F_\theta(z) = R - w_s \frac{\partial \langle \theta \rangle}{\partial z}$, $A = \frac{\Delta \theta}{\Gamma h + \Delta \theta}$, $w_s = \frac{A \phi_0}{\Delta \theta}$, $R = -\Gamma w_s$ (Convective fixed-point)	Van Driel and Jonker (2011) utilised the self-similarity of the CBL and the flux-ratio method to assign uniform values of w_s and R that balance the bulk heating and vertical growth of the CBL and enforce an assigned lapse rate, Γ , in the free atmosphere. Developed to work in the limit of free convection, no similar closure method or self-similarity for application to the SBL (van Driel and Jonker, 2011).	(vi)
$F_\theta(z) = R - w_s \frac{\partial \langle \theta \rangle}{\partial z} = \frac{\Delta \langle \theta \rangle}{\Delta t}$ (Frozen transient)	Volumetric source/ sink term and stabilising velocity are defined from the development of a transient simulation, such that the vertical growth and local heating/ cooling of the boundary layer are balanced. Can be applied to both the CBL and SBL. Discussed in detail in Section 4.5.2.	(vii)

flows. A range of simplifications, forcings and boundary conditions can be applied to form steady states. These steady-state methods affect the mean and turbulent statistics of the modelled flow. They must be formulated to produce physically realistic UBL dynamics whilst also satisfying the aims and computational demands of a given study. Steady-state methods in this context refer to the volumetric terms and top boundary conditions that can be applied such that the modelled boundary layer reaches a statistical steady state (periodic lateral boundary conditions are assumed and these methods are general to various bottom boundary conditions (under the condition that some statistically steady $\langle \phi_0 \rangle$ exists; e.g. constant surfaces heat fluxes and full three-dimensional radiative transfer models)).

Both the imposed thermal and flow forcings are important. Thermal forcings, both as defined within the literature and presented in this paper, are overviewed in Table 4.1 and discussed in detail in Sections 4.2.2 and 4.2.2. The flow forcings are presented in Section 4.2.2 and in Table 4.2. In the context of running steady-state urban LES, it is important to note herein the use of both the spatial and temporal ($\bar{\cdot}$) averaging operators (following the ergodic principle; Monin and Yaglom, 2013; Ghannam et al., 2015). Averaging over the horizontal extent of the LES domain alone is often insufficient to fully resolve the scales of turbulent motion.

Flow forcing

The flow forcings F_u and F_v require consideration as they directly affect the shear stresses τ_x and τ_y . Four flow forcings are used as part of this study (details provided in Table 4.2). Real UBL flow forcings arise from mean mesoscale pressure gradients and the Coriolis effect, $F_u = fv - \frac{1}{\rho} \frac{\partial p}{\partial x}$ and $F_v = -fu - \frac{1}{\rho} \frac{\partial p}{\partial y}$ where f is the Coriolis parameter (equivalent to forcing a). This results in an Ekman spiral through the UBL (under stable and neutral conditions), meaning that the direction and magnitude of the flow forcing changes with height. In neutral urban LES studies the rotationality and non-uniformity is typically circumvented by neglecting the Coriolis force and therefore simplifying the forcing term to a uniform pressure gradient $F_u = -\frac{1}{\rho} \frac{\partial p}{\partial x} = \text{const.}$ (forcing b ; Coceal et al., 2006; Xie et al., 2008). This simplification allows for the wind angle and friction velocity/ volume flow rate (depending on its formulation) to be user-defined. The effect of changing from an Ekman layer to a uni-directional flow under neutral conditions has been shown to have a minimal effect within the inner layer of the boundary layer but to cause significant changes to the turbulent structure in the outer layer due to the roll of vortex tilting (Ansorge and Mellado, 2014). The uniform forcing therefore only holds for analysis of the inner layer of the neutral UBL. In fact, it is not possible to model the free atmosphere/ residual layer above the UBL in a steady-state with a uniform forcing, as the flow accelerates uniformly

4.2 HOW TO CREATE STEADY-STATE UBLs

Table 4.2: A summary of the flow forcings (F_u and F_v) used in this study.

Form (name)	Comments	Ind.
$F_u(x, y, z, t) = f(v - v_g),$ $F_v(x, y, z, t) = -f(u - u_g),$ $f = 2\Omega \sin \Theta$ (Geostrophic)	Flow forcing defined as a function of the mesoscale pressure gradient and Coriolis force via geostrophic velocities (u_g and v_g) and the Coriolis parameter, f .	(a)
$F_u = \frac{u_*^2}{h} \cos \beta$ and $F_v = \frac{u_*^2}{h} \sin \beta$ (Uniform)	Uniform and unidirectional forcing defined by idealised mesoscale pressure gradients (using a reference friction velocity u_* ; neglects Coriolis force).	(b)
$F_{GD}(z) = [(f(u_g - \langle \bar{u} \rangle))^2 + (f(\langle \bar{v} \rangle - v_g))^2]^{1/2},$ $F_u = F_{GD} \cos \beta$, $F_v = F_{GD} \sin \beta$ (Geostrophic deficit)	Momentum forcing is defined using the absolute geostrophic deficit of a transient simulation. This acts as an approximation of the vertical variability of the flow forcing whilst neglecting its rotationality.	(c)
$F_u(z) = \frac{\partial \tau}{\partial z} \cos \beta,$ $F_v(z) = \frac{\partial \tau}{\partial z} \sin \beta,$ $\tau = u_*^2 (1 - z/h)^{3/2}$ (SBL stationary solution)	Flow forcing is predefined following the stationary solution of Nieuwstadt (1984) (using a reference u_*). Results in non-linear total vertical momentum flux profile.	(d)

in the absence of the Coriolis force. The modelled boundary layer will therefore be capped by the domain top in a steady state by definition when using a uniform pressure gradient. Enforcing a constant pressure gradient results in a linear shear stress profile. This forcing is therefore consistent with e.g. the mixed layer of the CBL. However the shear stress profiles of the SBL have been shown to be far more challenging to simplify or parametrise in such a way (Mahrt, 1999).

Forcings c and d similarly neglect the rotationality of the wind through the UBL and require the boundary layer to be capped, but they provide the capability to model non-linear shear stress profiles. Forcing c defines F_u and F_v using the magnitude of the geostrophic deficit of a transient simulation. Forcing d utilises the solution of Nieuwstadt (1984) for the homogeneous and stationary SBL. It defines the flow forcing such that the expected 3/2 power law shear stress profile is enforced (Glazunov, 2014).

Capped UBLs

The majority of neutral urban LES studies use a free-slip boundary condition at the top of the domain (domain height, l_z and $\tau_{l_z} = 0$) to cap the height of the modelled boundary layer such that $\frac{dh}{dt} = 0$ by construction and the boundary layer height is equal to the vertical height of the domain ($h = l_z$; hereafter referred to as capping the boundary layer or capped UBLs). The conditions for the integral properties of the boundary layer to reach

a steady state subsequently simplify to $\hat{F}_u = \langle \overline{\tau_x} \rangle_0$ and $\hat{F}_v = \langle \overline{\tau_y} \rangle_0$. This simplification has the additional advantage of being computationally efficient: the boundary-layer height can be predefined and set specifically for the problem of interest. The quiescent layer above the boundary layer which is often not of interest in targeted studies is neglected. Domain heights are typically ≈ 100 -200 m, using the surface layer assumption and assumed turbulent scaling with the building height to justify this simplification. Capping the boundary layer in this manner is similarly used in methods *i-v* in Table 4.1, although it is unclear whether these assumptions will hold under non-neutral conditions.

Capping the boundary layer and applying a uniform forcing have been routinely used for both convective and stable conditions. Li and Wang (2018) applied this condition with a zero flux top boundary condition for heat and no thermal forcing ($\phi_{l_z} = 0$ and $F_\theta = 0$; method *i*). These conditions do not equilibrate the inherent transiency of Equations 4.3 and 4.6; allowing the mean temperature profile to increase in time. Self-similar behaviour was assumed for the turbulence profiles once the temperature profile was increasing uniformly in time. By definition, the steady-state criteria are not satisfied by this method.

Following Equation 4.6, if $F_\theta = 0$ the only way to produce a steady state is to ensure that $\langle \overline{\phi_0} \rangle = \langle \overline{\phi_h} \rangle$. Constant flux or isothermal boundary conditions at the top of the domain can be applied to satisfy this condition (method *ii*; Li et al., 2010; Boppana et al., 2014; Chan and Liu, 2013). These conditions result in a uniform vertical heat flux profile over the LES domain, which is consistent with the established surface layer assumption ($h/10$) for the neutral case (uniform flux profiles). This description holds for the CBL but, by definition, the height of surface layer of the SBL is of similar order of magnitude to the building height. The changes in the scaling of turbulence under non-neutral conditions also challenge the justification for modelling the surface layer alone (also discussed in Section 4.2.2). For example, Inagaki et al. (2012) highlighted that coherent structures in the convective mixed-layer significantly impact the nature of flow within the UCL. The applicability of this assumption is analysed in detail in Sections 4.4.2 and 4.4.3.

Assigning a thermal forcing term $F_\theta \neq 0$ in Equations 4.3 and 4.6 provides the capability to produce steady states that feature non-uniform heat flux profiles. F_θ must be defined such that it does not affect the turbulent dynamics of the modelled flow. However this criteria is generally satisfied due to the slow transients associated with the CBL and SBL dynamics (consideration is required for time-dependant terms). Continuing under the assumption of a capped boundary layer, the condition for a steady state in Equation 4.6 becomes $\hat{F}_\theta = \langle \overline{\phi_{l_z}} \rangle - \langle \overline{\phi_0} \rangle$ and the local balance in Equation 4.3 becomes $F_\theta = \frac{\partial \langle \overline{\phi} \rangle}{\partial z}$ (equivalent to the relationship between flow forcing and shear stress). Under these conditions, a volumetric heat source/ sink term, $F_\theta = R$, can be defined to balance the bulk

and local cooling/ heating of the boundary layer. The magnitude and vertical distribution of this forcing term directly impacts the resulting heat flux profile. Three methods are defined in Table 4.1 that follow this methodology (methods *iii-v*).

Boppana et al. (2014) and Shen et al. (2017) imposed a constant, uniform profile of F_θ , which results in a linear heat flux profile (method *iii*). This profile is consistent with the expected linear heat flux within the convective mixed-layer and also with the stationary solution defined by Nieuwstadt (1984) for the SBL. In both of these studies, a zero flux top boundary condition was applied for heat, $\phi_{t_z} = 0$, analogous to modelling up to the top of the UBL. However the domain heights were considerably smaller than the typical height of the CBL. It is possible to apply this method with non-zero values of ϕ_{t_z} in order to simulate e.g. the role of entrainment at the top of the CBL or to enforce profiles of the turbulent heat flux that are consistent the CBL height but modelled in a smaller domain. If the surface heat flux is not known *a priori*, it is possible to define an equivalent thermal forcing by applying a time-dependent bulk nudging term $F_\theta = -(\hat{\theta} - \theta_i)/t_N$ (where θ_i is a predefined temperature profile and t_N is the relaxation time scale).

For typical meteorological conditions over cities, particularly for the SBL, heat flux profiles are non-linear. The ability to produce non-linear turbulent flux profiles using a non-uniform forcing can therefore be a useful tool (methods *iv* and *v*). Following Equation 4.3, the turbulent heat flux can be defined following $\langle \phi \rangle = \int \langle F_\theta \rangle dz$, with applied top and bottom boundary conditions (method *iv*; following a similar methodology to forcing *d* and still satisfying $\hat{F}_\theta = \langle \phi_h \rangle - \langle \phi_0 \rangle$).

F_θ can also be defined such that it is a function of both height and time. The mean temperature profile can be nudged towards a predefined profile following $F_\theta = -(\langle \bar{\theta} \rangle - \theta_i)/t_N$. Matsuda et al. (2018) applied nudging of this form over the top cells in the domain to produce steady-state unstable conditions. If applied over a limited number of cells, a uniform heat flux will be present up to the lowest nudged cell and the nudged cells act to form a buffer layer at the top of the domain (therefore acting equivalently to method *ii* but defining a buffer region between the bulk boundary-layer flow and the top of the domain). For the CBL, a steady-state mean temperature profile can be obtained but this forcing would behave fundamentally differently under stable conditions.

Time dependent thermal forcings are useful for application in simulations where the surface heat flux is not known *a priori* (e.g. with isothermal boundary conditions or a full three-dimensional radiative transfer models) or when the aim of the study is to reproduce e.g. a specific mean temperature profile. These forcings follow the form of ‘nudging’ or data assimilation that has been applied extensively in transient studies in the literature (Pleim, 2007). In the context of this work, the forcing serves to nudge the the potential

temperature towards a steady state as opposed to towards some transient profile as is typically done. In a steady state, the nudging term, as defined in Table 4.1, will result in a translation of the mean temperature profile as a function of the heat flux divergence and the relaxation time scale (Cai et al., 1997; Lakshmivarahan and Lewis, 2013). The relaxation timescale must also be sufficiently large to ensure that the nudging term does not directly affect the turbulent state of the flow, an effect that can be minimised by averaging over the largest possible spatial extent.

Uncapped UBLs

Uncapped UBLs refer to simulations where the domain top is not used to define the boundary layer top and therefore both the boundary layer and its interaction with the free atmosphere/ residual layer aloft are modelled. Sorbjan (1996) studied the impact of modelling ‘solid lid’ non-penetrative CBLs. A significant difference was identified between the turbulent structure of modelled boundary layers where entrainment through the inversion layer was captured and where the boundary layer was capped by a solid and adiabatic wall. If entrainment processes are to be incorporated faithfully in a steady-state formalism, the UBL must not be capped by the top of the domain.

Van Driel and Jonker (2011) derived a convective fixed-point solution to create steady states in uncapped simulations of the CBL. The vertical growth of the boundary layer was balanced by the addition of a stabilising velocity, w_s , in the thermal forcing term ($F_\theta = R - w_s \frac{\partial \langle \theta \rangle}{\partial z}$; method *vi*). The stabilising velocity is analogous to a subsidence velocity and provides a forcing component that is dependent on the local thermal stratification. The magnitude of the uniform profiles of R and w_s can be defined through the convective fixed-point solution that applies the flux-ratio method and mixed layer model to Equation 4.6 (equations provided in Table 4.1; Ball, 1960; Tennekes, 1973). The thermal forcings are also applied above the boundary layer where they act to further maintain the defined lapse rate, Γ , following $\Gamma = -\frac{R}{w_s}$. This method is designed for use with free as opposed to mixed or forced convection (the entrainment ratio will change for sheared CBLs; Liu et al., 2018) and there is no similar closure method for use with the SBL.

A novel ‘frozen transient’ method is developed as part of this study where non-uniform profiles of R and w_s are defined such that the method is suitable for both convective and stable stratifications (method *vii*). The frozen transient method is discussed in detail in Section 4.5.

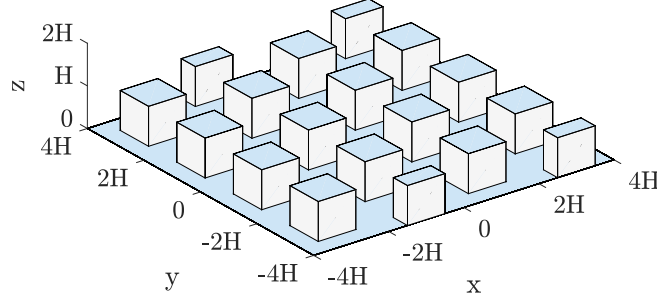


Figure 4.2: Representation of the staggered cubic array used across all simulations. Blue areas indicate road and roof levels where a constant heat flux is applied.

4.3 Large-eddy simulation set-up

The model used in this study is the Dutch Atmospheric Large-Eddy Simulation model (DALES-Urban; Heus et al., 2010; Tomas et al., 2015, 2016b). The SGS model used follows Vreman (2004). The immersed boundary method has been incorporated into DALES in order to provide the capability to model buildings within the domain (Tomas et al., 2015). Wall functions are used to model the dynamics close to the walls (see Section 2.3.5; Uno et al., 1995; Suter, 2018). The numerical scheme consists of a spatial discretisation on an Arakawa C-grid, utilising a second-order central-differencing scheme for all field variables and a third-order Runge-Kutta time integration scheme.

A series of simulations of both convective (-C) and stable (-S) conditions is carried out to evaluate the different steady-state methodologies (simulation details are provided in Table 4.3 and details of the applied flow forcings are provided underneath). Two transient simulations (tC and tS), applying a geostrophic flow forcing and no thermal forcing, are used to model the development of a typical CBL and SBL over a 10 hour time period. A suite of steady-state simulations (s-) are set up with the aim of reproducing the state of their corresponding transient simulation after 10 hours run time (hereafter referred to as the reference state):

- sC1-sC3 apply established simplifications from the literature to model the assumed surface layer of the CBL. The boundary layers are capped at $h/10$ and $h/5$, a uniform flow forcing is applied and methods *ii* and *iii* are used to enforce uniform or linear vertical heat flux profiles respectively.

- sC4-sC6 similarly cap the boundary layer and apply a uniform flow forcing. In these simulations the top heat flux is defined such that the vertical heat flux profile matches that of the reference state and the domain height is varied to investigate its effect on the modelled flows ($l_z = h/5, h/2$ and h).
- sC7-sC8 do not cap the boundary layer and correspondingly use a geostrophic flow forcing. Methods *vi* and *vii* are used to enforce a steady-state.
- sS1-sS2 apply methodologies as found in the literature to model the SBL. The boundary layers are capped, a uniform flow forcing is applied and methods *ii* and *iii* are used to enforce a uniform or linear vertical heat flux profile respectively.
- sS3-sS5 cap the boundary layer and apply different combinations of non-uniform flow and thermal forcings. sS3 satisfies the solution of Nieuwstadt (1984) by applying a uniform thermal forcing (method *iii*) and a 3/2 power law flow forcing (forcing *d*). sS4 uses the statistics of tS to obtain non-uniform profiles of both the thermal and flow forcing (method *vi* and forcing *c*). sS5 applies the 3/2 power law flow forcing and method *v* to nudge the mean temperature profile towards the temperature profile of the reference state.
- sS6 does not cap the boundary layer and correspondingly uses a geostrophic flow forcing. Method *vii* is applied to enforce a steady-state.

The surface heat flux ($\phi_{0,C} = 0.04$ and $\phi_{0,S} = -0.005 \text{ Km s}^{-1}$), friction velocity ($u_{*,C} = 0.45$ and $u_{*,S} = 0.16 \text{ m s}^{-1}$) and therefore the Obukhov length ($L_C = -163$ and $L_S = 63 \text{ m}$) are matched to that of the corresponding reference state in all convective and stable steady-state simulations. In simulations where a unidirectional forcing is applied, the wind angle is defined such that it matches that of the reference state at building height ($\beta_C|_{z=H} = 28^\circ$ and $\beta_S|_{z=H} = 51^\circ$). The boundary-layer heights, h , of the reference states, which are used to determine the domain heights, l_z , of the capped simulations, are $h_C = 1234 \text{ m}$ and $h_S = 120 \text{ m}$ (following the definition of h as the top of the inversion and using the height at which the mean velocities tend to their geostrophic values to calculate this). The mean and turbulent profiles of simulations tC and tS are provided in Section 4.4.1.

A base simulation set-up is defined such that the other simulation conditions remain constant whilst the forcings, top thermal boundary condition and domain configurations are varied as discussed. The base set-up applies periodic horizontal boundary conditions for both momentum and heat and a free slip condition at the top of the domain. A staggered cubic array is used, diagrammatically shown in Figure 4.2, with a building height $H = 16 \text{ m}$. Constant heat fluxes are defined at the road and roof top levels with no heat flux defined

4.3 LARGE-EDDY SIMULATION SET-UP

Table 4.3: Properties of the transient (t-) and steady-state (s-) convective (-C) and stable (-S) simulations. Indices for the flow forcing are outlined in Table 4.2 and indices for the thermal forcing refer to those in Table 4.1. *The surface heat flux was scaled from $5\phi_0$ to ϕ_0 over the first 1800 seconds of simulation time in order to avoid enhanced boundary layer development resulting from the initial conditions.

Sim.	Domain size [m]	Grid size [-]	ϕ_0 [Km s ⁻¹]	$\phi_{l_z}, (\theta_{l_z})$ [Km s ⁻¹ , (K)]	F_u, F_v	F_θ
tC	$2304 \times 1536 \times 1920$	$288 \times 192 \times 480$	0.040	(293.8)	(a)	-
sC1	$256 \times 256 \times 128$	$128 \times 128 \times 128$	0.040	0.040	(b)	(ii)
sC2	$512 \times 256 \times 256$	$256 \times 128 \times 128$	0.040	0.040	(b)	(ii)
sC3	$512 \times 256 \times 256$	$256 \times 128 \times 128$	0.040	0.000	(b)	(iii)
sC4	$512 \times 256 \times 256$	$256 \times 128 \times 128$	0.040	0.029	(b)	(iii)
sC5	$1280 \times 640 \times 640$	$320 \times 160 \times 320$	0.040	0.013	(b)	(iii)
sC6	$2304 \times 1536 \times 1152$	$288 \times 192 \times 288$	0.040	-0.008	(b)	(iii)
sC7	$2304 \times 1536 \times 1920$	$288 \times 192 \times 480$	0.040	(293.8)	(a)	(vi)
sC8	$2304 \times 1536 \times 1920$	$288 \times 192 \times 480$	0.040	(293.8)	(a)	(vii)
tS*	$384 \times 192 \times 144$	$192 \times 96 \times 144$	-0.005	(288.0)	(a)	-
sS1	$160 \times 192 \times 120$	$160 \times 192 \times 120$	-0.005	-0.005	(b)	(ii)
sS2	$160 \times 192 \times 120$	$160 \times 192 \times 120$	-0.005	0.000	(b)	(iii)
sS3	$160 \times 192 \times 120$	$160 \times 192 \times 120$	-0.005	0.000	(d)	(iii)
sS4	$160 \times 192 \times 120$	$160 \times 192 \times 120$	-0.005	0.000	(c)	(iv)
sS5	$160 \times 192 \times 120$	$160 \times 192 \times 120$	-0.005	0.000	(d)	(v)
sS6	$384 \times 192 \times 144$	$192 \times 96 \times 144$	-0.005	(288.0)	(a)	(vii)

^(a) Rotation rate of the Earth, $\Omega = 7.292 \times 10^{-5}$ rad s⁻¹, and latitude, $\Theta = 51^\circ$ N.

through the vertical building walls. The horizontal sizes of the computational domains are defined to be sufficiently large with respect to their respective vertical domain heights such that one can average over various large coherent structures. It is important to note that urban LES best practice requires a minimum of ≈ 10 grid cells per building height, H , to resolve flows within the UCL (Blocken, 2015). This criterion is not satisfied in some simulations, which highlights the advantage of capping the boundary layer at lower heights in urban LES studies (this criterion is discussed in more detail in Section 4.4.2).

The initial profiles of horizontal velocities and potential temperature also vary by simulation. Simulation tC applies an initial lapse rate, $\Gamma = -0.003$ K m⁻¹, in order to represent the free atmosphere, whereas simulation tS uses a uniform initial temperature profile of 288 K to represent the residual layer. Both transient simulations utilise uniform profiles of the specified geostrophic velocities ($u_g = 4$ m s⁻¹, $v_g = 0$ m s⁻¹) as initial conditions. Steady-state simulations that apply method *vii* (sC8 and sS6; see Section 4.5 for details) are run directly from the state of the corresponding transient simulation after 10 hours run time. Following van Driel and Jonker (2011), sC7 sets a uniform initial potential temperature

profile up to the defined boundary layer height h_C , an increase in potential temperature of the inversion strength, $\Delta\theta = 0.78$ K, at h_C , and an increase in potential temperature at the defined lapse rate, $-\Gamma$, for $z > h_C$. The other steady-state convective simulations (sC1-sC6) utilise a uniform initial potential temperature profile of 288 K. sC1-sC7 apply uniform initial velocity profiles that represent the geostrophic velocity adjusted to the wind angle at building height as discussed. The remaining steady-state stable simulations (sS1-sS5) use profiles of the mean potential temperature and magnitude of the wind speed (adjusting the wind angle) from the reference state. Using the values from the reference state helped to reduce the required simulation times in the presence of large timescales in the outer layer.

Statistics are obtained by spatially averaging in the horizontal directions (a mask is applied in the positions of the buildings; c.f. intrinsic spatial averaging; Xie and Fuka, 2018) and temporally averaging with a sampling time of 5 s. The transient simulations are averaged over a time-period of one hour and the steady-state simulations are averaged over a time period sufficient to produce converged statistics. For the convective simulations a maximum averaging period of $\approx 20T_C$ is used ($T_C = h_C / (gh_C\phi_0/\bar{\theta}_C)^{1/3} = 1041$ s) and for the SBL an averaging period of $\approx 10T_S$ ($T_S = h_S/u_{*,S} = 750$ s) is used across all simulations. The simulations are run until a negligible change is observed between the resulting mean and turbulent statistics over consecutive averaging periods.

4.4 Results

The two transient simulations are discussed first to provide a reference state for a typical urban CBL and SBL. Mean and turbulent profiles of the steady-state simulations are then plotted alongside those of the reference state in order to evaluate the range of applied steady-state methodologies. Deviations from the reference state in these profiles indicate a discrepancy in the representation of the modelled flow. The boundary conditions, forcings and simplifications applied to produce these steady states are reviewed and guidelines are outlined for best practice in modelling non-neutral steady-state UBLs in future studies. Much of the following analysis is equally applicable to generic boundary layers in a non-urban context, however the discussion and guidelines are based around modelling approaches for urban LES.

4.4.1 Transient non-neutral UBLs

Simulations tC and tS capture the development of a typical CBL and SBL over an urban area through the day and night respectively. The mean and turbulent statistics of the two

4.4 RESULTS

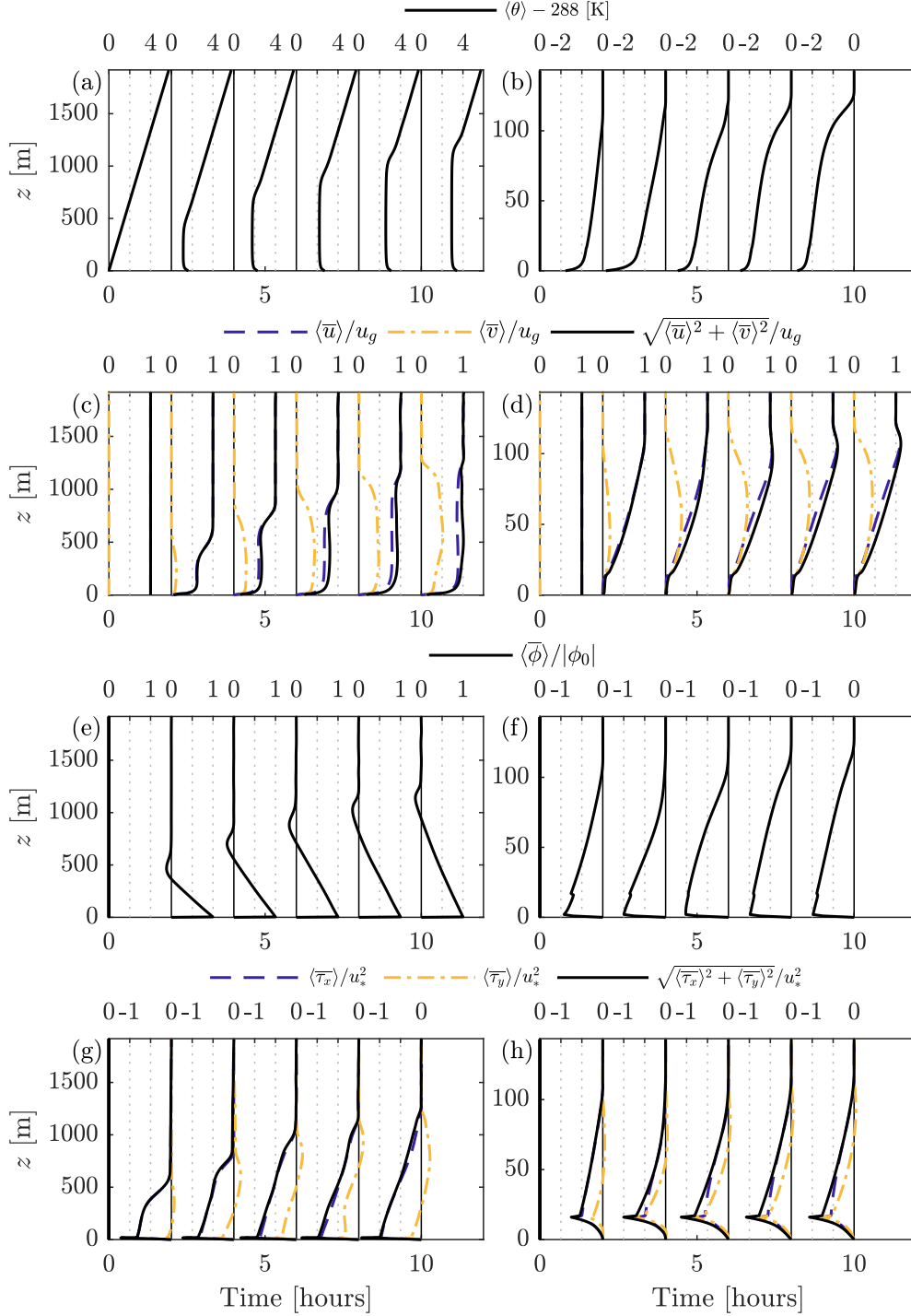


Figure 4.3: Development of the mean (a) potential temperature, (b) wind speed, (c) vertical heat flux and (d) shear stress profiles of the transient simulations tC (left) and tS (right).

developing non-neutral UBLs are shown in Figure 4.3. The CBL height grows in time, achieving a height $h_C = 1234$ m after 10 hours simulation time. This growth is driven by the formation of an inversion through which warm air is entrained down from the stratified free atmosphere aloft. The mean temperature and turbulent heat flux profiles exhibit self-similar behaviour consistent with classical mixed-layer theory; as has been found in urban field studies (Wood et al., 2010). The development of the velocity and turbulent momentum flux profiles is consistent with a weakly sheared CBL (Fedorovich and Conzemius, 2008). The wind rotates within the RSL and entrainment zone and is relatively uniform within the mixed layer. Park and Baik (2014) provide detailed analysis of a similar urban CBL.

The SBL grows to a quasi-equilibrium height, $h_S \approx 120$ m, within the first four hours of simulation time. This height is an order of magnitude smaller than the convective case. An inversion forms and strengthens, limiting turbulent entrainment through the boundary layer top. As the inversion strengthens, the cooling is redistributed across the boundary-layer height. A nocturnal jet forms towards the top of the velocity profile. The wind rotates down through the boundary layer, with a maximum wind angle, $\beta_S = 77^\circ$, within the UCL after 10 hours simulation time. The geostrophic deficit also varies with height as the wind profile increases up to the geostrophic velocity. The temperature and heat flux profiles do not exhibit self-similar behaviour. Classifying or applying canonical results and similarity theory to the SBL has been shown to be challenging in the literature (Mahrt, 1999; Barlow et al., 2011). The development of tS is typical of a weakly SBL, characterised by continuous turbulence and an elevated inversion. Approaching 10 hours simulation time, the turbulent profiles are relatively consistent with the stationary solution of Nieuwstadt (1984).

Three key length scales, boundary layer height, h , Obukhov length, L , and building height, H , are prevalent in the UBL dynamics. These two transient simulations provide typical reference cases of sheared convective and weakly stable conditions over urban areas (Kotthaus and Grimmond, 2018). In future investigations it would be useful to investigate more combinations of h , L and H , however applying the steady-state methods to these reference states covers the predominant cases of interest and also provides a platform for future works.

4.4.2 Steady-state convective UBLs

The development of simulation tC highlights several points of interest that require consideration when forming steady-state urban CBLs: 1) the large boundary-layer height and corresponding turbulent length scale, $h_C \gg H$, 2) the significant vertical growth of the boundary layer via turbulent entrainment at the boundary layer top, dh_C/dt , and 3) the

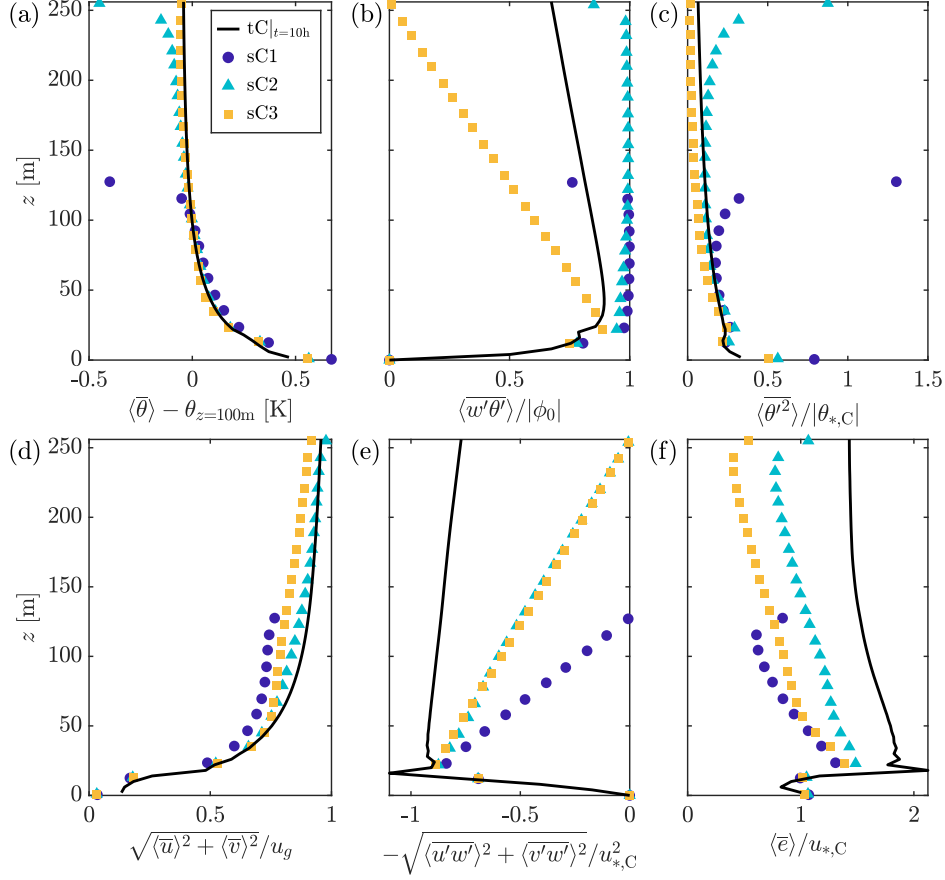


Figure 4.4: Mean and turbulent profiles of the steady-state convective simulations sC1-sC3 in comparison to the reference state $tC|_{t=10h}$. sC1-sC3 apply steady-state methods as seen in the literature.

applicability of mixed-layer theory and therefore the expected uniform mean profiles and linear turbulent flux profiles.

The behaviour of capped CBL simulations in which only the surface layer is considered will be explored first. sC1-sC3 apply methodologies as seen in the literature to model the CBL up to heights of $h_C/10$ or $h_C/5$. The resulting mean and turbulent profiles are shown in Figure 4.4. The application of a uniform flow forcing and enforcement of either uniform (method *ii*) or linear (method *iii*) vertical heat flux profiles are self-evident from the turbulent flux profiles. By definition, the limited domain heights and these forcings lead to deviations from the reference state in the turbulent flux profiles. The use of a non-zero top thermal boundary condition in sC1 and sC2 results in a small layer at the top of the domain with an unstable stratification and a corresponding local increase in the potential temperature variance. In sC1 this deviation is significant from as low as 60 m. sC3 does not exhibit the same thermal interaction with the domain top. However the

reduced turbulent heat flux leads to a corresponding reduction in the potential temperature variance (bulk reduction of 35% in comparison to the reference state). The increased potential temperature variances at the surface are a result of the differences in the modelled resolutions (Sullivan and Patton, 2011). The mean wind speeds follow similar profiles to the reference state although the steady-state simulations exhibit a reduction in the mean wind speed above the RSL (maximum difference in wind speed of 24% at 114 m in simulation sC1).

The most pronounced deviation from the reference state is the reduced magnitude of turbulent kinetic energy (TKE; e) at building height and above in all three simulations in Figure 4.4f. A maximum reduction of 61%, 44% and 72% is exhibited in simulations sC1-sC3 respectively. The magnitude of TKE is indicative of the intensity of the local turbulent motion and therefore e.g. the turbulent mixing (it is the defining parameter in terms of the vertical exchange of pollutants out of the UCL; Salizzoni et al., 2011). A reduction in TKE therefore signifies a fundamental change in the turbulent structure of these flows in comparison to the reference state and therefore a significant potential source of error in urban LES studies of unstable conditions.

The TKE reductions are a result of the limited domain heights. The reduced turbulent flux profiles directly affect the mechanical (sC1-sC3) and buoyant (sC3) production of turbulence above the RSL. But these profiles alone cannot account for the nature of the TKE reductions shown in Figure 4.4 (e.g. at building height). A more fundamental difference in the turbulent structure of the modelled flows exists that affects both the dissipation and transport of TKE within these boundary layers. Typically, within a mixed convective surface layer, large-scale eddy structures (e.g. temperature ramp structures; Wilczak, 1984) form and, within and just above this layer, these structures merge to produce the convective thermals that drive the formation of the mixed layer aloft. The relationship between the boundary layer height and the Obukhov length and their effect on TKE is discussed in Lenschow (1974). Within the convective mixed layer, there is near uniform spectral behaviour of the velocity components with height. However, underneath the mixed layer low frequency spectral components do not show such uniformity and exhibit a scaling with the dimensionless height z/L (Kaimal et al., 1976). The limited domain heights in simulations sC1–3 inhibit the formation of the convective mixed layer, which evidently affects the turbulent structure of the modelled flow. The domain heights of these simulations are equal to $-0.8L_C$ and $-1.6L_C$ indicating the prominence of mechanical over buoyant effects in these boundary layers. The scaling regions for the CBL dictate that $h/|L| \geq 5$ is the criteria to drive the CBL in a convective state (with the surface layer then defined at $-L/2$; Holtslag and Nieuwstadt, 1986). The importance of capturing the large-scale structures

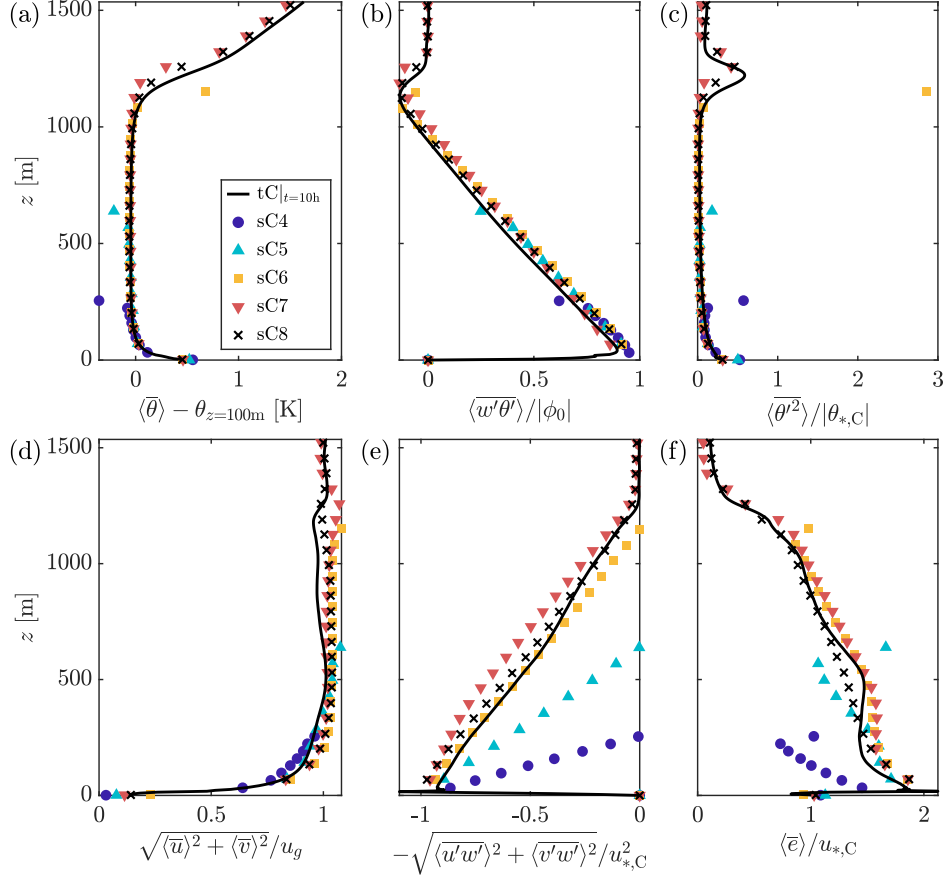


Figure 4.5: Mean and turbulent profiles of the steady-state convective simulations sC4-sC8 in comparison to the reference state $tC|_{t=10h}$. sC4-sC6 apply simplified conditions and vary the domain height between them. sC7-sC8 model uncapped steady-state CBLs.

of the convective mixed layers and their interaction with the surface layer has previously been highlighted in other LES studies (Mason, 1989; Inagaki et al., 2012). These results clearly indicate that modelling unstable conditions by significantly limiting the domain height results in flows that do not capture the turbulent dynamics of a realistic CBL.

Having established that it is not sufficient to resolve the surface layer only for a CBL, the following set of simulations use larger domain heights and more realistic thermal forcings. Figure 4.5 shows the results for simulations sC4-sC8. sC4-sC6 were set up similar to sC3 however method *iii* is applied such that the turbulent heat flux profile follows that of the reference state ($\phi_{l_z} = \phi_C|_{z=l_z}$) and the domain height is varied $l_z = h_C/5$, $l_z = h_C/2$ and $l_z = h_C$. sC7-sC8 do not cap the boundary layer and these results are discussed in Section 4.5.

The mean, turbulent flux and potential temperature variance profiles of sC4-sC6 follow

the trends identified in the analysis of sC1-sC3. sC4 matches the turbulent heat flux profile up to $h_C/5$ but exhibits the same systematic underestimation of the TKE in Figure 4.5f due to the impeded size of the boundary layer. sC5 uses a limited domain height, $l_z = h_C/2$, however does not exhibit the same reduction over the surface layer of the modelled flow. The TKE shows a good agreement up to a height of 270 m above which a small reduction is evident. This profile indicates that modelling up to a height of $h_C/2$ and $4.5L_C$ was sufficient to capture the convective nature of the boundary layer in this case and sufficient to realistically model the turbulent dynamics over the UCL. Following this finding and the assertion in Holtslag and Nieuwstadt (1986) that $h/L \geq 5$ is required to drive the convective state of the boundary layer, the scalings of $l_z \geq 5|L|$ and $l_z \geq h/2$ provide guidelines through which to avoid the systematic underestimation of TKE in future urban LES studies. However, the applicability of these scalings for other stability parameters, h/L , must be investigated to understand the generality of these scalings e.g. in the limit of free convection (Grylls et al., 2020). A comprehensive study should therefore be conducted in the future to further investigate this scaling for different h/L and in terms of the importance of the building height, H (Lenschow, 1974).

sC6 applied the same simplifications with a domain height equal to that of the reference state ($l_z = h_C$). The agreement shown between sC6 (as well as sC5) and the reference state in Figure 4.5 illustrates that simplifying the CBL by neglecting the Coriolis force and by capping the boundary layer is reasonable (given that the domain height is sufficiently large). These simplifications are possible due to the well mixed nature of the CBL. The changes in turbulent structure resulting from ‘solid-lid’ nonpenetrative convection (Sorbjan, 1996) are not evident within the potential temperature variance or TKE profiles of sC5 and sC6. The application of a negative heat flux at the top of the domain in simulation sC6 (which was not imposed by Sorbjan, 1996) acts to minimise these differences by modelling the entrainment of heat down from the free atmosphere.

The challenge for urban LES is that a trade-off exists between the physical size of the domain and the computational feasibility of a given simulation. High resolutions are required to effectively resolve flow within the UCL (1-2 m; Tseng et al., 2006; Xie and Castro, 2009). However, as has been highlighted, relatively large domain heights are necessary to effectively model the CBL. This criterion for the resolution was not satisfied in tC and sC6–8 but was obtained in the vertical direction in sC5. Clustering the grid towards ground level, such that the finest resolutions are obtained within the UCL and the grid is coarser towards the top of the domain, can help to alleviate this issue. The use of grid nesting presents an alternative tool to deal with the large vertical and horizontal scales but can introduce inconsistencies where the grids meet (Garcia-Menendez and Odman, 2011).

The discussed set of steady-state convective simulations encompass the range of set-ups that could be applied to model convective conditions in targeted urban LES studies. It is shown that capping the boundary layer and using a one-dimensional flow forcing are reasonable simplifications, particularly if a study is focussed upon the inner layer of the UBL. However a key finding is that the vertical extent of the domain must be equal or greater than half the expected boundary-layer height ($l_z \geq h/2$) and five times the Obukhov length ($l_z \geq 5|L|$) to avoid a systematic underestimation of TKE. In studies of e.g. a single infinite canyon it may seem superfluous to model up to heights of 600 m and above, however capturing the large scale structures of the convective mixed layer is fundamental to understanding the urban climate under convective conditions.

4.4.3 Steady-state stable UBLs

The SBL provides a different set of challenges in terms of modelling realistic steady-state conditions in urban LES. The difficulty in defining any generalised state of the SBL is alleviated by the use of a reference state that represents a typical weakly SBL (Mahrt, 1999). The modelled conditions also avoid the LES difficulties associated with runaway cooling and strongly stable conditions (Van de Wiel et al., 2012). The challenges arising from the form of the reference state are 1) the relatively small boundary-layer height ($h_S \approx 8H$), 2) the non-uniform mean and non-linear turbulent flux profiles, 3) the rotation of the wind down through the boundary layer and (4) the long time scales associated with the outer layer dynamics.

Figure 4.6 shows time series of the bulk wind speeds from all of the steady-state simulations. Simulation sS2 exhibits global intermittency over a time period of $\approx 40T_S$ which exceeds the defined sampling period ($10T_S$) and therefore does not satisfy the steady-state criteria defined in this study (Mahrt, 1999; Anson and Mellado, 2014). The intermittency in sS2 arises due to the use of a uniform flow forcing. The flow forcing of the reference state is a function of the geostrophic deficit, which is largest at the urban surface and reduces to zero at the boundary layer top. Despite providing the same friction velocity, the uniform flow forcing systematically underestimates the forcing within the UCL and therefore directly affects the local mechanical generation of turbulence. In this case, the underestimation permits the cooling induced by the surface heat flux to periodically dominate the flow dynamics. The use of this well established simplification is therefore shown to be fundamentally limited because it has resulted in dynamics that were not present in the reference state. It should be noted that for other SBL states (e.g. different Obukhov lengths), the same change in forcing may not instigate global intermittency, however it will similarly underestimate the mechanical generation of turbulence and therefore lead to a

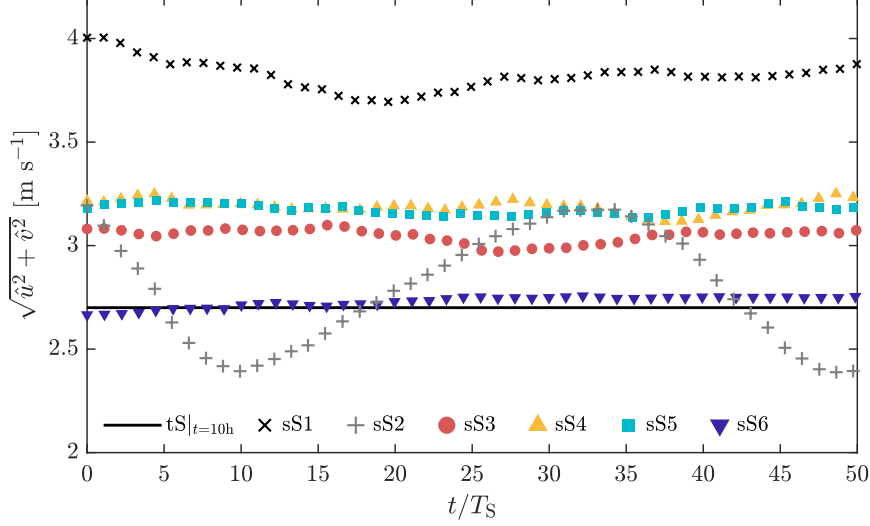


Figure 4.6: Time series of the bulk wind speed of the steady-state stable simulations sS1-sS6 in comparison to the reference state $tS|_{t=10h}$. sS1-sS2 apply simplifications as seen in the literature. sS3-sS5 use different steady-state methods to capture non-linear fluxes. sS6 models uncapped steady-state SBL.

different turbulent state of the boundary layer.

sS1 also applied a uniform flow forcing but alongside method *ii* which acts to enforce a uniform heat flux profile. The bulk wind speed exhibited in Figure 4.6 is 40% higher than that of the reference state’s bulk wind speed, indicating a fundamental problem with this steady-state methodology. The effect of this thermal forcing is shown more clearly in Figure 4.7, which exhibits the mean and turbulent profiles of the steady-state stable simulations (excluding sS2). The enforced vertical heat flux in sS1 leads to a lower and stronger inversion over which high wind speeds and potential temperature variances arise. The fundamental problem of enforcing a uniform heat flux to a SBL is evident from the turbulent heat flux profile in Figure 4.7b as the flux in the reference state reduces to zero at the boundary-layer height. A further problem in sS1 is indicated by the fact that the normalised turbulent heat flux is significantly less than one above the RSL, which is due to the prevalence of the subgrid stress term in the LES.

sS3-sS6 exhibit only negligible changes in bulk wind speed over time in Figure 4.6 and also show far better agreement with the reference state in Figure 4.7. The increased magnitude of the bulk wind speed in simulations sS3-sS5 is due to the neglect of the wind’s rotationality and therefore of the role of vortex tilting in these simulations (consistent with the findings of Ansorge and Mellado (2014); also discussed in Section 4.2.2). The increase

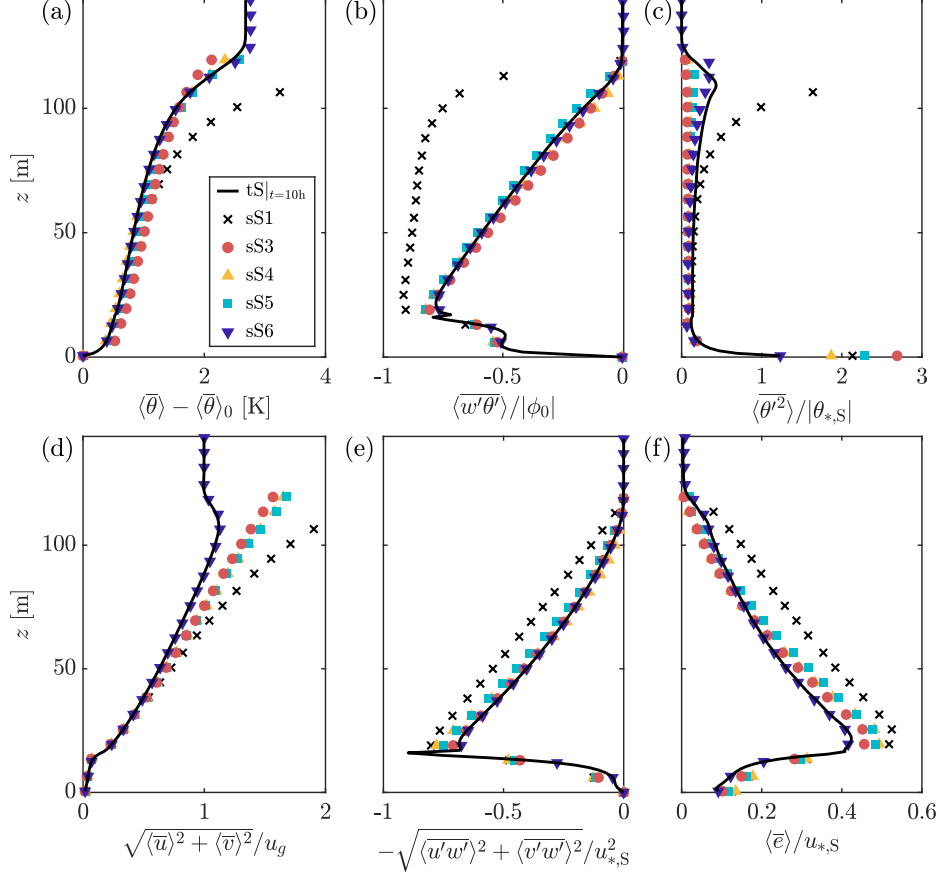


Figure 4.7: Mean and turbulent profiles of the steady-state stable simulations sS1 and sS3-sS6 in comparison to the reference state $tS|_{t=10h}$. sS1 applies simplifications as seen in the literature. sS3-sS5 use different steady-state methods to capture non-linear fluxes. sS6 models an uncapped steady-state SBL.

in the magnitude of wind speed in the outer layer of the modelled flows can be clearly seen in Figure 4.7. There is also a small overestimation in the turbulent momentum flux within the RSL that correspondingly leads to higher TKE in this region. However, the flow forcings applied in these simulations (forcings c and d) generally show a good agreement with the turbulent momentum flux and TKE profiles of the reference state. In terms of conducting targeted urban LESs, they present a significant improvement from the uniform flow forcing applied in sS1 and sS2 and in particular the agreement shown by the $3/2$ power law is an important finding as it can be defined *a priori* and provides the numerical control to specify the wind direction and friction velocity of a given simulation.

sS3-sS6 all cap the boundary layer with a zero heat flux top boundary condition and therefore do not capture the boundary layer's interaction with the residual layer aloft. As a result of this, these simulations do not capture the local increase in the potential

temperature variance over the inversion in Figure 4.7c. Apart from this deviation, the applied thermal forcings (methods *iii-v*) all reproduce the mean temperature and turbulent heat flux profiles of the reference state well. sS3 simply uses a uniform thermal forcing, which alongside the $3/2$ power law enforces flux profiles that follow Nieuwstadt (1984)’s solution for the SBL. This agreement may not be surprising due to the quasi-stationary state of the boundary layer at the reference state, but the ability to apply these simplified forcings to reproduce the turbulent statistics of a realistic reference SBL in a steady state is significant. The difference between the performance of sS2 and sS3, which only differ by the applied flow forcing, further indicates the importance of applying the $3/2$ power law forcing here. sS4 and sS5 illustrate successful applications of non-uniform thermal forcings (derived from tS and through nudging respectively). The resulting non-uniform thermal forcings capture the non-linear details of the vertical heat flux, providing a small improvement in terms of the mean temperature profile in comparison to sS3. The application of the nudging term alongside the $3/2$ power law illustrates a methodology that can be useful in studies attempting to reproduce a specific mean temperature profile e.g. from observation.

The typical heights of the SBL ($\approx 100 - 200$ m) mean that the neglect of the interaction with the residual layer and the deviations in the outer layer dynamics will be significant in some urban studies. A prevalent current example of this is studies of the role of tall buildings in the urban climate (building heights may even exceed the height of the SBL). Simulation sS6 applies method *vii* to capture the SBL in its entirety as well as the residual layer aloft and therefore presents a method that can be beneficial to these studies. This method and these results are discussed in detail in Section 4.5.

For targeted LES studies where the dynamics at the top of the SBL are not of interest and a simplified representation of the SBL is advantageous, the most significant finding in this section is the limitation of using a uniform flow forcing. The solution to this problem is the application of the $3/2$ power law flow forcing. In terms of the thermal forcing, three methods were presented that achieved reasonable results in this context by applying volumetric source terms. The uniform thermal forcing of method *iii* is the simplest and easiest to implement in urban LES.

4.5 Steady-state uncapped non-neutral UBLs

The discussion above focused upon simulations where the boundary layer was capped by the top of the domain. It is of interest to form steady states where the interaction with the quiescent layer above the UBL is captured. In terms of the CBL, it was shown by Sorbjan (1996) that the turbulent structure of the boundary layer is different when modelling

penetrative (uncapped) as opposed to ‘solid-lid’ nonpenetrative (capped) convection. It was also shown in Section 4.4.3 that the outer layer flow was significantly misrepresented when capping the SBL and that typical SBL heights are of similar magnitude to tall buildings.

4.5.1 Fixed-point solution method

The fixed-point solution of van Driel and Jonker (2011) was discussed in Section 4.2.2 and in Table 4.1 (method *vi*). It outlines a method through which uncapped freely convective UBLs can be modelled in a steady state. The advantage of this method is that the magnitude of the stabilising velocity and volumetric source term ($F_\theta = R - w_s \frac{\partial \langle \theta \rangle}{\partial z}$; shown diagrammatically in Figure 4.1) can be defined to produce a mean temperature profile with a predefined boundary-layer height and inversion strength *a priori*. However this method is limited due to its employment of the entrainment ratio as this term changes under sheared convective conditions (Liu et al., 2018) and because no such simplification and closure scheme exists in the stable case. Method *vi* was applied to reproduce the mean temperature profile of the convective reference state. The resulting profiles of the applied thermal forcings are shown in Figure 4.8a and b. The steady-state mean and turbulent profiles from the corresponding simulation (sC7) are shown in Figure 4.5. A steady-state CBL was achieved with good agreement to the reference state despite the sheared nature of the reference CBL. A small increase in the boundary-layer height is shown and the velocity profile exhibits a maximum value within the entrainment zone.

4.5.2 Frozen transient method

A novel method to freeze the state of the atmosphere in a specific statistical state is presented below (method *vii*). The method works in both stable and convective situations (unlike method *vi*) and only requires information about the average potential temperature profile of a transient simulation and its time derivative. Following van Driel and Jonker (2011), this method uses a thermal forcing consisting of both a stabilising velocity and a volumetric source/ sink term. However, instead of relying on a parametrisation of the UBL to obtain estimates for w_s and R , the frozen transient method relies on the fact the normal velocity v_n of an isosurface of a scalar ψ is given by (Holzner and Lüthi, 2011; van Reeuwijk and Holzner, 2014)

$$v_n = -\frac{1}{|\nabla\psi|} \frac{\partial\psi}{\partial t}, \quad (4.7)$$

where $v_n = \vec{v} \cdot \vec{n}$ and $\vec{n} = \nabla\psi/|\nabla\psi|$ is the normal to the isosurface. For the case of a transient UBL, the aim is to create a steady state case using information of the potential

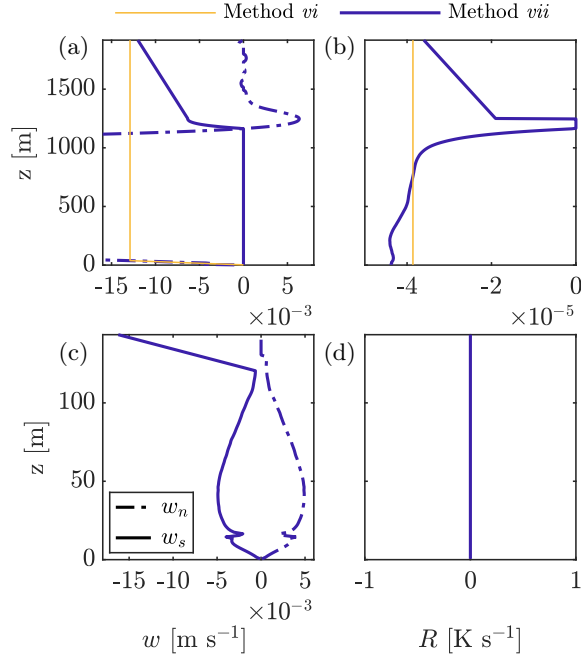


Figure 4.8: Profiles of the vertical velocity of the potential temperature profile w_n (calculated from the transient simulations using Equation 4.8; a and c), stabilising velocity w_s (a and c) and volumetric source/sink term R (b and d), applied for steady-state methods *vi* and *vii* in simulations sC7-sC8 (top) and sS6 (bottom). Note that method *vi* does not utilise w_n and is not applicable to SBLs and is therefore not plotted in c and d.

temperature $\langle \bar{\theta} \rangle(z, t)$ only. Setting $\psi = \langle \bar{\theta} \rangle$ and using the homogeneity of the problem, Equation 4.7 simplifies to define the vertical velocity w_n of the potential temperature profile as

$$w_n(z) = - \left| \frac{\partial \langle \bar{\theta} \rangle}{\partial z} \right|^{-1} \frac{\partial \langle \bar{\theta} \rangle}{\partial t}, \quad (4.8)$$

where $w_n = v_n$ has been introduced to emphasise that the isolines of potential temperature move in the vertical direction only. If a statistically stationary steady state is required, then in principle it will suffice to set the stabilising velocity to $w_s = -w_n$ such that the resulting volumetric thermal forcing term, $w_s \frac{\partial \langle \bar{\theta} \rangle}{\partial z}$, balances the development of the mean potential temperature profile. However, care must be taken in the values that are obtained for w_n : 1) in growing boundary layers, we require that $w_s < 0$; and 2) large values of w_s must be avoided to ensure that it will not modify the turbulent statistics. We thus define a maximum allowable stabilising velocity $w_{n,max} = \eta w_*$ where $\eta = 0.1$ was used in this study and w_* is a turbulent velocity scale (defined as the Deardorff velocity scale for the convective case and equal to the friction velocity for the stable case). The stabilising

velocity over the boundary-layer height $0 < z < h$ can then be defined according to

$$w_s(z) = \begin{cases} 0 & \text{if } w_n < 0 \\ -w_n & \text{if } 0 \leq w_n < w_{n,max} \\ -w_{n,max} & \text{otherwise.} \end{cases} \quad (4.9)$$

In the absence of radiative forcing or subsidence, the vertical velocity of the potential temperature profile is zero by definition above the boundary layer. However maintaining a negative stabilising velocity above the boundary layer ($z > h$) acts as a secondary system to impede the vertical growth of the boundary layer. Applying the stabilising velocity above the boundary layer is particularly important in sheared flows where the effects of the thermal forcing must also act to equilibrate the development of the velocity profile. The most robust steady states are achieved by linearly increasing the stabilising velocity from the boundary-layer top to the domain top. The conditions enforced in Equation 4.9 and the possibility of non-zero lapse rates, Γ , above the boundary layer (as in simulation tC) necessitate an additional thermal forcing term. A volumetric term, $R(z)$, can be defined that 1) absorbs the remainder of the unsteadiness (arising due to the conditions in Equations 4.9; $w_s \neq -w_n$) and 2) enforces the lapse rate above the boundary layer ($\Gamma = -\frac{R}{w_s}$; also used in van Driel and Jonker (2011) and equivalent to the radiative equilibrium with a constant large-scale divergence). This term can be derived by substituting $\frac{\partial \langle \bar{\theta} \rangle}{\partial t} = -F_\theta$ in Eq. 4.8 giving

$$R = (w_n + w_s) \left| \frac{\partial \langle \bar{\theta} \rangle}{\partial z} \right|. \quad (4.10)$$

Practically, there is a challenge associated with obtaining the vertical velocity of the potential temperature profile: the averaging period must be large enough that the effects of the smallest scale eddies are averaged out but small enough that the vertical development of the boundary layer does not significantly alter the time-averaged statistics. Maximising the horizontal extent of the domain of the transient simulation is advantageous to minimise the associated averaging errors. An averaging period of 1 hour worked for both the stable and convective transient simulations used in this study.

The mean temperature profiles of tC and tS were used to ‘freeze’ the state of these simulations in time at the reference state following this methodology. Figure 4.8 shows the calculated vertical velocity of the potential temperature profile, the stabilising velocity and the volumetric source/ sink profiles which are applied in sC8 (Figure 4.8a and b) and sS6 (Figure 4.8c and d). In the convective case, the defined criteria (Equations 4.9 and 4.10) partition the thermal forcing between 1) a relatively uniform volumetric cooling (that shows agreement with the R profile of method *vi*), 2) a stabilising velocity that sharply

decreases over the entrainment zone (with a lower peak than w_s from method *vi*; partly due to the inaccurate entrainment ratio in *vi* and partly due to the discussed limitations of the applied temporal averaging) and 3) a linear decrease in both w_s and R that forces the flow in the free atmosphere to the predefined lapse rate, $\Gamma = -0.003 \text{ K m}^{-1}$. Note that w_n reaches large negative values within the convective mixed layer in Figure 4.8a. This occurs as $\partial\langle\bar{\theta}\rangle/\partial z$ tends to zero within the convective mixed layer and highlights the importance of the maximum value, $w_{n,max}$, used in Equation 4.9. In the convective case, w_s and R therefore act to balance the two growth mechanisms identified in Equation 4.6 independently. The challenges associated with parametrising the SBL are evident in that a similar partition is not possible for the SBL. The profiles in Figure 4.8c and d illustrate that the stabilising velocity is used to balance the non-linear development of the potential temperature profile in this case. The stratification is large enough and the magnitude of the vertical velocity development is small enough in the SBL that the criteria for $w_{n,max}$ is not used and therefore $R = 0$. The stabilising velocity is largest towards the centre of the SBL where the stratification is weakest. The stabilising velocity linearly decreases up through the residual layer aloft.

The resulting steady-state mean and turbulent profiles of sC8 and sS6 are shown in Figures 4.5 and 4.7. Both simulations show a good agreement with the reference state and therefore this method is shown to have effectively ‘frozen’ a developing convective and stable urban LES. The set-up of these simulations means that the vertical distribution and directionality of the flow forcing (inclusive of the Coriolis force) and the process of entrainment have therefore been captured in a steady state. Whilst this method demands a ‘run-up’ transient simulation, a large domain size for the CBL and does not provide control over e.g. the wind direction, it is the only method through which a range of convective and stable UBLs can be modelled faithfully in a steady state. The use of a ‘run-up’ simulation can be advantageous in the stable case where predefining e.g. the boundary-layer height and turbulent flux profiles is not trivial. For the CBL, this method provides the capability to model the process of penetrative convection in a steady state and accounts for the effect of shear in the entrainment zone (which may limit the application of van Driel and Jonker (2011)’s solution under more strongly sheared conditions). A growing area of interest in urban LES studies is the effect of tall buildings and this method provides the capability to study their interaction with the SBL in the specific case where the building height exceeds that of the domain height.

4.6 Conclusion

Thermal effects play an integral role in the urban environment and fundamentally alter the dispersion of urban air pollutants. However their incorporation into urban LES studies is complicated by corresponding changes in the state of the overlying UBL (fundamental differences in its mean and turbulent structure and the introduction of slow transients). Modelling non-neutral UBLs in statistical steady states is key to obtaining converged statistics and to reducing the degrees of freedom of a given problem. Steady-state methodologies are therefore necessary to balance this inherent transiency. Studies in the literature have typically applied the same simplifications, forcings and boundary conditions as for the well-established neutral case (e.g. the surface layer assumption). Few studies have considered the altered demands arising from the fundamentally different forms of the convective and stable UBL and subsequently there is a lack of coherence on how best to produce realistic steady states. Accurately modelling the state of the UBL is imperative towards understanding the resulting changes to pollution dispersion within and above the UCL. A comprehensive investigation was therefore conducted to determine best practice guidelines (specifically the applied forcing terms, boundary conditions and computational domain sizes; Blocken, 2015) for the modelling of realistic steady-state convective and stable conditions in urban LES.

The boundary conditions and forcings that can be applied to enforce a steady state were reviewed in Section 4.2 and Table 4.1. The resulting steady-state methodologies were contextualised via an integral description of the UBL and the formulation of a generalised thermal forcing term, F_θ . A defining characteristic of these methodologies was the difference between those that cap the top of the boundary layer (ensuring $\frac{dh}{dt} = 0$ by definition) and those that model the UBLs interaction with the quiescent layer aloft. A novel frozen transient method was developed as part of this study that provides a tool to model uncapped steady-state UBLs under both convective and stable conditions.

Two transient simulations of the developing CBL and SBL over an idealised urban morphology were used to provide a realistic reference state. The mean and turbulent profiles of a series of steady-state simulations (set up to reproduce the conditions of the reference state) were then analysed to assess the advantages and shortcomings of a range of steady-state methodologies. Table 4.4 outlines the main findings from this analysis and the guidelines for best practice in future studies.

The results indicated that capping the UBL (restricting the growth of the UBL such that the boundary layer height is equal to the domain height) is suitable in studies where the dynamics within the inner layer or RSL are primarily of interest. This methodology enables user control over e.g. the boundary-layer height, wind direction and friction velocity

Table 4.4: Table summarising the main challenges, results and guidelines regarding the modelling of capped and uncapped steady-state non-neutral UBLs in LES (where capped refers to simulations where the domain top is used to define the height of the modelled boundary layer, $h = l_z$).

Sim.	Highlights
CBL	- Challenges: magnitude of the boundary-layer height and turbulent length scale within the mixed layer and their importance for the turbulent dynamics within and above the UCL. - Results: 1) limiting boundary-layer height to $h/10$ and $h/5$ resulted in reductions in TKE of 61% and 44% respectively, 2) uniform flow and thermal forcings are reasonable simplifications given nature of the mixed layer and 3) domain heights, $l_z \geq h/2$ and $l_z \geq 5 L$, are required for the formation of large-scale convective structures and to obtain realistic representation of TKE over inner layer. - Guidelines: Uniform flow and thermal forcings (top thermal boundary condition set to match that of targetted CBL at the height of the domain top) and minimum domain heights of $l_z \geq h/2$ and $l_z \geq 5 L$ (grid stretching advantageous to maintain high-resolution within UCL).
	- Challenges: Magnitude of vertical growth of the boundary layer $\frac{dh}{dt} \gg w_*$ and resolution requirements within the UCL. - Results: Convective fixed-point solution and frozen transient method both shown to provide a good agreement with the reference state. - Guidelines: Apply either method <i>vi</i> (sets mean potential temperature profile <i>a priori</i> but consideration required on entrainment ratio under sheared conditions) or method <i>vii</i> (use ‘run-up’ simulation and ensure that averaging period does not significantly affect w_n over the entrainment zone).
SBL	- Challenges: Difficulty to categorise or define typical SBL state over urban area and non-uniformity of the flow forcing and wind angle. - Results: 1) Neglecting rotationality of the wind results in a significant over prediction of wind speed in the outer layer, 2) application of a uniform flow forcing leads to underestimation of mechanical generation of turbulence over urban roughness and resulted in fundamental misrepresentation of the modelled flow in sS2 (global intermittency) and 3) several methods of varying complexity were shown to successfully reproduce non-linearities in the turbulent flux profiles, providing good agreement within the inner layer (methods <i>iii-v</i>) and forcings <i>c</i> and <i>d</i>. - Guidelines: Simplest method that also provides numerical control is application of a uniform thermal forcing term (method <i>iii</i>) and a $3/2$ power law forcing (both follow the solution of Nieuwstadt (1984) for the stationary weakly SBL).
	- Challenges: Defining any generalised state of the SBL, parametrising the growth of the SBL (e.g. determining boundary-layer height/ entrainment flux <i>a priori</i>). - Results: Only the frozen transient method, outlined as part of this study, is capable of capturing a steady-state uncapped SBL. - Guidelines: Apply method <i>vii</i> to a transient developing SBL, consideration is required on the surface heat flux and geostrophic velocity to avoid intermittency/ runaway cooling at the surface.

and can be set up to minimise the computational demands of a given simulation. However, care needs to be taken in terms of the domain height and the applied flow and thermal forcing in order to obtain the correct mean and turbulent statistics (simulations citing the same Obukhov length or Richardson number could produce different flow structures; see Table 4.4 for details). In studies where capturing the UBL in its entirety or the UBL's interaction with the quiescent layer aloft is of importance, uncapped steady states are necessary.

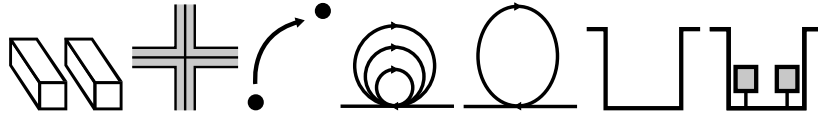
The methods reviewed and developed in this chapter (and more generally in this thesis) are based on statistical steady states in domains with periodic boundary conditions. However, other applications may demand an inflow-outflow configuration. In these cases, a steady-state driver simulation may be executed to obtain a fully realistic turbulent flow field, of which one plane is then used as the inflow boundary condition for the actual simulation (thereby avoiding having to resort to synthetic turbulence at the inflow boundary; Tomas et al., 2015). A pertinent example of this would be the application of the method outlined in Section 4.5 to study the interaction between tall buildings and the SBL e.g. low level inversions. A steady-state driver simulation using this method would enable this problem to be studied with a realistic SBL and even if the building height exceeded the UBL depth.

The methods developed in this study are also applicable to achieve steady states in other situations. Indeed, the issue of transient statistics is prevalent for *any* scalar in a periodic domain, including moisture and pollutants (methods from this chapter are similarly applied to achieve steady-state profiles of the water vapour specific humidity in Chapters 5 and 6). As has been shown, consideration is necessary to define a meaningful steady state (e.g. realistic vertical profiles). However, with this in mind, the methods reviewed and presented in this chapter outline pathways with which to achieve the required steady state in a straightforward manner.

Chapter 5

A minimal model for trees in urban large-eddy simulations

A minimal tree model is presented in this chapter through which the integrated effects of trees within the urban environment (drag, transpiration, shading and deposition) can be modelled at a ‘grey-scale’. A bulk parametric study is conducted and the model is verified against previous numerical studies. The effect of trees on urban air quality is investigated under both neutral and convective atmospheric conditions.



5.1 Introduction

Trees are an integral part of the urban form. By definition, many urban areas are forests and as such the urban canopy layer can be viewed as dichotomous: composed not only of bluff and opaque buildings but also of flexible and permeable trees (where ‘forest’ implies >10% tree cover; Grey et al., 1978; Rowntree, 1984; Oke, 1989). The presence of trees in the urban microclimate affects the local exchanges of momentum, radiation, moisture, heat, noise and pollution. Trees can therefore provide many functions, e.g. shade in the summer time, shelter from winter winds, flood risk protection and noise attenuation (Mullaney et al., 2015; Bozovic et al., 2017). They have also been shown to have both societal and environmental benefits (Willis and Petrokofsky, 2017; Donovan, 2017). However, the roles of trees in mitigating poor urban air quality and the urban heat island (UHI) effect have

been more challenging to quantify in comparison to these other benefits. Their complex interactions with the surrounding microclimate mean that they can have both beneficial and detrimental effects on these two significant urban challenges.

For example, trees actively remove pollutants from the urban atmosphere via enhanced rates of deposition due to their relatively large surface area and, depending on the species, surface properties (introduced in Section 1.5.4; Sæbø et al., 2012). However, they also impose drag on the surrounding urban flow field and subsequently can have adverse effects on pollutant dispersion (in particular in respect to the vertical exchange with the urban boundary layer aloft; discussed in Section 1.5.2; Salim et al., 2015). The role of trees in urban pollution dispersion is often characterised by this balance between their dispersive and depositional properties (Buccolieri et al., 2018). Janhäll (2015) reviewed these two dominant effects and concluded that there is a need for more integrated studies where they are both considered simultaneously. Recent studies that have investigated these effects present results where trees have both helped and hindered the local air quality (Jeanjean et al., 2017; Santiago et al., 2017). Abhijith et al. (2017) reviewed the existing field, experimental and numerical studies on trees and urban air pollution, and reported that on average, across all studies considered, trees had a detrimental effect ($\approx 20\text{-}96\%$ increase in local pollutant concentrations). Buccolieri et al. (2018) reiterated this viewpoint in stating that whilst the problem is case-specific, in the majority of cases the reduced ventilation induced by trees outweighs their active removal of pollutants from the urban atmosphere.

A key conclusion from all three review papers discussed above is that there is a need to study the thermal effects of trees (Janhäll, 2015; Abhijith et al., 2017; Buccolieri et al., 2018). Tree canopies alter the energy balance of the local microclimate. As a result, the distribution and magnitude of buoyancy sources and sinks within the urban canopy layer are different whether a tree is present or not. These thermal effects can therefore significantly affect the dispersion of pollutants.

The thermal effects of trees have predominantly been studied with a focus on their potential to act as tools to mitigate the UHI effect (Oke, 1982). The cooling potential of trees can be attributed to two main processes: 1) transpiration that increases the net latent heat flux and reduces the net sensible heat flux over urban areas (this effect can be pronounced in urban areas due to the advection of generally warmer and drier air through isolated canopies; the oasis effect; Akbari et al., 1990; Grimmond and Oke, 1991) and 2) shading that reduces the net radiative heat incident on surrounding urban surfaces and therefore decreases surface temperatures and heat storage (Oke, 1989; Smithers et al., 2018). Numerous field studies have empirically investigated these cooling effects. But due to the natural variability and case-specificity of the problem, the magnitude and spatial

and temporal extent of this cooling is highly variable across these field studies and it is challenging to attribute cooling to particular processes (Bowler et al., 2010).

In recent years, trees have been incorporated into existing numerical models over a range of scales. Similar to the study of their effect on air quality, a range of modelling approaches have been followed to capture the thermal effects of trees with particular effects often neglected. Yang et al. (2019) review the treatment of trees in both energy balance and computational fluid dynamics (CFD) models and highlight the processes and characteristics (transpiration, radiation transmittance etc.) that are not captured in each of the discussed models. Saaroni et al. (2018) indicate that less than 20% of the 89 field, experimental and numerical studies on tree’s thermal effects that they review directly consider the energy balance of the tree canopy. Tan et al. (2018), Wang et al. (2018) and Rahman et al. (2019) all express the importance of considering both radiative and transpirational effects simultaneously. Specifically, there is a need to be able to attribute cooling between these two processes as that is seen as the key to understanding the differences in tree’s cooling potential between species, times of the year, positions and in different climates.

CFD modelling is a key tool in developing our understanding of these thermal effects due to its ability to resolve the unsteady and turbulent urban flow field and to capture horizontal heterogeneity and exchanges that can be challenging to define in mesoscale and energy balance models. The discussed range of modelling approaches is particularly evident across the CFD literature. For example, the majority of non-urban studies of tree canopies use a volumetric source of heat to model the divergence of net radiation down through the tree canopy (Shaw and Schumann, 1992). Conversely, Li and Wang (2018) and Salim et al. (2018) neglect the effects of heat exchange within the canopy and consider only the reduced radiative heat flux incident on shaded urban surfaces. In contrast, Gromke et al. (2015) neglect radiative exchanges completely but capture the canopy’s bulk transpirational cooling power via a comparison with case-specific field data ($P_c=250 \text{ W m}^{-3}$). This parametrisation has since been used as a benchmark in other studies (Moradpour et al., 2017). These fundamentally different modelling approaches illustrate the necessity to consider energy balances at the scale of interest.

Coupled tree and energy balance models have been incorporated into both RANS (Huttner, 2012; Manickathan et al., 2018) and LES (Matsuda et al., 2018) to good effect, with the ENVI-Met model most widely used in practice (Tan et al., 2016; Wang and Akbari, 2016; Morakinyo et al., 2017). These studies further illustrate the importance of capturing both radiative and transpirational thermal effects. There are numerous challenges associated with capturing the full complexity of this problem. Introducing a three-dimensional radiative transfer model can significantly increase the computational demands of a model

and increases the complexity and degrees of freedom within a given simulation. Resolving the leaf temperature, which has been solved both iteratively and numerically in time in the literature, also increases computational demands and introduces additional free parameters to the problem.

In this chapter, a minimal tree model for urban large-eddy simulation (LES) is presented that is capable of capturing the complex thermal effects of urban tree canopies. Importantly, it 1) minimises the number of free parameters that are introduced to an already complex problem and large parameter space, 2) simplifies the problem such that it is analogous to the application of idealised constant surface heat fluxes (yet is still driven by radiative conditions), 3) avoids the need to resolve the leaf temperature and 4) formulates the thermal effects of the tree such that the contribution of different cooling mechanisms can be quantified. The minimal tree model is therefore capable of capturing the effects necessary to study the role of buoyancy redistribution in pollution dispersion and trees' cooling effects at the microclimate scale. The level of abstraction applied to the minimal tree model is consistent with the simplified approach often applied to the study of non-neutral urban flows (applied in Chapter 4; Boppana et al., 2014) and therefore provides a method through which to conduct targeted simulations of urban trees and the capability to isolate particular phenomena. Section 5.2 describes the formulation of this model. A simplified parametric study is conducted in Section 5.3 to explore the system dynamics. Section 5.4 verifies components of the model and also presents further verification cases for future studies. Results are presented for a base case scenario in Section 5.5, analysing four scenarios with and without trees and under neutral and convective conditions. Finally conclusion are drawn in Section 5.7.

5.2 Minimal tree model

The minimal tree model is devised for urban LES at street-level resolutions. The challenge here is that at $O(1)$ m resolutions, trees are resolved partially. This means that the classical macro-scale parametrisations of tree behaviour, in which the tree processes are fully parametrised, cannot be used. However, a large part of the tree still needs to be modelled as it is computationally prohibitive and physically undesirable to resolve the entire tree at the micro-scale. Thus, borrowing a term from the atmospheric community, there is a need for a 'grey-zone' tree model, in which the tree is partially modelled (scales of tree modelling shown diagrammatically in Figure 5.1).

The formulation of a grey-zone tree model requires a consistent and spatially inhomogeneous representation of the effects of the tree canopy (therefore capable of capturing the

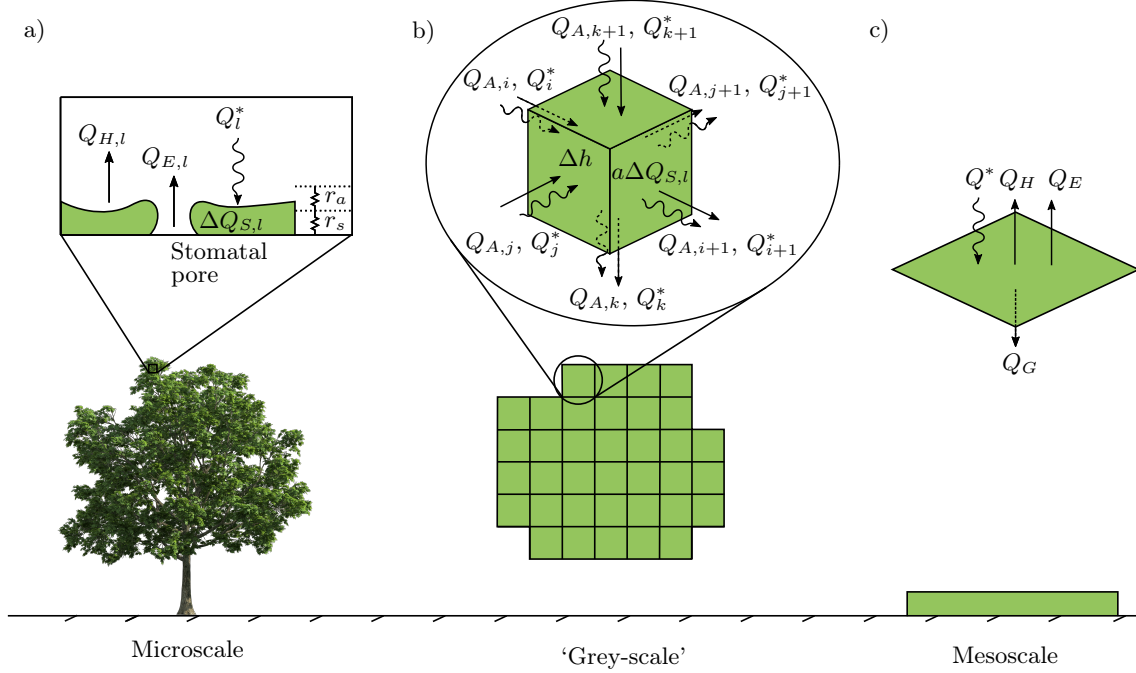


Figure 5.1: Diagrammatic representation of the different scales of tree modelling. a) Microscale representation with individual leaf energy balances, b) the grey-scale approach followed in this thesis that parametrises the microscale effects at the resolution of an LES model and c) mesoscale where the effects of individual trees occur at a subgrid scale and the net effects are calculated as a bulk energy balance.

intrinsic variability of tree effects in urban LES). In practice this means representing the drag, thermal, moisture, radiative and deposition processes of the tree canopy as sink/source terms at the designated resolution. The tree canopy is modelled by homogenising its presence within cells of the computational domain such that they have two constituent parts: air and the tree's biomass (the geometry method; Yang et al., 2019). The micro-scale tree-air interactions occur at a sub-grid scale and are therefore must be resolved through a set of volumetric source and sink terms (S_{u_i} , S_φ , S_θ and S_q) that can be applied directly into the right-hand side of uDALES' governing equations (Equations 2.3 and 2.4).

These micro-scale interactions can be captured at the 'grey-scale' by applying the concept of coarse graining and parametrising the combined effects of a given surface area of leaves on the corresponding volume of air. Specifically, the minimal tree model defines these volumetric terms as functions of the properties of the surrounding air and a set of representative parameters. It is important to note that the parameters must be able to encompass the natural variability associated with the problem (e.g. different species and climates) and be investigated through field and experimental studies such that accurate values can be obtained.

An example of such a parameter is the leaf area density, a (m^2/m^3), that defines the one-sided surface area of leaves over the volume of air that they are present in. This term acts as an inverse length scale that relates fluxes at the leaf surface to those over the surrounding volume of air. It is possible to obtain values for the leaf area density both experimentally and in the field and this term is capable of capturing both species and seasonal variability (Jeanjean et al., 2017).

By modelling the sensible and latent heat exchange between the tree canopy and the surrounding air, the minimal tree model expands upon the majority of existing tree models in urban CFD that largely focus upon drag and depositional effects under neutral conditions (Moonen et al., 2013; Santiago et al., 2017). Capturing this heat transfer by resolving an energy balance at the ‘grey-scale’ and therefore modelling the fluxes of both temperature and moisture provides a more complete method in comparison to studies where empirical parametrisations are used (Gromke et al., 2015; Moradpour et al., 2017) or particular phenomena, e.g. shading, are neglected (Li and Wang, 2018). Other studies where an energy balance is modelled to capture the thermal effects of trees include the work of Manickathan et al. (2018) and Matsuda et al. (2018). The main simplifications and assumptions applied to form the minimal tree model are: 1) a big-leaf approach (assuming that the values obtained from a given cell are representative of the average conditions of all leaves and that these do not differ at a subgrid scale), 2) simplifying the radiative budget to a one-dimensional problem and 3) applying a uniform stomatal resistance. The formulation of the discussed source terms is outlined below.

5.2.1 Drag

The volumetric term for drag, S_{u_i} , is well-established in the literature. Drag is defined as a function of the local wind velocity and the drag coefficient, C_d . This term captures both the viscous (Darcy) and inertial losses

$$S_{u_i} = -aC_d|u|u_i \quad (5.1)$$

where $|u|$ is the absolute wind speed and C_d is a drag coefficient. Typical values of C_d range from 0.1-0.3 depending on the tree species; $C_d = 0.2$ has been widely applied in the literature for non-species specific studies (Buccolieri et al., 2018).

Many studies also define additional terms to capture the turbulent kinetic energy (TKE) production and enhanced dissipation resulting from the application of drag to the mean flow (e.g. following the closure scheme of Wilson and Shaw, 1977). Buccolieri et al. (2018) reviews the range of closure schemes and coefficients applied across different studies to capture these effects and evaluates the performance of models with and without these ad-

ditional terms. There are too few studies to conclude whether these sub-grid scale terms lead to better predictions but LES studies where they are neglected achieve very good agreement with the CODASC wind-tunnel experiments (Moonen et al., 2013). LES captures most of the dynamic scales so providing a subgrid TKE term is much less important than for RANS in which the entire energy spectrum needs to be modelled. The minimal tree model therefore neglects these additional terms and empirical coefficients.

5.2.2 Deposition

The volumetric term for deposition, S_φ , adapts the classical approach from mesoscale models (introduced in Section 1.5.4) to a volume of leaves using the leaf-area density

$$S_\varphi = -au_d\varphi \quad (5.2)$$

where u_d is the deposition velocity and φ is the pollution concentration. The deposition velocity is a conductance term that must capture the aerodynamic, laminar boundary layer and surface resistances to pollutant deposition. Values of u_d therefore vary hugely between species, pollutants and also due to e.g. ambient humidity and atmospheric stability and there is currently insufficient data to produce a robust parametrisation (Janhäll, 2015). Sæbø et al. (2012) found that u_d could vary by 10-20 times depending on the leaf hairiness. Comprehensive studies have been conducted into the magnitude of constant values of u_d for different tree species, pollutants and under different conditions (Janhäll, 2015; Santiago et al., 2017). Typical values are less than 0.01 m s^{-1} for most pollutants and tree species. A value of 0.005 m s^{-1} is applied throughout this thesis (similar values have been applied to separate studies of NO_x , $\text{PM}_{2.5}$ and PM_{10} ; Buccolieri et al., 2018).

5.2.3 Canopy energy balance

It has been established that to effectively capture the thermal effects of trees it is necessary to consider the surrounding energy balance system (Yang et al., 2019). The presence of a tree canopy fundamentally alters the energy balance of the local urban microclimate due to 1) radiative exchanges within the canopy and between the canopy, the sky and the surrounding buildings and 2) sensible and latent heat exchanges between the tree and the surrounding air. Figure 5.1 highlights the relevant energy balances at the different scales of the problem. At the micro-scale (Figure 5.1a), one can define a leaf surface energy balance following

$$c_{pl} \frac{dT_l}{dt} = Q_l^* - Q_{H,l} - Q_{E,l} \quad (5.3)$$

where c_{pl} is the heat capacity of a leaf, T_l is the leaf surface temperature and Q_l^* , $Q_{H,l}$ and $Q_{E,l}$ are the net radiative, sensible and latent heat fluxes respectively. The second and

third terms on the right hand side of Equation 5.3 define the transfer of energy between the leaf and the surrounding air. Applying the big-leaf approach (Dai et al., 2004) at the grey-scale by integrating over a volume of tree biomass (Figure 5.1b), Equation 5.3 becomes

$$\frac{d}{dt} \int I dV = \oint Q^* dS - \int a Q_{H,l} dV - \int a Q_{E,l} dV. \quad (5.4)$$

where I is the internal energy of the tree biomass and Q^* is the net radiative flux defined over the surface of the control volume. The leaf area density, a , translates the sensible and latent heat flux from individual leaf surfaces to a volumetric term. In terms of pollution dispersion and the UHI effect we are primarily interested in how this balance affects the enthalpy of the surrounding air. In the LES domain, cells where the tree canopy is present have two constituent parts: moist air and the tree's biomass. As such we can define a corresponding energy balance for the specific enthalpy of moist air, h_v , over the same control volume

$$\frac{d}{dt} \int h_v dV = \oint Q_A dS + \int a Q_{H,l} dV + \int a Q_{E,l} dV \quad (5.5)$$

where Q_A is the advective heat flux. Equation 5.5 is inherently coupled with Equation 5.4 and summed these two equations define the 'grey-scale' energy balance as depicted in Figure 5.1b. The advective term in Equation 5.5 is captured by construction in the LES model. The specific enthalpy of moist air is a function of both the potential temperature, θ , and water vapour specific humidity, q_v , which are modelled in uDALES (see Section 2.3). Correspondingly, the latent heat flux represents the energy transferred to vapourise liquid water at the leaf surface and results in a source of q_v in the air

$$S_{q_v} = a \frac{Q_{E,l}}{\rho L_v} \quad (5.6)$$

where ρ is the air density and L_v is the latent heat of vapourisation. The sensible heat flux is the energy supplied to warm or cool the surrounding air and therefore can be defined as

$$S_{\theta} = a \frac{Q_{H,l}}{\rho c_p} \quad (5.7)$$

where c_p is the heat capacity of the air. The minimal tree model must therefore obtain values of $Q_{E,l}$ and $Q_{H,l}$ following the leaf surface energy balance (Equation 5.3). All four terms in this equation can be defined as a function of the leaf temperature however the following methodology outlines a method through which resolving this additional term can be avoided.

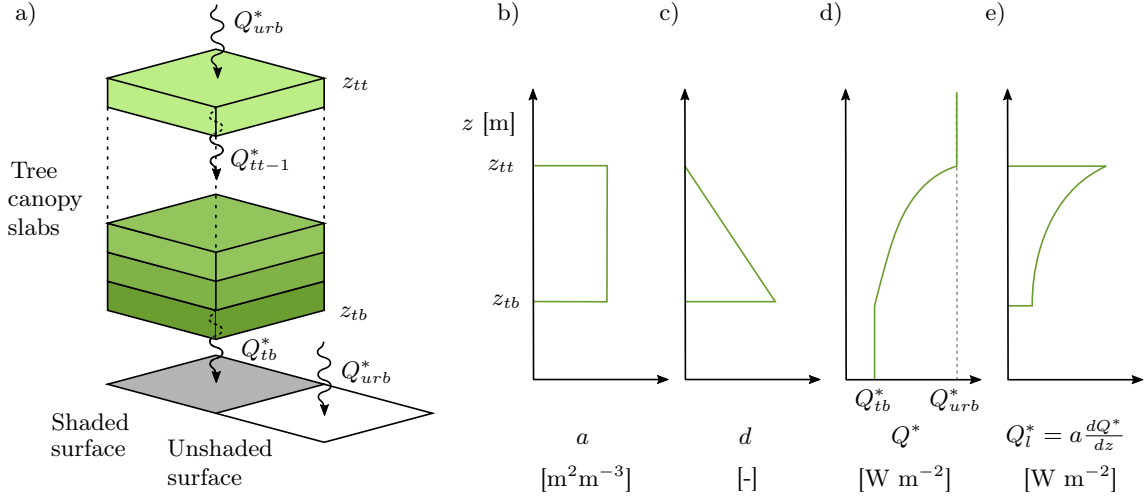


Figure 5.2: a) Diagrammatic representation of the one-dimensional radiative budget and vertical profiles of b) leaf area density, c) leaf area index, d) Net radiation and e) net radiation incident on the leaf surface.

Radiative budget

Short- and long-wave radiation is absorbed, reflected, transmitted and emitted throughout the tree canopy. The radiation budget over a volume of leaves is three-dimensional, involves multiple scattering and is a function of the leaf temperature itself. Matsuda et al. (2018) use the radiosity method to solve a three-dimensional radiative transfer model. This approach captures complex horizontal exchanges of radiation (e.g. between the adjacent buildings) however it is also computationally intensive and introduces numerous additional free parameters to the problem.

A common simplification when considering the radiative budget of a tree canopy is to reduce this to a one-dimensional problem by assuming relative horizontal homogeneity within the canopy (Monteith and Unsworth, 2013) and that the radiative budget is dominated by the incoming radiation from above. This simplification is consistent with the application of constant surface heat fluxes at the road and rooftop levels for unshaded surfaces. Similar assumptions are made in the urban studies of Li and Wang (2018) and Manickathan et al. (2018). Following this methodology, simulations can be partially driven by the assigned radiative conditions. The urban form can be split into unshaded surfaces where the incident net radiative energy is transferred unimpeded and shaded surfaces where the shading effect of the tree results in reduced incoming net radiative energy (see Figure 5.2).

Above the shaded surfaces, the tree canopy is simplified to a series of horizontal slabs where the incoming radiative flux from above is larger than the outgoing flux to the layer

below. The attenuation of radiation through the tree canopy is a function of e.g. the leaf orientation, albedo, transmissivity and emissivity. An established method to simplify this radiative exchange through the tree canopy is the application of the Beer-Lambert law that relates the attenuation of radiative fluxes to the properties of the medium through which it is travelling (Brown and Covey, 1966; Shaw and Schumann, 1992)

$$Q^*(z) = Q_{urb}^* e^{-\alpha d(z)} \quad (5.8)$$

where Q_{urb}^* is the net radiation above the urban area, α is the extinction coefficient and d is the cumulative leaf area index defined as $d(z) = \int_z^{z_{tb}} a(z') dz'$. This equation relates the attenuation of radiation through the tree canopy to the properties of the canopy itself. The attenuation coefficient is the product of the cumulative leaf area index and the extinction coefficient. The extinction coefficient is therefore a non-dimensional parameter that captures the multiple scattering and absorption of radiation within the canopy (as a function of the leaf albedo, emissivity, transmissivity and orientation). Analysis was performed of the performance of this term against more complex radiative approaches in Appendix A.4 (Zhao and Qualls, 2005, 2006). The net radiation above the urban area is defined following established mesoscale parametrisations (defined as a function of the time of day, day of year, cloud cover, surface albedo and surface emissivity; Kasten and Czeplak, 1980; Holtslag and Nieuwstadt, 1986). The same set of parametrisations are applied for the minimal tree model as used in SIRANE and these are outlined in Appendix A.1.

Assuming a uniform leaf area density over the tree canopy, Figure 5.2 displays example profiles of the leaf area index, net radiation and net radiation at the leaf surface. Figure 5.2e indicates how leaves at the top of the tree receive the largest net radiative flux. Given the leaf area density over a specific layer and the vertical size of that layer, the net radiation at the leaf surface Q_l^* is given by

$$Q_l^*(z) = \frac{1}{a} \frac{dQ^*}{dz}. \quad (5.9)$$

Heat storage

The heat storage term in Equation 5.4 encompasses both the change in internal energy of the tree canopy and the photosynthetic heat component. The thermal properties of trees and the ability to regulate leaf temperatures via transpiration mean that in comparison to the other materials found in urban areas, a tree's thermal inertia and therefore storage term is relatively low (the photosynthetic component is generally assumed to be negligible). Oliphant et al. (2004) investigated the heat storage term within deciduous forest canopies and found that generally both the internal energy and photosynthetic storage terms are

negligible (maximum 5% of total storage term inclusive of soil and air in the canopy). Many studies neglect heat storage within the tree canopy completely and the same simplification is applied in the minimal tree model ($\Delta Q_{S,l} = 0$; Manickathan et al., 2018).

Latent and sensible heat fluxes

The net radiation on the leaf surface, Q_l^* , therefore quantifies the available energy for sensible and latent heat exchange between the leaves and the surrounding air. Figure 5.1a diagrammatically shows this relationship and also highlights the aerodynamic resistance, r_a , and stomatal resistance, r_s , terms that can be used to define the heat and water vapour transfer coefficients. The aerodynamic resistance r_a captures the resistance to turbulent exchange within the leaf's boundary layer and can be approximated by (Thom, 1968; Dauzat et al., 2001)

$$r_a = C \left(\frac{l}{|u_i|} \right)^{1/2} \quad (5.10)$$

where l is the leaf size, $|u|$ is the wind speed and C is a proportionality coefficient (Parlange and Waggoner (1972) empirically defined $C \approx 130 \text{ s}^{1/2} \text{ m}^{-1}$ by studying leaves in a wind-tunnel). The stomatal resistance r_s captures the regulatory control exhibited by the leaf on the size of the stomatal openings. The stoma are pores that facilitate gas exchange and as such determine the rate of transpiration from the leaves of the tree. There are numerous parametrisations of the stomatal resistance as reviewed by Damour et al. (2010) that aim to capture the physiological processes occurring within the tree (soil water availability, temperature, shortwave irradiation, CO_2 concentration etc.). For simplicity, uniform values of stomatal resistance are applied in this study. For deciduous trees the minimum stomatal resistance r_s is in the range $150\text{-}450 \text{ s m}^{-1}$ (Jones, 2013). The sensible and latent heat fluxes between the leaf and surrounding air then follow

$$Q_{H,l} = \frac{2}{r_a} \rho c_p (T_l - \theta) \quad (5.11)$$

$$Q_{E,l} = \frac{1}{r_a + r_s} \frac{\rho R_a L_v}{p_0 R_v} (\varepsilon_{v,l} - \varepsilon_v) \quad (5.12)$$

where $\varepsilon_{v,l}$ is the vapour pressure at the leaf surface (Pa) and ε_v is the vapour pressure of the surrounding air (Pa). The factor 2 in Equation 5.11 is due to the definition of the leaf area as the one-sided area (most leaves are hypostomatous meaning that stoma are situated on the underside of the leaf only whereas sensible heat exchange occurs on both sides of the leaves). Classically, the vapour pressure at the leaf surface is assumed to equal the saturation vapour pressure at the temperature of the leaf surface $\varepsilon_{v,l} = \varepsilon_s(T_l)$ (Robitu et al., 2006). Both the sensible and latent heat fluxes are therefore a function of the leaf temperature.

The necessity to model the leaf temperature can be avoided following the derivation of the classical Penman-Monteith equation. Equation 5.12 can be substituted into Equation 5.3 by partitioning the vapour pressure difference between the leaf surface and the surrounding air to the vapour pressure deficit of the surrounding air, $D = \varepsilon_s(\theta) - \varepsilon_a$, and a term that is proportional to the temperature difference between the leaf surface and the surrounding atmosphere $s(T_l - \theta)$ (where s is the slope of the curve relating saturation pressure to temperature; Jones, 2013). The sensible heat flux can then be substituted into this equation and this term can then be substituted into the energy balance for the leaf resulting in

$$Q_{E,l} = \frac{sQ_l^* + \frac{2}{r_a}\rho c_p D}{s + 2\gamma \frac{(r_a + r_s)}{r_a}} \quad (5.13)$$

where γ is the psychrometric constant. The full derivation is provided in Appendix A.5. The form of this equation is helpful to understand tree cooling. The first term in the numerator relates to the transpiration that occurs due to the available energy from the net radiation incident on the leaf surface. The second term defines the transpiration that occurs due to the advection of drier air over the leaf surface (or the ‘oasis’ effect). McNaughton and Jarvis (1983) rearranged the classical Penman-Monteith equation to define a decoupling factor, Ω , that determines the relative significance of these two terms. Applying the same methodology to Equation 5.13 gives

$$Q_{E,l} = \Omega \frac{s}{s + 2\gamma} Q_l^* + (1 - \Omega) \frac{\rho c_p}{\gamma r_s} D, \quad (5.14)$$

where

$$\Omega = \left(1 + \frac{2\gamma}{s + 2\gamma} \frac{r_s}{r_a}\right)^{-1} \quad (5.15)$$

from which we can define the first and second terms on the right-hand side of Equation 5.14 as the radiative component of the latent heat flux, $Q_{Er,l}$, and the advective component of the latent heat flux, $Q_{Ea,l}$. The decoupling factor is therefore proportional to the ratio between the stomatal and aerodynamic resistances (with the limits that if $r_s/r_a \ll 1$ then $\Omega \approx 1$ and if $r_s/r_a \gg 1$ then $\Omega \approx 0$). It changes depending on the relative significance of atmospheric versus surface processes (Oke et al., 2017). Typical bulk values for trees are ≈ 0.2 due to their elevated positions and therefore strong coupling to a large proportion of the ABL (suggesting that the latent heat flux is primarily driven by its advective component; Oke et al., 2017). Higher values of the decoupling factor Ω are typical of e.g. grass that are more responsive to their available energy (McNaughton and Jarvis, 1983). The decoupling factor determines this relationship however the available energy at the leaf surface and the vapour pressure deficit are defined by the radiative budget and local transfers of momentum and moisture respectively.

Finally, the leaf surface energy balance can be closed by rearranging Equation 5.3 for the sensible heat flux ($\Delta Q_{S,l} = 0$ as discussed above)

$$Q_{H,l} = Q_l^* - Q_{E,l}. \quad (5.16)$$

5.2.4 Urban surface energy balance

The energy balance of the tree canopy is therefore driven partially via the assigned net radiation above the urban surface Q_{urb}^* . The aim of the minimal tree model is to act alongside simplified uniform surface heat fluxes and also to capture the shading effect of the tree canopy. It is therefore necessary to define an urban surface energy balance that estimates the sensible heat flux from the unshaded and shaded urban surfaces from Q_{urb}^* and Q_{tb}^* respectively (see Figure 5.2). Following from the one-dimensional treatment of the radiative budget and assuming the urban surfaces are dry ($Q_{E,urb} = 0$), an energy balance can be defined for the unshaded road and roof surfaces following

$$Q_{urb}^* = Q_{H,urb} - \Delta Q_{S,urb} \quad (5.17)$$

where Q_{urb}^* is defined following the methodology discussed in Section 5.2.3, $Q_{H,urb}$ is the sensible heat flux from the ground- and roof-level surfaces and $\Delta Q_{S,urb}$ is the heat storage term of the roads/ buildings.

In order to define a constant surface heat flux $\phi_{0,\theta} = \frac{Q_H}{\rho c_p}$, the heat storage term for the unshaded surfaces is parametrised as a function of the net radiation above the urban area following the Objective Hysteresis Model (OHM; Grimmond and Oke, 1999, 2002)

$$\Delta Q_{S,urb} = A_1 Q_{urb}^* + A_2 \frac{\partial Q_{urb}^*}{\partial t} + A_3 \quad (5.18)$$

where A_1 , A_2 (h) and A_3 (Wm^{-2}) are constants that can be defined empirically or analytically following Sun et al. (2017). In this study, average empirical values for paved/ impervious surfaces are used ($A_1 = 0.70$, $A_2 = 0.33$ and $A_3 = -38$). At the shaded surfaces the net radiative flux in Equation 5.17 is Q_{tb}^* ($< Q_{urb}^*$) and the corresponding heat storage term is scaled linearly by the ratio Q_{tb}^*/Q_{urb}^* . The sensible heat fluxes underneath the trees are therefore smaller than unshaded surfaces as a function of the shading effect of the canopy.

5.3 Bulk parametric study

Despite simplifying the problem significantly and minimising the number of additional free parameters, the energy balance component of the minimal tree model introduces relatively

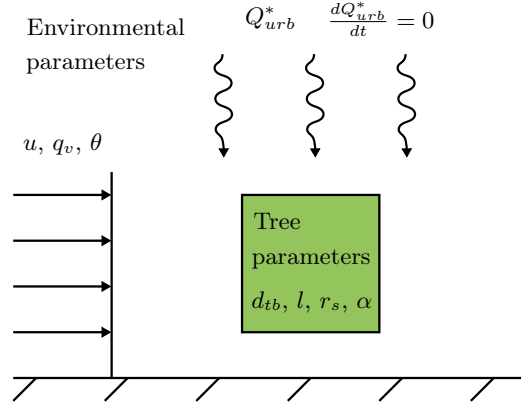


Figure 5.3: Diagram of the idealised set up of a single row of trees in a crossflow used to conduct the bulk parametric study.

complex system dynamics. It is therefore advantageous to first explore the main processes and sensitivities of the defined energy balance system (tree canopies and urban surfaces combined). In this section, trees' thermal effects are first discussed in the context of the minimal tree model formulation outlined above. A bulk sensitivity analysis of the system is then presented focussing on the leaf area index d_{tb} and the net radiation Q_{urb}^* .

As introduced in Section 5.1, the thermal effects of tree canopies are generally simplified into two dominant mechanisms: transpirational cooling (indicative of negative sensible heat fluxes between the tree canopy and the surrounding air) and shading (characterised by reduced sensible heat fluxes from the urban surface and heat storage within the urban form). In terms of the minimal tree model, the necessary condition for a volume of leaves to cool the surrounding air is that the latent heat flux at the leaves' surfaces is larger than the net radiative flux absorbed by them $Q_{E,l} > Q_l^*$. Thus resulting in a negative sensible heat flux $Q_{H,l}$ and volumetric cooling term S_θ (transpirational cooling; see Equation 5.16). Conversely if $Q_{E,l} < Q_l^*$ then $Q_{H,l}$ is positive and the tree canopy warms the surrounding air. The latent heat flux $Q_{E,l}$ is decoupled into advective ($Q_{Ea,l}$; a function of the local vapour pressure deficit D) and radiative ($Q_{Er,l}$) components in Equation 5.14. It is therefore a function of the net radiative flux Q_l^* itself meaning that the weighting of this relationship is significant (partly captured by the decoupling factor Ω). The radiation absorbed by the tree canopy also leads to a reduction in the radiative flux incident on the shaded surface beneath the canopy. The greater the attenuation of net radiation through the tree canopy, the more significant the shading effect ($Q_{H,shade} < Q_{H,urb}$ where $Q_{H,shade}$ is the sensible heat flux at ground-level directly underneath the tree). The buoyancy effect of the tree canopy is determined by three effects: 1) the volumetric source/ sink of potential temperature within the tree canopy, 2) the volumetric source of water vapour within the

5.3 BULK PARAMETRIC STUDY

Table 5.1: Bulk environmental and tree parameters used in the base and comparison cases for the parametric study.

Parameters	Environmental				Tree			
	u	q_v	θ	Q_{urb}^*	d	l	r_s	α
Units	[m s ⁻¹]	[kg kg ⁻¹]	[K]	[W m ⁻²]	[-]	[m]	[s m ⁻¹]	[-]
Base case	1	0.0094	293	300	6	0.1	250	0.4
Following Shashua-Bar et al. (2009)	1	0.0094	305.2	300	6	0.05	150	0.4

tree canopy (that acts to reduce the density of the surrounding volume of air; increasing the virtual potential temperature; Equation 2.6) and 3) the reduced surface sensible heat flux underneath the tree canopy. The trees' cooling and buoyancy effects are therefore a function of both the surrounding environmental parameters (which vary both spatially and temporally) and the assigned parameters of the tree canopy itself.

Manickathan et al. (2018) conduct a parametric study in RANS to investigate the sensitivity of a tree's transpirational cooling to both environmental and tree parameters. An idealised set-up of a single row of trees in a cross-flow is used in this investigation (depicted in Figure 5.3). A base case scenario is devised over which the system parameters are varied. Parameters that directly affect the exchange of moisture between the leaves and the surrounding air (e.g. relative humidity and stomatal resistance) exhibit fairly straightforward relationships with this transpirational process. For example, if the oncoming air is less humid, the latent heat flux is increased and as such the sensible heat flux is low and the tree acts to cool the surrounding air. However, at high humidity the exchange of moisture is limited and the tree canopy exhibits net positive sensible heat fluxes. Parameters that affect the latent and sensible heat exchange but not the radiative budget of the tree canopy follow this general relationship. The sensitivity of the bulk tree energy balance to the leaf area index d_{tb} and net radiation Q_{urb}^* is more complex.

The main differences between the tree model implemented in RANS by Manickathan et al. (2018) to the minimal tree model presented here are that it solves the leaf temperature iteratively and it provides a different treatment of the radiative budget (the canopy shading effect is neglected). Before discussing LES results, a similar parametric study is conducted to expand on the results of Manickathan et al. (2018) using the capabilities of the minimal tree model. The same set-up as in Manickathan et al. (2018) is used to conduct this study but with the highly idealised condition of uniform environmental and tree parameters (see Figure 5.3). Table 5.1 displays the base case parameters that were used, which are

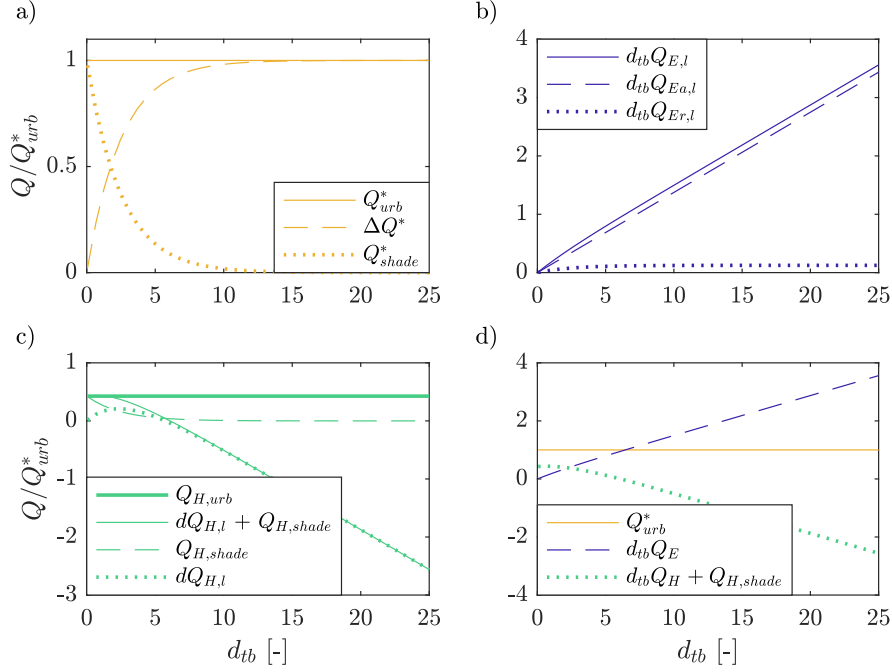


Figure 5.4: Plots illustrating the sensitivity of the calculated a) radiative, b) latent, c) sensible and d) combined energy balance of the bulk minimal tree model to the leaf area index d_{tb} .

conductive of a scenario where both the shading and transpirational cooling effects are relevant to the canopy energy balance.

Figure 5.4 shows the sensitivity of the net energy balance to the assigned leaf area index, d_{tb} (representative of the height and/or leaf area density of the tree canopy). Figure 5.4a indicates the shading effect of the tree canopy. Up to $d_{tb} \approx 5/\alpha$ the net absorbed radiative flux increases and correspondingly the net radiative flux absorbed by the shaded surface underneath the tree decreases. Above this threshold value, a further increase in d_{tb} results in no change as the canopy has reached its maximum shading effect. Figure 5.4b shows the quasi-linear relationship between the latent heat flux and d_{tb} . The bulk latent heat flux over the canopy is broken down into advective and radiative components following Equation 5.14. The radiative contribution to the latent heat flux increases up to $d_{tb} \approx \frac{5}{\alpha}$ but is relatively small across all d_{tb} for the base case conditions. The advective component increases linearly with increasing leaf area index d_{tb} . This relationship is what defines the transpirational cooling effect. Parameters such as the relative humidity, wind speed and stomatal resistance act to define the gradient of this line. Figure 5.4c shows the predicted sensible heat fluxes at the shaded and unshaded surfaces and over the tree canopy. Comparing the sum of the shaded surface and tree canopy to the unshaded surface provides a method to understand the cooling effect of the tree and also to partition this

between the shading and the transpirational cooling effects. The shading effect increases up to $d_{tb} \approx 5/\alpha$ as seen by the reduced sensible heat flux from the shaded urban surface. At high leaf area indices the transpirational cooling effect is shown to dominate as the sensible heat flux decreases at the same linear rate discussed above and shown in Figure 5.4b. A more complex energy balance regime is observed for lower leaf area indices where the sensible heat flux from the tree canopy is positive (the net radiation absorbed by the leaves exceeds the latent heat flux). This phenomenon is important to note and the magnitude and range of d_{tb} over which this is significant depends on both the net radiation (increases this effect at low d_{tb} and also increases the relative importance of tree shading) and the parameters that directly affect the latent heat flux (an increase in the gradient $\partial Q_{E,l}/\partial a$ such that this dominates over radiative warming of the canopy or a decrease where transpiration is limited and the this warming effect is more significant).

The empirical relationship outlined by Gromke et al. (2015) ($P_c = 250 \text{ W m}^{-3}$ per unit of leaf area density) acts under the assumption that the advective transpirational cooling effect is dominating the canopy energy balance. This relationship is defined via a comparison with the field study of Shashua-Bar et al. (2009) which was conducted in a very hot and dry climate with ample water supply to the trees. Considering the conditions of this field study, the same relationship between leaf area density and transpirational cooling can be obtained by approximating the environmental and tree parameters from this study (applied parameters shown in Table 5.1) and inputting them into bulk minimal tree model. In this case study (relative humidity of 35% and low stomatal resistance) the transpirational cooling effects dominate the energy balance system and the empirical relationship of Gromke and Ruck (2012) holds. However, evidently the magnitude of this volumetric cooling ratio is highly case specific and its applicability to other conditions is therefore limited.

Returning to the base case set-up, Figure 5.5 presents a sensitivity analysis with respect to the net radiative flux over the urban area. The use of the decoupling factor Ω is evident in Figure 5.5b where the increase in the net latent heat flux is directly attributed to the radiative component $Q_{Er,l}$. For high net radiative fluxes (typical of sunny, midday conditions), the base case scenario is shown to lead to net positive sensible heat fluxes in Figure 5.5c (although the magnitude of the total sensible heat flux remains lower than that of the unshaded surface). This finding can be better explained by the relationship shown in Figure 5.5d: as the net radiative flux increases, the corresponding increase in the latent heat flux is much smaller and as such the sensible heat flux rises at a faster rate. The increase in the latent heat flux is shown to be only a function of the radiative component of this term at the leaf surface and therefore this effect is a function of the decoupling

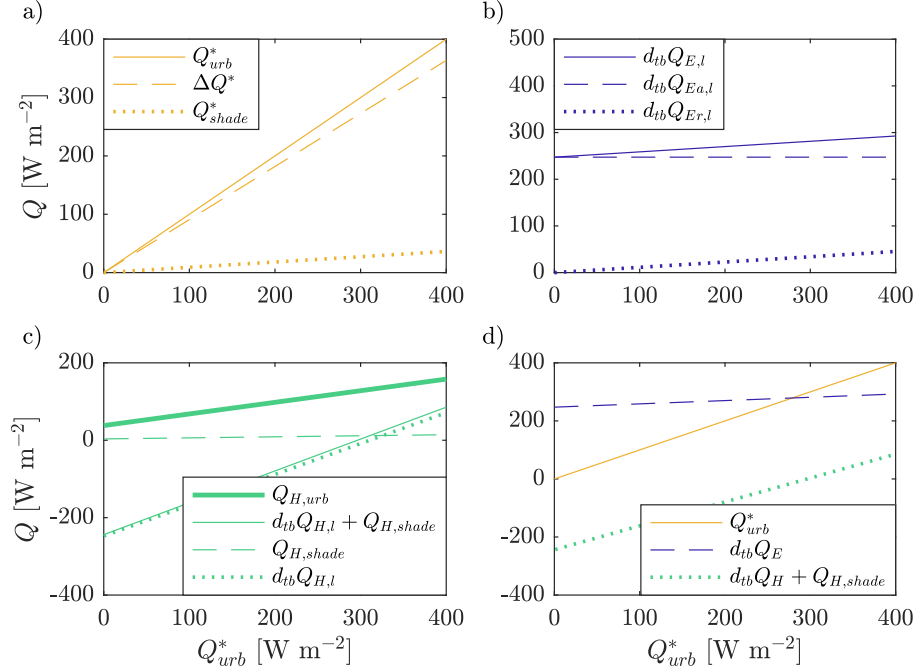


Figure 5.5: Plots illustrating the sensitivity of the calculated a) radiative, b) latent, c) sensible and d) combined energy balance of the bulk minimal tree model to the net radiation.

factor, Ω , and partly of the ratio between the aerodynamic and stomatal resistances.

The above analysis provides an initial insight into the additional free parameters introduced to a given urban simulation by the minimal tree model. It also highlights the mechanisms through which existing observational studies produce highly case specific results. The results discussed in this section are highly idealised. In application within a CFD model, the vertical inhomogeneity of the net radiative flux and the three-dimensional variability of the other environmental parameters (u , q_v and θ) means that similar balances to those discussed here occur at the ‘grey-scale’ within the tree canopy.

5.4 Verification

The challenges associated with the scaling of vegetation for experimental studies mean that there is a paucity of validation cases to apply the minimal tree model to (particularly ones that include thermal effects; Gromke et al., 2015). In the following section we therefore verify the formulation of the minimal tree model against existing numerical studies. In doing so, we also present results that can be used to evaluate the performance of future vegetation models. Figure 5.6 illustrates the three simulation set-ups that are explored in this section: a full-canopy, half-canopy and a single row of trees.

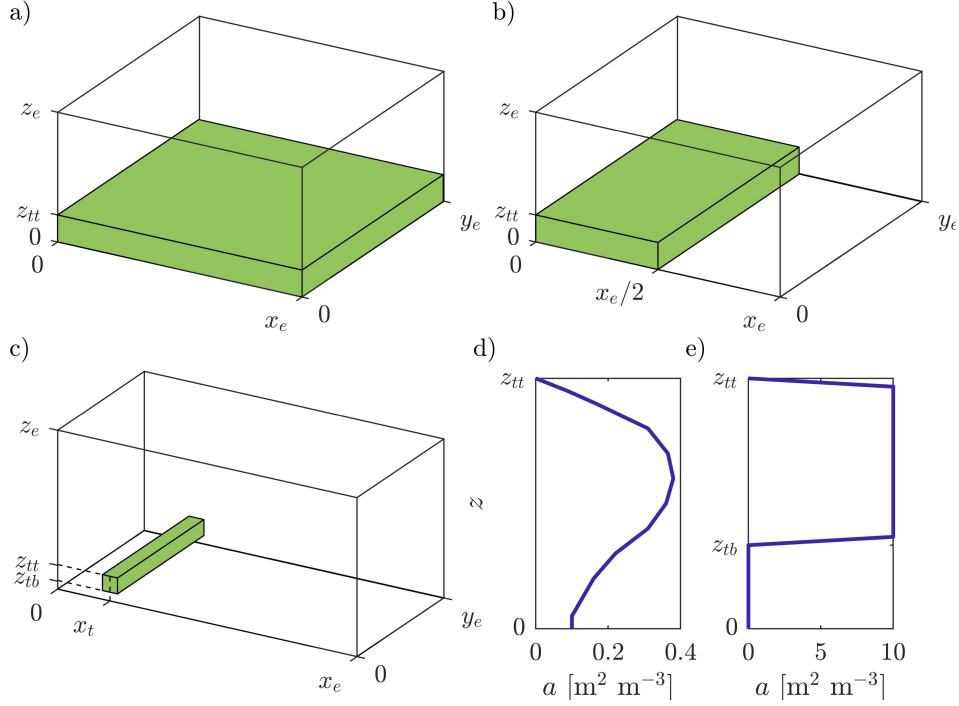


Figure 5.6: a) Full-canopy, b) half-canopy and c) a single row of trees (following Manickathan et al., 2018) domain and canopy set-ups for the verification simulations. d) and e) Leaf area density profiles applied within this set of simulations.

5.4.1 Full-canopy

The full canopy set-up has been studied extensively both to better understand the mesoscale effects of forest canopies on the ABL and to verify the drag applied across various vegetation models (Shaw and Schumann, 1992; Xie and Li, 2005; Gu et al., 2010). The simulation set-up of Shaw and Schumann (1992) is followed in defining a domain size of $192 \times 96 \times 60$ m with a horizontally homogeneous tree canopy of height $H = 20$ m. The cell size is 1 m in all directions. A constant volume flow rate is set in the streamwise direction enforcing a bulk wind speed of 2 m s^{-1} , periodic boundary conditions are defined in the horizontal directions and a free-slip condition is set at the top of the domain. Neutral conditions were used for the case of the drag validation. The wall function is applied at the bottom of the domain with a roughness length of 0.02 m. The tree canopy properties are a non-uniform vertical profile of leaf area density with a leaf area index d_{tb} of 2 (as shown in Figure 5.6d) and a drag coefficient of 0.15. The full-canopy simulation was run up for a period of 8000 s and results were taken over a further 2000 s averaging period with a sampling time of 2 s.

Figure 5.7 compares the mean velocity and Reynolds stress profiles obtained in uDALES

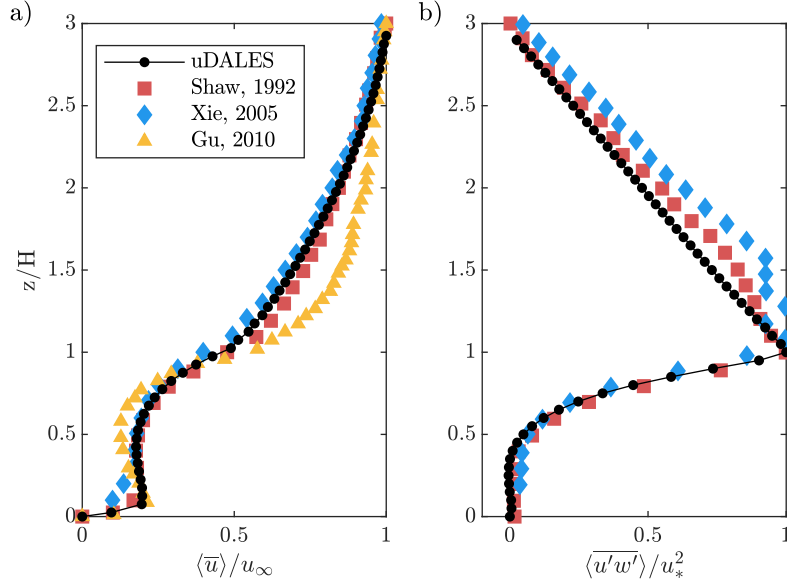


Figure 5.7: Time and spanwise averaged profiles of (a) mean streamwise velocity and (b) turbulent momentum flux for the full-canopy simulation. Comparison against three other numerical studies.

and compared against the results of Shaw and Schumann (1992), Xie and Li (2005) and Gu et al. (2010). Good agreement is provided both within and above the tree canopy. These profiles show qualitative agreement with those found in field studies of forest canopies. The mean wind speed is near-logarithmic above the canopy, there is an exponential decay of velocity in the upper half of the canopy, the parameter $u(0.25H)/u(1.4H) = 0.27$ agrees with observation (equivalent value of 0.28 in Cionco, 1979) and there is a reversal in the velocity gradient in the lower half of the canopy (Shaw and Schumann, 1992).

5.4.2 Full- and half-canopy comparison

Shaw and Schumann (1992) incorporated thermal effects into their full-canopy investigation by introducing a source term, S_θ , as a function of the divergence of net radiation through the tree canopy. This methodology is equivalent to neglecting the latent heat flux and any ground heat flux in the minimal tree model. Xie and Li (2005) developed upon this study by investigating the half-canopy simulation set-up displayed in Figure 5.6b. Two cases are considered in this investigation. The first case follows the same set of assumptions as Shaw and Schumann (1992) in defining constant volumetric heat sources throughout the tree canopy (this case aims to reproduce strong radiative conditions). The second case reverses the sign of the volumetric source terms such that the tree canopies act to cool the surrounding air (this case aims to reproduce weak radiative conditions where

transpirational cooling dominates). With this simplified approach, reasonable agreement was obtained with the field study of Gao et al. (1989).

The minimal tree model provides the capability to reconsider these full- and half-canopy set-ups, this time with a full energy balance model. Two simulations are run using the minimal tree model, one with a full-canopy (FC) and one with a half-canopy (HC) set-up. The domain size for both simulations is $192 \times 192 \times 96$ m with a resolution of 1 m in all directions. The same boundary conditions for momentum, flow forcing and tree canopy properties are assigned as discussed in Section 5.4.1. Non-neutral conditions were modelled in these simulations with periodic boundary conditions applied for potential temperature and specific humidity. Uniform initial profiles of $\theta = 288$ K and $q_v = 0.007$ kg kg⁻¹ are defined (relative humidity of 67%). The bottom boundary condition for heat is set following Section 5.2.4 and a steady state is enforced by assigning constant values at the domain top ($\theta(h) = 288$ K and $q_v(h) = 0.007$ kg kg⁻¹; therefore following the surface layer assumption as defined in Chapter 4 with uniform turbulent heat and moisture flux profiles once the flow is fully developed). Using the values outlined in Xie et al. (2003), the net radiation is set to 256 W m^{-2} ($\frac{dQ_{urb}^*}{dt} = 0 \text{ W m}^{-2}\text{h}^{-1}$ for consistency) and the extinction coefficient is 0.6. The leaf size is 0.15 m and the stomatal resistance is 200 s m^{-1} . Both simulations were run up for a period of 14400 seconds before averaging was done for a period of 7200 seconds with a sampling time of 2 seconds.

Figure 5.8 displays the vertical profiles of time and spanwise averaged streamwise velocity, potential temperature and water vapour specific humidity for both simulations. Due to the streamwise homogeneity of the full-canopy simulation, the profiles are uniform in the x -direction. The velocity profile has a similar shape as in the full-canopy case in absence of convection (Figure 5.7). The main difference is that the convective nature of the flow results in enhanced vertical mixing above the tree canopy. The half-canopy simulation is inhomogeneous in the streamwise direction. The drag imposed from the tree acts to reduce the wind speed below $z = H$. Towards the end of the tree canopy ($x = 96$ m), the velocity profile approaches that of the full-canopy simulation. Without the presence of the tree canopy, the velocity profile recovers from the exponential decay and countergradient over the latter half of the domain. The flow speeds up and approaches a near-logarithmic profile towards the end of the domain. The velocity profiles are in good agreement with those of Xie and Li (2005).

The profiles of potential temperature and specific humidity form as a result of the minimal tree model's energy balance. In the full-canopy case, it is evident that the tree has a net warming effect in the top layer of the tree canopy ($z > 0.5H$). Over this region, the net radiative flux incident on the leaves of the canopy exceeds the latent heat flux (which

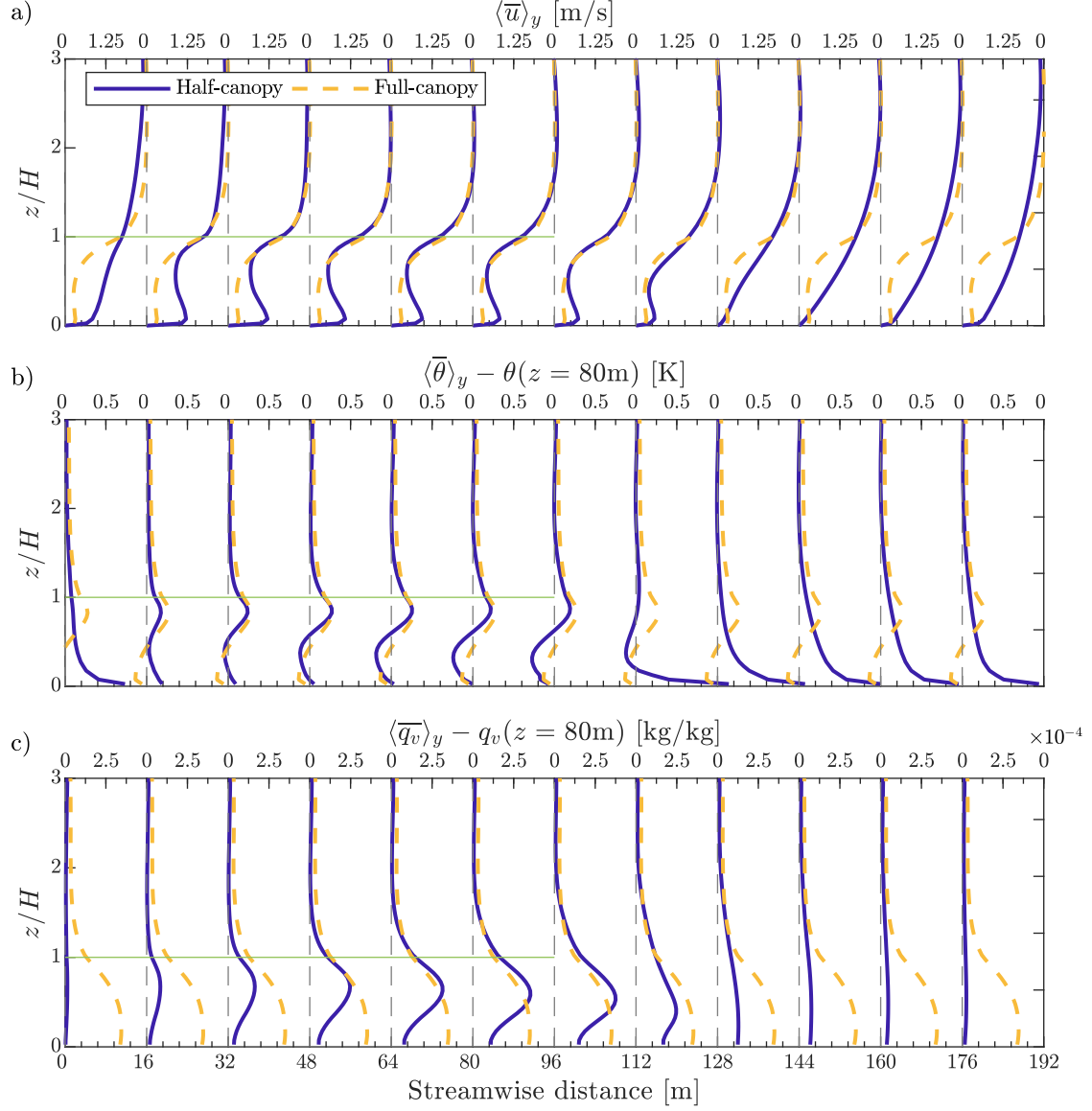


Figure 5.8: Spanwise and time averaged a) streamwise velocity, b) potential temperature and c) water vapour specific humidity for both the half- and full-canopy simulations. The green line indicates the spatial extent of the tree canopy in the half-canopy simulation.

is a function of both this radiative flux and the vapour pressure deficit). The attenuation of radiation down through the tree canopy is such that below this height transpirational cooling is the dominant effect and the air is cooled by the canopy. In the full canopy case the advective component of the latent heat flux is driven by the vertical exchange of less humid air down into the tree canopy. Figure 5.8c clearly shows that the specific humidity is larger over the tree canopy and quickly mixed into the flow overhead. The increased humidity within the canopy results in lower rates of transpiration. Despite these differences the latent heat flux is dominated by the advective component as opposed to that relating to the available energy at the leaf surface. For the simple full-canopy case, a tree canopy exhibits both the heating and cooling effects that were initially investigated in Xie and Li (2005).

In the half-canopy simulation, the advection of drier air into the tree canopy is not limited to vertical exchange. The step change between the modelled unshaded urban surface and the tree canopy leads to the advection of less humid, warmer air into the tree canopy at higher velocities, a phenomena that is called the ‘oasis’ effect. The latent heat flux is therefore larger than in the full canopy simulation, which is evident in the rate of change in the specific humidity in 5.8c up to $x = 96$ m. As the humidity rises along the streamwise direction through the tree canopy, the magnitude of the leading edge ‘oasis’ effect diminishes and towards the end of the canopy ($x \approx 80$ m) the energy balance approaches that of the full canopy simulation. The temperature of the incoming air to the tree canopy is relatively increased (in comparison to simulation FC) due to the sensible heat flux from the unshaded surface. The larger latent heat flux however leads directly to larger cooling of the air in the lower layers of the tree canopy. The air is quickly cooled within the tree canopy and is cooler than the full canopy simulation at $x = 96$ m. Despite the increased latent heat flux within the half-canopy simulation, the top of the tree canopy (that receives the most radiative energy) still acts to warm the surrounding air. But the tree layer over which this is the case is relatively reduced in comparison the full-canopy case ($z > 0.6H$).

The tree energy balance results in system dynamics that were not captured in the study of Xie and Li (2005). However certain phenomena identified by Xie and Li (2005), such as the presence of an elevated inversion in temperature towards the top of the tree canopy can be observed in both cases. This simplistic set-up exhibits the details and sensitivities associated with the thermal effects of trees. Small changes in environmental parameters such as the wind speed and relative humidity have significant effects on the expected latent and sensible heat fluxes. The tree canopies are shown to both warm and cool the surrounding air indicating that the the relationships between the local latent heat $Q_{E,I}$ and

net radiative Q_l^* fluxes discussed in Section 5.3 both apply for the modelled conditions. It is important to note that under these fairly strong radiative conditions the rates of heating/cooling can vary spatially within a single tree canopy. The vertical distribution of the net radiative flux is particularly important in this regard. The set-ups provided in this section can act as a reference point for future model verifications.

5.4.3 Single row of trees

The final verification set-up models an isolated row of trees using LES. The set-up mimics that of Manickathan et al. (2018) (as discussed in Section 5.3 and shown in Figure 5.6c). Manickathan et al. (2018) neglect the tree shading effect but their study provides a simulation set-up that enables a verification of the tree canopy energy balance model (with adjustments made considering the differences between the two models and tree modelling approaches).

In order to model a fully-developed, neutral upwind boundary layer (without the effects of the tree wake), a precursor simulation was used to define the velocity profile at the inlet. The methodology for driver simulations was discussed in Chapter 2. The domain size of the driver simulation is $20 \times 10 \times 10$ m with a resolution of 0.05 m in all directions. A constant volume flow rate is assigned with a bulk wind speed of 1.35 m s^{-1} . Periodic boundary conditions are assigned in the horizontal directions, a free-slip condition is applied at the domain top and the roughness length of the ground surface is 0.018 m. The driver simulation is run-up for 1000 s and a further 1500 s are used to drive the inlet of the single-row-of-trees simulation.

The same domain size and top and bottom boundary conditions for momentum are assigned in the single-row-of-trees simulation as the driver. Uniform profiles of potential temperature ($\theta = 303.15 \text{ K}$) and specific humidity ($q_v = 0.016 \text{ kg kg}^{-1}$) are assigned at the inlet and a convective outflow condition is enforced at the outlet plane. Periodic spanwise boundary conditions and zero-flux top and bottom boundary conditions are applied for potential temperature and specific humidity. The urban surface energy balance discussed in Section 5.2.4 is switched off (zero surface heat flux) in order to enable a direct comparison. The tree is 0.5 m above the ground, 1 m wide in the streamwise direction, 1 m tall and is positioned 3 m from the inlet boundary (see Figure 5.6c). The drag coefficient $C_d = 0.2$, the decay coefficient $\alpha = 0.78$, the leaf area density $a = 10$ and is uniform over the tree height (see Figure 5.6e), the net radiation above the canopy $Q^* = 797 \text{ W m}^{-2}$, the leaf size $l = 0.1 \text{ m}$ and the stomatal resistance $r_s = 150 \text{ s m}^{-1}$.

Figure 5.9 shows the instantaneous, mean and root-mean-square fields from the single-row-of-trees simulation. The wake of the tree can be seen to extend downstream from the

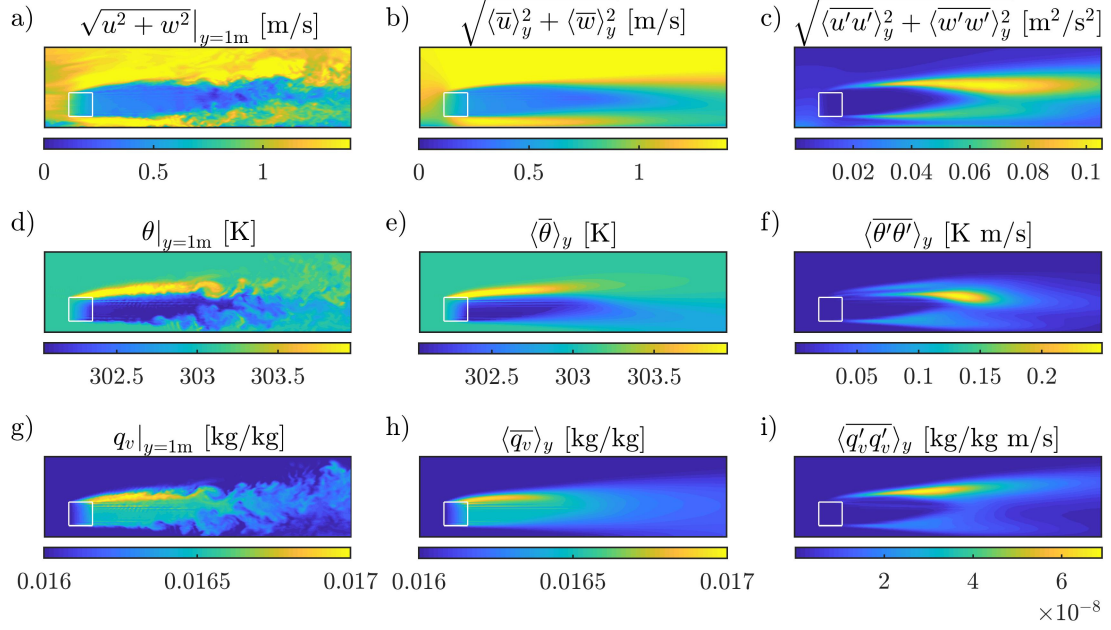


Figure 5.9: Instantaneous, mean and root-mean-square fields of wind speed (a, b and c), potential temperature (d, e and f) and water vapour specific humidity (g, h and i) for the single-row-of-trees simulation. The white box indicates the position of the tree canopy.

tree canopy. The mean profiles are qualitatively similar to the mean values obtained from the RANS model in Manickathan et al. (2018).

Figure 5.10a compares the net radiative, sensible heat and latent heat fluxes at the leaf surfaces at the centre of the modelled tree ($x = 3.5$ m) from uDALES and compares them to the results obtained in the RANS simulation of Manickathan et al. (2018). The fluxes are averaged in time and in the spanwise direction in uDALES. A good agreement is shown between the two models. The radiative budget applied in the minimal tree model captures the same exponential decay of radiative energy down through the tree canopy. The modelled sensible and latent heat fluxes are also very similar. This finding illustrates that the application of the Penman transformation produces equivalent results to a model in which the leaf temperature is resolved through an iterative process (this finding is not surprising as the iterative approach also estimates the leaf temperature based upon the sensible heat flux that is solved via the same leaf energy balance equation). This agreement has also been verified extensively by applying both techniques within the bulk model discussed in Section 5.3 and comparing the results. The small differences that are evident between the two models may be partly associated with these different modelling approaches but also occur due to the challenges in reproducing the same turbulent boundary layer as

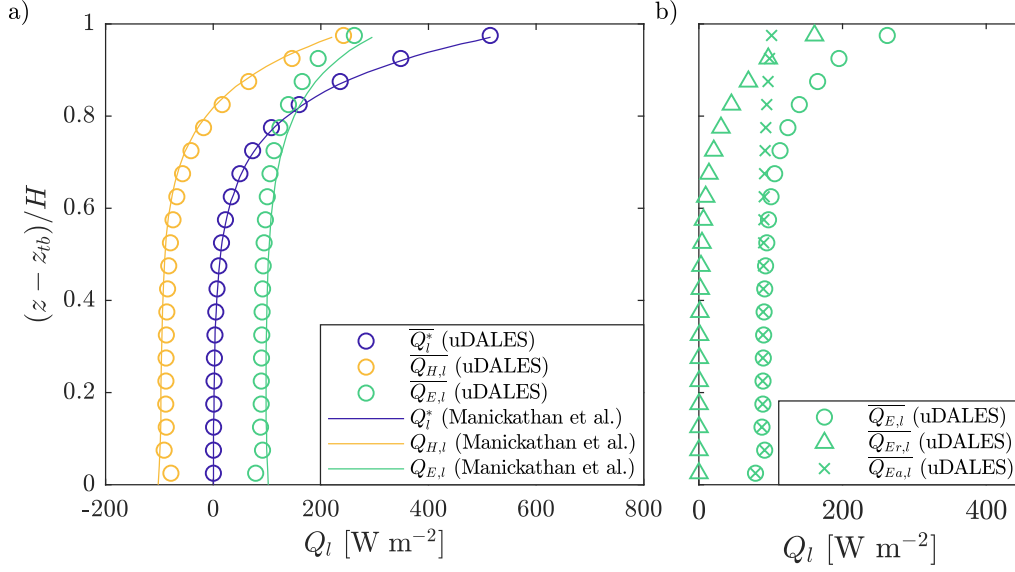


Figure 5.10: a) Net radiative, sensible and latent heat fluxes and b) total, advective and radiative components of the latent heat fluxes on the leaf surfaces at $x = 3.5$ m in the single-row-of-trees case. Comparison against values obtained by Manickathan et al. (2018).

the RANS simulation in LES. The oncoming wind speed is not perfectly matched which results in small deviations in the drag characteristics of the tree and to the aerodynamic resistances. However, these differences are shown to be minimal in Figure 5.10a.

Similar to the case discussed in Section 5.4.2, the net radiation on the leaf surfaces is larger than the latent heat flux at the top of the tree canopy and therefore the sensible heat flux is positive. As the net radiation decays through the tree canopy, this effect is reversed and the sensible heat flux is negative. The latent heat flux is decomposed into its radiative and advective components in Figure 5.10b. The advective component is relatively uniform across the height of the tree due to the uniform upwind profiles of potential temperature and specific humidity. The radiative component results in an increase in the total latent heat flux towards the top of the canopy. These findings concur with the analysis introduced in Figure 5.5b. The breakdown of these two terms further indicates how the advective cooling effect acts independently to the radiative balance. For this case, a change in e.g. the relative humidity of the oncoming air acts to directly change the magnitude of $Q_{Ea,l}$. This point further elaborates on the discussion within Section 5.3 that, under conditions where the advective component of the latent heat flux is much larger than the net radiative energy incident on the leaf surface, this process will dominate throughout the tree canopy. As this term decreases and is of similar magnitude to the radiative flux, a regime exists where the tree can both warm and cool the air in different positions. Within this regime,

the decoupling factor is of interest. The ratio between the radiative component of the latent heat flux and net radiative flux is important in terms of the energy balance at the top of the tree and can either minimise or maximise the heating effect that has been shown here and in Section 5.4.2.

5.5 Trees in infinite canyons

The variability in trees' physical effects discussed in Sections 5.3 and 5.4 above is amplified within the urban environment where localised heterogeneity further complicates the problem (particularly in terms of its case-specificity). The minimal tree model provides the capability to study the integrated (dispersive, depositional and thermal) effects of trees and therefore this inherent variability. In this section, an investigation is conducted into the role of trees within an infinite urban canyon set-up. This set-up without trees has been studied extensively in the literature and provides a platform through which to explore the sensitivity of tree's combined effects to other key parameters. A base case set-up is defined for which analysis is provided for a given tree set-up under neutral and convective conditions and with and without depositional effects. The following section presents the simulation set-up and results of this base case which presents the application of the minimal tree model to an urban environment.

5.5.1 Simulation set-up

A simulation set-up is devised that enables systematic analysis of the effect of trees on air quality under both neutral and convective conditions. Infinite canyons are modelled with an aspect ratio of 1 and a canyon height of 32 m (see Figure 5.11). The base case tree set-up is composed of two trees on the wind- and lee-ward sides of each canyon as shown in Figure 5.11a and b. The constant leaf area density and cuboid forms of the tree canopies provide an idealised set-up that 1) facilitates a simplified configuration for analysis and 2) has been used widely in existing studies of urban trees (Salim et al., 2011a; Li and Wang, 2018). Non-uniform leaf area densities and more complex tree canopy forms (see Chapter 6) can also be modelled using the minimal tree model and are also of interest to gain a holistic understanding of the effects of urban trees. One configuration (tree size, shape, parameters) is considered in this study, however a more comprehensive study will be required in the future to fully investigate the relevant parameter space. A pollutant line source is positioned at the bottom centre of each canyon (Gaussian distribution with a standard deviation of 0.5 m) and a normalised emission rate of $1 \text{ g m}^{-1}\text{s}^{-1}$.

Four simulations are run for the base case scenario analysis: neutral (N), neutral with

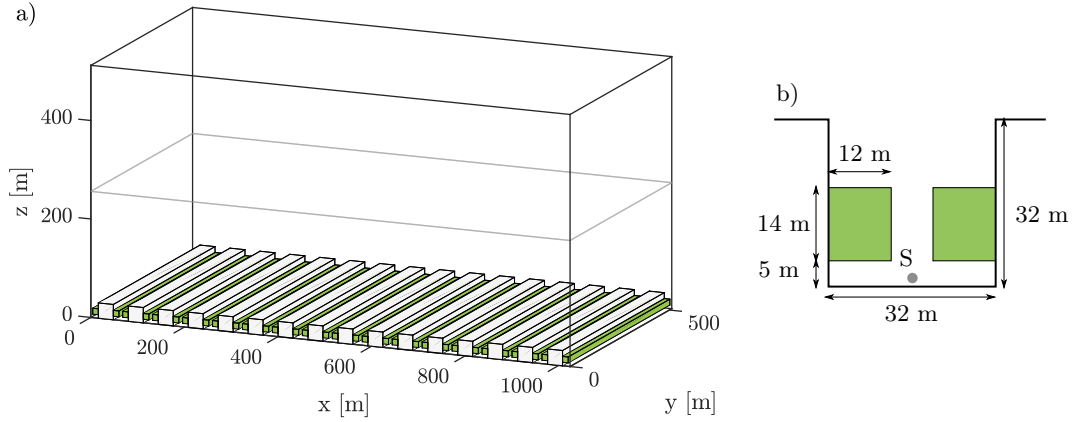


Figure 5.11: a) Domain and canopy set-up applied for the simulations of trees in infinite urban canyons (the grey line represents the domain height used for the neutral simulations). b) Diagrammatic representation of the tree configuration within each street canyon.

trees (NT), convective (C) and convective with trees (CT). The main simulation parameters are outlined in Table 5.2. Values are assigned that are typical of large urban trees following the literature (Jones, 2013; Buccolieri et al., 2018). The radiative conditions defined for the convective case are that of a summer’s day at noon with low cloud cover (conductive of strong net irradiation at the urban surface and a low zenith angle; these conditions are approximated following the parametrisations outlined in Appendix A.1; CERC, 2001). A friction velocity of 0.3 m s^{-1} is enforced across all simulations using a constant pressure gradient forcing. $q_{v,0}$ and θ_0 indicate the assigned values for uniform initial profiles of water vapour specific humidity and potential temperature.

Incorporating tree’s integrated effects on the momentum, temperature, moisture and pollutant fields necessitates careful consideration in terms of the applied boundary conditions. Following the methodology applied throughout this thesis, periodic boundary conditions are applied in the spanwise directions for momentum, temperature and moisture such that a statistically stationary and horizontally homogeneous UBL is modelled. Applying the findings of Chapter 4, a domain height, l_z , is set that is greater than half the predicted convective boundary layer (CBL) height ($h > h_C/2$) in simulations C and CT. Using the meteorological conditions approximated for the convective, no trees base case: $h_C \approx 1024 \text{ m}$ (estimated using mesoscale parametrisations; Batchvarova and Grynning, 1991; CERC, 2001). A domain height of 512 m is therefore defined for the convective cases. The same scaling and subsequent systematic reduction of turbulent kinetic energy does not apply in the neutral case and as such the domain height in simulations N and NT is set to 256 m for computational efficiency (indicated by the grey line in Figure 5.11a).

5.5 TREES IN INFINITE CANYONS

Table 5.2: Environmental and tree parameters used in the four simulations of the trees in infinite canyons study: neutral (N), neutral with trees (NT), convective (C) and convective with trees (CT).

Sim.	Environmental					Tree				
	u_* [m s ⁻¹]	$q_{v,0}$ [kg kg ⁻¹]	θ_0 [K]	Q_{urb}^* [W m ⁻²]	$\frac{dQ_{urb}^*}{dt}$ [W m ⁻² hr ⁻¹]	a [m ² m ⁻³]	l [m]	r_s [s m ⁻¹]	α [-]	u_d [m s ⁻¹]
N	0.3	-	-	-	-	-	-	-	-	-
NT	0.3	-	-	-	-	1	0.15	-	-	0.005
C	0.3	-	288.15	450.2	15.47	-	-	-	-	-
CT	0.3	0.00735	288.15	450.2	15.47	1	0.15	200	0.4	0.005

The grid is stretched in the z -direction in simulations C and CT such that the grid size is the same as simulations N and NT but a resolution of 1 m is retained up to $z = 50$ m. The maximum vertical cell size is 3.21 m at the top of the domain. The streamwise length of the domain is set to $2h$ for these two convective simulations resulting in a relatively large domain for an investigation of infinite canyons (the same streamwise length is defined for the neutral simulations to enable a direct comparison of the developing pollutant fields).

Steady-state methodology *iii* from Chapter 4 is followed to produce realistic steady-state convective conditions. The heat flux at the top of the domain is set to equal half of net heat flux into the fluid domain from the unshaded surfaces, shaded surfaces and tree canopies combined. This calculation is made by integrating over the relevant areas and volumes: $\phi_{\theta,h} = \frac{\int \phi_{\theta,urb} dA + \int \phi_{\theta,shade} dA + \int S_{\theta} dV}{2A}$ (where A is the horizontal extent of road and roof top surfaces within the domain). A uniform volumetric cooling term is applied throughout the domain to account for the resulting imbalance in the total heat flux in and out of the domain and to enforce the expected linear profile of turbulent heat flux in the CBL: $R = -\frac{\phi_{\theta,h}}{h_M}$ (where h_M is the vertical size of the domain weighted by the masking matrix over the buildings). In a typical stationary CBL, one expects a flux of moisture from the ‘surface’, a relatively uniform profile of humidity over the convective mixed-layer and a flux of the same sign over the entrainment zone where moisture is transferred to the free atmosphere above (Stull, 2012). To replicate these expected profiles in uDALES, the flux at the top of the domain is defined to equal the integrated flux from the tree canopies $\phi_{q_v,h} = \frac{\int S_{q_v} dV}{A}$ (resulting in a uniform profile of the turbulent moisture flux; equivalent to method *ii* in Chapter 4).

The concentration fields require a different treatment. Assuming that the pollutant field is also in equilibrium with the modelled stationary UBL implies that there is a region

upwind with a self-similar emissions rate over which the pollutant has mixed across the boundary layer depth. The validity of this assumption can be understood by considering the time and length scales over which this mixing would need to occur. The eddy turnover time is a characteristic time scale that is representative of this mixing process. $\tau \approx \frac{h}{u_*}$ or $\tau \approx \frac{h}{w_*}$ for neutral or freely convective conditions respectively where $w_* = ((g/\theta_0)h\phi_{\theta_v,0})^{1/3}$ is the Deardorff scale. Inputting the values associated with simulations N and C and using $h = 512$ m for both calculations, the corresponding eddy turn-over times are 1707 s and 380 s respectively. Given a typical wind speed of 5 m s^{-1} these timescales relate to corresponding upwind distances of 8.5 km and 1.9 km under neutral and convective conditions respectively. The assumption for stationarity in the pollutant field is therefore more reasonable under convective conditions. The highlighted difference means that such an assumption is not applicable in a study where neutral and convective conditions are directly compared. For this reason, and more generally due to the typical variability in emissions at the discussed scales, inflow-outflow boundary conditions are assigned for the pollutant scalar fields across all simulations. The pollutant fields therefore develops in the streamwise direction.

A uniform background concentration is assigned at the inlet boundary to represent the upwind air quality (as is done in Chapter 3). The deposition of pollutants onto the tree canopies introduces a sink term to Equation 2.4. The rate of deposition is a function of the surrounding pollutant concentration. Different pollutants have different source attributions to road emissions and exist at different ratios in terms of background and roadside concentrations. In the following study, the passive scalar pollution field is decomposed into two terms: the background concentration (φ_b ; assigned as a uniform profile of 1 at the inflow boundary) and the emitted concentration (φ_e ; assigned as a uniform profile of 0 at the inflow boundary). Given the linearity of the scalar conservation equation (Equation 2.4; neglecting chemistry) and the volumetric deposition term (Equation 5.2), different pollutants or different emission rates can be explored via the same set of results using $\varphi = \omega\varphi_b + (1 - \omega)\varphi_e$ to define the total pollution concentrations where ω is an assigned weighting. This method allows for more complex depositional effects to be explored from smaller datasets and, to the author's knowledge, is novel to the work conducted in this thesis. It presents a useful tool in studying depositional or active removal processes in the urban environment.

Simulations are run up until the UBL has reached a steady-state. Statistics are then taken with a sampling time of 2 s and sampling period of 6000 s or larger.

5.5.2 Results

Flow field

Figure 5.12 and 5.13 show the variation in flow profile and velocities within the domain for the four simulated cases. Focussing first on the difference between the neutral and convective cases without trees, it is apparent that the wind speed above the UCL is higher for the neutral case in both of these figures. The friction velocity is matched across these simulations and the large domain-size turnovers present in the convective case result in increased drag that, given the same flow forcing, results in lower bulk wind speeds. The enhanced mixing in the convective UBL also results in practically uniform velocity profiles above the UCL, unlike the neutral case where a logarithmic profile is exhibited. Despite the reduced wind speeds above the UCL, simulation C exhibits higher in-canyon velocities than simulation N (canyon-average absolute wind speed of 0.55 m s^{-1} as opposed to 0.48 m s^{-1} in the neutral case; 14% higher). The canyon vortex in this simulation is consistent with the thermally reinforced recirculation regime identified in the study of bottom heated canyons of Kim and Baik (2001). The streamlines at the top of the canyon in Figure 5.13c curve upwards over the top of the canyon (a phenomenon discussed by Allegrini et al., 2014) and this enhanced vortex diameter further illustrates the effect of buoyancy on the canyon vortex (shown to weaken the shear layer in Li et al., 2010). Given equal wind speeds above the UCL, the convective case would exhibit significantly higher in-canyon velocities in comparison to the neutral case (the flow reinforcement has acted to balance out the relative wind speed deficit in these two simulations). Similar effects have been exhibited for ground heating of canyons with different aspect ratios (a regime change due to heating was only exhibited for an aspect ratio of 0.5; Li et al., 2012).

The effect of trees is to reduce the velocities inside the canyons for both the neutral and convective cases. This observation is congruent to expectations as the drag force exerted by the tree leaves results in lowered in-canyon velocities (canyon-averaged absolute wind speeds reduced by 62% and 72% with trees for neutral and convective conditions respectively). The blocking effect of the trees is shown to be significant and of similar magnitude in both simulations NT and CT. Figure 5.13b and d indicate that the presence of trees has also significantly altered the canonical canyon vortex exhibited by simulations N and C. The centre of the vortex is moved significantly as the top of the windward tree crown acts to inhibit flow down the facade of the windward building in both simulations. A smaller secondary vortex also forms in the lower leeward corner of the canyon in both simulations NT and CT. Whilst the positions of the centres of these vortices are similar for both neutral and convective conditions, there is an apparent difference in the structure

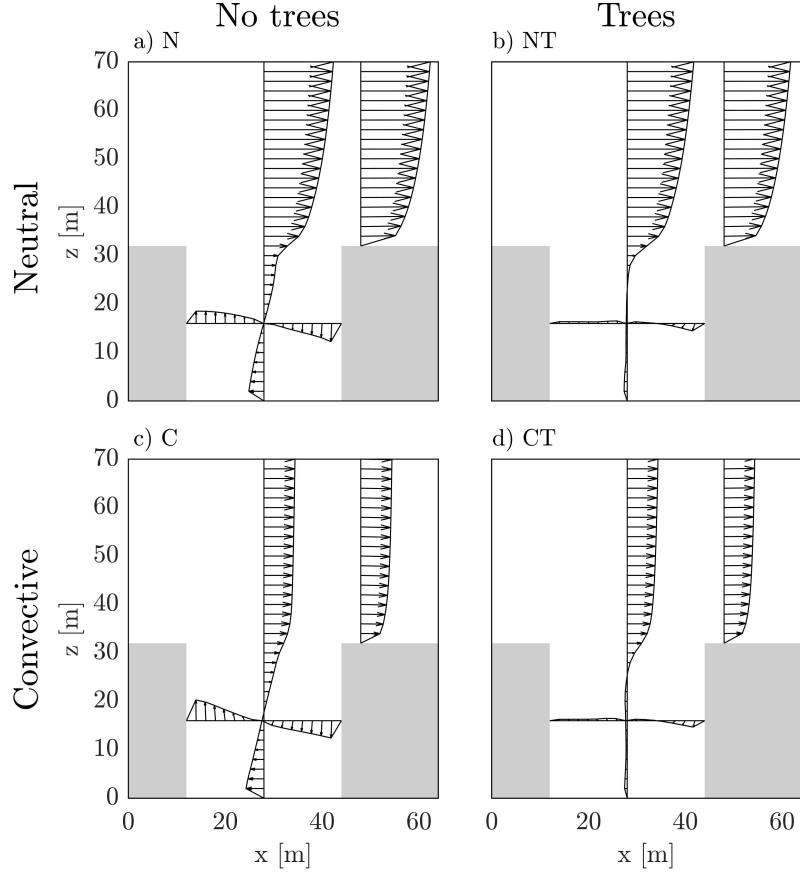


Figure 5.12: Quiver plots of the time and spanwise averaged flow fields for the a) neutral, b) neutral with trees, c) convective and d) convective with trees simulations.

of the vortices as shown in Figure 5.13b and d. The streamlines illustrate that the flow structure is comparatively stretched in the horizontal direction and that there is a distinct shift in the flow over the leeward tree canopy in simulation CT. This difference illustrates that buoyancy has a non-negligible effect on the flow within the canyon although the similarities in terms of the vortex centres suggest that it is still secondary to the direct effects of drag. The reduced wind speeds in the canyons result in a larger velocity deficits across the shear layer. This change therefore directly affects one of the prevalent velocity scales that defines this transfer between the canyon and overlying boundary layer (Salizzoni et al., 2011).

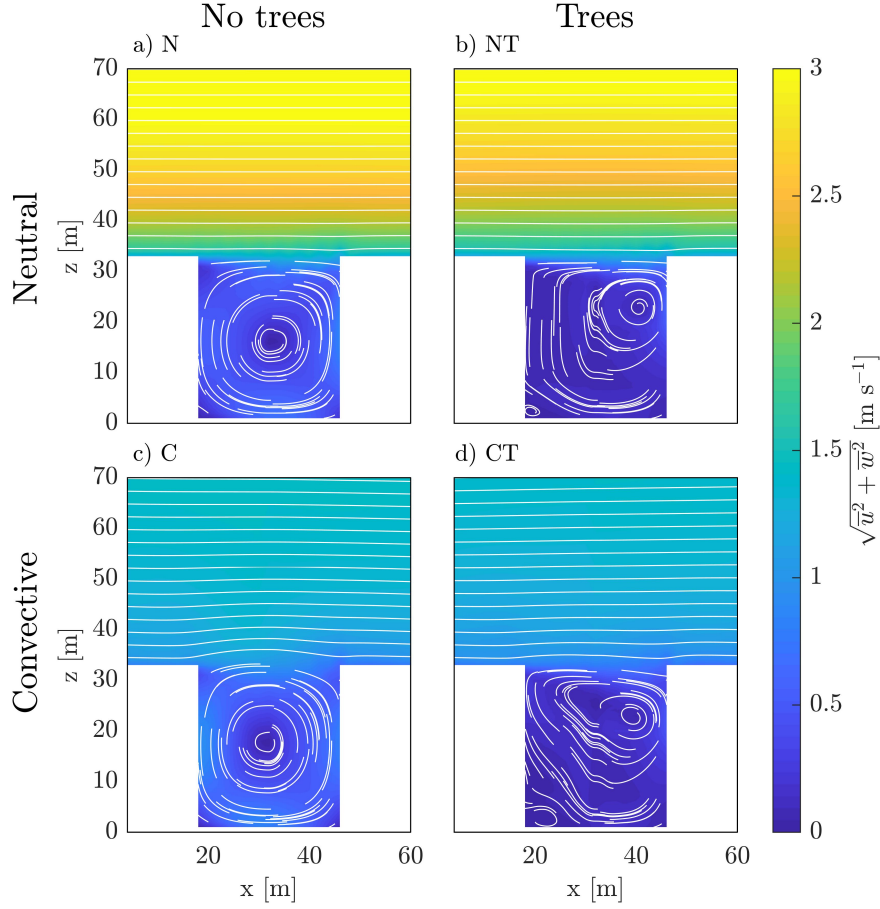


Figure 5.13: Streamlines and plots of the time and spanwise averaged flow field and wind speed for the a) neutral, b) neutral with trees, c) convective and d) convective with trees simulations.

Temperature and humidity

Figure 5.14 shows the spanwise and time-averaged potential temperature fields for the two convective simulations. Figure 5.14a clearly shows the increased temperatures arising from the bottom heating of the canyon. The reinforced canyon vortex results in efficient mixing within the canyon which is evident by the relatively homogeneous temperature field above the lowest 5 m of the canyon. The effect of trees is to redistribute and alter the sources/sinks of buoyancy within the canyon. Figure 5.14b illustrates increased temperatures at the tree crowns tops (smaller than the maximum temperature shown in simulation C) and decreased temperatures down through the canopy and at pedestrian level beneath. The canyon-averaged temperature in simulation CT is 0.22 K cooler than in simulation C and the pedestrian-averaged (at $z = 1.5$ m) is 0.83 K cooler. These results are consistent with the temperature difference found in field studies (Bowler et al., 2010). In terms of

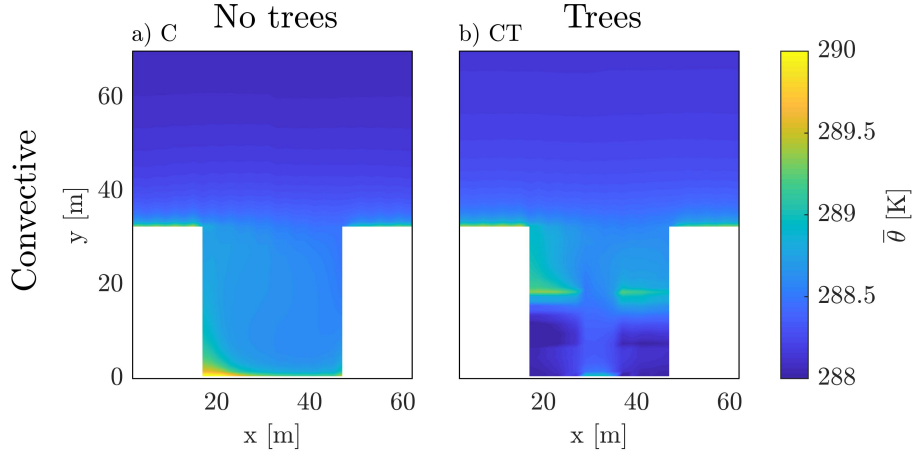


Figure 5.14: Plots of the time and spanwise averaged potential temperature for the a) neutral, b) neutral with trees, c) convective and d) convective with trees simulations.

pedestrian thermal comfort, the cooling effect of the trees is much larger as a result of the direct benefits of tree shading on a pedestrian.

For the relatively strong radiative conditions ($Q_{urb}^* = 450.2 \text{ W m}^{-2}$) and leaf area index ($d = 12$) modelled in this base case, the heat flux from the shaded surfaces is 166 W m^{-2} less than the unshaded surfaces. This results in a cooling power per unit length of the street canyon of -3998 W m^{-1} due to the tree shading effect. Figure 5.15 displays the spanwise and time averaged volumetric sources and sinks of the water vapour specific humidity, temperature and the emitted and background scalar components. Figure 5.15d illustrates that the tree canopy itself acts as both a source and sink of sensible heat, as a heat source at the canopy top and a sink towards the bottom of the canopy (following a similar trend to that exhibited in Sections 5.4.2 and 5.4.3). The total average sensible heat flux from the two tree canopies to the surrounding air is 2684 W m^{-1} . The net effect of the tree canopy is therefore to heat the surrounding air. Under the modelled conditions the cooling affect of the tree is therefore attributed to it's shading as opposed to transpirational cooling effect (although the latent heat flux acts to minimise the magnitude of the net sensible heat flux). This behaviour is indicative of the regime discussed for lower $d_t b$ in Figure 5.4 and higher Q_{urb}^* in Figure 5.5. This finding highlights the difficulty in attributing the cooling effect of trees to particular mechanisms found in previous studies. It also reiterates that the net radiation is a key variable in terms of the this attribution. For a lower net radiation, the shading effect would be reduced and in turn the radiative flux onto the leaves would be smaller and transpirational cooling would dominate. Therefore, the presence of tree would still act to cool the surrounding microclimate but via a different mechanism.

The rate of transpiration from the tree leaves in simulation CT is therefore not suffi-

ciently large to offset the strong irradiation onto the leaves at the top of the canopy. The volumetric sources of moisture from the tree canopies are displayed in Figure 5.15a, b and c (broken down into radiative and advective components). The total source of water vapour specific humidity is $0.003 \text{ kg kg}^{-1}\text{m}^{-1}\text{s}^{-1}$ of which 73% is attributed to the advective component of the latent heat flux. It is important to note therefore that the proportion due to the available energy at the leaf surface is non-negligible and that the latent heat flux is not spatially homogeneous throughout the tree canopy as has been assumed in previous studies. The advective component is shown to be relatively uniform throughout both tree canopies (in comparison to total the range of S_{qv} between both canopies) and the radiative component is shown to be predominantly determined by the decay of radiation in the z -direction. Analysing these components over a smaller range indicates that both of these terms also vary spatially as a direct function of the decoupling factor Ω . An increase and decrease of the advective and radiative components respectively is evident towards the top of the windward tree canopies where higher velocities result in a lower decoupling factor (Ω is 0.38 at the top of the windward tree and 0.52 at the bottom of the leeward tree; relatively high values for Ω relating to the low in-canyon velocities and the use of a minimum stomatal resistance). However, the magnitude of this change is small in terms of the net canopy energy balance.

The tree's effect on buoyancy can be understood by the change in virtual potential temperature, which is a function of both potential temperature and the water vapour specific humidity (see Equation 2.6). The maximum and minimum volumetric source/sink terms of virtual potential temperature from the tree canopies in simulation CT are 0.0795 and -0.017 K s^{-1} respectively. The magnitude of the volumetric source of water vapour (maximum source term $2.1 \times 10^{-5} \text{ kg kg}^{-1}\text{s}^{-1}$) has a negligible effect on these values indicating that the latent heat flux from tree canopies does not directly affect the buoyancy of the surrounding air. The distribution of S_θ is therefore a good indicator of the buoyancy sources introduced by the tree canopy. This source therefore acts to alter the flow field in terms of the positive buoyancy source at the canopy top and the negative source towards the bottom. The streamlines in Figure 5.13d illustrate the buoyancy effect on the flow structure within the canyon.

The case of an infinite canyon and horizontally homogeneous tree canopies is not conducive of the 'oasis' effect as the relatively low rates of vertical exchange lead to correspondingly higher values of specific humidity within the UCL. As the trees simultaneously act to cool the surrounding air, this case set up can result increased relative humidities and therefore vapour pressure deficits (in comparison to the initial values; canyon-average relative humidity of 72.3 % in simulation CT). The generally low wind speeds present in the

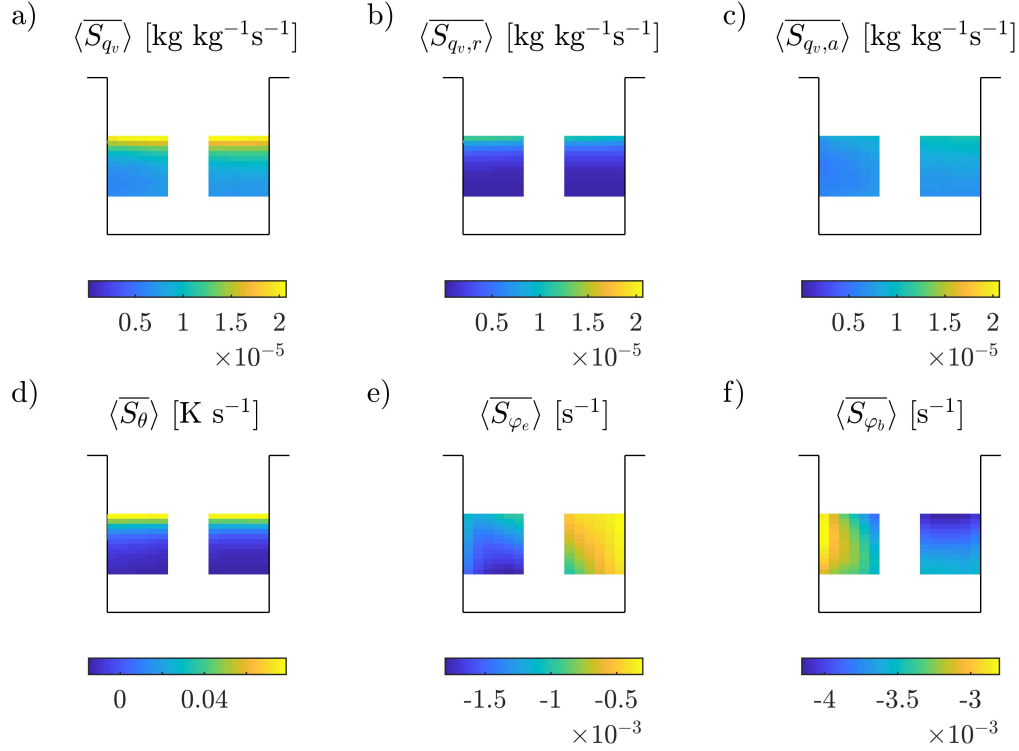


Figure 5.15: Plots showing the time and spanwise averaged volumetric sources and sinks of a) water vapour specific humidity, b) the radiative component of water vapour specific humidity, c) the advective component of water vapour specific humidity, d) potential temperature, e) the emitted component of the pollutant field and f) the background component of the pollutant field for the tree canopies in simulation CT. The 8th canyon from the inlet boundary is used for S_{φ_e} and S_{φ_b} .

canyon in simulation CT also acts to reduce the average aerodynamic resistance leading to reduced latent and sensible heat fluxes. One may expect the latent heat flux and therefore transpirational cooling to be relatively increased in more complex morphologies and with sparser tree canopies. Further work is required to gain a more holistic understanding of the transpirational and shading effects of trees (encompassing the entire parameter space) but these results suggest that the minimal tree model is a good tool with which to do this.

Pollution

Figure 5.16 shows the streamwise development of the emitted passive scalar field, φ_e , for simulations N and C. The combination of higher wind speeds and less vertical mixing in the neutral case results in significantly different downwind dispersion characteristics. The pollutant plume can be seen to mix over the height of the domain after approximately 600 m for the convective case in Figure 5.16b whereas it reaches a height of only 100 m

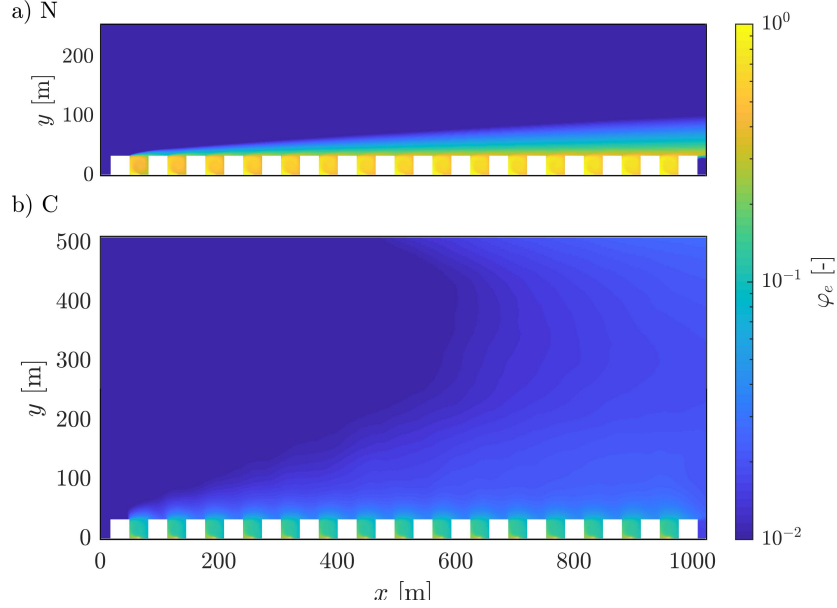


Figure 5.16: Plots of the time and spanwise averaged emitted components of the pollutant concentration in the a) neutral and b) convective simulations.

under neutral conditions in Figure 5.16a (relating back to the eddy turnover times discussed above). The differences exhibited by the neutral and convective cases illustrate the difficulties in directly comparing pollution dispersion under different atmospheric stabilities and simultaneously highlight the importance of capturing thermal effects in studies of urban pollution dispersion. The canyon-averaged pollutant concentrations increase in the streamwise direction in both of these simulations as a result of the higher above canyon concentrations and subsequent detrainment (5.5% and 6.2% larger in the fifteenth canyon from the inlet boundary in comparison to the first for simulations N and C respectively). The 8th canyon from the upwind side of the domain is used for the following analysis.

As discussed in Section 5.5.1, a weighting, ω , can be applied to the background (φ_b) and emitted (φ_e) scalar fields to study the effects of trees on different pollutants or under different emission rates. The example applied in this analysis, is that of capturing ‘effective’ roadside NO_x and $\text{PM}_{2.5}$. NO_x emissions are predominantly due to road transport and as such one typically expects much larger values close to busy roads than in quieter roads or parks (as illustrated in Chapter 3). $\text{PM}_{2.5}$ is also associated with vehicular emissions but due to a combination of other source attributions and different chemical interactions, it generally exists more homogeneously within the urban microclimate. London wide air quality data can be used to provide reference values of the roadside-background concentration ratios that characterise this effect (King’s College London, 2017). The average

roadside-background concentration ratios in London for NO_x and $\text{PM}_{2.5}$ are 3.22 and 1.18 respectively (using monthly averages taken at 12:00 over a period of a year; King’s College London, 2017). The weighting factor can be applied in post-processing to obtain a similar ratio between the average pollutant concentration at pedestrian level and the assigned background concentration at the inlet ($\langle \bar{\varphi} \rangle_{z=1.5\text{m}} / \varphi_{b,x=0\text{m}}$). This process was followed using simulation C as the reference case.

The weighting factor for ‘effective’ NO_x is calculated as $\omega = 0.11$. Figure 5.17 shows the resulting time and spanwise averaged pollutant fields for the four base case simulations. The difference between air quality under neutral and convective conditions is reiterated in this figure by the requirement to use different colour bars to illustrate the distribution of pollutants within the canyon. The canyon-averaged concentration in simulation N is 3.1 times larger than the canyon-averaged concentration in simulation C. The reason for the magnitude of this difference is that whilst the friction velocities are matched in these simulations (which is the dominant scaling in defining vertical exchange in the neutral case), the Deardorff velocity scale is also an important scaling under convective conditions. For the CBL modelled here, the Deardorff velocity scale is 1.35 m s^{-1} which is significantly larger than the specified friction velocity ($u_* = 0.3 \text{ m s}^{-1}$). The Obukhov length is 14.2 m, which also indicates the dominance of buoyancy in the modelled CBL. The effect of this scaling is evident in the measured exchange velocities which are 0.04 and 0.24 for simulations N and C respectively. The magnitude of these exchange velocities is consistent with the empirical parametrisations applied within SIRANE that, using the modelled boundary layer properties, predict corresponding values of 0.08 and 0.17 m s^{-1} (calculated as a function of the parametrically defined standard deviation in vertical velocity; see Section 2.2).

Figure 5.17b and d illustrate the combined drag and deposition effects of trees on the pollutant fields. Both simulations with trees exhibit higher concentrations on the leeward side of the canyon. Simulation NT shows a particularly large hotspot of pollution at pedestrian level on the this side where a small secondary circulation was shown to exist in Figure 5.13. The increased concentrations are a direct result of the drag imposed on the flow within the street canyons. In simulation NT the depositional effects of the tree are evident in that the concentration on the windward side of the canyon is lower than in comparison to simulation N. The position of the tree canopy in this base case scenario is such that the majority of the emissions flow through the windward tree canopy relatively quickly and before they are significantly diluted. A large proportion of the emitted pollutant is deposited through this process in simulation NT. The review of Abhijith et al. (2017) highlights a number of studies that found the same asymmetry when studying infinite canyons with a perpendicular wind angle of incidence. The same asymmetrical effect

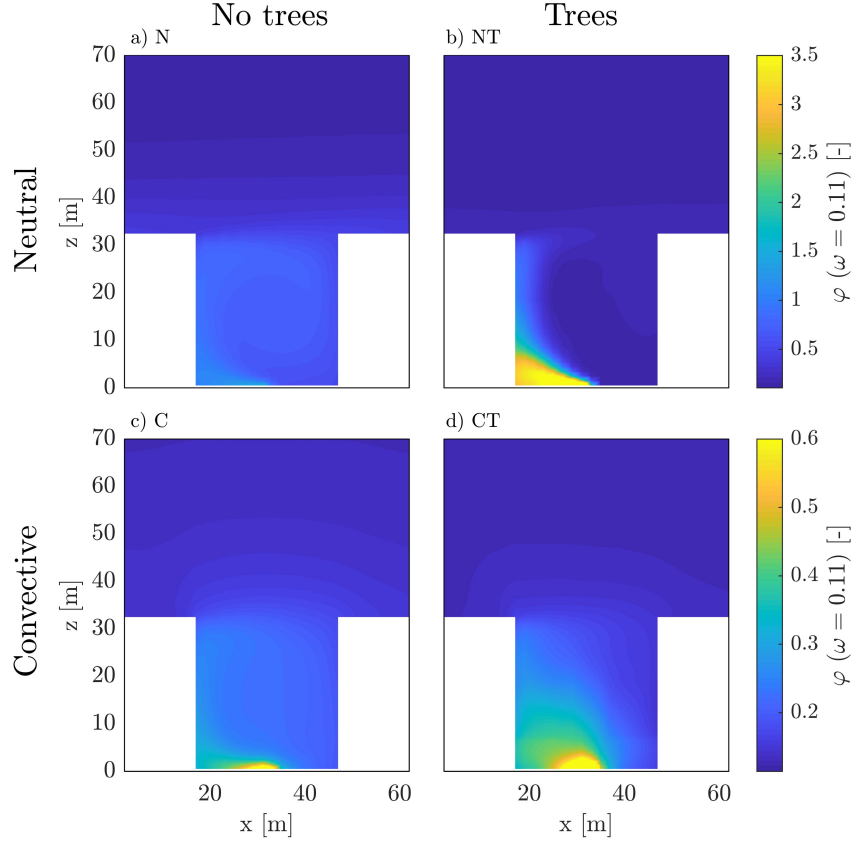


Figure 5.17: Plots of the time and spanwise averaged pollutant concentrations for the a) neutral, b) neutral with trees, c) convective and d) convective with trees simulations. The weighting factor $\omega = 0.11$ and the results are shown of the 8th canyon from the inlet boundary.

is apparent between simulations C and CT but to a lesser extent. The buoyancy sources in simulation CT were shown to result in a different flow structure and it is suggested that more of the pollutant is transported closer to the centre of the canyon and therefore not through the windward tree canopy. The sink of φ_e in simulation CT is displayed in Figure 5.15. The largest sink of pollutant is in the leeward tree canopy and towards the centre of the canyon, which agrees with this hypothesis. The increased vertical exchange in the convective simulation also means that the emitted component of the scalar field has a lower residence time within the canyon. This difference between neutral and convective conditions significantly alters the canyon-averaged effects of the trees. Under neutral conditions, the presence of trees results in a 24% reduction in canyon averaged pollutant. Contrastingly the trees result in an 8% increase in concentration for the convective case. This finding highlights the sensitivity of the role trees play in urban air quality. It also indicates that the depositional effects of trees is more effective under conditions where one

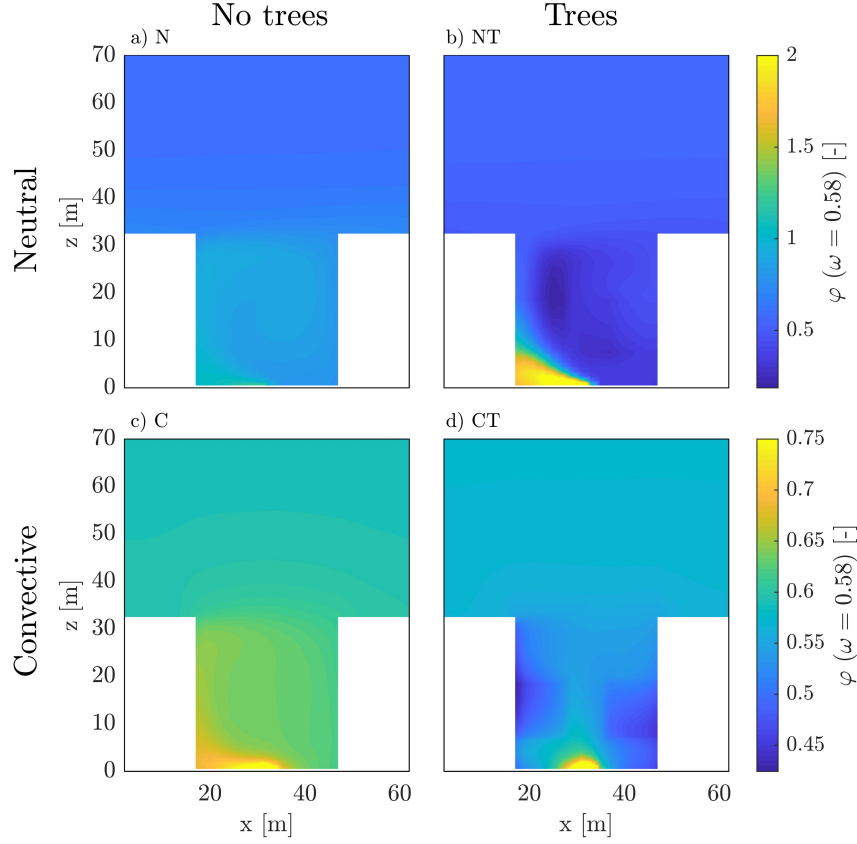


Figure 5.18: Plots of the time and spanwise averaged pollutant concentrations for the a) neutral, b) neutral with trees, c) convective and d) convective with trees simulations. The weighting factor $\omega = 0.58$ and the results are shown of the 8th canyon from the inlet boundary.

would expect poor air quality (higher concentrations and lower wind speeds resulting in increased deposition).

Increasing the weighting factor to 0.58 increases the relative importance of the background concentration on the pollutant field and, as discussed, reproduces the ratio between roadside and background concentrations of PM_{2.5}. Figure 5.18 provides the same analysis as above with the altered weighting. The same pollutant hotspot with very high concentrations is found in the lower leeward corner of the canyon in simulation NT. However it is evident that, apart from that hotspot, the simulations with trees are shown to have considerably reduced pollutant concentrations. The canyon averaged concentrations are reduced by 40% and 18% due to the presence of trees under neutral and convective conditions respectively (again illustrating improved performance under neutral conditions). In simulation N the deposition of pollutants onto the tree canopies is such that the concentration is lower in some positions within the canyon than above. This effect is caused by

polluted background air being entrained into the canyon where it is deposited onto the leaf surfaces.

The main difference, in comparison to the results shown in Figure 5.17, is that the relatively high background concentration means that the distribution of pollutant deposition within the canopies is fundamentally changed. If the pollution levels are more associated with the direct emissions, due to road transport (ω is small), as was the case in Figure 5.17, then the most effective deposition occurs when the tree is very close to emissions source and before the emitted pollution is diluted with cleaner ambient air. This positioning aspect of using trees and green infrastructure to mitigate poor air quality has been discussed in e.g. Morakinyo et al. (2017). If the pollutant field is generally at a higher concentration and less associated with direct emissions this effect is diminished. Figure 5.15f shows the volumetric sink of the background component of the modelled pollutant field. The largest sink of pollution is on the windward tree canopy however the magnitude of the sink term is generally more uniform between the two canopies than the sink of the emitted component. The removal of background air pollution is therefore more efficient than of the emitted pollutant field as the proximity to the emissions source and local transport of the emissions is irrelevant. The same effect therefore applies to trees in quieter streets and parks. It is important to note that generally the most harmful levels of pollutants are associated with direct emissions and hotspots close to specific emission sources. It is therefore necessary to study the absolute reduction in pollutant levels as well percentage terms. However, the application of the weighting factor in this study has highlighted a phenomena of urban trees that has hitherto rarely been considered. As in Section 5.5.2, further work is required to gain a more holistic understanding of the role of trees in urban air quality (encompassing the full parameter space) however these results again reiterate that the minimal tree model and the roadside-background concentration ratio present useful tools with which to do this.

5.6 Future work

The scenario discussed in Section 5.5 presents a show-case study into the integrated role of trees within infinite canyons using urban LES. Typical environmental and tree parameters were used to produce generalised results. However, as highlighted in Section 5.3, the role of the trees is highly sensitive to a number of the specified variables. For example, the size and positioning of the trees in Section 5.5 is conducive of high levels of deposition and drag within the street canyon. In particular, having the tree canopies adjacent to the building walls is likely to amplify these effects (and stops potential channeling of the flow

between the building and tree canopy). A comprehensive sensitivity study will therefore be conducted in the future to explore the effects of e.g. different street aspect ratios, tree configurations, radiative conditions, stomatal resistances and deposition velocities.

Of particular importance is the tree’s sensitivity to deposition velocity and stomatal resistance. Both of these parameters have been shown to vary significantly within the literature and there is a need for more experimental studies to accurately determine values for e.g. different tree species (Sæbø et al., 2012; Jones, 2013; Buccolieri et al., 2018). Moreover, the assigned values of these two parameters within the minimal tree model are critical to the resulting tree effects on air quality and cooling. The deposition velocity is a function of environmental (dynamics of the flow field, moisture in the air), tree parameters (leaf thickness and hairiness) and properties of the pollutant of interest (particle size). There is currently not enough data to produce a full parametrisation of all of these effects (Janhäll, 2015; Santiago et al., 2017). Damour et al. (2010) presents a review of existing parametrisations that capture the stomatal resistance as a function of e.g. the net radiation, vapour pressure, leaf temperature, CO₂ concentration and soil water availability. Integrating such a model within the minimal tree model would better capture the variation of stomatal resistance within the tree canopy however also adds additional complexity where gaining an initial understanding with a uniform value is a necessary initial step.

Other important effects that were neglected here but could be added in later iterations of the model are the resuspension of pollutants and the emission of volatile organic compounds from tree canopies. Resuspension occurs when particles that are captured on a leaf surface are re-emitted into the atmosphere. Nowak et al. (2013) estimated resuspension of PM_{2.5} as 4.5-12% and Hong et al. (2018) incorporated resuspension into a CFD model using a volumetric source term. Beyond this, further work is required to ascertain the importance of capturing the SGS TKE generation of the tree canopy. In order to do so, more experimental and field validation cases are required.

Finally a further addition to the model, which increases its complexity and number of free parameters but would be advantageous in future investigations, is to extend the radiative model to capture short- and longwave radiative exchanges independently and to incorporate these within a three-dimensional urban energy balance model. Following the work of Suter (2018), this development would be possible by treating the canopy edges as ‘facades’ and assuming that radiative exchanges occur within the canopy along the cardinal directions. The multiple scattering model of Zhao and Qualls (2006) (discussed in Appendix A.4) could then be applied and incorporated into the existing radiative transfer model of uDALES.

5.7 Conclusion

Trees are an integral part of the urban form and their presence within the UCL affects the transfer of momentum, radiation, temperature, moisture and pollutants. A minimal tree model has been presented through which the integrated effects of trees within the urban environment (drag, transpiration, shading and deposition) can be modelled at a ‘grey-scale’. The model is devised so that the number of additional free parameters is minimised and idealised, systematic studies can be conducted (working alongside the application of a simplified constant heat flux boundary condition). The minimal tree model resolves the latent and sensible heat fluxes from the tree canopy without using a model for the leaf temperature by applying the Penman transformation. The latent heat flux is decomposed into an advective and radiative term following an adapted form of the decoupled Penman-Monteith equation. Tree shading is captured via the attenuation of net radiation down through the canopy and by modelling the heat storage at the urban surfaces using the objective hysteresis model.

A parametric study was conducted that develops upon the work of Manickathan et al. (2018) on the sensitivity of tree’s transpirational cooling effects. The cooling potential of the tree canopy was shown to derive from the balance between the net radiation incident on the leaf surfaces and the transpiration rate, which is a function of both the net radiation and the ambient vapour pressure deficit. It was shown that, over certain ranges of e.g. leaf area index, the transpirational cooling effect can dominate such that other processes are near negligible. However, other regimes exist where the tree shading effect is more significant in terms of the net cooling and where the tree canopy exhibits a net positive heat flux. The canopy energy balance is a complex function of both the assigned tree and environmental parameters and the demonstrated sensitivity was indicative of the case-specificity seen with urban tree studies in the literature. However, the ability of such a simple, bulk model to capture these effects indicated that the application of the minimal tree model within coarser pollution dispersion models should be possible. The bulk model was able to reproduce the relationship between volumetric cooling and leaf area density presented in Gromke et al. (2015) (highlighting the case specificity of this empirical parametrisation).

The application of the minimal tree model in uDALES was verified using existing numerical studies. Full-canopy, half-canopy and single row of tree simulations were conducted that verified the applied drag and energy balance models. For the range of conditions studied, the tree canopies were shown to act as both sources and sinks of temperature, with the sensible heat flux predominantly varying over the height of the modelled canopy. The ‘oasis’ effect in which enhanced rates of transpiration and subsequently cooling occur was illustrated in the half-canopy simulation. The full-canopy and half-canopy simulations present

extensive and repeatable set-ups that could be applied for future model verifications.

The minimal tree model was applied within a simplified infinite canyon set up in order to conduct a show-case investigation into its role within the urban canopy layer and its effects on urban air quality. Neutral and convective conditions were modelled with and without tree canopies. For the case considered in this study, trees were shown to significantly affect the flow structure within the canyon (67% average reduction in the wind speed). The tree canopies resulted in low wind speeds and the formation of a secondary vortex under both neutral and convective conditions. The sensible heat flux from the tree canopies altered the flow structure for the convective case, particularly in terms of the flow direction around the windward tree canopy. The presence of trees under convective conditions resulted in a cooling of the air. The canyon- and pedestrian-averaged temperatures were reduced by 0.22 and 0.83 K respectively in these simulations. As a result of the strong radiative conditions, the cooling effect was attributed largely to the tree shading effect (the net sensible heat flux from the tree canopy was positive). This behaviour is consistent with a tree regime exhibited in the parametric study. The in-canopy spatial variability of sensible and latent heat fluxes was shown to be affected by the decoupling factor. However, these differences, due to variability in e.g. aerodynamic resistance, were small in comparison to the decay of radiation vertically through the tree canopy.

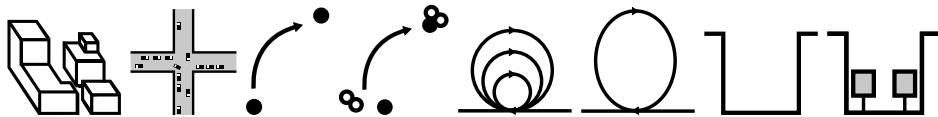
A novel method was used to study the tree's effects on air quality by splitting the pollutant fields into background and emitted components and applying a weighting factor to reproduce different effective pollutant fields. For a low weighting factor (indicative of high local emissions), the presence of a tree resulted in a hot spot of poor air quality within the canyon in these simulations. For the case considered, the canyon-averaged pollutant concentration of effective NO_x was reduced by 24% and increased by 8% due to the presence of trees under the neutral and convective conditions respectively. A finding that highlights that the depositional performance of trees is likely to be improved under atmospheric conditions that are conducive of poor urban air quality. But also that indicates that the thermal effects (reduced surface heat flux and elevated buoyancy sinks) may further inhibit the transport and dilution of pollutant emissions from pedestrian level. A higher weighting factor was applied to indicate the change in the performance of trees when the pollutant field is less directly affected by the local traffic based emissions. Trees were shown to be more effective in reducing local pollution concentrations in situations where this is the case (e.g. quieter roads and pollutants that exist more homogeneously).

The infinite canyon study presents a show-case investigation into urban trees using LES. More extensive studies are required using the minimal tree model to explore the large parameter space and complex system sensitivities.

Chapter 6

Simulating air pollution in the urban microclimate II: atmospheric stability and trees

Convective atmospheric conditions and trees are introduced into the case study presented in Chapter 3 (by applying the methods and models outlined in Chapters 4 and 5). The large-eddy simulations (LES) showcase the model capabilities developed as part of this work and the advancements towards realistically modelling air pollution in the urban microclimate. Fundamental insight is obtained by directly comparing LES results (e.g. with and without trees) and a further evaluation of the operational model SIRANE is conducted.



6.1 Introduction

Real urban environments are inherently heterogeneous; composed of buildings, trees, green spaces and bodies of water that combine to form complex morphologies and networks of anthropogenic emissions that emit heat and pollutants into the urban air. The best practice guidelines for the production of steady-state non-neutral atmospheric conditions in urban large-eddy simulations (LES; see Chapter 4) and the minimal tree model (see Chapter 5) provide tools to amalgamate some of this additional complexity to the case study introduced in Chapter 3. The following chapter therefore presents a showcase of the

model capabilities developed in this thesis, encompassing all of the five elements of urban air quality identified in Chapter 1 (morphology, emissions, chemistry, atmospheric stability and trees).

The majority of studies that use computational fluid dynamics models to study urban pollution dispersion aim to isolate particular phenomena and processes of interest by simplifying the problem and reducing the degrees of freedom (as discussed in Section 1 and done in Chapters 4 and 5). There are very few investigations where several of the elements of urban air quality have been considered simultaneously, particularly studies of urban pollution dispersion using LES. Moradpour et al. (2017) study the influence of trees on reactive pollution dispersion within a semi-realistic morphology for neutral and stable atmospheric conditions (using a Reynolds-Averaged Navier-Stokes (RANS) model). The trees impose drag on the surrounding flow field and their thermal effects are approximated following the empirical cooling parametrisation of Gromke et al. (2015) (there is a discussion on the applicability of this parametrisation in Section 5.3; deposition effects are neglected). The trees result in downward flows and stable stratifications. Simulations are run for a variety of leaf area densities a and street-canyon aspect ratios. The reactive NO and NO₂ concentrations are shown to be dominated by their dispersion within the urban flow field. Maximum concentrations of NO and NO₂ coincide with minimum concentrations of O₃ (this phenomenon was also exhibited in Chapter 3). Trees are shown to generally lead to increases in NO_x concentrations although the tree behaviour is shown to be highly case-specific to the modelled aspect ratios and leaf area densities. The vegetation generally causes the pollutants to tend closer to a chemical equilibrium within the urban canopy layer (UCL). Jeanjean et al. (2017) investigate the effect of trees on inert pollutant dispersion within a realistic urban morphology with semi-realistic emissions over different seasons (using OpenFOAM with a RANS turbulence model). The focus of the analysis is on the dispersive versus drag effects of the trees. Trees are, once again, shown to generally lead to increases in pollutant concentrations. This effect is particularly pronounced for high wind angle of incidences (for lower angles trees are shown to have more positive effects). Kurppa et al. (2018) study the dispersion of inert pollutants in a realistic morphology with semi-realistic emissions under both neutral and stable conditions and with and without trees (using the LES model PALM). The variation in building heights results in increased vertical exchange out of the urban canopy layer (UCL). Stable conditions are shown to result in twice as high pedestrian-level pollutant concentrations in comparison to the neutral case. Only the drag effects of trees are considered which are shown to result in higher pollutant concentrations and decreased vertical exchange. A methodology is presented to analyse the large amount of output data obtained from the study of such heterogeneous

urban areas using LES.

The following study (alongside the work presented in Chapter 3) simulates both inert and reactive pollution dispersion under neutral and convective conditions over a realistic urban morphology with realistic emissions and with and without trees. A limited number of cases are simulated here and therefore the results are primarily presented as a showcase of the model capabilities developed in this thesis. However, the intrinsic variability of the case study region (e.g. the range of different street aspect ratios, street types, wind angle of incidences and emissions) and the extrinsic control exhibited by carefully varying specific elements of urban air quality between each simulation, enable some generalised results and relevant findings to be obtained despite the relatively small number of total simulations. Studying the combined effects of all of these elements provides the opportunity to gain a better understanding of how these determinants of the life cycle of urban air pollutants interact and how the interplay between them acts to define air quality at the microclimate scale. In addition, the evaluation of SIRANE (also introduced in Chapter 3) is extended to investigate the operational pollution dispersion model’s performance under convective atmospheric conditions and with trees.

The changes made to the simulations presented in Chapter 3 in order to capture both convective conditions and the presence of trees within the modelled domain in both SIRANE and uDALES is outlined in Section 6.2. The results are provided in Section 6.3 with two main forms of analysis: 1) direct comparisons between LES with systematic differences (e.g. neutral versus convective conditions; Section 6.3.1) and 2) a further evaluation of the predictive ability of SIRANE (Section 6.3.2). Finally conclusions are drawn in Section 6.4.

6.2 Case study

The case study was first introduced in Chapter 3. It involved equivalent simulations with uDALES (denoted by DA) and SIRANE (denoted by SI) over the case study region under neutral atmospheric conditions with south-westerly and westerly wind directions. The case study region is a 672×1344 m area in South Kensington, London, UK. It encompasses a range of road types, street aspect ratios and street orientations and also has a substantial ‘urban forest’. The morphology of the case study region is obtained by processing LIDAR data to conform to the Cartesian grid and IBM in uDALES (see Section 3.3.1). Traffic emissions are obtained in pre-processing using a traffic microsimulation and instantaneous emissions model (see Section 3.3.2). Further details of the morphology, meteorological conditions and emissions are provided in Section 3.3 and in Table 3.1.

The south-westerly simulations presented in Chapter 3 (hereafter denoted by simula-

tions DA N and SI N) are used as a starting point for four further simulations in this chapter (two in uDALES and two in SIRANE). Simulations SI C and DA C develop upon the previous simulation set-ups by enforcing convective atmospheric conditions (with the friction velocity still matched to the neutral case; $u_* = 0.33 \text{ m s}^{-1}$). Simulations SI CT and DA CT develop further upon these set-ups by also incorporating the presence of trees within both SIRANE and uDALES. Simulations DA C and DA CT are run up for a time of 3600 s and averaged over a further period of 10800 s. The changes applied to the simulation set-ups in uDALES and SIRANE for the four additional simulations are outlined below.

6.2.1 Atmospheric stability

The meteorological conditions over London are generally non-neutral (Kotthaus and Grimmond, 2018). The urban boundary layer (UBL) is typically less stable and larger in height than the corresponding rural planetary boundary layer (Roth, 2000; Barlow, 2014). Field campaigns over London indicate the prevalence of convective atmospheric conditions with mixing layer heights for momentum and aerosols often exceeding 800 m. Under convective conditions, the measured turbulence profiles show good agreement with canonical profiles (e.g. mixed layer similarity theory; Barlow et al., 2011). Kotthaus and Grimmond (2018) study observational data of London’s UBL over a six year and calculate the frequency of different atmospheric states. This investigation found that convective, cloudy conditions are most prevalent during the day over Central London. A typical convective boundary layer (CBL) on a partly cloudy summer’s day is therefore the targeted condition for the following case study.

The atmospheric stability in SIRANE is determined by the approximated Obukhov length of the surface layer, which acts as a switch in categorising the state of the overlying UBL (convective for $L < 0$; stable for $L > 0$ and neutral for $|L| \rightarrow \infty$). The Obukhov length is a function of the friction velocity and net sensible heat flux (Equation 1.6), which are both determined via parametrisations based upon the meteorological inputs into SIRANE (Soulhac et al., 2011). A mesoscale urban energy balance is defined via various parametrisations to define the net sensible heat flux of the urban area. The net radiation is calculated following the process outlined in Appendix A.1 (the same parametrisation as used in the minimal tree model). The heat storage term is estimated as a function of the incoming radiation (Soulhac et al., 2011). The latent heat flux is calculated using the Priestley-Taylor coefficient, which depends on the soil saturation rate and the presence of vegetation in the modelled domain (Priestley and Taylor, 1972). The profiles of e.g. standard deviation of the vertical velocity (σ_w ; that is the applied scaling for the exchange velocity) are then defined by different functions for stable and neutral conditions (both as

a function of the friction velocity) and for convective conditions (as a function of both the friction and Deardorff velocities). This methodology follows reviews on canonical boundary layer profiles and the parametrisations applied within ADMS (Holtslag and Van Ulden, 1983; Fisher et al., 2001; CERC, 2001; Soulhac et al., 2011).

The same date and time (7th July, 1 pm) and cloud cover ($Cld = 6$) are used within simulations SI C and SI CT as applied for SI N in Chapter 3. Neutral conditions were enforced in simulations SI N by defining a net urban surface albedo of 1. This value was reduced to 0.6 for simulations SI C and SI CT to produce a net surface sensible heat flux, $Q_{H,urb} \approx 100 \text{ W m}^{-2}$. The change in atmospheric stability necessitates changes to the reference values of wind speed and potential temperature at the measuring height ($z = 30 \text{ m}$) because the estimated mean vertical profiles are altered. In order to match the friction velocity in simulation SI C to that in simulation SI N, despite the change in boundary layer profiles, the reference velocity is reduced from 2.46 to 1.76 m s^{-1} . To ensure that the $\text{NO} + \text{O}_3$ reaction rate (k_2) also matched the neutral case, the reference temperature at the same height was changed from 293 to 290.5 K (a similar process was done for simulation SI CT with small differences in the values; see Section 6.2.2). The corresponding boundary layer properties of simulation SI C (as calculated within SIRANE) are a CBL height, $h_C = 1200.1 \text{ m}$ and an Obukhov length of -32.3 m .

These conditions are reproduced in simulation DA C by enforcing a sensible heat flux at all roof and road surfaces ($\phi_{\theta,0} = 0.0796 \text{ K m s}^{-1}$; following the same one-dimensional radiative budget simplification applied in Chapters 4 and 5). The lateral boundary conditions for temperature and moisture are periodic (boundary conditions for momentum and the scalar fields are periodic and inflow-outflow respectively as defined in Section 3.3.4; background concentration levels are assigned at the inlet planes). Steady-state method *iii* from Chapter 4 is then followed to produce a realistic, statistically steady-state CBL within uDALES in simulations DA C and DA CT. The modelled domain height is set to 600 m ($l_z \approx h_C/2$). The grid is stretched in the vertical direction with a maximum cell size of 4.39 m at the top of the domain (minimum vertical cell size of 2.15 m over the lowest 100 m of the domain). The grid is stretched using a hyperbolic tangent function with a stretching constant of 0.88 (Vinokur, 1983). The increased vertical size of the domain means that the constant pressure gradient assigned to force the flow in a south-westerly wind direction is adjusted to $\rho^{-1}\partial p/\partial x = \rho^{-1}\partial p/\partial y = 0.000128 \text{ m s}^{-2}$ in both simulations DA C and DA CT (this ensures that the friction velocity is matched to simulation DA N). The grid size remains the same as in Chapter 3 ($384 \times 768 \times 192$). The top boundary condition for heat is set to half that from the urban surface ($\phi_{\theta,h} = \phi_{\theta,0}/2$). A uniform volumetric sink of potential temperature ($R = -6.965 \times 10^{-5} \text{ K s}^{-1}$) is defined throughout the domain also

following the best practice guidelines outlined in Chapter 4. A similar process is followed for simulation DA CT but with the net sensible heat flux recalculated as the combined flux from the shaded and unshaded urban surfaces and the tree canopies (see Section 6.2.2). Simulation DA CT also has a flux of moisture into the domain from the tree canopies. A steady-state is enforced by applying an equivalent flux condition at the top of the domain ($\phi_{q_v,h} = \phi_{q_v,0}$) and therefore producing a uniform turbulent moisture flux profile over the domain height (consistent with a typical CBL; Stull, 2012).

6.2.2 Trees

Numerous trees are present in the defined case study region (an aerial photograph is shown in Figure 6.1a). Greater London is, by square meter, the ‘greenest’ city in Europe with 40% of its surface area made up of public green spaces (BOP Consulting, 2013). Inner London has a tree canopy coverage of 13% (corresponding to a total of 1,587,000 trees; Rogers et al., 2015). Numerous different tree species are present in the case study region. One of the most numerous is *Platanus Acerifolia*, commonly called the ‘London Plane’, which is well suited to the urban environment due to its relatively high tolerance to pollutant exposure.

SIRANE does not account for the drag or depositional effects of trees. The one way in which vegetation is captured within the model is via the Priestley-Taylor coefficient in the net surface energy balance discussed above. The percentage of canopy coverage of the case study region is 14.2% (similar to London’s average) and therefore the Priestley-Taylor coefficient is increased by 0.142 between simulations SI C and SI CT (Soulhac et al., 2011). The net latent heat flux from the urban area therefore increases in comparison to simulation SI C and as a result of this change the net sensible heat flux is reduced from 97.9 to 79.3 W m⁻² between simulations SI C and SI CT. Subsequently, the Obukhov length (-39.6 m) and boundary layer height (1081.7 m) are also different. As discussed in Section 6.2.1 above, minor adjustments are required in the reference wind speed and potential temperature to ensure that the friction velocity and NO+O₃ reaction rate remain the same across all simulations ($u(z = 30\text{m}) = 1.81 \text{ m s}^{-1}$ and $\theta(z = 30\text{m}) = 290.8 \text{ K}$ in simulation SI CT).

In order to input trees into uDALES, data is required on the positioning of tree canopies within the case study region. Each Borough of London has compiled a list of tree species and positions; however it is not exhaustive and does not include all the necessary information to capture their positions at the scale of the LES model. Tree positions can also be obtained from aerial photographs (such as those shown in Figure 6.1a) however these do not indicate the vertical size of the tree canopies. A process was therefore developed to obtain

the three-dimensional positions of tree canopies over the case study region by processing LIDAR (Light Detection and Ranging) and Digital Terrain Model datasets (DTM; 0.5 m resolution; Environmental Agency, 2017). The LIDAR data is a point cloud in which each data point has its three dimensional position, an intensity value (a dimensionless measure of the return strength of the laser pulse and therefore partly a function of the reflectivity of the surface struck by the laser pulse) and a classification (standard LAS format file classifications).

A plan view of the LIDAR intensity data over the case study region is shown in Figure 6.1b. The available LIDAR data is taken from the 12th April 2012 (this date presents a challenge in terms of the targeted summer conditions in this case study when the leaf area density and extent of the tree canopies is expected to be relatively larger). The low point density of the available dataset and the partial inapplicability of the applied classification system to urban areas (most points are incorrectly classified as ‘low’ or ‘high vegetation’) means that a bespoke processing procedure is necessary. The process of converting this data set to a three-dimensional representation of the tree canopies rasterised onto the Cartesian grid used in uDALES is as follows:

- 1 Raw LIDAR data → Ground normalised point cloud data set
 - 1.1 Extract point cloud and DTM data over case study region. Change to a projected coordinate systems and rebase the origins (DTM heights shown in Figure 6.1c).
 - 1.2 Subtract the DTM heights from the LIDAR point heights so that ground level is normalised.
- 2 Ground normalised point cloud → Tree canopy point cloud
 - 2.1 Remove all LIDAR points with height < 4 m and with classifications of 2 (ground) and 3 (low vegetation). This step removes noisy data close to the urban surface. A minimum bottom height of the canopy is therefore set to 4 m.
 - 2.2 Apply a building mask (using the plan area of the urban morphology processed for uDALES; Figure 3.2) with an additional buffer region of 3.5 m. This step removes all points positioned above and in close proximity to the buildings. The buffer region acts to remove noisy data produced by building facades. Also apply a further 12 m buffer region to the domain edge (this mask is similarly applied to the emissions and morphology; Section 3.3.4). A plan view of the point cloud data prior to this step with the buffer mask overlaid is shown in Figure 6.1d.

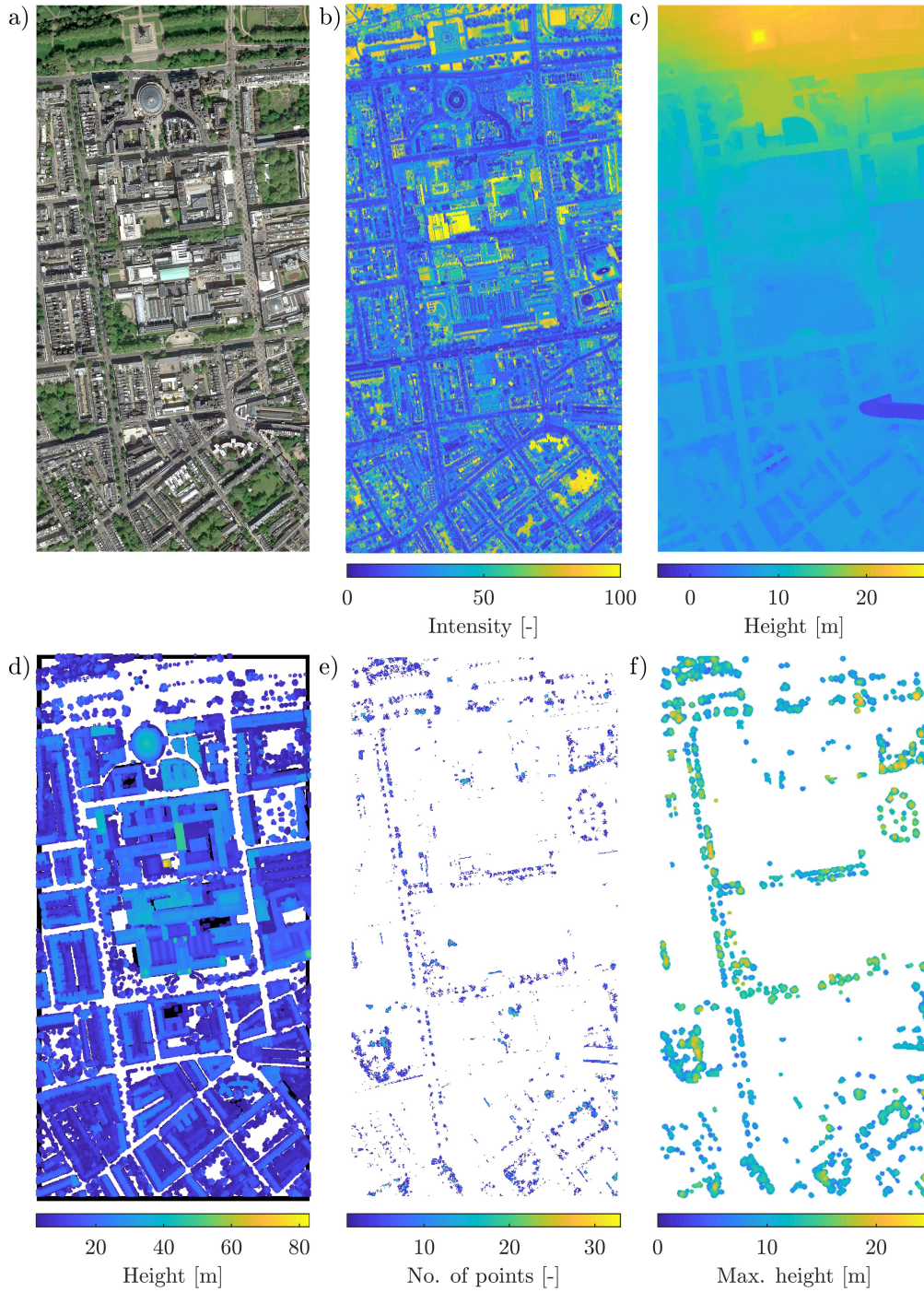


Figure 6.1: a) Aerial photograph, b) LIDAR intensity values, c) Digital Terrain Model, d) processed point cloud (at 2.2) underlaid by building and buffer mask in black, e) processed point cloud (at 2.4) and f) canopy heights as inputted into uDALES.

- 2.3 Remove LIDAR points with an intensity > 40 . The magnitude of this value is dataset specific and obtained via trial and error. This step is effective at removing the remaining non-canopy LIDAR points from the dataset (identified as a result of their higher reflectivity).
- 3 Tree canopy point cloud $\rightarrow$ Cartesian representation for uDALES
 - 3.1 Aggregate point cloud data to the nearest cell centres in the x - y plane of uDALES. Create two-dimensional arrays of the number of LIDAR points, maximum canopy heights and minimum canopy heights in each cell. Figure 6.1e displays the array of number of points at this stage. It indicates that the LIDAR data used in this study does not provide a dense representation of the tree canopies (therefore the data could not be used to estimate the leaf area density) and that the tree canopies are reduced in size due to the Spring-time sampling date.
 - 3.2 Nullify data in cells with one tree canopy neighbour or two tree canopy neighbours on opposing sides. This step removes remaining noisy data. For future studies with higher density datasets, an additional step would be to remove cells with a number of points below a threshold value.
 - 3.3 Smooth the dataset by applying a weighted average. The maximum and minimum canopy heights are defined as a weighted mean of the surrounding tree canopy and empty cells (within a radius of 5.5 m). Weighting is applied via the number of LIDAR points present within each cell (empty cells are defaulted to the mean canopy height of the averaging area and 0.1 points).
 - 3.4 Finally, manual adjustments are made via a qualitative comparison with the aerial view in Figure 6.1a.
 - 3.5 Process for input into uDALES. Figure 6.1f shows the resulting two-dimensional array of canopy maximum heights. Using these heights and the corresponding set of minimum heights, the input file for uDALES is configured.

A three-dimensional representation of the trees and urban morphology in simulation DA CT is provided in Figure 6.2. Uniform tree parameters are assigned for the canopies within uDALES. Typical values from the literature are applied (equivalent to those applied in Section 5.5). The leaf area density a is $1 \text{ m}^2 \text{ m}^{-3}$ (which is similar to values that have been applied to model London Planes in previous studies; Jeanjean et al., 2017), the leaf size l is 0.15 m, the stomatal resistance r_s is 200 s m^{-1} , the extinction coefficient α is 0.4 and the deposition velocity u_d is 0.005 m s^{-1} . The same deposition velocity is assigned

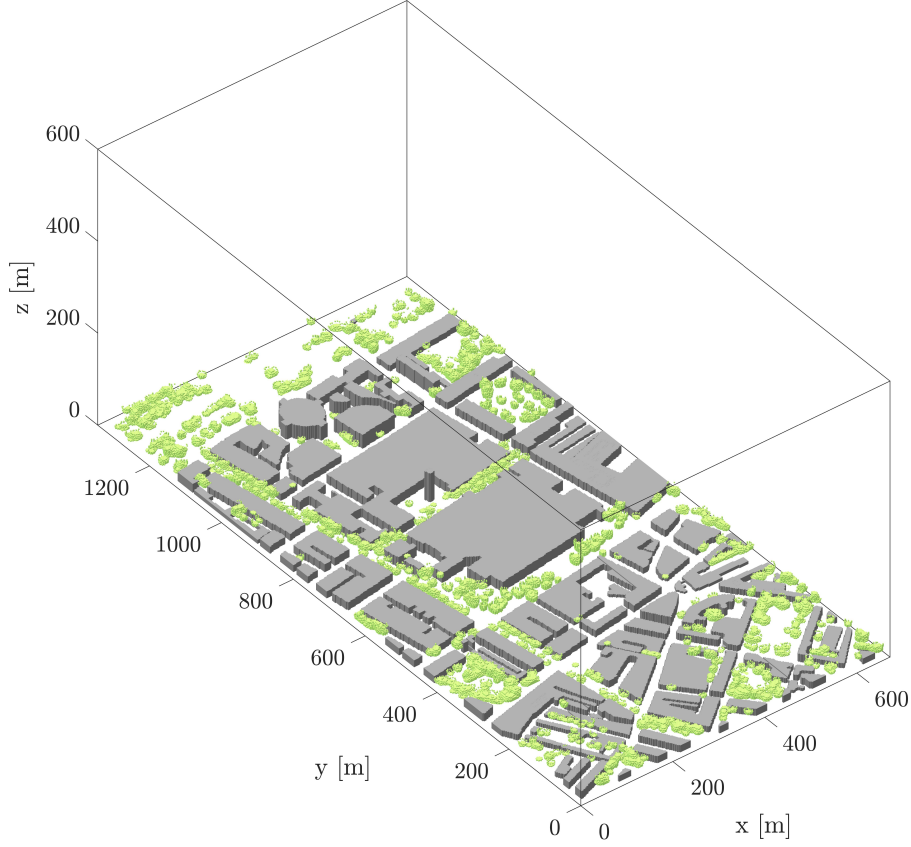


Figure 6.2: Domain configuration of simulation DA CT showing the modelled urban morphology (grey) and tree canopies (green).

to the pollutant fields of inert NO_x and reactive NO , NO_2 and O_3 . This value has been applied to study NO_x in previous studies (Santiago et al., 2017). The net radiation Q_{urb}^* is 195.5 W m^{-2} (the change in net radiation for application to the objective hysteresis model is -2.29 W m^{-2}). A uniform initial profile of the water vapour specific humidity $q_v = 0.00728 \text{ kg kg}^{-1}$ is assigned resulting in an initial relative humidity of 65%. It is important to note that there is a significant range of applicable values and that the ones specified here are simply the most representative as found in the literature.

6.3 Results

The incorporation of convective atmospheric conditions and trees into uDALES and SIRANE simulations enables two forms of analysis. Firstly, uDALES simulations can be compared directly to one another with the carefully specified changes between each simulation attributed to the differences in the results. Qualitative analysis and integrative statistics are used to investigate how the changes between each of the simulations affect the modelled air quality. Simulation DA C is compared to simulation DA N, providing insight into the changes in air quality over the case study region arising from the extrinsic switch from neutral to convective conditions. Simulation DA CT is then compared to simulation DA C to investigate how the presence of trees (that are intrinsically variant within the modelled microclimate) impacts the resulting pollutant concentrations. The same averaging procedures that are applied to evaluate SIRANE in Chapter 3 are used to conduct this analysis. The defined ‘boxes’ (see Figure 3.2) provide effective control volumes to obtain integrative statistics from the LES data and the canyon- and pedestrian-averaged concentrations and along-canyon velocities are also used for analysis in this chapter.

Secondly, equivalent simulations run in uDALES and SIRANE (e.g. simulation DA C and SI C) are compared to provide further evaluation of SIRANE’s predictive performance (specifically how it performs under convective conditions and with trees). Statistical metrics of model performance are used to provide quantitative analysis (the fractional bias (FB), normalised mean square error (NMSE) and fraction in a factor of 2 (FAC2); refer to Chapter 3; Chang and Hanna, 2004).

The notation for the different averaging procedures applied to the uDALES dataset is as follows (the further spatial averaging is applied in post-processing to the time-averaged statistics; consistent with the analysis in Section 3.4). DA-s denotes canyon-averages that are calculated as the spatial averages of the cells in uDALES that fall within each of SIRANE’s boxes. The two-dimensional field that is also denoted by DA-s illustrates a plan view of these canyon-averaged values and, outside of the street-network, takes values at $z = 20$ m (if a building height exceeds 20 m then the first cell above the building is used). DA-p are the horizontally averaged values of uDALES at a height of 1.8 m over each of the defined ‘boxes’ (pedestrian-averaged values). DA-lp apply the same spatial averaging procedure but only over the leeward half of the ‘box’ (also at a height of 1.8 m; leeward-averaged values). DA-wp are equivalent to this term but on the windward side of the canyon (windward-averaged values).

6.3.1 uDALES-uDALES comparison

Neutral versus convective conditions

The initial focus of this analysis is on the difference between simulations DA N and DA C, which provides insight into the effects of convective atmospheric conditions and ground heating on pollutant dispersion within a realistic urban environment. Figure 6.3a shows the percentage change in pedestrian-level concentrations of inert NO_x over the case study area. It is evident that the pollutant concentrations are, for the most part, significantly lower under convective conditions in these two simulations. This finding is expected due to the increased vertical exchange out of the urban canopy layer (UCL) onset by the change in the boundary layer structure (due to the buoyant production and transport of turbulent kinetic energy (TKE)). The mean and turbulent boundary layer profiles (up to a height of 200 m) are shown in Figure 6.4. Figure 6.4f illustrates the magnitude of the difference in the mean TKE just above and within the UCL for convective conditions (the maximum mean TKE, $\langle \bar{e} \rangle$, is 2.89 times larger in simulation DA C than DA N). Figure 6.3b shows a scatter plot comparing the pedestrian-averaged concentrations of these two simulations. The spread of the concentrations displayed in this plot indicates that the change in pollutant concentrations between neutral and convective conditions is non-proportional (meaning $[\text{NO}_x]_{\text{DA-C}}/[\text{NO}_x]_{\text{DA-N}} \neq \text{const.}$; the canyon-averaged values show a similar effect). One may expect that if the only difference between these two conditions was the increased average rate of vertical exchange with the overlying UBL then these concentrations would decrease proportionally between simulations DA N and DA C. Evidently the applied surface heat flux and overlying CBL have affected the in-canyon concentrations in a non-proportional way. The mean reductions in canyon- and pedestrian-averaged NO_x concentrations between simulation DA C and DA N are 17% and 16% respectively. Figure 6.3c compares the two datasets using box plots. The bulk statistics illustrate the same trends, which are also shown to apply to the asymmetry of pollutant concentrations on the lee- and windward sides of the street canyons. The mean ratio between the lee- and windward-averaged concentrations in simulation DA N is 1.21 whereas in simulation DA C this ratio is slightly reduced to 1.18.

Despite the magnitude of the mean concentration reduction, there are regions of the case study area (particularly close to intersections) where the concentration is higher under convective conditions. The flow fields of simulations DA N and DA C are analysed to investigate this phenomenon. Figure 6.5a shows a scatter and box plot of the canyon-averaged along-canyon velocities in simulations DA N and DA C (the along-canyon velocities are calculated as the mean wind speed acting along the street axis of each of the defined

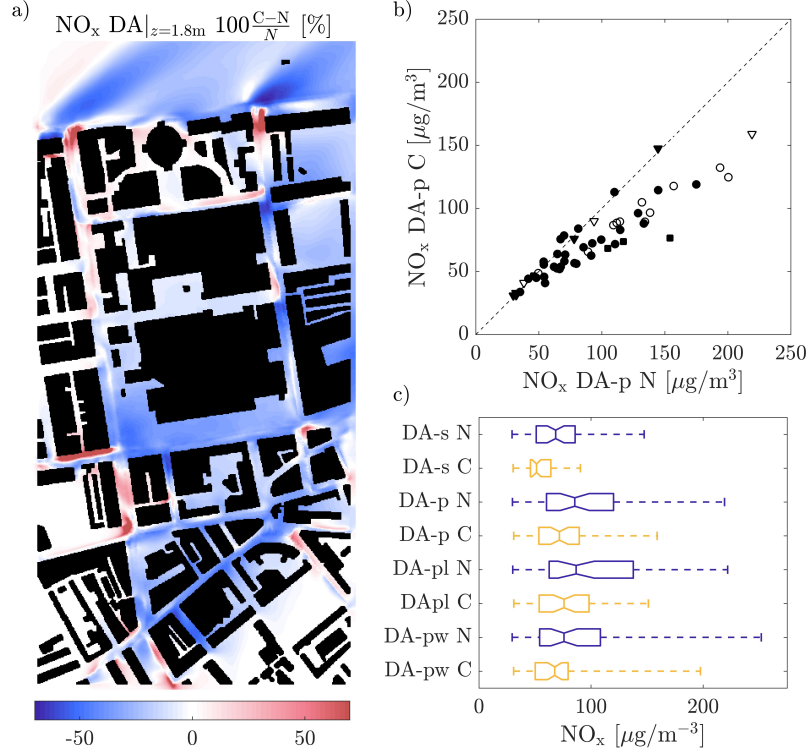


Figure 6.3: a) Percentage reduction of pedestrian-level concentrations of inert NO_x between simulations DA N and DA C. b) Scatter and c) box plots showing the pedestrian-averaged concentrations in simulations DA N and DA C. Triangles represent streets that are connected to the upwind side of the domain, squares represent short streets (length $\approx$ width) and circles are typical street canyons that do not enter in the two previous categorisations. Empty markers denote streets adjacent to an open space.

boxes). It is clear that the velocities under convective conditions are lower in these simulations. This effect is caused by lower mean wind speeds in the modelled boundary layer flow in simulation DA C (shown in Figure 6.4d). This difference is a result of the two simulated boundary layers having the same friction velocities but the drag being relatively higher in the convective case and is consistent with the differences shown between the neutral and convective cases in Section 5.5.2. The scatter plot indicates that the change in along-canyon velocities is also non-proportional between simulation DA N and DA C. The non-proportionalities indicate that the flow structures within the UCL and roughness sublayers must exhibit some fundamental differences. It is hypothesised that these changes are caused by 1) local changes to the interactions of the overlying boundary layer with the flow within the UCL (e.g. the momentum transfer between the UCL and overlying boundary is spatially different under convective conditions, that are characterised by large-scale thermals which interact with the local wakes of buildings within the roughness sublayer, as opposed to neutral conditions, that are dominated by local scale eddies that are predom-

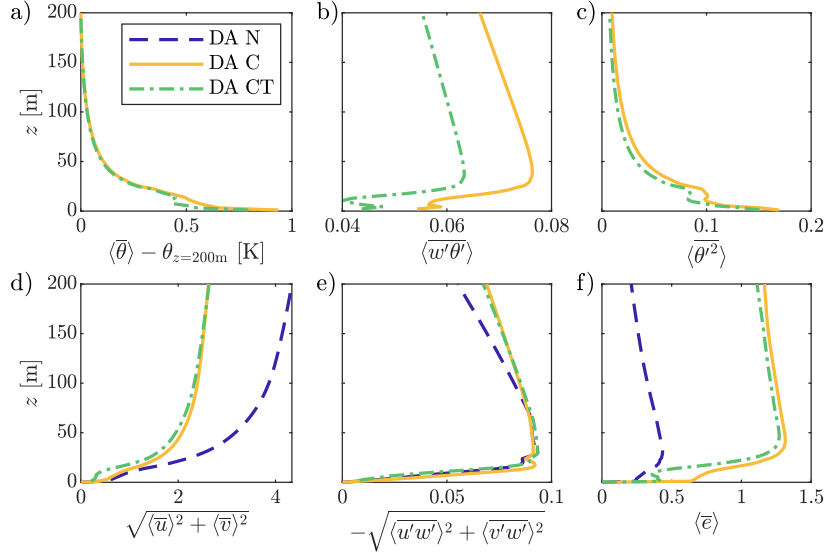


Figure 6.4: Vertical profiles up to $z = 200$ m of a) potential temperature, b) turbulent heat flux, c) potential temperature variance, d) wind speed, e) turbulent momentum flux and e) turbulent kinetic energy for simulations DA N, DA C and DA CT.

inantly related to the upwind turbulent foot print) and 2) changes to the in-canyon flow structures (e.g. it has been shown that infinite canyons of varying aspect ratios with ground heating exhibit different numbers of canyon vortices and different flow regimes dependant on the surface heat flux; Li et al., 2012).

Figure 6.5b and c focuses on the time-averaged flow fields at pedestrian level over an area towards the north-eastern edge of the case study region. A significant proportion of this region is shown to have equivalent or higher pedestrian-level concentrations under convective conditions in Figure 6.3a. The higher mean wind speeds in the neutral case are evident from these plots. The quiver plots also indicate that the flow fields at the the major intersections in this region are fundamentally different between the two simulations. The non-proportional changes to the along-canyon wind speeds mean that the volume fluxes meeting at intersections do not have the same ratios and subsequently fundamentally different exchanges occur. For example, for the neutral case (Figure 6.5b) the flow up the large south-northerly street interacts with the westerly flow across the top of the focus area resulting in the horizontal advection of pollutants out of this street. However, for the convective case (Figure 6.5c) the same intersection is shown to result in reduced wind speeds and a subsequent stagnation point at which an accumulation of pollutants (hotspot) occurs. Similar processes can be identified throughout the domain where relative changes in along-canyon velocities result in regions where the advective transport out of the canopy

6.3 RESULTS

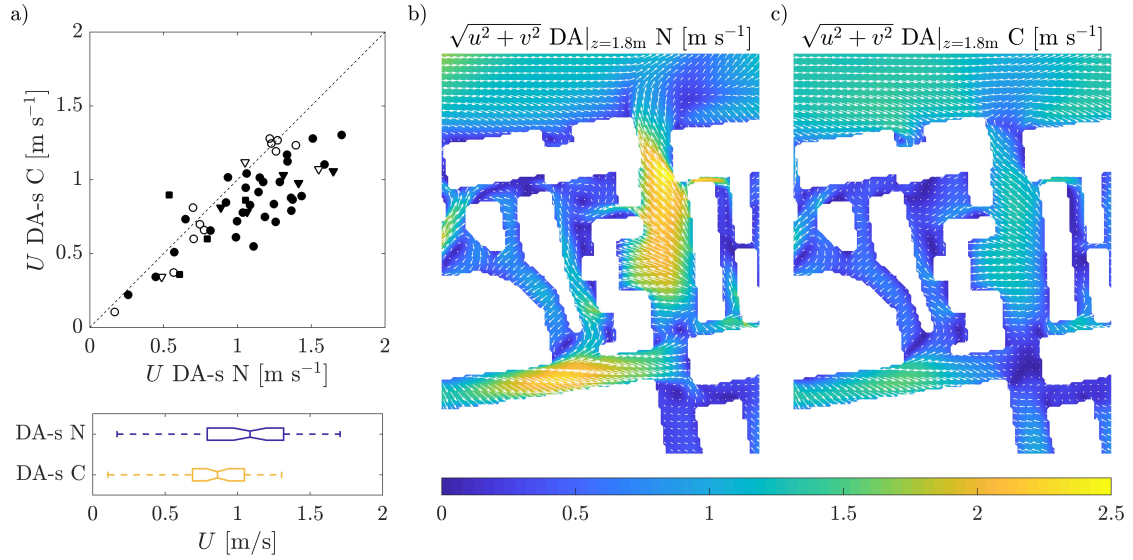


Figure 6.5: a) Scatter and box plot of canyon-averaged along-canyon velocities for simulations DA N and DA C. Wind speeds and quiver plot at pedestrian-level for b) simulation DA N and c) DA C. The markers are consistent with Figure 6.3.

(be that horizontally, as in the discussed example, or vertically) are fundamentally different between simulations DA N and DA C.

Figure 6.6 displays scatter and box plots comparing the calculated pedestrian-averaged concentrations for reactive NO, NO₂ and O₃ (similar trends are found for the canyon-averaged values). The change in concentrations of these reactive pollutants is defined by both the direct changes in their dispersion by the altered flow field under convective conditions and also by the effects that these dispersive changes have on their respective chemical states. It is shown that convective conditions lead to decreased concentrations of NO and NO₂ and increased concentrations of O₃ in these simulations. The reductions in NO and NO₂ can be explained primarily by the change in the dispersion characteristics as the emissions of NO and NO₂ are more mixed more efficiently with the overlying boundary layer. Figure 6.7a and b show the canyon-averaged and above canyon values of the photostationary steady-state (PSS; Equation 1.11) defects for simulations DA N and DA C. The canyon-averaged values are on average 12.5% higher under convective conditions indicating that the pollutants are further from the PSS. Two mechanisms affect the value of the PSS in this comparison: 1) the mixing of pollutants that, if enhanced, allows an equilibrium to be reached more quickly and 2) the decreased residence times of the emitted NO and NO₂ within the UCL that decreases the average amount of time pollutants have to reach a PSS within the UCL. The overall increase in the PSS defect indicates that the

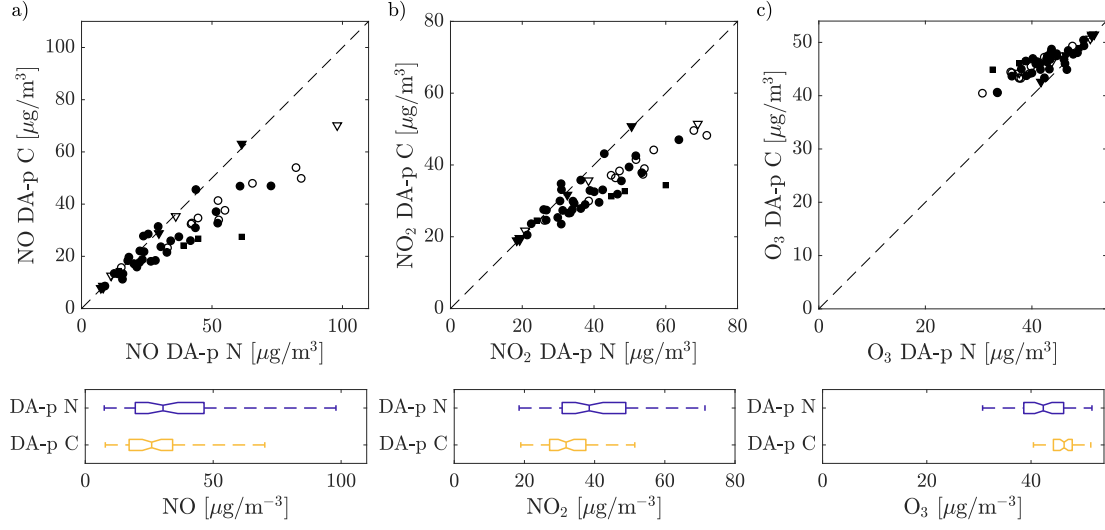


Figure 6.6: Scatter and box plots of canyon-averaged concentrations of reactive a) NO, b) NO₂ and c) O₃ for simulations DA N and DA C. The markers are consistent with Figure 6.3.

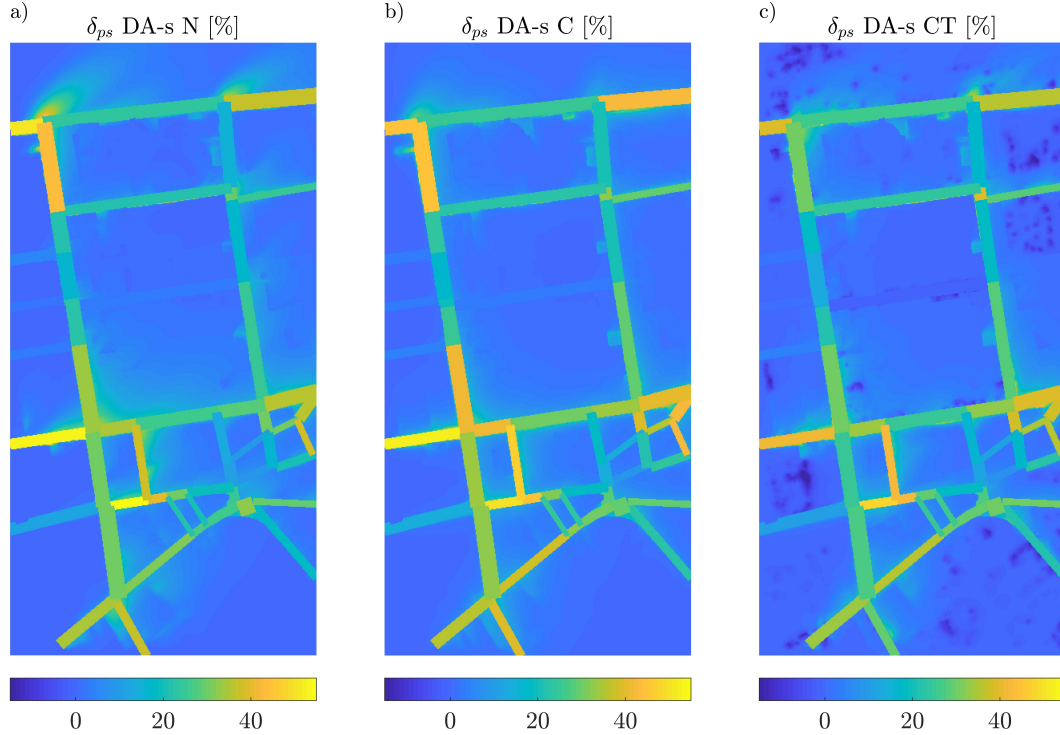


Figure 6.7: Canyon-averaged and above canyon PSS defects for simulations a) DA N, b) DA C and c) DA CT.

latter has a more pronounced effect in the discussed case study. The relative increase in O_3 concentrations under convective conditions therefore occurs as less of the background concentration reacts with the NO rich emissions source to produce more NO_2 within UCL.

Convective with and without trees

Simulation CT incorporates the presence of trees in the case study region, including their drag, depositional and thermal (both shading and transpirational) effects. From Chapter 5 we obtained the general understanding that trees interact with emissions: driven by the balance between their dispersional (drag and buoyancy effects) and depositional influences. Whilst their drag and depositional effects are relatively straightforward to envisage, it is necessary to understand tree's case-specific thermal effects to gain an understanding of how they alter buoyancy between simulations DA C and DA CT. The net cooling effect of the trees in simulation DA CT is evident from both the reduction in the vertical potential temperature profile for $z < 25$ m (Figure 6.4a) and the significant reduction in the turbulent heat flux profile (17.1% reduction in peak $\overline{w'\theta'}$; Figure 6.4b). The relative contributions of this cooling effect (following the same calculations performed in Chapter 5) are -12.5 and -5.3 $W\ m^{-2}$ due to tree shading and transpirational cooling effects respectively. Both phenomena are therefore prevalent. The tree canopy tops generally exhibit a positive sensible heat flux due to the relatively strong irradiation at the tree crowns. However the transpiration rate dominates throughout the rest of the canopy resulting in an overall more significant cooling effect. In terms of pollution dispersion, the tree canopies in simulation DA CT therefore both reduce the sensible heat flux at the urban surfaces and introduce elevated sources of negative buoyancy within the UCL that can be expected to inhibit vertical exchange and potentially to reduce deposition onto the tree canopy. A full analysis of the tree's combined cooling effects over the case study region is beyond the scope of this chapter which focuses on air quality.

Figures 6.8 and 6.9 show the percentage and absolute changes in canyon-averaged and pedestrian-level NO_x concentrations respectively. The overriding trend in both of these figures is that the concentrations along the main roads of the case study region are generally increased whilst the concentrations away from these busy streets and close to tree canopies are reduced (with notable exceptions). Comparing the percentage and absolute reductions indicates that the absolute increase in concentrations close to the busy roads and intersections is more significant than the reduction seen in 'background' areas. These results therefore indicate that, in this case study, the drag and thermal effects of the tree canopies are the dominant processes close to traffic emissions and therefore that in these positions trees lead to a degradation in NO_x concentrations (as qualitatively shown by the

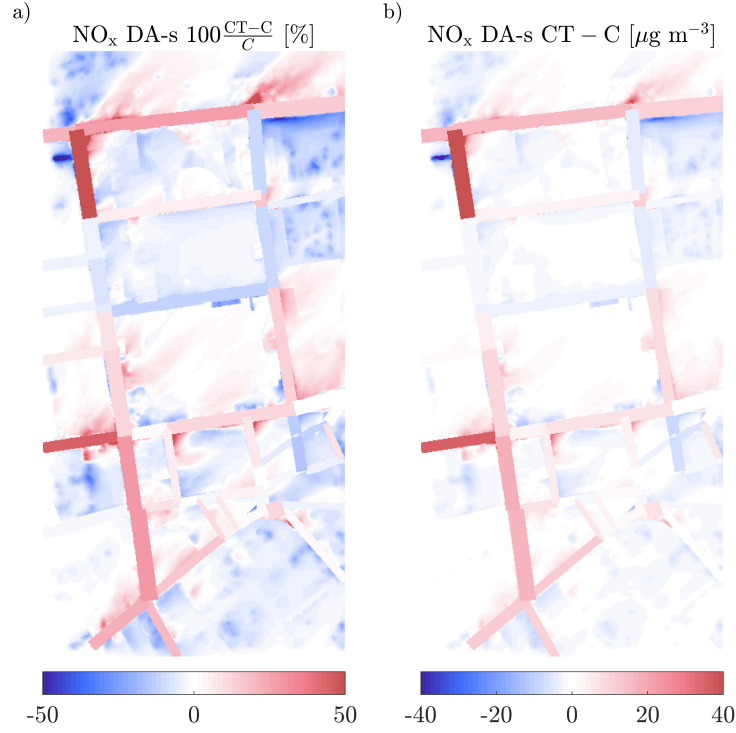


Figure 6.8: Canyon-averaged and above canyon a) percentage and b) absolute changes in inert NO_x concentrations between simulations DA C and DA CT.

trend of higher concentrations with trees in areas close to both tree canopies and high emissions in Figures 6.8 and 6.9). Conversely, further away from the direct emissions of NO_x, these pollution dispersion inhibiting phenomena are not of consequence and therefore, in these regions (pedestrianised streets, squares and parks etc.), the active removal of pollutants by trees is shown to improve the local air quality in this case study. These findings agree with the analysis provided in Section 5.5.2 where the emissions ratio was altered to explore the interaction of the tree canopies with pollutants existing at different roadside-background concentration ratios. The same approach applies fairly well to the results of simulation DA CT where e.g. along the quasi-pedestrianised east-westerly street in the centre of the domain (with zero emissions and therefore $\omega = 0$) a 15.4% reduction in canyon-averaged NO_x is observed but at the main intersections with high emissions (and therefore high effective ω) the NO_x concentrations are shown to be as much as 50% higher (maximum increase of 87.9%). Away from the traffic emissions, the tree canopies therefore act to clean the polluted air entrained into the street canyon from above or advected from surrounding streets (approximately at the background concentration) and therefore the canyon-averaged pollutant concentration is lower due to the presence of trees. Another

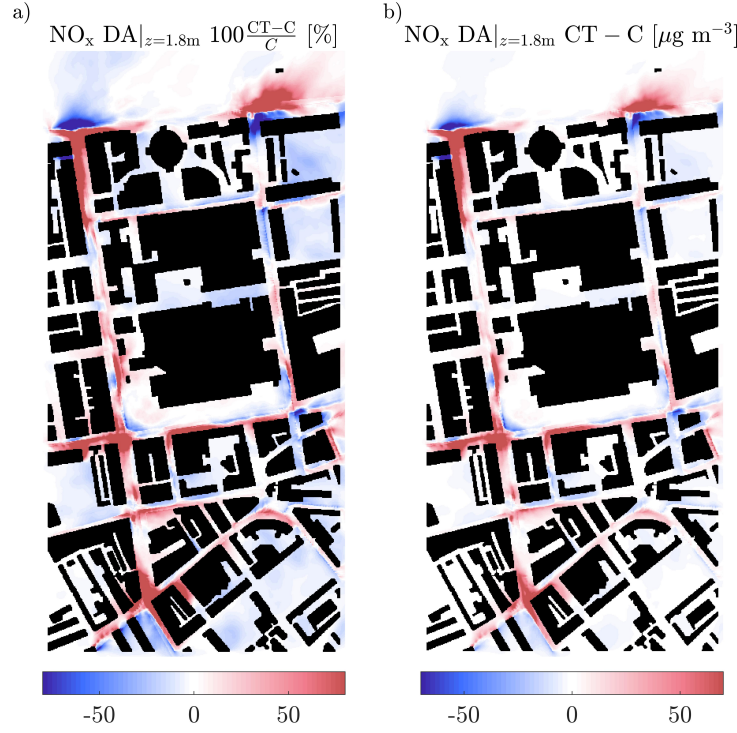


Figure 6.9: Pedestrian-level a) percentage and b) absolute changes in inert NO_x concentrations between simulations DA C and DA CT.

effect of the trees in simulation DA CT is that the air above the UCL is, on average, less polluted than without trees as the net flux of pollutants from the urban area is lower by construction. This effect is particularly pronounced close to green areas such as squares (as shown in Figure 6.8).

Figure 6.10 shows scatter plots that compare the canyon-averaged along-canyon velocities and NO_x concentrations from simulations DA C and DA CT. A canopy volume fraction, λ_l , is defined that is tree canopy-‘box’ volume ratio of each part of the defined street-network. The drag imposed by the tree canopies is evident in Figure 6.10a where the streets with $\lambda_l > 0$ are shown to have lower along-canyon velocities in simulation DA CT. Figure 6.10b further illustrates that the overriding trend in this case study is an increase in the canyon-averaged pollutant concentration due to trees. The streets with the largest concentrations are also shown to have the largest increases in NO_x concentrations due to the presence of trees. Figure 6.10c shows the box plot analysis inclusive of pedestrian-averaged concentrations. In general, the minimum and lower quartiles are positioned similarly between simulations C and CT but the upper quartile and maximum concentration are shifted to significantly higher values in simulation CT (with the excep-

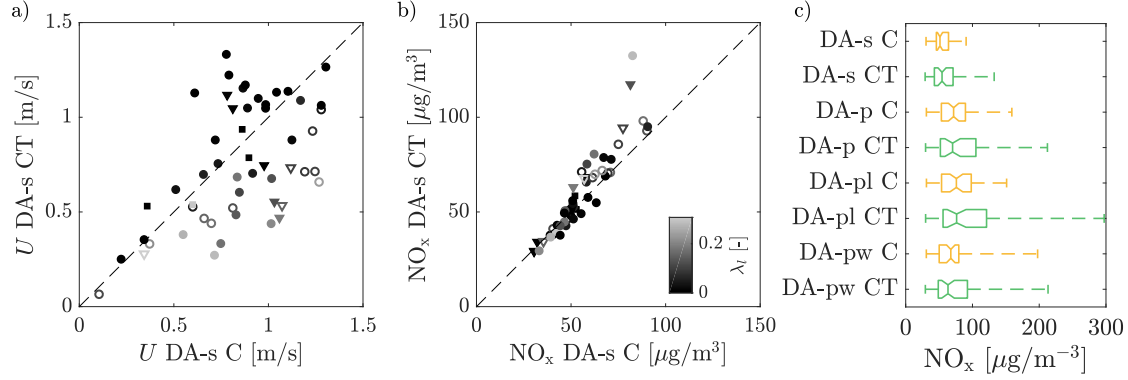


Figure 6.10: Scatter plots of canyon-averaged a) along-canyon velocity and b) inert NO_x for simulations DA C and DA CT. c) Box plots of the canyon-, pedestrian, leeward- and windward-averaged concentration of simulations DA C and DA CT. The markers are consistent with Figure 6.3.

tion of the windward averaged concentration where the maximum values are similar). In fact the asymmetry ratio of the pollutants is generally more significant with trees with a tendency for larger concentrations on the leeward side of the canyon and lower concentrations on the windward (the asymmetry ratios are 1.18 and 1.24 for simulation DA C and DA CT respectively; Abhijith et al., 2017).

The pedestrian-averaged concentrations of reactive NO , NO_2 and O_3 are compared in Figure 6.11. Similar trends are evident for NO and NO_2 as for inert NO_x suggesting the dispersion effects of trees are more significant than the corresponding change in the chemical state of the system for these two pollutants. The change to the chemistry can again be seen via the PSS defect in simulation DA CT (shown in Figure 6.7c). Focussing on the canyon-averaged values, there is a net reduction in PSS defect of 13.9% between simulations DA C and DA CT. This finding indicates that the pollutants are closer to a chemical equilibrium, which occurs because the trees lead directly to increases in the residence time of pollutants in the UCL (a similar conclusion was drawn in the investigation of Moradpour et al., 2017, where they attribute this effect to enhanced mixing). Pedestrian-averaged O_3 is therefore 7.2% lower on average as the net change in the chemical effect is that more of the background O_3 is converted to NO_2 within the UCL (on top of this O_3 is also lost via deposition). Negative PSS defects can be seen in the vicinity of the tree canopies. Deposition is a function of the surrounding concentration and therefore, depending on the assigned background concentrations, trees will result in deviations away from chemical equilibrium as a function of the higher concentration species. As a result of the higher background ozone concentration in this case study, the effect of deposition is to lead to negative values of the PSS defect. These findings are consistent with our understanding of the chemical system presented in this thesis. However in practice trees emit VOCs

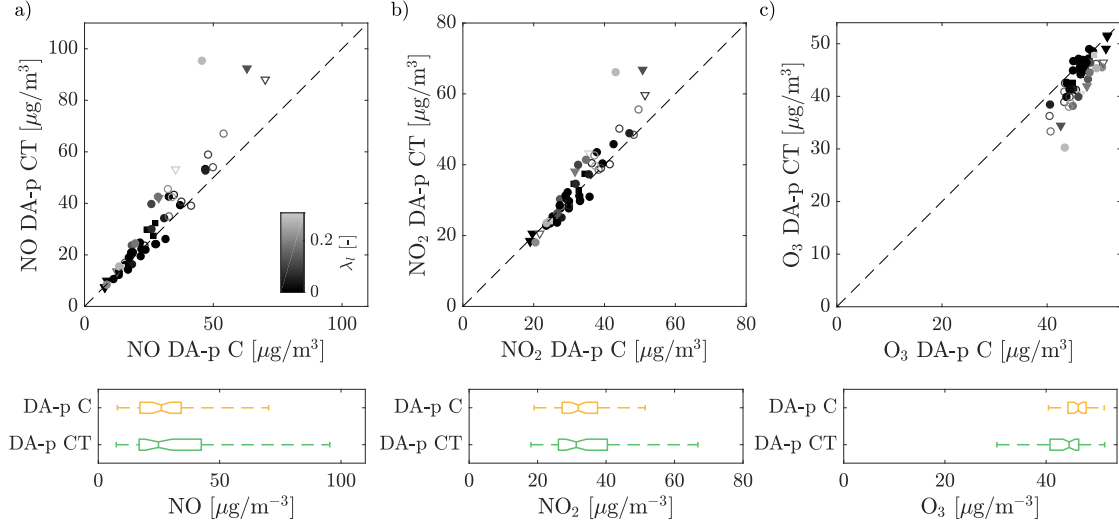


Figure 6.11: Scatter and box plots of pedestrian-averaged a) NO, b) NO₂ and c) O₃ for simulations DA C and DA CT. The markers are consistent with Figure 6.3.

that interact with the modelled chemical cycle and lead to more complex chemical system dynamics.

6.3.2 uDALES-SIRANE comparison

With an understanding of how convective conditions and the presence of trees altered the results of simulations DA C and DA CT, a further evaluation of SIRANE can be conducted. Table 6.1 shows the metric for model performance of the neutral (N; south-westerly case from Chapter 3), convective (C) and convective with trees (CT) simulations. Figure 6.12 displays scatter and box plots of the predicted canyon-averaged NO_x concentrations and along-canyon velocities in SIRANE and uDALES for these three set-ups. The trends exhibited by the convective dataset are qualitatively similar to those obtained in the neutral case (similar values of NMSE). The fractional bias (FB=-0.12) is 50% lower than the neutral case indicating that SIRANE has more of a tendency to overpredict the concentrations under convective conditions (this trend is evident in the box plot of Figure 6.12a). The parametrisations defining the vertical profiles of the CBL in SIRANE have therefore reasonably approximated the changes in the downwind dispersion of NO_x above roof level and the its enhanced ventilation out of UCL under convective conditions ($\sigma_w(z)$; with only a small decrease in predictive ability).

The along-canyon velocities under convective conditions in SIRANE are shown to be overestimated in Figure 6.12b (an overestimation was shown under neutral conditions in Chapter 3 due to the neglect of pressure gradients and secondary flows and the FB is

Table 6.1: Overview of the statistical indices used to quantify the performance of SIRANE’s canyon-averaged predictions against the results of uDALES for a south-westerly wind direction under neutral (N), convective (C) and convective with trees (CT) conditions. The statistical indices are defined in Table 3.2.

Index	Simulation	Along-canyon velocity, U	Inert NO_x	Reactive		
				NO	NO_2	O_3
FB	N	-0.18	-0.08	0.03	-0.18	0.14
	C	-0.39	-0.12	0.00	-0.22	0.13
	CT	-0.51	-0.06	0.11	-0.21	0.07
NMSE	N	0.11	0.08	0.12	0.08	0.03
	C	0.23	0.05	0.05	0.08	0.02
	CT	0.44	0.05	0.11	0.07	0.01
FAC2	N	0.94	1.00	0.96	1.00	1.00
	C	0.91	1.00	1.00	1.00	1.00
	CT	0.59	1.00	1.00	1.00	1.00

twice as low under convective conditions). The box plots of SI N and SI C indicate that, despite the change in atmospheric conditions, there is a negligible change in the predicted along-canyon velocities by SIRANE. The along-canyon velocity is parametrised in SIRANE by the balance between its forcing (defined using the friction velocity and wind angle of incidence) and the drag imposed by the canyon walls (Soulhac et al., 2008). Significantly, the entrainment from the UBL aloft is a function of only the friction velocity and the verification of this parametrisation was conducted using a RANS model under neutral conditions. Therefore the change in the turbulent nature of the UBL flow arising from the effects of buoyancy is not considered. However, as discussed above, both the in- and above-canyon flow structure is significantly altered when modelled in LES. Developing upon the parametrisation for along-canyon velocity under non-neutral conditions is therefore an area for potential improvement in SIRANE in the future.

As discussed above, the only difference between simulations SI C and SI CT is the increase in the Priestley-Taylor coefficient that approximated a 18.6 W m^{-2} decrease in the net sensible heat flux. It is shown in Section 6.3.1 that the average reduction over the case study area between simulations DA C and DA CT (due to shading and transpirational cooling combined) is 17.8 W m^{-2} and therefore the Priestley-Taylor coefficient provides a very good estimation of the thermal effects of the trees in this case. However, the reduction in the net sensible heat flux results in only small changes to SIRANE’s canyon-average predictions. The dataset SI CT is therefore similar to SI C and the above analysis

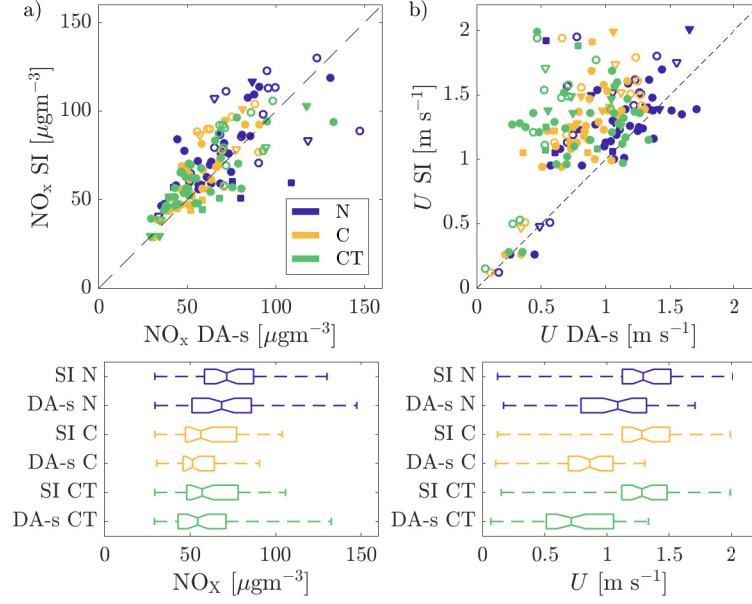


Figure 6.12: Scatter and box plots of canyon-averaged a) inert NO_x and b) along-canyon velocity comparing results from uDALES and SIRANE for neutral, convective and convective with trees conditions. The colours signify the conditions modelled in both the SIRANE and uDALES simulations (N - neutral, C -convective and CT - convective with trees). The markers are consistent with Figure 6.3.

applies with the superposition of the trees of the tree effects in the results of simulation DA CT. The FB for NO_x is therefore slightly reduced as the higher concentrations in uDALES offset SIRANE's systematic overprediction. The reduced along-canyon velocities due to trees result in a significantly worse prediction of along-canyon velocity by simulation SI CT (FB = -0.51, NMSE = 0.33 and FAC2 = 0.59). A potential development within SIRANE would be to incorporate a value similar to the devised canopy volume fraction, λ_t , that acts as an additional source of drag within vegetated parts of the street network (applying a drag term analogous to that discussed in Section 5.2.1). The similarity of the NMSE values for the predictions of NO_x despite the negligible changes in along-canyon velocities indicate that the errors arising from this flow parametrisation apply similarly under all three conditions and that the integrative nature of these spatially averaged statistics makes SIRANE's prediction more robust by construction. Overall, the accuracy of SIRANE's NO_x predictions highlight the effectiveness of the boundary layer parametrisations (particularly for σ_w) and also, in light of the errors in along-canyon velocity, the importance of accurately capturing the emission levels within operational air quality models.

Figure 6.13 displays the canyon-averaged concentrations of reactive NO, NO_2 and O_3 . On the whole, similar trends as those outlined under neutral conditions in Chapter 3 apply for both the convective and convective with trees datasets (that is the assumption of

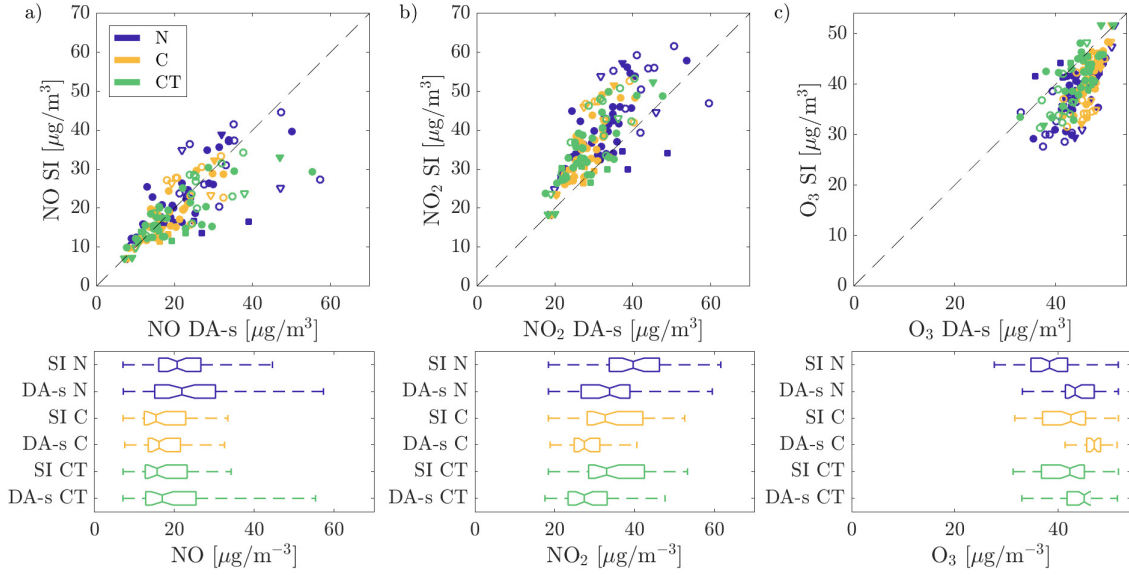


Figure 6.13: Scatter and box plots of canyon-averaged a) NO, b) NO₂ and c) O₃ comparing results from uDALES and SIRANE for neutral, convective and convective with trees conditions. The colours signify the conditions modelled in both the uDALES and SIRANE simulations (N - neutral, C -convective and CT - convective with trees). The markers are consistent with Figure 6.3.

photostationarity in SIRANE leads to a systematic over- and under prediction of NO₂ and O₃ respectively). The small changes in the PSS defects shown in simulations DA C and DA CT impose small changes to the magnitude of this systematic bias in SIRANE. For convective conditions the effect is amplified due to the lower UCL residence times and vice versa for the simulation with trees. The tendency for PSS defects to decrease as a result of the presence of trees suggests that the errors arising due to the assumption of photostationarity in SIRANE will be reduced by other drag and turbulence inducing components within the UCL (e.g. the mixing induced by moving vehicles and other roughness elements such as parked cars). Thus, for neutral or stable boundary layer stratifications, one can expect the PSS defect to also be lower.

Table 6.2 displays the calculated correction factors for simulations DA C and DA CT (the linear relationships between the canyon- and pedestrian-averaged values; see Chapter 3). The R^2 values remain relatively high in the results of both DA C and DA CT indicating that there is a statistically significant linear relationship between the pedestrian-level and canyon-averaged concentrations. The correction factors exhibit a small increase for NO_x, NO and NO₂ under convective conditions (in comparison to neutral) indicating a change in the average in-canyon variability. The presence of trees in simulation DA CT leads to further increases in the correction factor for NO_x, NO and NO₂. This effect occurs as the emissions on vegetated streets are mixed more slowly by the canyon vortex and

6.4 CONCLUSION

Table 6.2: Overview of the correction factors, m , and corresponding R^2 values for the linear regressions of DA-p against DA-s for each pollutant. Results are shown for simulations DA N, DA C and DA CT. All linear regressions were defined to intercept the background concentration following $\phi_{\text{DA-p}} = \phi_b + m (\phi_{\text{DA-s}} - \phi_b)$.

Pollutant		Simulation	m	R^2
Inert	NO _x	N	1.62	0.92
		C	1.75	0.88
		CT	1.81	0.93
Reactive	NO	N	1.75	0.93
		C	1.90	0.89
		CT	1.93	0.92
	NO ₂	N	1.39	0.93
		C	1.47	0.89
		CT	1.57	0.93
	O ₃	N	1.16	0.94
		C	1.15	0.86
		CT	1.08	0.88

hotspots can occur at pedestrian level on the leeward side of the canyon (see Chapter 5). For O₃ the correction factor is decreased due to the presence of trees which occurs due to the increased residence times resulting in a more homogeneous distribution of O₃ within the canyon. The magnitude of these changes show that the correction factors defined in Chapter 3 are not universal (it is expected that changes in the chemical balance will also be prevalent in altering this term for reactive pollutants). However, there is still value in applying a term to account for the systematic underestimation of pedestrian-level exposure by canyon-averaged concentrations and that the magnitude of this term does not vary hugely for the conditions studied here.

6.4 Conclusion

LES of a case study region in South Kensington, London were compared under neutral and convective conditions and with and without the presence of trees. The LES showcased the model capabilities developed in this thesis by incorporating all five of the elements of urban air quality. It resulted in a final realistic simulation that faithfully models the urban microclimate (modelling a real urban morphology, realistic emissions, atmospheric chemistry, convective conditions and trees). Comparable simulations were also run in the

operational pollution dispersion model SIRANE, facilitating an evaluation of predictive performance under convective conditions and in the presence of vegetation.

The case study simulation set-ups introduced in Chapter 3 were extended by 1) systematically altering the modelled atmospheric stability (neutral to convective conditions); and 2) incorporating the presence of trees. The incremental nature of these changes to the simulation set-ups capitalised on the numerical control provided by studying the problem via operational and LES pollution dispersion models. Whilst the results discussed in this chapter are case-specific to the defined study area and limited by the number of different set-ups (only one convective state, wind direction, friction velocity and tree configuration are investigated), the intrinsic variability of the studied microclimate means that interesting findings and some more general conclusions can be drawn on the effects of convective atmospheric conditions and trees on the air quality within a ‘realistic’, heterogeneous urban environment.

Direct comparisons between the LES cases enabled targeted analysis. The onset of convective conditions resulted in an overall decrease in pollutant concentrations as expected (a 16% reduction in pedestrian-averaged concentrations). However the street-by-street changes were shown to be non-proportional indicating that 1) the interaction of the convective boundary layer with the RSL and UCL is different to that under neutral conditions and 2) flow structures within the RSL and UCL are fundamentally altered by the effects of ground heating. Along-canyon velocities were shown to change in a similar non-proportional manner. The residence times of the NO_x emissions are reduced as a result of the enhanced vertical exchange. This change directly leads to higher PSS defects under convective opposed to neutral conditions (a net 12.5% increase in canyon-averaged PSS defects).

The presence of trees in the case study area:

- reduced along-canyon velocities;
- reduced the vertical exchange of pollutants out of the UCL and the transport of pollutants away from pedestrian level;
- reduced the net ground heating due to shaded surfaces;
- imposed elevated buoyancy sources and sinks within the UCL;
- actively removed pollutants from the urban atmosphere.

The intrinsic variability of the morphology, emissions and tree canopies in the case study region enabled a wide range of complex conditions to be analysed within the integrative statistics of simulation DA CT. Despite this inherent variability, several important trends

were identified for the conditions investigated in this case study. Firstly, that the presence of trees close to busy roads leads to a degradation of NO_x air quality at pedestrian level (an average increase in pedestrian-averaged NO_x concentrations of 9.7% and hotspots with increases as high as 87.9%). Secondly that the presence of trees away from busy roads leads to a reduction in the local NO_x concentrations (15% reduction in a quasi-pedestrianised street). Finally that, of these findings, the absolute concentration increases close to busy roads are considerably larger than the absolute reductions in e.g. pedestrianised streets and squares (for the studied tree and environmental parameters and for NO_x that exists at a relatively high roadside-background concentration ratio). The drag and thermal sinks imposed by the tree canopies were also shown to increase pollutant residence times resulting in a reduction in the PSS defect within the UCL (reduction in the canyon-averaged PSS defect of 13.9%).

Comparable simulations from uDALES and SIRANE were used to develop upon the evaluation of SIRANE conducted in Chapter 3. The parametrisations of the mean and turbulent characteristics of the overlying CBL were shown to perform similarly to those under neutral conditions ($\text{FB} = -0.12$, $\text{NMSE} = 0.05$ and $\text{FAC2} = 1.00$). It was highlighted that the parametrisation for the turbulent entrainment at roof level, that affects the along-canyon velocity, is negligibly altered by a change in atmospheric stability. This leads to a larger overprediction of along-canyon velocities in SIRANE for convective in comparison to neutral conditions ($\text{FB} = -0.39$). The Priestley-Taylor coefficient resulted in a very accurate prediction of the net cooling effect of trees in SIRANE. However the neglect of tree's drag, depositional and local thermal effects within the street-network combined to impose additional variability on its predictive ability between simulations DA CT and SI CT. SIRANE also systematically over- and under-predicted reactive NO_2 and O_3 (as was found for the the neutral case in Chapter 3). The magnitude of this systematic bias is affected by the PSS defect that, as discussed above, changed for convective and convective with tree conditions. It is notable that additional roughness and turbulent generation within real urban canyons will reduce the PSS defect and therefore decrease the error introduced by SIRANE's assumption of photostationarity.

The approach followed in this chapter allows for results and insight to be obtained on the elements of urban air quality over a highly complex case study region. The LES results obtained in this study open up a broad range of potential further analyses. For example, a more detailed analysis of the efficacy of each individual tree canopy's cooling and deposition potential in relation to its e.g. size, proximity to emissions and position within the urban morphology would be beneficial in the future. Also a further neutral simulation with trees would enable a direct comparison of the changes in pollutant concentrations

between neutral with and without trees and convective with and without trees cases that would provide a good indication of the importance that the modelled thermal effects of trees have in determining the local air quality. In general, conducting more simulations in the future that further explore the sensitivities of and interplay between the five elements of urban air quality would be advantageous. As more conditions are studied, the scope and range of possible analyses quickly increases.

The combined intrinsic variability of the modelled morphology, emissions and trees in simulation DA CT generally made the production of generalised results and formal analysis more challenging. By simplifying one or more of these elements, a more targeted attribution of the determinants of local air quality can be achieved (whilst maintaining the intrinsic variability of the other elements for analysis). A study that follows this approach and systematically varies between realistic and idealised morphologies, emissions and tree configurations as well as between different extrinsic atmospheric and chemical states presents the best method to further study the complex interactions of these different elements of urban air quality.

Chapter 7

Conclusion and future work

7.1 Overview

Urban air quality presents the largest single environmental health risk (World Health Organization, 2016) and has adverse effects across the three capitals of sustainability (environmental, economic and social; Newman, 1999). With continuing urbanisation and business-as-usual emission regulation policies, mortalities due to urban air quality will continue to rise in the period up to 2050 (Lelieveld et al., 2015). It is necessary to consider the combined life cycle (emission, dispersion, reaction and removal) of urban air pollutants in order to develop a holistic understanding of this problem. Our ability to understand and to realistically model the life cycle of harmful pollutants within the urban atmosphere is integral towards the formation of both short- and long-term solutions to the challenges of urban air quality. Yet our understanding of and ability to accurately model the dominant processes and phenomena determining pollution concentrations in our cities remains limited.

The main aim of this thesis was therefore to develop the model capabilities to realistically simulate air pollution in the urban microclimate; with a focus on accurately resolving 1) urban morphologies, 2) emissions, 3) chemistry, 4) atmospheric stability and 5) trees (namely the five elements of urban air quality as identified in Chapter 1). The inherently heterogeneous and multi-scale nature of the urban climate culminates in a highly complex and computationally demanding research problem. A conceptual methodology, in which relevant spatial and temporal scales are used to classify between e.g. intrinsic and extrinsic variability of a system, was devised in Chapter 1. This methodology provided the overarching framework of this research; helping to systematically tackle the challenges associated with modelling the urban microclimate and ultimately to achieve this research aim.

Large-eddy simulation (LES) models present the optimal tool for resolving the un-

steady, turbulent urban flow field and are capable of modelling the urban environment at the microclimate scale up to very high resolutions. A significant proportion of the work was therefore focused upon developing the model capabilities to simulate the five elements of urban air quality using urban LES:

- Validating the use of the LES model, uDALES, to simulate pollution dispersion within and above realistic urban morphologies (Chapter 2).
- Conducting a comprehensive review of and establishing best practice guidelines for the formation of steady-state non-neutral urban boundary layers using LES (Chapter 4).
- Developing a minimal tree model to capture the integrated (drag, transpiration, shading and deposition) effects of urban trees using LES (Chapter 5).
- Developing uDALES and the pre- and post-processing tools necessary to simulate and analyse all five elements via both idealised and realistic studies (e.g. incorporating the chemistry of the null cycle, coupling a traffic microsimulation model and processing LIDAR data to capture the forms of real buildings and trees; Chapters 2-6).

The case study presented in Chapters 3 and 6, where all five elements and the interplay between them were studied over a real urban microclimate, represents the culmination of these model developments and signifies that this main research aim has been achieved with regards to urban LES. Incorporating all five elements of urban air quality into one LES investigation presents a significant contribution towards realistically modelling and fully resolving air pollution in the urban microclimate and these advancements in urban LES modelling facilitate a plethora of impactful studies in the future (discussed in more detail in Sections 7.2 and 7.4). The results obtained from this case study, as well as those from the targeted studies on atmospheric stability and trees, also provided fundamental insight into the role of and interplay between each of the five elements in determining air quality at the microclimate scale.

Comparable simulations were run over the case study region using the operational pollution dispersion model, SIRANE, thus facilitating a novel method of model evaluation (Chapters 3 and 6). The use of an operational model, in addition to uDALES, extended the scope of the work covered in this thesis; spanning the gap between the high-resolution, computationally intensive modelling techniques typically used in research and the highly parametrised, city-scale modelling that is used by practitioners. The results obtained from SIRANE contextualised the role of urban LES in this research area and also unearthed

several forms of systematic bias in SIRANE that can be used to help improve operational modelling in the future.

The contributions of this work are outlined in Section 7.2 where they are broken down in the context of each of the five elements of urban air quality. A discussion on the developing role of LES in this research area is presented in Section 7.3 and finally recommendations are made for future work in Section 7.4.

7.2 Contributions

The main contributions of this thesis are encapsulated by the breadth of the case study presented in Chapters 3 and 6. To conduct such a study, where all five of the elements of urban air quality were systematically modelled and analysed using two different pollution dispersion models, the conceptual methodology, best practice guidelines, model capabilities and tools for analysis presented in this thesis were imperative. Also, by encompassing sufficient intrinsic variability in terms of e.g. street orientations, aspect ratios, emission levels and tree positions, it was possible to conduct generalised analysis on each of the elements from a limited number of simulations in this case study. Such results are integral towards our understanding of e.g. pedestrian-level exposure to urban air pollutants and the methodology followed here presents a key pathway towards obtaining a complete understanding of urban air quality in the future.

The greatest contribution of this work is the platform that this methodology and these developments provide for future studies into urban air quality and the solutions to it. The targeted study of trees in infinite canyons in Chapter 5 presents a comprehensive initial stride towards an exhaustive study using the presented minimal tree model where the sensitivity of that system and therefore vital questions over trees' thermal and air quality effects in cities can be fully understood. The best practice guidelines outlined from the investigation into the modelling of statistically steady-state non-neutral urban boundary layers in Chapter 4 also provide a reference point for future studies of stable and convective conditions in urban LES. The 'frozen transient' method, introduced in the same chapter, provides a novel tool through which previously problematic studies can now be conducted (e.g. studying the interaction of tall buildings with low-level inversions). Using uDALES in its updated form, one is now able to investigate other key questions regarding the solutions to poor urban air quality as a result of this work, e.g. the localised impacts of urban design, the mitigation potential of green infrastructure and the feasibility of innovative active removal technologies. Further discussion on future work is provided in Section 7.4.

The evaluation of SIRANE indicated that, given accurate emissions data, its predictive ability for canyon-averaged inert NO_x and dispersion above the UCL was robust to the wind directions, atmospheric stabilities and the presence of trees studied in the case study. However, several forms of systematic error were identified in this evaluation and the corresponding suggested improvements provide an additional operational contribution to the research presented in this thesis. Details of the contributions of this thesis, with regards to both LES and operational modelling, are broken down in terms of each of the five elements of urban air quality in the remainder of this section.

Morphology · The typically bluff and heterogeneous range of buildings that amalgamate to define the morphology of an urban area are instrumental in defining the complex flow structures (and therefore the pollution dispersion characteristics) within the urban canopy layer (UCL). Both idealised and realistic urban morphologies were studied in this thesis. Staggered cubic array (Chapters 2 and 4) and infinite canyon (Chapter 5) set-ups were used to treat the morphology as an extrinsic property of the system at the microclimate scale. This permitted targeted studies where other elements, parameters and processes were isolated and analysed.

uDALES was validated against wind tunnel data in Chapter 2 and was shown to provide a good agreement with the dispersion of passive scalars over a real urban morphology. A realistic urban morphology was obtained directly from LIDAR data for the case study conducted in Chapters 3 and 6. A pre-processing routine was developed (first introduced by Suter, 2018) to extract the form of the buildings at the resolutions required for LES. Additions were made to this scheme to adhere, where possible, to the guidelines outlined by Blocken (2015).

A novel approach to obtain bulk statistics from LES of complex urban morphologies was devised and applied to analyse LES outputs in Chapters 3 and 6. The explicit definition of a network of control volumes (representative of individual street segments and equivalent to those used in the operational model SIRANE) served to reduce the inherent complexity of the flow within the realistic urban morphology to its essential features (mean concentrations, pedestrian-level exposure, exchange with the atmosphere etc.). These averaging procedures therefore enabled bulk statistics to be gained from a given simulation with the morphology as an intrinsic variable. The resulting statistics facilitated both an evaluation of SIRANE and analysis of the effects of convective conditions and trees on pollution dispersion within a realistic urban morphology.

SIRANE was shown to systematically overestimate the along-canyon velocities within its street network due to its neglect of secondary flows at intersections and pressure

gradients within the UCL. A strong correlation was exhibited between the pedestrian- and canyon-averaged pollutant concentrations within a realistic morphology from uDALES despite the wide range of angles of incidence and street orientations that were captured. A correction factor was explored to account for SIRANE's systematic underestimation of pedestrian-level exposure, which occurs due to its use of canyon-averaged concentrations.

Insight was also obtained into the flow structures within heterogeneous urban morphologies. The heterogeneous nature of the urban morphology was shown to result in a dominance of advective as opposed to turbulent fluxes of pollutants at roof level. Also the in-canyon flow structures were shown to fundamentally change between the simulations of neutral and convective conditions (the non-proportional nature of this change was hypothesised to relate to the interaction of the boundary layer eddies with the wakes of buildings in the roughness sublayer and changes in the vortical structures and flow regimes in the UCL due to ground heating).

Emissions · Emissions due to road transport are the most ubiquitous within urban areas and often the most harmful in terms of pedestrian exposure. The majority of the thesis focussed upon NO_x traffic emissions and other less prevalent or more spatially homogeneous emissions were captured via the assigned background concentration. The capability to model idealised point and line sources (applied in Chapters 2 and 5) and realistic networks of emissions (derived from the traffic microsimulation model VISSIM; discussed in Chapter 3) were introduced into uDALES.

The approach taken to study the dispersion of traffic emissions within the urban microclimate was to first model the other prognostic fields (velocity, u_i , potential temperature, θ , and specific humidity, q_v) in a statistical steady state such that the urban boundary layer (UBL) is stationary and horizontally homogeneous. Next, uniform profiles were assigned to the background concentration at the upwind boundaries and an outflow condition was set at the downwind boundaries such that an internal pollutant boundary layer forms within a given simulation. The dispersion characteristics are therefore consistent with a single boundary layer profile throughout the domain, which helps to isolate particular phenomena and minimise the degrees of freedom of the problem. This approach also presents a suitable and flexible method to study downwind dispersion under varying atmospheric stabilities as the time and length scales of mixing vary between these different atmospheric states.

The pollutant fields were split into two separate components in Chapter 5: direct emissions and background concentrations. This novel method allows for a range of pollutants that exist at different roadside-background concentration ratios or a range of emission rates to

be studied from only two outputted scalar fields from LES. It presents an instrumental tool for future studies of active removal processes in the urban environment (be that from vegetation or other innovative technologies).

The use of a traffic microsimulation model (augmented by local traffic counts) provided a good spatial representation of traffic emissions within the case study region and accurately captured e.g. pedestrianised areas (used in both Chapters 3 and 6). The intrinsic variability of the emissions in the case study domain permitted more complex analysis and allowed for key features, such as the formation of pollutant hot spots close to intersections, to be explored. The instantaneous three-dimensional pollutant fields from these simulations are actively being analysed to investigate pathways of pedestrian exposure through the case study region by a research group in the Laboratoire de Mécanique des Fluides et d'Acoustique at the École Centrale de Lyon. This analysis provides insight into the timescales of dispersion within the UCL and the real-time exposure of e.g. pedestrians and cyclists. Accurately capturing the spatial (and in the future temporal) variability of the emissions in this way will be crucial to this work going forwards.

Chemistry · Chemical reactions that occur at similar timescales to the dispersion of pollutants within the UCL alter the in-canyon variability of pollutants. The chemistry of the null cycle was introduced into uDALES following a fully-implicit scheme (outlined and validated in Appendices A.2 and A.3 respectively).

These reactions were shown to be significant in determining the concentrations of NO, NO₂ and O₃ over the case study area in Chapters 3 and 6. An understanding of the net effect of this chemistry scheme was obtained by considering the magnitude and spatial distribution of the photostationary steady-state (PSS) defect (a measure of the local chemical imbalance). This parameter was shown to effectively capture the relationship between the dispersion and chemical transformations of pollutants within and above the UCL and was found to be predominantly determined by the magnitude of emissions, emissions ratio, rate of mixing and vertical exchange. General trends were identified such as an average increase in PSS defects under convective conditions (due to a reduction in residence times) and a decrease in PSS defects due to the presence of trees (conversely due to larger residence times). SIRANE applies the assumption that pollutants reach a PSS over each of its hourly time steps and this simplification was shown to result in a systematic over- and under prediction of NO₂ and O₃ respectively. Integrating the chemistry scheme of SIRANE with its bulk dispersion model is imperative to negate these errors in the future.

Incorporating more complex chemical schemes, in particular introducing volatile organic compounds (VOCs) into urban pollution dispersion models, is an active area of research in

the research group. The challenge in applying mechanism reduction schemes to this problem is that concentrations are inherently imbalanced close to emissions within the UCL and these methods focus on equilibrium states. Moreover, existing reduced chemical schemes necessitate 51 or more different species to be modelled (Bright et al., 2013), which is currently too computationally expensive to implement within the LES conducted in this thesis.

Atmospheric stability · The stability of the atmosphere defines the mean and turbulent states of the UBL and is a key factor in determining the flow structures within the RSL and UCL. This meteorological condition, which is determined by the balance between the mechanical generation of and buoyant production/ suppression of turbulence, is treated as an extrinsic property of the urban microclimate. Following the thesis methodology, the modelling approach applied in this thesis was to capture the state of the UBL in a statistical steady state (thus simplifying the problem and obtaining converged statistics). The majority of urban LES studies simplify the problem by assuming neutral atmospheric conditions and investigations that do consider stable or convective boundary layers generally apply the same simplifications and forcings as used for this well-established neutral case. A study was therefore conducted into the best practice for modelling non-neutral UBLs in LES (with periodic boundary conditions) in Chapter 4. It was illustrated that stable and convective atmospheric conditions demand different modelling approaches. A distinction was made in the guidelines between studies that 1) are primarily focussed on dynamics within the RSL and UCL that classically cap the modelled boundary layer (boundary layer height is equal to the domain height; thus enabling greater user control over e.g. boundary layer height, wind direction, friction velocity) and 2) studies where the interaction of the UBL with the quiescent layer aloft is important. The resulting best practice guidelines are summarised in Table 4.4. A novel method (the ‘frozen transient’ method) that allows one to model uncapped convective and stable UBLs in a statistically steady state is presented as a part of this study. This method has numerous potential applications for future work including studies into the interaction of tall buildings with low-level inversions under stable stratification.

The best practice guidelines for convective atmospheric conditions were followed in Chapters 5 and 6. This ensured that the turbulent kinetic energy of the modelled convective boundary layers was not underestimated in the studies of trees in infinite canyons and convective atmospheric conditions over the case study region. Both of these studies highlighted the importance of considering different atmospheric stabilities. Indeed, the air quality was shown to change drastically between neutral and convective conditions (68% and 17% lower canyon-averaged concentrations exhibited in Chapters 5 (infinite canyons)

and 6 (case study region) respectively). The analysis of the case study results in Chapter 6 indicated that the flow structure within the UCL changed non-proportionally due to a change from neutral to convective atmospheric stability of the overlying boundary layer. The parametrisation for along-canyon velocity in SIRANE was shown not to capture the differences in turbulent entrainment at roof level arising from the altered boundary layer properties.

Trees · Trees are an integral part of the urban form and their presence within the UCL affects the transfer of momentum, radiation, temperature, moisture and pollutants. Trees have the potential to act as mitigation tools to both the urban heat island effect and poor urban air quality. However their combined drag, thermal and depositional effects generally result in complex, case-specific changes to their local microclimate that are fairly poorly understood and these effects have rarely been considered simultaneously.

A minimal tree model was presented in Chapter 5 that captures the drag, shading, transpirational and depositional effects of urban trees. The model avoids the need to resolve the leaf temperature and minimises the number of additional free parameters introduced into the system. A bulk parametric study was conducted that highlights the attribution of tree's cooling potential to their shading and transpirational effects. The implementation of the minimal tree model in uDALES was verified against existing numerical simulations and the results from a half-canopy case were presented that can be used for future model verifications.

A show-case study was conducted into the effects of trees under both neutral and convective conditions within infinite canyons in Chapter 5. For the environmental and tree parameters modelled in this study, the trees were shown affect the local flow field and temperature by:

- reducing in-canyon wind speeds (on average by 67%);
- leading to the formation of a small secondary vortex on the leeward side of the canyon;
- reducing the pedestrian-level air temperature by 0.83 K (shading as opposed to transpiration was the dominant cooling mechanism for the modelled set-up);
- resulting in elevated sources/ sinks of buoyancy (positive sensible heat fluxes towards the tree crown due to strong irradiation and negative sensible heat flux throughout the rest of the canopy due to transpirational cooling).

The effect of trees on local pollutant concentration was shown to vary due to both the incorporation of thermal effects/ onset of convective conditions and the background-roadside concentration ratio of the pollutants themselves. Using a weighting factor to specify this

ratio, the differences between tree and no tree cases were shown to result in both degradations and improvements in pedestrian-level concentrations. The effectiveness of trees to improve urban air quality was shown to be strongly related to their proximity to and the strength of the local emission sources. For pollutants that exist relatively homogeneously within the urban environment or in quieter streets, the results suggested that the detrimental impact of trees on vertical exchange and pollutant transfer away from pedestrian level is of less importance and their depositional effects dominate. The thermal effects of trees were shown to reduce the surface heat flux in shaded areas and produce elevated sources and sink of buoyancy that alter the structure of the recirculation within the canyon, these effects combine to exacerbate the reduced vertical exchange introduced by the drag of the imposed canopy. Overall, this showcase study indicated that the depositional effects of trees were shown to be more beneficial under atmospheric conditions conducive of poor air quality and in urban areas away from busy roads.

The results in Chapter 5 showed good agreement with the results obtained in Chapter 6 where tree canopies were implemented within a realistic urban morphology with realistic emissions. Over the case study region, trees were shown to lead to larger NO_x concentrations and hotspots at pedestrian-level close to busy roads and intersections whilst reducing concentrations on pedestrianised streets and in squares and parks.

7.3 Role of large-eddy simulations

The work conducted in this thesis is indicative of LES models' changing role in the research area. LES present the optimal tool towards accurately modelling urban environments. However LES codes are very rarely used operationally due to their high computational demands. Reynolds-Averaged Navier-Stokes (RANS) models are able to model larger domains over larger time-scales but do not capture the inherent unsteadiness of the turbulent urban flow field and are inherently limited by the accuracy of their turbulence model. Operational models, such as SIRANE, are necessary for city-scale modelling however the accuracy of these models is coupled directly with developments from field, wind and numerical studies in this research area.

One of the key elements of this thesis was the incorporation of thermal effects to the modelling of urban air quality and these were shown to have significant effects on pollution dispersion. Hanjalić and Kenjereš (2008) and Kenjereš and Hanjalić (2009) discuss the challenges associated with capturing thermal effects, in particular large-scale thermal structures, in RANS models. As discussed, UBLs are generally non-neutral and therefore LES, which is better equipped to capture these thermal effects, have additional value for

this reason.

Another challenge highlighted by the work conducted in this thesis is that a large number of simulations of increasing complexity are required to fully encompass and analyse the parameter space associated with simulating air pollution in the urban microclimate. As the complexity of these simulations increase, the time-resolving nature of LES becomes more important to accurately capture the dominant dynamics (more complex morphologies and energy balance systems resulting in more complex and bimodal flow behaviour). However as the parameter space grows, so does the required number of increasingly complex simulations, which suits the computationally cheaper qualities of RANS models.

Research developments such as the application of reduced order modelling or the transition to graphics processing units for urban LES present pathways through which such extensive studies will be made more feasible in the future. These developments, which improve the computational efficiency of running LES studies, also inherently make the operational use of LES more feasible (alongside general increases in computational capacity). Accurate modelling of the change in air quality due to e.g. the development of a tall building in a city centre can be the deal-breaker on multi-million pound schemes and is therefore invaluable to developers and urban planners. This relationship should be able to drive significant advancements in the application of urban LES to these problems in the near future.

Coupled to these future studies is the necessity to validate both RANS and LES more thoroughly and in particular against field data (complex thermal effects and vegetation are very challenging to scale for wind tunnel experiments). There are numerous large-scale research projects that bring together these different research disciplines for studies of urban environments (DAPPLE, MAGIC, DIPLOS, UFM SIG etc.). These projects are integral to the future development of this research area. A particularly beneficial future study would be to conduct a comprehensive intercomparison of the various existing urban LES models (such as that conducted for LES of the stable boundary layer; Holtslag, 2003). The main models seen in the literature differ in both their numerical approaches (treatments of the grid and urban surface) and simulation set-ups (grid nesting, inflow generation etc.). An intercomparison, ideally against a benchmark field campaign, would also be advantageous towards developing more stringent and generalised best practice guidelines for urban LES.

7.4 Future work

As highlighted above, there is significant scope for future work following the work conducted in this thesis. To develop on the case study presented in Chapters 3 and 6, a more extensive

study is required where each of the elements of urban air quality is systematically varied between being treated as realistic or idealised/ intrinsic or extrinsic. A fine balance is required to systematically analyse the relevant parameter space in its entirety and the interplay between different elements whilst limiting all superfluous sources of complexity where possible. The key aspect of such an investigation is our ability to numerically control the variability of each of the elements of urban air quality between each simulation (e.g. switching systematically between idealised and realistic treatments and therefore extrinsic and intrinsic variabilities). This method would encompass the full parameter space (in terms of the main determinants of urban air quality) and enable a wealth of analysis. The necessity for a validation against field data and a future urban LES intercomparison was also already discussed in Section 7.3 but is also a key point of interest for future work in this area.

One important feature of the urban microclimate, that was simplified throughout the work conducted in this thesis, is the urban energy balance. Sensible and latent heat exchanges between urban surfaces and the surrounding air were modelled through idealised boundary conditions (constant heat fluxes assigned at road- and roof-level in Chapters 4, 5 and 6). In real urban environments, these exchanges are determined by complex three-dimensional radiative transfers, the thermal properties of the urban form, the urban flow field and anthropogenic emissions. These processes lead to highly heterogeneous and transient thermal environments with non-uniform fluxes of temperature and moisture corresponding to complex distributions of buoyancy sources and sinks throughout the UCL (characterised by phenomena such as radiation trapping, differential heating and heat storage). The intrinsic variability of the urban energy balance at the microclimate scale therefore affects the dispersion of pollutants within and above the UCL and could be considered as a sixth element of urban air quality in future studies. Suter (2018) developed the model capabilities to capture three-dimensional radiative transfer, heat storage and a variety of different urban surface properties in uDALES (including green roofs). These model developments were implemented in parallel to the work presented in this thesis. The respective model capabilities have since been integrated such that this sixth important determinant of air pollution in the urban microclimate can now be incorporated within future studies. When simplified to idealised boundary conditions (as was done in this thesis), the energy balance acts as an extrinsic property of the studied microclimate whereas when explicitly resolved it results in another intrinsic element of the system. Even a single further simulation of the case study area using the urban energy balance model would quickly enable an enhanced understanding of the importance of accurately capturing this element over urban areas (via a direct comparison with the then idealised simulation

DA C of Chapter 6).

A modelling approach has been devised such that a later iteration of the minimal tree model can be coupled to the implemented three-dimensional radiative transfer model (treating the edges of tree canopies as equivalent ‘facades’ and capturing short- and long-wave radiative transfer through the canopy in the cardinal directions following the multiple scattering models of Zhao and Qualls, 2005, 2006). This development would improve the predictions of the minimal tree model by capturing more realistic radiative conditions throughout the canopy (realistic sky view factors and horizontal radiative exchanges with the surrounding buildings). The net radiation at the leaf surfaces was shown to be an important parameter in Chapter 5.

The next step with the data obtained in this thesis is also to better understand what these results mean for human exposure to urban air quality. This includes the pedestrian exposure pathways studies that are now taking place (as discussed in Chapter 7.2). But also gaining a better understanding of indoor-outdoor pollutant exchange and therefore e.g. to contextualise the potential improvements in air quality shown to be provided by trees in quieter streets and for pollutants that exist more homogeneously within the urban environment.

Specific further studies and model developments could be recommended for each of the six elements of urban air quality (uneven building heights, incorporation of VOCs, vehicle turbulence generation etc.). For brevity, two important future studies are recommended here.

Tree sensitivity · Expand upon the idealised study of trees in infinite canyons introduced in Section 5.5. Conduct a more comprehensive sensitivity study to provide similar analysis for a range of tree configurations, aspect ratios, deposition velocities, stomatal resistances, relative humidities etc. Also further work is required to improve the values of the main parametric terms that are integral to determining trees’ thermal and depositional effects (deposition velocity, aerodynamic resistance and stomatal resistance). Finally, as discussed, integrating the minimal tree model with the three-dimensional radiative transfer model in uDALES would be a significant future research development.

Passive and active pollutant removal · After studying the life cycle of urban air pollutants, it is evident that there are two options for the short-term flexible solutions to urban air quality discussed in Chapter 1: enhanced vertical exchange and direct removal from the urban atmosphere. Passive pollution removal can be studied in terms of ‘smart flushing techniques’. How can urban design be configured to maximise the advective flux of pollu-

7.4 FUTURE WORK

tants out of the urban canopy layer in the ‘hot spot’ positions where this is needed most? Can the differential heating effect be utilised to enhance vertical exchange out of canonical urban canyons? Active removal by nature-based solutions such as trees, green walls and green roofs and technologies such as outdoor air purifiers, photocatalytic pavements also require further investigation.

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Appendix A

Appendices

A.1 Net radiation parametrisation

SIRANE's meteorological pre-processor uses the observational inputs of the model to estimate the net sensible heat flux from the urban surface, the boundary layer height and other important boundary layer characteristics (Soulhac et al., 2011). The parametrisations for the net radiation are also used in the minimal tree model in Chapter 5.

Assuming stationary conditions and homogeneity over the urban surface, an urban surface energy balance is defined

$$Q_{urb}^* = Q_{H,urb} + Q_{E,urb} + Q_{G,urb} \quad (\text{A.1})$$

where Q_{urb}^* is the net radiation, $Q_{H,urb}$ is the net sensible heat flux, $Q_{E,urb}$ is the net latent heat flux and $Q_{G,urb}$ is the ground heat flux. The net radiation over the modelled area is defined as

$$Q_{urb}^* = K_{\downarrow} - K_{\uparrow} + \Lambda_{\downarrow} - \Lambda_{\uparrow} \quad (\text{A.2})$$

where $K_{\downarrow}$ is the incoming shortwave radiation, $K_{\uparrow}$ is the outgoing shortwave radiation, $\Lambda_{\downarrow}$ is the incoming longwave radiation and $\Lambda_{\uparrow}$ is the outgoing longwave radiation. The incoming shortwave radiation (during the day) is given by (Kasten and Czeplak, 1980)

$$K_{\downarrow} = (990 \sin(\zeta) - 30) \left(1 - 0.75 \left(\frac{Cld}{8} \right)^{3.4} \right) \quad (\text{A.3})$$

with

$$\sin(\zeta) = \sin(\Omega) \sin(\iota) + \cos(\Omega) \cos(\iota) \left(\frac{2\pi}{24} (t_{HTU} - 12) \right), \quad (\text{A.4})$$

$$\iota = 23.45 \sin \left(\frac{2\pi}{365} (D + 284) \right) \quad (\text{A.5})$$

where D is the day number, t_{HTU} is the hour of the day, ι is the declination angle of the sun, Ω is the latitude and Cld is the cloud coverage index (octas). The reflected shortwave radiation is estimated using a bulk urban surface albedo, A . The incoming longwave radiation from the clouds and atmosphere and outgoing longwave from the urban form are estimated following Holtslag and Van Ulden (1983). The net radiation over the urban area can then be defined as (Soulhac et al., 2011)

$$Q_{urb}^* = \frac{(1 - A)K_{\downarrow} + (0.94 \times 10^{-5}T_0^2 - E)\sigma T_0^4 + 60(Cld/8)}{1.12} \quad (A.6)$$

where E is the bulk emissivity of the urban area, T_0 is a reference air temperature and σ is the Stefan-Boltzmann constant. Typical values of the net albedo $A = 0.18$ and emissivity $E = 0.88$ are assigned throughout this thesis (Soulhac et al., 2011).

A.2 Null cycle chemical scheme implementation

A backward Euler approach is followed to obtain a fully-implicit scheme for the reactions introduced in Equations 3.3-3.5. The change in concentrations between the vector of the reactive pollutants, $\underline{\varphi}$, between time steps n and $n + 1$ (and times t and $t + \Delta t$) can be defined using a Taylor series expansion around $\underline{\varphi}^n$ as

$$\frac{\underline{\varphi}^{n+1} - \underline{\varphi}^n}{\Delta t} = \underline{f}(\underline{\varphi}^{n+1}) \approx \underline{f}(\underline{\varphi}^n) + \underbrace{\frac{\partial \underline{f}}{\partial \underline{\varphi}}}_{A} \bigg|_{\underline{\varphi}^n} (\underline{\varphi}^{n+1} - \underline{\varphi}^n) \quad (A.7)$$

where $A = \frac{\partial \underline{f}}{\partial \underline{\varphi}}$ is the Jacobian and therefore

$$\frac{\underline{\varphi}^{n+1} - \underline{\varphi}^n}{\Delta t} = (I - A\Delta t)^{-1} \underline{f}(\underline{\varphi}^n). \quad (A.8)$$

Applying this definition to define the volumetric reaction terms introduced in Equations 3.3-3.5 gives

$$\begin{bmatrix} \epsilon_{NO} \\ \epsilon_{NO_2} \\ \epsilon_{O_3} \end{bmatrix}_n = [I - \Delta t A]^{-1} \begin{bmatrix} -k_3[NO][O_3] + J_{NO_2}[NO_2] \\ k_3[NO][O_3] - J_{NO_2}[NO_2] \\ -k_3[NO][O_3] + J_{NO_2}[NO_2] \end{bmatrix}_n \quad (A.9)$$

where

$$A = \begin{bmatrix} -k_3[O_3] & J_{NO_2} & -k_3[NO] \\ k_3[O_3] & -J_{NO_2} & k_3[NO] \\ -k_3[O_3] & J_{NO_2} & -k_3[NO] \end{bmatrix}_n. \quad (A.10)$$

Conducting the matrix multiplication and further simplifying then yields:

$$\begin{bmatrix} \epsilon_{\text{NO}} \\ \epsilon_{\text{NO}_2} \\ \epsilon_{\text{O}_3} \end{bmatrix}_n = \frac{-k_3[\text{NO}][\text{O}_3] + J_{\text{NO}_2}[\text{NO}_2]}{1 + (([\text{NO}] + [\text{O}_3])k_3 + J_{\text{NO}_2})\Delta t}\bigg|_n \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}. \quad (\text{A.11})$$

The numerics follow a splitting scheme with the calculation performed at the end of each time step (after advection and diffusion) within uDALES. It is important to note that consideration is required on the units of the concentrations and the reaction rates. In uDALES the concentrations and reaction rates are converted to mol m^{-3} for this calculation and reverted back to g m^{-3} following it.

A.3 Chemistry validation

As highlighted by Han et al. (2018), there are no applicable experimental studies to directly validate the implementation of a chemistry scheme within an urban LES model. The validation used by Han et al. (2018) is reproduced here.

uDALES was set up to replicate the wind tunnel experiment of Pavageau and Schatzmann (1999). Periodic horizontal boundary conditions for velocity, an outflow condition at the downwind boundary for scalars and prescribed upwind concentrations for scalars ($\text{NO} = 0 \mu\text{gm}^{-3}$, $\text{NO}_2 = 0 \mu\text{gm}^{-3}$ and $\text{O}_3 = 195 \mu\text{gm}^{-3}$) were defined to allow a steady-state to form over a series of infinite canyons. A line source emitted $281 \mu\text{gs}^{-1}\text{m}^{-1}$ of NO_x ($\text{NO}_2/\text{NO}_x = 0.1$) at the lowest cell in the centre of one of the canyons. The simulation time was two hours, with statistics taken over the final 30 minutes (Han et al., 2018).

Figure A.1 shows the wind- and leeward profiles of NO_x ($= \text{NO} + \text{NO}_2$; a passive pollutant following Equations 3.3 and 3.4) and the passive scalar of Pavageau and Schatzmann (1999). The agreement shown in this figure indicates that uDALES captures the dispersion of a passive pollutant in an idealised urban canyon and that the applied chemistry scheme satisfies the assertion that the null cycle has no net chemical effect on the NO_x concentration. The incorporation of the chemistry scheme as described in Section 3.2.2 has therefore been shown to be capable of modelling reactive pollutant dispersion (Han et al., 2018).

A.4 A note on the tree canopy radiation budget

A simplified one-dimensional radiative transfer budget was introduced in Section 5.2.3. This scheme has the advantage that the leaf temperatures within the tree canopy do not have to be resolved and the simulation can be driven by the assigned net radiation over the

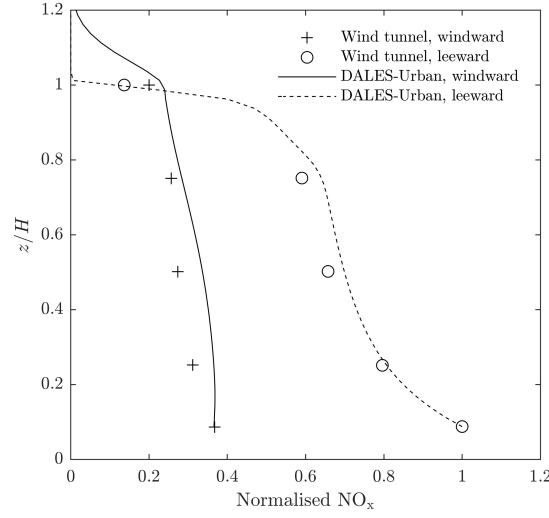


Figure A.1: Vertical profiles of the spanwise- and time averaged NO_x ($\text{NO} + \text{NO}_2$ of a reactive simulation following Han et al., 2018) and passive scalar (experimental results of Pavageau and Schatzmann, 1999). Profiles were taken at a distance of $0.03H$ from each wall (where H is the building height) and normalised by the concentration on the leeward profile at $z = 0.08H$.

urban area (in line with a simplified constant surface heat flux boundary condition). The attenuation of radiation through the tree canopy is defined through the Beer-Lambert law (Equation 5.8), which models an exponential decay in net radiation as a function of the cumulative leaf area index d and an extinction coefficient α (Brown and Covey, 1966; Shaw and Schumann, 1992). This equation encompasses the absorption, reflection, transmission and emission of both short- and longwave radiation by the leaves of the tree canopy. The simplification provided by this one-dimensional radiation budget can be contextualised by considering the radiative transfers within tree canopies in more detail. In particular, it is important to understand the physical meanings of the applied net radiation and extinction coefficient used in the minimal tree model in Chapters 5 and 6.

The incoming shortwave radiation can be decomposed into direct, $K_{\downarrow,B}$, and diffuse, $K_{\downarrow,D}$, radiative components. Following the parametrisation of Kasten and Czeplak (1980), $K_{\downarrow,D} = K_{\downarrow} \left(0.3 + 0.7 (Cld/8)^2 \right)$ where $K_{\downarrow}$ can be defined from Equation A.3. The directionality of these two radiative fluxes is different by construction and therefore so is their attenuation through the tree canopy. The interception of direct shortwave radiation can be determined by the Beer-Lambert law with the extinction coefficient defined as a function of the leaf distribution within the canopy (e.g. an ellipsoidal leaf distribution; Campbell and Norman, 2012). The interception of diffuse incoming shortwave radiation can be obtained by integrating the same function over all of the relevant hemispherical di-

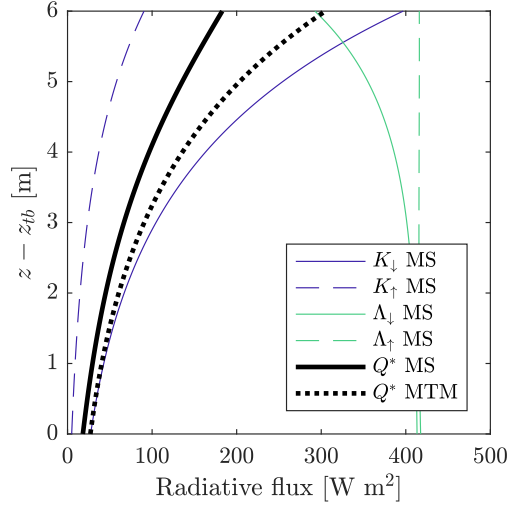


Figure A.2: Comparison of the radiative fluxes through the base case idealised tree canopy using the radiative budget of the minimal tree model (MTM) law and multiple scattering (MS) models of Zhao and Qualls (2005, 2006).

reactions (for which analytical solutions exist for simple leaf distributions; Zhao and Qualls, 2005). The direct and diffuse shortwave radiation that is intercepted by leaves within the tree canopy is either absorbed by the leaf or scattered (via reflection from the leaf surface and transmission through the leaf surface) as diffuse radiation. The scattered shortwave radiation is then transferred in multiple directions through the canopy (the directionality of this scattering process is also partly a function of the leaf distribution). The scattered radiation is then typically intercepted by the surrounding leaves resulting in a continuous process of multiple scattering.

The longwave radiation transfer within the tree canopy also results in multiple scattering processes through similar mechanisms. There is no incoming direct component of the longwave radiation flux but there is an additional emission of longwave radiation from the leaves as a function of their temperature.

Zhao and Qualls (2005, 2006) outline modelling approaches to capture these multiple scattering processes for both short- and longwave radiation. These models are devised such that the multiple scattering processes between different layers of the tree canopies can be set up as a set of linear simultaneous equations. The radiative model can therefore be solved without iteration and moreover the equations can be manipulated into a tri-diagonal matrix system that allows them to be solved efficiently (see Zhao and Qualls (2005, 2006) for details).

The multiple scattering models for short- and long-wave radiation are implemented

within the bulk tree model that was used in the parametric study in Section 5.3. The leaf temperature is solved following an iterative process similar to that outlined by Manickathan et al. (2018). The base case tree and environmental parameters outlined in Table 5.1 are used where applicable in this multiple scattering model. The backward scattering fraction, $r = 0.5$, the leaf albedo, $A_l = 0.4$, and the leaf emissivity, $E_l = 0.96$. The day of the year is 250, the latitude is 51° , the time of day is 12:00 and the cloud cover index, $Cld = 6.2$. The extinction coefficient, $\alpha = 0.7$, is set to the same value for diffuse and direct radiation and higher than the base case scenario for the minimal tree model (for reasons discussed below).

Figure A.2 displays the vertical profiles of the radiation fluxes through the tree canopy, comparing the net radiation calculated through the use of the minimal tree model (MTM) and the multiple scattering (MS) model. It is important to note two main findings from this analysis:

- The extinction coefficient applied for the Beer-Lambert law for net radiation differs in its definition for incoming short- and longwave radiation in the MSM. In the latter case, its value is representative of the leaf distribution and the interception of radiation. In the Beer-Lambert law the extinction coefficient must also represent the scattering processes within the tree canopy and therefore must be relatively decreased. For the discussed base case, an extinction coefficient of 0.4 results in a similar decay of net radiation using the Beer-Lambert law as an extinction coefficient of 0.7 in the multiple scattering model. For this reason, a smaller than average extinction coefficient is used in both Chapters 5 and 6.
- The net radiation above the tree canopy is overestimated using the minimal tree model (for this base case). This value is defined using the parametrisations in Appendix A.1 for the minimal tree model. However, this parametrisation does not consider the change in the net albedo, emissivity and surface temperature above the tree canopy. In future iterations of the model this overestimation can be partially avoided by 1) calculating a different value of net radiation above the tree canopy and 2) altering the applied parametrisation such that it can better represent differences between the tree canopy and urban surfaces.

This analysis indicates that the Beer-Lambert law is capable of capturing the dominant trend in terms of the attenuation of radiation through the tree canopy. But it is also important to note that further attention is required on the assigned value of the net radiation. More extensive investigations are necessary to fully understand the sensitivities of the multiple scattering radiation budget. However, it presents a future model development

that can improve the accuracy of a tree model in urban LES. Future work will also aim to integrate the application of the multiple scattering radiation model for tree canopies within the three-dimensional radiative transfer model developed for uDALES by Suter (2018).

A.5 Tree canopy Penman-Monteith derivation

The equations for the latent and sensible heat fluxes between a leaf and the surrounding air were established in Chapter 5

$$Q_{H,l} = \frac{2}{r_a} \rho c_p (T_l - \theta), \quad (\text{A.12})$$

$$Q_{E,l} = \frac{1}{r_a + r_s} \frac{\rho R_a L_v}{p_0 R_v} (\varepsilon_{v,l} - \varepsilon_v). \quad (\text{A.13})$$

where the right-hand sides of the equations are composed of resistance terms for the pathway between the leaf surface and bulk air (r_s is the stomatal resistance and r_a is the aerodynamic resistance), unit conversion terms (ρ is the density of air, c_p is the heat capacity of the air, R_a and R_v are the gas constants of dry air and water vapour respectively, p_0 is the atmospheric pressure and L_v is the latent heat of vaporisation) and finally a vapour pressure, ε , or temperature difference (absolute temperature, T , and potential temperature, θ).

The vapour pressure at the leaf surface is at saturation point and therefore $\varepsilon_{v,l} = \varepsilon_s(T_l)$ where ε_s is the saturation vapour pressure. Both Equations A.12 and A.13 are therefore a function of the leaf temperature. It is possible to avoid the need to model the leaf temperature by following the Penman transformation (Penman, 1948). The first step is to partition the surface-air vapour pressure deficit into two terms (using a Taylor series expansion; Jones, 2013)

$$\varepsilon_s(T_l) - \varepsilon_v = [\varepsilon_s(\theta) - \varepsilon_v] + [\varepsilon_s(T_l) - \varepsilon_s(\theta)] = D + s(T_l - \theta) \quad (\text{A.14})$$

where $s = \frac{\partial \varepsilon_s}{\partial T}$ is the slope of the curve relating saturation vapour pressure to temperature and D is the vapour pressure deficit of the ambient air. It is assumed that s is approximately constant over the defined range of temperatures.

Substituting Equation A.14 into Equation A.13 gives

$$Q_{E,l} = \frac{1}{r_a + r_s} \frac{\rho R_a L_v}{p_0 R_v} [D + s(T_l - \theta)]. \quad (\text{A.15})$$

Now both the latent and sensible heat fluxes can be defined as a function of the leaf-air temperature difference ($T_l - \theta$) (Equations A.12 and A.15). Rearranging Equation A.12

for $(T_l - \theta)$ and substituting into Equation A.15 then gives

$$Q_{E,l} = \frac{1}{r_a + r_s} \frac{\rho R_a L_v}{p_0 R_v} \left[D + \frac{s Q_{H,l}}{\frac{2}{r_a} \rho c_p} \right]. \quad (\text{A.16})$$

$Q_{H,l}$ can be defined by rearranging the leaf energy balance equation (Equation 5.16 in Chapter 5)

$$Q_{H,l} = Q_l^* - Q_{E,l}. \quad (\text{A.17})$$

Substituting this relation into Equation A.16 and rearranging gives

$$Q_{E,l} = \frac{s Q_l^* + \frac{2}{r_a} \rho c_p D}{s + 2\gamma \frac{(r_a + r_s)}{r_a}} \quad (\text{A.18})$$

where $\gamma = \frac{p_0 c_p R_v}{R_a L_v}$ is the psychrometric constant which relates the partial vapour pressure to the air temperature (Jones, 2013). Equation A.18 is an adapted form of the original Penman-Monteith equation (Penman, 1948). The above derivation avoids the necessity to model the leaf temperature and has been applied widely across many fields and at many spatial scales (Jones, 2013).

The saturation vapour pressure is calculated using the empirical Clausius-Clapeyron relation of Buck (1981) which accounts for the variability of L_v with temperature and is accurate over the range of temperatures found in urban areas

$$\varepsilon_s = 610.8 \exp \left(\frac{17.27(T - 273.15)}{T - 35.85} \right). \quad (\text{A.19})$$

The slope of the curve relating saturation vapour pressure to temperature is given by (Bittelli et al., 2008)

$$s = \frac{4098 \varepsilon_s}{(T - 35.85)^2}. \quad (\text{A.20})$$