

IMPERIAL

Here Comes the Sun

Modelling the Diurnal Cycle of Urban Microclimates using
Large-Eddy Simulation

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Statement of Originality

This thesis represents work that is my own, with other work referenced where appropriate.

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¹Spoiler alert: it’s not good.

Abstract

This thesis involves upgrading uDALES, a large-eddy simulation (LES) model with a surface energy balance (SEB) scheme, and using it to study microscale urban boundary layer (UBL) processes over a diurnal cycle. The upgraded code (v2.0) has two main new features: an improved parallelisation that substantially increases the scalability, and a high-fidelity surface treatment that can capture geometries that are not aligned with the Cartesian computational grid. uDALES v2.0 is validated against other models and experiments, and demonstrated to offer better accuracy than previous versions.

Subsequently, uDALES v2.0 is used to investigate the microclimate in a realistic masterplan in a hot, arid climate. Analysis of the bulk SEB shows that while behaviour is primarily driven by radiation, thermal inertia is important as well. Moreover, the flow behaviour in the wake of the buildings is shown to be more important than the surface temperature in determining the local air temperature. This case is compared with a set of simulations that each represent one hour of the day and in which the SEB reaches a steady state. The lack of thermal inertia in the steady-state simulations results in systematic differences in the SEB and surface temperature over the diurnal cycle.

Finally, uDALES v2.0 is coupled to a mesoscale model (MetUM) for a diurnal cycle of the UBL in London, considering both idealised and realistic geometrical configurations. Comparing the models, the daytime convective boundary layer is similar overall, though there are differences in the near-surface wind speed, and the nocturnal boundary layer generally shows less good agreement. The bulk SEB is predicted similarly, whereas the surface temperature exhibits a consistent discrepancy. The SEB for the various uDALES geometries are closer to each other than to MetUM. The models exhibit fair agreement with observations near the surface, and poorer agreement at higher altitude.

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Acronyms

ABL atmospheric boundary layer

CFD computational fluid dynamics

DNS direct numerical simulation

FFT fast Fourier transform

HPC high-performance computing

IBM immersed boundary method

ISL inertial sub-layer

LSM land-surface model

LES large-eddy simulation

MRT mean radiant temperature

RANS Reynolds-averaged Navier-Stokes

RSL roughness sub-layer

SEB surface energy balance

UBL urban boundary layer

UCL urban canopy layer

UCM urban canopy model

UHI urban heat island

Symbols

Constants

δ	Kronecker delta [-]
ε	Levi-Cevita epsilon [-]
κ	von Kármán constant [-]. Value used: 0.41.
σ	Stefan-Boltzmann constant [$\text{W m}^{-2} \text{K}^{-4}$]. Value used: 5.67×10^{-8} .
Ω	diurnal cycle angular frequency [rad s^{-1}]. Value used: $\frac{2\pi}{86400}$.
g	gravity of Earth [m s^{-2}]. Value used: 9.81.
$\mathcal{L}_v$	latent heat of vaporisation of water [J kg^{-1}]. Value used: 2.26×10^6 .

Fields, Coordinates, & Properties

α	shortwave albedo [-]
Γ	distance [m]
δ	thermal penetration depth [m]
ϵ	longwave emissivity [-]
ζ	spatial coordinate [m]
η	spatial coordinate [m]
θ	air potential temperature [K]
θ_a	air potential temperature adjacent to the surface [K]
θ_v	air virtual potential temperature [K]
θ_τ	surface characteristic temperature [K]
Θ	zenith angle (typically solar) [rad or °]
$\varkappa$	diffusivity (typically thermal) [$\text{m}^2 \text{s}^{-1}$]
λ	thermal conductivity [$\text{W m}^{-1} \text{K}^{-1}$]
λ_c	complete aspect ratio [-]

λ_f	frontal area fraction [-]
λ_p	plan area fraction [-]
ν	kinematic viscosity [$\text{m}^2 \text{s}^{-1}$]
ξ	spatial coordinate oriented from the surface exterior to the interior [m]
π	kinematic pressure correction [$\text{m}^2 \text{s}^{-2}$]
Π	fluid masking function [-]
ρ	density [kg m^{-3}]
τ	shear stress [Pa] or time lag [h]
τ_s	surface shear stress [Pa]
v	distance [m]
ϕ	scalar flow variable [various]
φ	flow variable [various]
Φ	azimuth angle (typically solar) [rad or $^\circ$]
χ	spatial coordinate [m]
ψ	view factor [-]
ω	Angular frequency [rad s^{-1}]
a	facet section area [m^2]
A_c	total three-dimensional surface area [m^2]
A_f	facet area [m^2]
A_f	windward area of buildings [m^2]
A_p	plan area of surface type (typically buildings) [m^2]
A_t	total plan area [m^2]
b	building width [m]
c	canyon width [m]
c_p	specific heat capacity (typically of air) [$\text{J kg}^{-1} \text{K}^{-1}$]
C	volumetric heat capacity [$\text{J m}^{-3} \text{K}^{-1}$]
C_m	momentum transfer (drag) coefficient [-]
C_h	heat transfer coefficient [-]
d	distance to the surface [m]
D	facet thickness [m]
$\mathcal{D}$	diffuse shortwave radiation [W m^{-2}]
D_{sky}	diffuse shortwave radiation from the sky [W m^{-2}]

$\mathbf{e}$	unit vector [-]
E	latent heat flux [W m^{-2}]
$\mathcal{F}_m$	momentum stability function [-]
$\mathcal{F}_h$	heat stability function [-]
F	large-scale momentum forcing [m s^{-2}]
G	conductive heat flux [W m^{-2}]
h	building height [m]
H	sensible heat flux [W m^{-2}]
I	direct normal irradiance [W m^{-2}]
k	turbulent kinetic energy [$\text{m}^2 \text{s}^{-2}$]
K	shortwave radiation [W m^{-2}]
K_m	momentum eddy diffusivity [$\text{m}^2 \text{s}^{-1}$]
K_h	thermal eddy diffusivity [$\text{m}^2 \text{s}^{-1}$]
L	longwave radiation [W m^{-2}]
L_{sky}	diffuse longwave radiation from the sky [W m^{-2}]
L_x	domain length in the x direction [m]
L_y	domain length in the y direction [m]
L_z	domain length in the z direction [m]
$\hat{\mathbf{n}}$	unit vector normal to the surface [-]
N	buoyancy frequency [s^{-1}]
N_f	number of facets [-]
N_l	number of facet layers [-]
N_x	number of grid points in the x direction [-]
N_y	number of grid points in the y direction [-]
N_z	number of grid points in the z direction [-]
p	kinematic deviatoric pressure [$\text{m}^2 \text{s}^{-2}$]
P	probability density [-]
$\mathbf{p}$	point [m]
$\hat{\mathbf{p}}$	unit vector in the local spanwise direction [-]
Pr_t	turbulent Prandtl number [-]
q	specific humidity [kg kg^{-1}]
$\hat{\mathbf{q}}$	unit vector [-]

q_τ	surface characteristic specific humidity [kg kg^{-1}]
q_a	specific humidity adjacent to the surface [kg kg^{-1}]
Q	heat storage [W m^{-2}]
r	resistance (e.g. aerodynamic) [s m^{-1}]
$\hat{\mathbf{r}}$	unit vector [-]
R	radiation [W m^{-2}]
$\mathcal{R}$	reflected radiation [W m^{-2}]
RH	relative humidity [%]
Re	Reynolds number [-]
Ri_b	bulk Richardson number [-]
Ri_f	flux Richardson number [-]
Ri_g	gradient Richardson number [-]
$\hat{\mathbf{s}}$	vector to the sun [-]
S	source or sink of atmospheric quantity [various]
$\mathcal{S}$	direct solar radiation [W m^{-2}]
t	time [s]
$\hat{\mathbf{t}}$	unit vector in the local streamwise direction [-]
T	surface temperature [K]
T_s	surface (exterior) temperature [K]
$\mathbf{u}$	velocity [m s^{-1}]
u	streamwise velocity component [m s^{-1}]
u_τ	surface characteristic (shear/friction) velocity [m s^{-1}]
u_x	velocity component in the x direction [m s^{-1}]
u_y	velocity component in the y direction [m s^{-1}]
u_z	velocity component in the z direction [m s^{-1}]
u_a	streamwise velocity component adjacent to the surface [m s^{-1}]
u_i	Cartesian velocity component in the x_i direction [m s^{-1}]
v	spanwise velocity component [m s^{-1}]
V	computational cell volume [m^3]
w	vertical velocity component [m s^{-1}]
x_i	generalised Cartesian coordinate ($i = 1, 2, \text{ or } 3$) [m]
x	horizontal spatial coordinate [m]

$\hat{\mathbf{x}}$	unit vector in the x direction [-]
y	horizontal spatial coordinate [m]
$\hat{\mathbf{y}}$	unit vector in the y direction [-]
z	vertical spatial coordinate [m]
$\hat{\mathbf{z}}$	unit vector in the z direction [-]
z_0	momentum roughness length [m]
$z_{0,h}$	heat roughness length [m]
z_d	displacement height [m]

Subscripts

τ	surface characteristic quantity
a	atmospheric quantity adjacent to the surface
f	facet index
g	facet index
i	Cartesian direction index
j	Cartesian direction index
k	Cartesian direction index
l	spatial index
m	spatial index
s	quantity at surface exterior
0	quantity at at $z=z_0$, or at surface exterior
∞	initial or free-stream value

Operators

$\bar{\cdot}$	time average
$\cdot'$	deviation from time average, or rotation
$\langle \cdot \rangle$	horizontal average

Chapter 1

Introduction

1.1 Motivation

It is expected that the global average temperature will increase by at least 1.5°C by 2050 (Masson-Delmotte et al., 2022) and that the fraction of people living in cities will increase from around a half to two-thirds (United Nations, 2023). To illustrate, by 2050 the climate of London, UK is expected to resemble that of Barcelona, Spain (Bastin et al., 2019) and could be home to over one million more people (Greater London Authority, 2023). In this context, urban residents face particular environmental challenges, e.g. the urban heat island (UHI) effect, in which the temperature in cities tends to be higher than in the surrounding rural area (Oke et al., 2017). Excess heat, particularly coupled with humidity, is uncomfortable at best and lethal at worst (Heaviside et al., 2017), and can damage infrastructure and impact wildlife (Chapman et al., 2013; Solecki and Marcotullio, 2013). Tall buildings can exhibit high wind speed at their base, which is a safety concern (Xu et al., 2017). Cities also tend to have poorer air quality, largely due to greater emission of pollutants within the city itself (Enenkel et al., 2020). Given the trends in climate change and urbanisation trends, these issues are likely to become ever more salient. It is therefore crucial to study air flow, heat transfer, and pollutant dispersion in the built environment in order to provide insight into wind, thermal comfort, and air quality. The applications range from the small scale, such as assessing design strategies for pedestrian comfort and climate change mitigation, to the large scale, such as improving weather forecasting for urban areas (Erell, 2008; Lai et al., 2019; Masson et al., 2020a; Lobaccaro et al., 2021; Yang et al., 2023; Aghamolaei et al., 2023; Lean et al., 2024).

Indeed, urban climatology is inherently challenging because of the wide range of relevant spatial and temporal scales — from a single building facade to an entire city; from a gust of wind to the passing of the seasons (see Fig. 1.1). Such a range of scales is due to both the sheer number of physical processes involved and the very nature of the built environment itself. Cities often exhibit significant variation in how they are structured and what they are made of — their so-called form and fabric — both in the sense of comparing multiple cities and within a single one. They tend to be highly heterogeneous, meaning their form and fabric vary significantly over short distances, causing environmental conditions to follow suit. It is therefore necessary to consider small-scale variation in environmental conditions, often referred to as microclimate, when designing buildings and other public spaces. The net result of local conditions across the city may result in some overall effect (e.g. UHI), thus potentially interacting with larger-scale conditions (Oke et al., 2017).

A combination of observations, experiments (physical modelling), and numerical modelling are used to study urban climates (Barlow, 2014). Given the increasing capabilities of high-performance computing (HPC) systems, numerical models are being developed to take advantage of these resources (Ching, 2013; Lateb et al., 2016; Krayenhoff et al., 2021). Some models are designed primarily to resolve processes at the local-scale and mesoscale, at which the effects of urban areas are parameterised (Masson, 2006; Martilli, 2007; Dudhia, 2014; Kwok and Ng, 2021), while others are designed to model processes at the microscale, at which the surface is explicitly resolved (Blocken, 2015; Toparlak et al., 2017; Jänicke et al., 2021; Mirzaei, 2021; Tominaga, 2024). Due to the multiscale nature of urban environmental processes, it is common to couple models with differing spatial resolution together, in particular when using microscale models to study large urban areas (Kadaverugu et al., 2019).

Atmospheric flows are governed by the Navier-Stokes equations, which can be solved numerically using computational fluid dynamics (CFD). Incorporating heat transfer at the surface requires modelling the surface energy balance, including the net radiation, convection, evaporation, and conduction. Modelling pollutant dispersion potentially involves chemical reactions of various aerosols. There are standalone tools for modelling air flow, heat transfer, and pollutant dispersion individually, but as these processes fundamentally interact, multi-physics modelling tools have been developed that have some

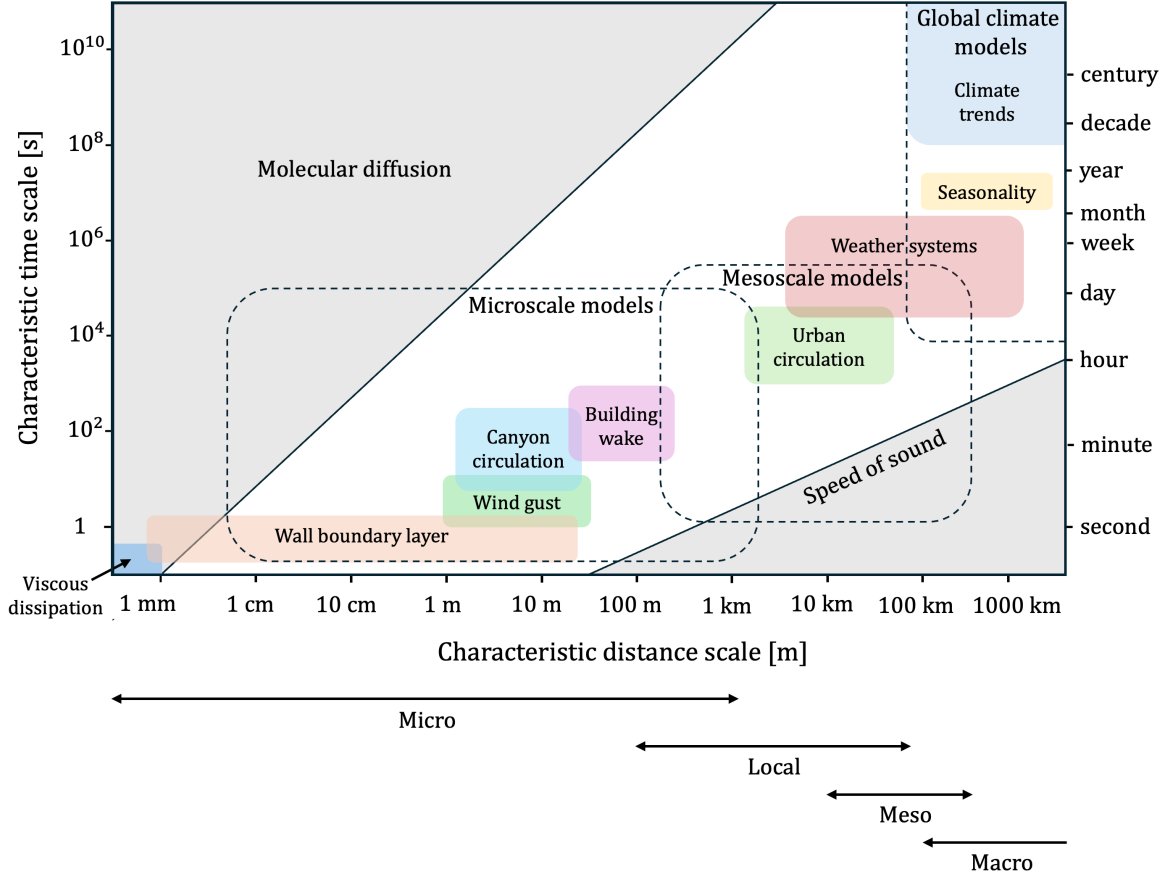


Figure 1.1: Scales associated with various urban environmental processes (adapted from Oke et al., 2017), as well as the range of models used to simulate them.

degree of coupling between physical processes (e.g. Maronga et al., 2020; Watanabe et al., 2021; Suter et al., 2022).

The key process driving the multi-physics, multiscale surface-atmosphere interaction is the diurnal cycle of solar radiation, which acts as the principal energy input to the system (Oke, 1988b; Garratt, 1994). Therefore, in order to accurately capture the behaviour of this system, is it necessary to consider how it evolves over several days.

The focus of this thesis is modelling urban processes over a diurnal cycle at high resolution, fidelity, and computational performance. In this context, high-resolution refers to resolving atmospheric flow at the microscale, and in particular using the large-eddy simulation (LES) approach for the CFD solver. Moreover, high-fidelity refers to using a geometry representation in a manner that is consistent with the actual urban form. Finally, high-performance means using efficient numerical algorithms, and thereby enabling high-resolution simulations on relatively large timescales, which for high-resolution tools is on the order of days. Applying these criteria strictly, there are no LES-based models

that are able to perform simulations with sufficient resolution, fidelity, and performance so as to enable the practical study of urban environments over a diurnal cycle. This is because at present, not all are capable of the high performance required, and none are capable of a high-fidelity representation of any given input geometry.

This thesis initially presents the development of an LES model, namely uDALES v2.0, whose performance and geometry representation fill this gap. Then, after validating the model, in particular the novel high-fidelity surface treatment, its capabilities for studying urban microscale processes are demonstrated in two diurnal cycle case studies. The first of these is based on a realistic masterplan in a hot, arid, coastal environment, with a focus on understanding the processes influencing the urban microclimate, in particular thermal inertia. The second involves simulating both idealised and realistic representations of a large area of central London, and includes a direct comparison with a mesoscale model.

The remainder of Chapter 1 formalises key concepts relating to urban form and fabric (Sect. 1.2) and the physical processes occurring at the surface and in the atmosphere aloft (Sect. 1.3), including a description of their characteristic evolution over diurnal cycle. Approaches taken to numerically modelling urban environments are then discussed, with a particular focus on microscale models, including a discussion of the existing literature on their use for simulating diurnal cycles (Sect. 1.4). Finally, the scope of the thesis is discussed in greater detail in the context of the literature (Sect. 1.5).



Figure 1.2: A sunset in London, UK. Note the high variation in the size, shape, and material composition of the buildings and other features making up the surface.

1.2 Urban surfaces

Urban environments are relatively heterogeneous in terms of their form (morphology) and fabric (materiality) in comparison to rural areas (Oke et al., 2017). Rigorously defining and quantifying the heterogeneity of Earth’s surface is challenging because it is a scale-dependent concept (Yu et al., 2023), and is beyond the scope of this thesis. However, this heterogeneity can be intuitively appreciated visually, such as in Fig. 1.2, which demonstrates the high variation in morphological and material properties of a typical large city. In order to make sense of this heterogeneity, an urban environment can be thought of as being composed of a hierarchical set of units (Oke et al., 2017). These are shown in Table 1.1, with examples of man-made, vegetative and aquatic features. The morphology and materiality of the urban surface can then be characterised using the unit that is appropriate for the scale of the problem at hand.

A set of quantities that can be used to characterise urban morphology are the fraction of the land area that is taken up by a particular cover type. This is known as the plan area fraction, and has the general form of $\lambda_p = A_p/A_t$, where A_t is the total plan area and A_p is the plan area occupied by e.g. buildings, vegetation, or impervious ground (roads etc). There are similar quantities used to indicate the morphological structure: the frontal area fraction $\lambda_f = A_f/A_t$, where A_f is the windward area of the buildings; and the complete aspect ratio $\lambda_c = A_c/A_t$, where A_c is the total surface area of the environment in three-dimensional space (Oke et al., 2017). In addition to these indicators, simplified urban morphologies such as cubic arrays or street canyons can be characterised by the dimensions and ratios associated with the buildings and streets (Oke, 1988a). Finally, the sky view factor (ψ_{sky}) is the fraction of the sky that is visible at a particular location, which can be an informative quantity with respect to radiation (Grimmond et al., 2001).

Table 1.1: Urban surface units with example features (adapted from Oke et al., 2017).

Unit	Features
Facet	Roof, wall, road, lawn, pond
Element	Building, tree
Canyon	Street (including buildings), row of trees, canal
Block	City block, park, wood, pond
Neighbourhood	City centre, residential area, industrial zone, greenbelt, forest, lake
City	Built-up area, urban forest
Urban region	City plus surrounding countryside

Urban materiality can be characterised by the properties that are relevant to the physical processes occurring in urban environments (discussed in Sect. 1.3). These include radiative properties such as absorptivity, reflectivity, transmissivity, and emissivity; and thermal properties such as heat capacity and conductivity. There are also aerodynamic properties, such as surface roughness length (z_0) and displacement height (z_d) (Garratt, 1994). Since these are not intrinsic properties of the surface, and are instead defined by the interaction with the flow, they are neither strictly morphological nor material in the same sense as other properties. Note that properties can be considered at any scale so long as there is a meaningful bulk definition. At the microscale, the properties of buildings and individual facets may be relevant, whereas at the local- and meso-scales, blocks and neighbourhoods are the appropriate urban units.

1.3 Urban physics

1.3.1 Atmospheric flow

As with any fluid flow, the fundamental physical processes within the Earth’s atmosphere are the conservation of mass, momentum, and energy, as well as moisture and other aerosols. Atmospheric flows are turbulent, with a high Reynolds number (Re) — a dimensionless number that characterises the ratio of inertial forces to viscous forces. This means that the turbulence exhibits a wide range of spatial and temporal scales of motion (Garratt, 1994). Macroscale processes determine the synoptic weather patterns that provide the backdrop for urban processes, which tend to be at the micro-, local-, and meso-scales. In addition to the showing the scales of various atmospheric processes associated with urban areas, Fig. 1.1 also shows the typical range of mesoscale and microscale models (which are discussed in Sect. 1.4).

The effect of the surface morphology on the flow is predominantly in the form of shear stress/drag: the surface acts as a sink of momentum via skin friction as well as form drag caused by the flow adjusting to the presence of obstacles (Cermak, 1976). Meanwhile, the materiality of the surface determines its heating or cooling, which acts as a source or sink of buoyancy and results in thermal circulation (Fan et al., 2017; Mei and Yuan, 2022). The surface therefore acts as both a source of mechanical and thermal turbulence.

The part of the atmosphere directly above the Earth’s surface is referred to as the

atmospheric boundary layer (ABL), which over an urban area is also referred to as an urban boundary layer (UBL). The UBL can be conceptually divided into further vertical layers (depicted in Fig. 1.3) based on how they are influenced by the urban surface, which can be linked to the units discussed in Sect. 1.2. At the lowest level is the urban canopy layer (UCL), which exists below building height and exhibits microscale variation according to facets (Oke et al., 2017). The UCL is contained within the roughness sub-layer (RSL), which extends above building height but still exhibits microscale variation due to individual elements and street canyons. The flow in the RSL is dominated by microscale morphological features, meaning the behaviour is often case-specific. It is common to study flow over simplified, idealised urban geometries in order to identify flow behaviour that may generalise to other urban environments (e.g. Xie et al., 2008;

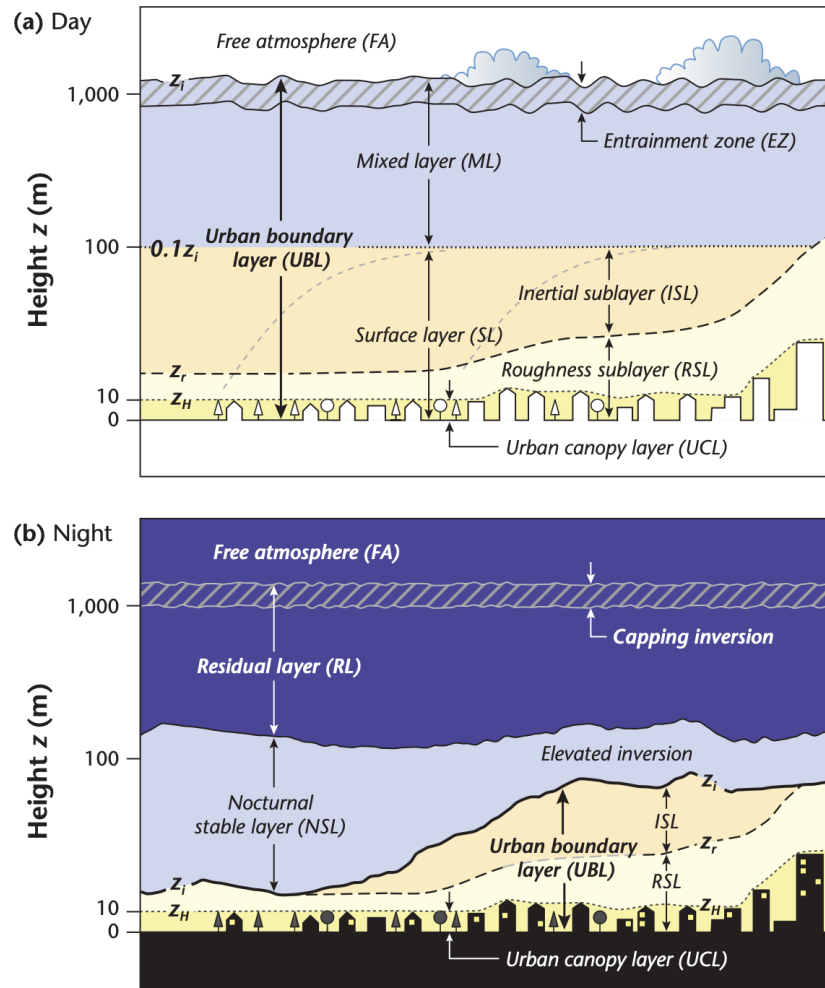


Figure 1.3: Structure of a typical urban boundary layer during (a) daytime and (b) nighttime (from Oke et al., 2017). Here z_H , z_r , and z_i refer to the height of the buildings, the roughness sub-layer, and the temperature inversion respectively.

Cai, 2012; Boppana et al., 2013; Carpentieri and Robins, 2015; Makedonas et al., 2021). On the scale of a block or neighbourhood, the surface appears more homogeneous and the influence of smaller-scale features on the flow becomes blended via turbulent mixing. There may be an inertial sub-layer (ISL) that varies at the local scale and in which theoretical boundary layer formulations are expected to hold (such as Monin-Obukhov similarity theory; Garratt, 1994). Local-scale properties such as λ_f and λ_p (the plan area fraction of built elements) have been used to characterise the flow in the ISL in terms of aerodynamic properties such as z_0 and z_d (Grimmond and Oke, 1999a). The RSL and ISL together make up the surface layer, defined by the fact that it is strongly affected by the form and fabric of the surface, and tends to exhibit vertical gradients of atmospheric properties. Above this there may be a mixed layer, where atmospheric properties are approximately uniform as a result of enhanced turbulent mixing due to buoyancy-driven processes. The mixed layer is also influenced by processes at the scale of the entire urban region and synoptic weather patterns. The ABL develops horizontally, with the variation of surface properties resulting in internal boundary layers. This means that characterising the internal structure of real UBLs in terms of the layers previously described is challenging, particularly because the layers potentially vary on different spatial (and temporal) scales (Barlow, 2014). Stability is a key concept used to characterise the structure of the ABL. This refers to the tendency of the atmosphere to discourage (if stable) or encourage (if unstable) vertical turbulent fluid motion, and is particularly useful for describing the evolution over a diurnal cycle (see Sect. 1.3.3).

1.3.2 Surface thermal processes

The surface energy balance (SEB) refers to the proportion of the various processes that transfer thermal energy to and from the surface. Radiation can be absorbed, reflected, and transmitted, and comes in the form of shortwave radiation originating from the sun and longwave radiation originating from terrestrial objects. The temperature difference between the surface and the air adjacent to the surface is associated with a sensible heat flux. Similarly, the difference in moisture between the surface and the air, resulting in evaporation, is associated with a latent heat flux. Therefore, the sensible and latent heat fluxes directly express the coupling between the state of the surface and that of the atmosphere. In cities, there are also anthropogenic (sensible) heat fluxes due to

human activities, e.g. HVAC systems, transportation, and machinery. Finally, conduction across the surface results in heat storage, which determines the temperature evolution. Note that surface temperature changes tend to be delayed and damped compared to the forcing (primarily due to solar radiation — see Sect. 1.3.3), which is referred to as thermal inertia. While the SEB is strongly influenced by the radiative and material properties of the surface, morphology also plays a role via shading and scattering of radiation.

In addition to providing realistic surface temperatures and moisture levels when determining sensible and latent heat fluxes in studies of UBL processes, modelling the SEB in urban environments is particularly relevant to the concept of thermal comfort. Thermal comfort is defined as ‘the condition of mind that expresses satisfaction with the thermal environment and is assessed by subjective evaluation’ (Oke et al., 2017). When considering thermal comfort, the energy balance of the human body is the determining factor, but this is challenging to model. Comfort indices such the universal thermal climate index (UTCI) or physiologically equivalent temperature (PET) (Epstein and Moran, 2006) attempt to capture this based on environmental conditions — wind speed, temperature, humidity, and radiation — though thermal comfort can also be studied in terms of these underlying factors individually. The effect of radiation in urban environments can be captured using a quantity called the mean radiant temperature (MRT). For a given location in the environment, one can imagine a hypothetical enclosure surrounding it, and from the enclosure receiving black-body radiation corresponding to a certain temperature. The MRT is defined such that the hypothetical radiation received is equal to the actual radiation at the location, which is determined in part by the SEB — this is discussed in further detail in Sect. 2.2. In addition to the energy balance, vegetative and aquatic surfaces also have a water balance, which is affected by the latent heat flux and other processes such as precipitation, and is outside the scope of this thesis.

1.3.3 Diurnal cycle

When the synoptic wind speed is low and the sky is relatively cloud-free, local-scale thermal effects strongly influence the structure of the ABL, and it varies in a characteristic manner over a diurnal cycle. The evolution is primarily driven by the response of the surface to the forcing due to solar radiation, as this is the dominant flux in the SEB. A depiction of the characteristic diurnal cycle of urban and rural ABLs is shown in Fig. 1.4.

the surface sensible heat flux tends to become negative at night, which causes the surface layer to cool and stabilise, forming a stable boundary layer. However, in urban areas the surface sensible heat flux has been observed to remain positive, so the surface layer may remain unstable (Oke et al., 2017). Regardless, the UBL tends to cool at night, and an inversion can develop above the surface layer due to atmospheric radiative transfer acting as a heat sink (Garratt and Brost, 1981; André and Mahrt, 1982). Note moisture is not important to the development, and in fact clouds can disrupt the characteristic evolution (by reducing solar radiation at the surface).

1.4 Urban environmental modelling

In general, when using numerical modelling approaches to study physical phenomena, it is necessary for the model to resolve or parameterise the processes that are important to the problem at hand, and to simulate these using a domain size and spatial and temporal resolution that capture the range of scales present in the problem (using an appropriate numerical scheme). Given these considerations, modelling a diurnal cycle of the UBL is a challenging task even for the idealised conditions described in Sect. 1.3.3 because of the relatively large number of relevant processes and the wide range of scales, though there are typically trade-offs in performance between model complexity (number of physical processes) and fidelity (surface representation) with the grid resolution and domain size.

Regarding processes, to model diurnal cycles it is necessary to simulate both the atmospheric flow and the SEB (see Sects. 1.3.1 and 1.3.2 respectively), including their coupling, with the sensible and latent heat fluxes acting as boundary conditions to the governing equations for the fluid.² The surface sensible heat flux is particularly important for capturing the characteristic diurnal cycle evolution as it directly influences atmospheric stability. In order to accurately capture thermal processes, it is necessary to simulate the entire diurnal cycle continuously (rather than at fixed times of day). This is because of thermal inertia: the state of the surface, i.e. the temperature, at a given time is affected not only by the forcing at that time, but also by the state history. Therefore, to avoid transient effects, simulations should be run for multiple days in order to ensure that the state is independent of the initial conditions.

²These processes are formalised in Sects. 2.1 and 2.2.

Regarding timescales, a diurnal cycle is relatively long compared to other aerodynamics applications (such as automotive, aeronautical, and wind turbine engineering). There are longer time scales associated with climate processes that are captured by larger-scale models (see Fig. 1.1), but these are outside the scope of this thesis. The largest length scale that it is necessary to consider here is that of the convective motion within the atmosphere, i.e. the height of the boundary layer, which is typically $\mathcal{O}(100 \text{ m} - 1 \text{ km})$ (Garratt, 1994). Capturing horizontal variation greater than this size is not necessary in general unless city-scale phenomena (e.g. UHI) are of interest. The smallest scale is in principle that of the smallest eddies in the flow, on the Kolmogorov scale, at which turbulent kinetic energy is dissipated into thermal energy via molecular viscosity (Pope, 2001). However, all models parametrise turbulence below some threshold, as explicitly resolving the smallest scales at all spatial locations is currently not practical for atmospheric flows.

Global climate models (GCMs), e.g. NCAR CAM (Neale et al., 2010), HadGEM (Collins et al., 2011), and CESM (Kay et al., 2015), can be used to simulate all the processes pertaining to the surface-atmosphere system over a diurnal cycle (and longer). However, this is achieved by using a low horizontal spatial resolution of $\mathcal{O}(10 \text{ km} - 100 \text{ km})$, meaning even the largest urban units may not be resolved. The vertical resolution is higher, typically $\mathcal{O}(10)$ levels within the ABL, though all turbulence is parameterised and the vertical structure is not captured in detail, particularly near the surface. Also, the land-surface model (LSM) used within a GCM typically does not treat urban surfaces very differently to other surface types, despite the substantial differences in morphological and material characteristics. In order to gain insight into processes within the UBL, it is necessary to use higher-resolution, higher-fidelity modelling approaches that are designed specifically to capture urban surfaces.

Single-column models (SCMs) are used to simulate atmospheric conditions at a single spatial location, hence only explicitly resolve processes in the vertical direction, with horizontal interactions parameterised. They are frequently integrated within GCMs (e.g. SCAM; Gettelman et al., 2019), and mesoscale models (see below). As they are generally less computationally expensive than these other modelling tools, they can be used in a lightweight manner in order to inform the parameterisations employed by more complex tools, including those for urban processes (McNorton et al., 2021). The resolution used

in SCMs is typically sufficient to study the vertical structure of the ABL over a diurnal cycle, however these models are inappropriate for studying processes for which horizontal variation is relevant.

Mesoscale models are designed to capture local- and mesoscale variation in the ABL, and thus can in principle resolve processes below the city scale. Examples include WRF (Skamarock et al., 2019), COSMO (Baldauf et al., 2011), MesoNH (Lafore et al., 1998), and the Met Office Unified Model (MetUM; Walters et al., 2019).³ These models resolve the flow using a horizontal resolution of $\mathcal{O}(100 \text{ m} - 10 \text{ km})$ and typically use domain nesting, where a higher-resolution simulation of the area of interest is contained within a lower-resolution simulation of the surroundings performed by a larger-scale model. The vertical resolution is higher, typically $\mathcal{O}(10 \text{ m} - 100 \text{ m})$. This is generally sufficient to resolve the upper layers of the ABL as described in Sect. 1.3. However, given the low horizontal resolution, the effect of surface features smaller than the block and neighbourhood scale must be aggregated in some manner. A dedicated urban canopy model (UCM) within an LSM can be used to calculate surface fluxes by considering a simplified representation of the urban environment. Examples of LSMs used in mesoscale models include NOAH (Niu et al., 2011, used by WRF), SURFEX (Masson et al., 2013, used by MesoNH), and JULES (Best et al., 2011, used by MetUM).

In an LSM, the SEB is generally modelled separately for each land cover type, or ‘tile’. Given that there is at least one tile per grid cell, the fluxes are combined in some way and applied at some forcing height(s) within the atmosphere. An UCM subdivides the surface into extra tiles to represent urban land cover, accordingly modifying the properties to be representative of urban environments in bulk (see Sect. 1.2). Statistical indicators such as the building plan area fraction (λ_p) and frontal area fraction (λ_f) are used to characterise the morphology of the surface and define a simplified geometry representation. This is used to determine aerodynamic properties (e.g. z_0) that influence the surface shear stress. Furthermore, for the SEB, the radiative terms can be determined using a less expensive method than would generally be required for a realistic urban environment by using a simplified geometry representation (Schoetter et al., 2023). In a one-tile/slab representation, the urban surface simply consists of a homogeneous one-dimensional (flat) surface.

³The distinction presented here between global-scale and mesoscale models, and non-urban and urban LSMs, is not clear in practice due to the variation in nesting and model coupling configurations.

A two-tile representation might consider e.g. roofs and street canyons, each with different properties. It is also possible to use a canyon scheme with four tiles, consisting of a roof, a road, and two walls. The details of these schemes are variable, though it is consistently a two-dimensional representation, with the canyon being infinite in length. More complex schemes use a three-dimensional but nonetheless simplified geometry; usually cubic arrays. The representation of vegetation within UCMs, including coupling with built features, also varies by model (Lipson et al., 2024). Furthermore, the vertical structure of the UCL can be modelled using single or multiple levels. Examples of UCMs included in LSMs are TEB (Masson, 2000, used by SURFEX), SLUCM (Kusaka et al., 2001, used by NOAH), and MORUSES (Porson et al., 2010*a*, used by JULES). There are also UCMs that are primarily designed to be run as standalone tools, such as UT&C (Meili et al., 2020), SUEWS (Järvi et al., 2011; Ward et al., 2016), and UrbClim (De Ridder et al., 2015), though some have also been coupled with mesoscale models (e.g. Sun et al., 2024).

Mesoscale models typically include parameterisation schemes for all the physical processes within the UBL, and so they are often used for diurnal cycle studies (e.g. Bohnenstengel et al., 2011; García-Díez et al., 2016; Brousse et al., 2016; Sharma et al., 2017; Martilli et al., 2024). However, the success of UCMs in capturing urban surface behaviour is mixed (Lipson et al., 2024). For example, the simplified geometry representation may cause errors in the radiative transfer compared to realistic geometries with similar morphometric indicators (Schoetter et al., 2023). There are also challenges with the representation of atmospheric processes that govern the structure of the UCL and RSL, which may influence the structure of the ISL as well (Barlow, 2014). In particular, the application of surface drag and heat fluxes (Schoetter et al., 2020; Sützl et al., 2021*a,b*), as well as the parameterisation of turbulent and dispersive mixing (Blunn et al., 2022; Nagel et al., 2023), are increasingly important as model configurations approach hectometric (100 m) resolution (Lean et al., 2024). Fundamentally, even sophisticated, multi-layer UCMs with relatively high vertical resolution are not capable of resolving microscale phenomena due to their low horizontal resolution, so it is advantageous to explicitly resolve them.

Microscale models use a spatial resolution of $\mathcal{O}(1\text{ m} - 10\text{ m})$, explicitly resolving the flow over the smallest urban features. The geometry can be specified arbitrarily (without assuming any particular morphology), and the material properties and SEB are considered on a per-facet basis, thus in principle enabling the full variability of real urban morphology

and materiality to be captured. When studying microscale urban processes, it is common to model the atmospheric flow and SEB separately, using a simplified (one-way) coupling with respect to the surface heat exchanges when thermal processes are of interest (Blocken, 2015; Toparlar et al., 2017; Jänicke et al., 2021). Standalone tools for modelling the SEB include SOLWEIG (Lindberg et al., 2008), TUF-3D (Krayenhoff and Voogt, 2007; Nice et al., 2018), and RayMan (Matzarakis et al., 2007). These tend to have sophisticated radiation models capable of modelling a wide range of features, and are well-equipped to predict thermal comfort indices (see Sect. 1.3.2).

The most popular CFD solvers used for simulating air flow in urban environments are based on discretisation and numerical solution of the governing equations (rather than alternatives such as the lattice Boltzmann method; Aidun and Clausen, 2010). Two common approaches for this are the finite-difference method, which involves approximations for the gradient terms, and the finite-volume method, which involves the fluxes at cell faces (derived via integration over cell volumes). Standard CFD packages (e.g. OpenFoam, ANSYS Fluent, Star-CCM+, Code_Saturne) are widely-used, though bespoke codes have been used for the purpose of conducting wind loading (Thordal et al., 2019) and pedestrian comfort studies (Blocken et al., 2016), as well as research into fundamental urban boundary layer processes (Tominaga, 2024). As previously mentioned, direct numerical simulation (DNS) of the governing equations (without any turbulence modelling) is not practical for atmospheric flows due to the excessively large number of grid points that would be required to resolve the smallest scales of motion. Instead, many studies use the Reynolds-averaged Navier-Stokes (RANS) approach, which involves parameterising turbulent fluctuations and only solving for the mean flow (Ferziger et al., 2019). Turbulence is often parameterised with a one-point closure (Pope, 2001), and it is challenging for RANS models to accurately simulate non-neutral flow conditions such as those within the ABL over land (Hanjalić, 2002). Moreover, these models often fail to reproduce unsteady flow features, leading to inaccurate prediction of quantities like turbulent kinetic energy for flows that involve time-dependent modulation (Moonen et al., 2012; van Hooff et al., 2017; Blocken, 2018; Vita et al., 2020). Two-moment closures and unsteady RANS approaches have been developed to address these problems, but these are rarely used in urban applications (Toparlar et al., 2015; Tominaga, 2015; Gao et al., 2018; Antoniou et al., 2019; Hadžiabdić et al., 2022). Alternatively, LES resolves the mean flow as well as

all turbulence with a length scale greater than the filter size (typically equal to the grid resolution), with small-scale turbulence parameterised using subgrid-scale models (Ferziger et al., 2019). Since LES resolves the energetic scales of the turbulence, it is expected to be more accurate than RANS (Murakami, 1993; Baker, 2007), but the computational cost is generally significantly higher (Chen, 2009).

Multi-physics urban CFD tools have been developed to include two-way coupling between the flow and the SEB, with each modelled at varying levels of sophistication depending on the tool (see Table 1.2). RANS-based tools tend to have a high-fidelity surface treatment as they are typically designed to study microclimate; examples include SOLENE-Microclimate (Musy et al., 2015, 2021), urbanMicroclimateFoam (Kubilay et al., 2018), and the model described in Wong et al. (2021). In contrast, LES-based tools have typically evolved from codes designed to simulate atmospheric phenomena in the upper ABL (such as clouds), and therefore tend to have a wider set of atmospheric parameterisations (than RANS-based tools); examples include PALM (Resler et al., 2017; Maronga et al., 2020; Krč et al., 2021), City-LES (Watanabe et al., 2021; Kusaka et al., 2024), and uDALES (Suter et al., 2022).

The high resolution used in microscale models introduces the challenge of modelling wall (facet) boundary layers, which consist of the viscous sub-layer close to the wall, and the log-law layer further from the wall, with the buffer layer between them (Pope, 2001). This is generally achieved using two approaches: either resolving the viscous sub-layer, placing the first computational mesh point adjacent to the wall within it (known as the low- Re approach), or by placing the first point within the log-law layer (known as the high- Re approach), typically using wall functions to parameterise the wall boundary layer. Given the relatively large range of scales for urban studies, particularly over a diurnal cycle, the low- Re approach is very computationally expensive in practice, and so some variation on the high- Re approach is generally used. The use of wall functions to parameterise wall boundary layers is conceptually similar to the approach taken in mesoscale models to parameterise the atmospheric surface layer, with the relevant aerodynamic properties used in the parameterisations, namely the roughness (characterised by z_0 for example), pertaining to individual facets, rather than urban neighbourhoods.

When using RANS, the most popular option for representing the geometry is to use a body-fitted computational mesh, i.e. a mesh that conforms to the geometry and is typi-

cally refined near the surface (Ferziger et al., 2019, depicted in Fig. 1.5). In the high- Re approach, the parameterisation of near-surface processes is either accounted for by using explicit wall functions, or is handled implicitly by some turbulence models (Ferziger et al., 2019). In contrast, when using LES the more common approach is to use a Cartesian grid combined with an immersed boundary method (IBM) (Verzicco, 2023, also depicted in Fig. 1.5.). First developed by Peskin (1972), the use of an IBM involves modifying the governing equations of cells inside the solid and/or close to the surface, which does not necessarily conform to the computational cell edges, in order to set the desired boundary conditions. The use of a fully Cartesian mesh avoids challenges associated with unstructured meshes, such as the effect of cell geometry (Hefny and Ooka, 2009). Also, using an equidistant Cartesian grid increases the computational performance because solving for the pressure can be carried out using the highly efficient fast Fourier transform (FFT) algorithm (Schumann and Sweet, 1988).

IBMs are traditionally discussed in the context of DNS (Mittal et al., 2008; Verzicco, 2023), in which the flow near the wall is fully-resolved, and so quantities can be linearly interpolated across the boundary. However, this is not the case with LES (using the high-

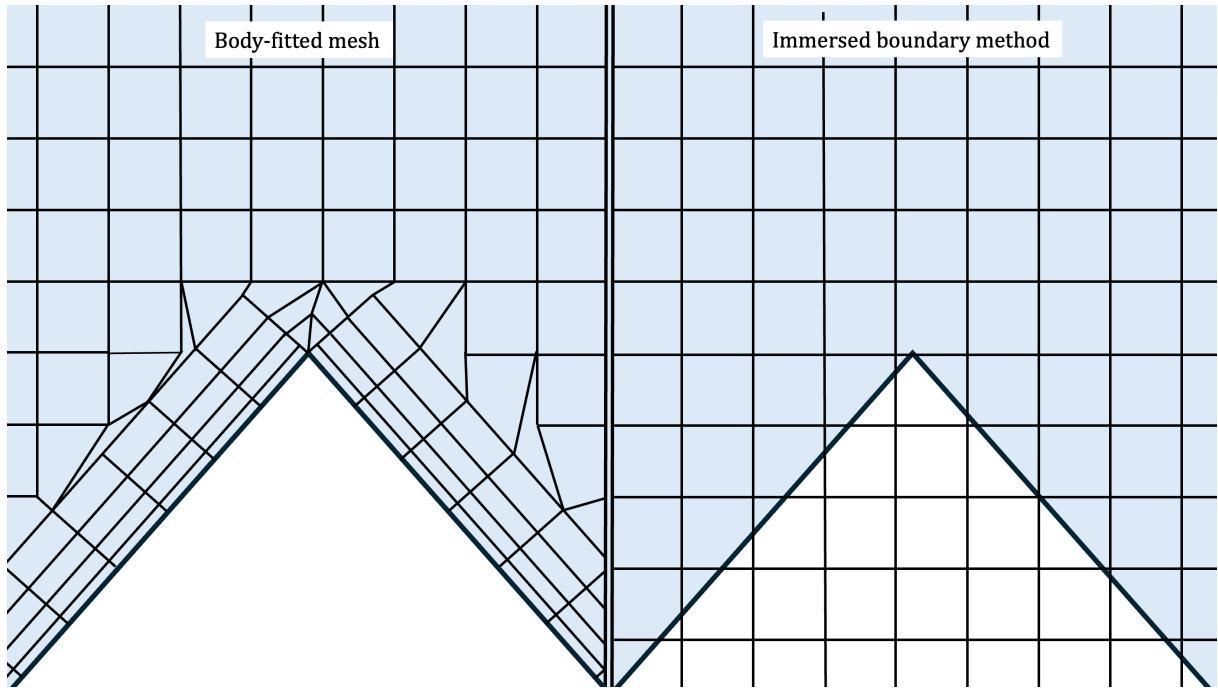


Figure 1.5: Left: body-fitted mesh approach, in which the mesh conforms to the surface of the solid (and there are no cells inside the solid); right: immersed boundary method, in which the mesh does not necessarily conform to the surface, instead the governing equations for cells inside the solid and/or fluid cells near the boundary are modified.

Table 1.2: Geometry representation and CFD approach used for urban microscale modelling tools that include an SEB scheme. The RANS-based codes use the finite volume method, and LES-based ones use the finite difference method; with second-order accuracy.

Model	Geometry representation	CFD approach
ENVI-met	Voxel	RANS
MITRAS	Voxel	RANS
SOLENE-Microclimate	Unstructured mesh	RANS (Code_Saturne)
urbanMicroclimateFoam	Unstructured mesh	RANS (OpenFoam)
City-LES	Voxel	LES
PALM	Voxel	LES
uDALES v1.0	Voxel	LES

Re approach); instead wall functions are used to predict the variation in near-surface quantities. Since the wall function approach typically assumes that the walls conform to the edges of the computational cells, there is an inherent challenge in combining them with an IBM (whose *raison d'être* is to capture non-grid-aligned surfaces). To circumvent this challenge, all the major LES-based urban microscale models specify the geometry using voxels, i.e. there is a boolean (true/false) value for each Cartesian grid cell corresponding to whether it is fluid or solid, and the immersed boundary aligns with the edges of the cells. Realistic, complex urban geometries may become distorted by the voxelisation process, which is particularly problematic for radiation, as this is strongly influenced by the surface area and orientation (Salim et al., 2022). Since shortwave radiation is the key process driving the diurnal cycle (see Sect. 1.3.3), this is a major limitation of models that represent the surface using voxels.

It is challenging in general to use microscale models for diurnal cycle studies. Firstly, the simulations are computationally expensive due to the relatively long runtime and domain size required, particularly with LES. Secondly, while they have sophisticated surface schemes, they do not typically capture as many atmospheric processes as mesoscale models, and often don't include atmospheric radiative transfer for example, which may impact the nocturnal boundary layer stability (as described in Sect. 1.3.3; Angevine et al., 2020). One way of making diurnal cycle studies more straightforward is to simply neglect the variation in the stability of the ABL and assume it is neutral, and so it is not an issue if processes that influence the stability are missing. Also, the lack of convection (on the scale of the boundary layer depth) means that the domain size can be smaller. Studies using this approach tend to use RANS, and thus avoid the problems associated with using this flow solution method for non-neutral situations (e.g. Maggiorotto et al., 2014; Salata

et al., 2017; Fabbri et al., 2020; Toparlar et al., 2015; Imbert et al., 2018). Neglecting variation in atmospheric stability is a better assumption for cases where there is no strong thermal forcing from the surface; for example in coastal urban environments with the wind coming predominantly from the ocean. This is because the surface temperature variation of the ocean tends to be relatively small over the diurnal cycle compared to the land due to the high thermal mass of water (Garratt, 1994).

It is also common to force microscale models in some way with data that includes all the relevant processes. This can be either from observations (e.g. Qu et al., 2011), or one-way coupling with a mesoscale model (e.g. Kaoru et al., 2011; Resler et al., 2020; Geletič et al., 2021; Anders et al., 2023). For studies of realistic geometries, it is common to use inflow-outflow boundary conditions, and apply forcing data directly as the inlet boundary condition. For studies of idealised, repeating geometries, such as flat terrain, infinite canyons, or cubic arrays, it is appropriate to use periodic boundary conditions, in which case the data can be used to ‘nudge’ the flow (e.g. Allaerts et al., 2020). Multiscale tools that incorporate both mesoscale and microscale models in a two-way coupled manner (e.g. Hellsten et al., 2021) are theoretically and practically challenging, and therefore rare.

When using LES, it is necessary to have a method for generating resolved turbulence at the inflow boundaries (Tabor and Baba-Ahmadi, 2010). One approach for doing this is synthetic turbulence generation (STG; e.g. Xie and Castro, 2008), which involves adding fluctuations to the mean flow applied at the inlet. This has been used in conjunction with coupling with mesoscale models via nesting (Kadasch et al., 2021; Lin et al., 2021), as described previously in this section. However, STG used in this context requires a run-up region for turbulence to develop, thus impacting performance. An alternative to STG is to use a precursor simulation, which involves computing a database of real turbulent flow and applying it at the inlet of the main simulation (e.g. Suter et al., 2022; Grylls et al., 2019; Lim et al., 2022). Precursor simulations typically use periodic boundary conditions, and are attractive because unlike STG, all turbulence statistics of the flow are representative of real turbulence. The precursor technique can also be simpler to implement as it requires less prior information. However, the drawback is the need to carry out another simulation either prior or simultaneously, and given the flow is strongly determined by the surface, trial and error with respect to the geometry is often required to obtain the desired turbulence statistics (if trying to match specific data). The use of

precursor simulations in diurnal cycle studies is rarer due to the fact that modelling heat transfer and non-neutral atmospheric stability is more challenging (e.g. Li et al., 2018).

Due to the challenges involved, diurnal cycle studies using microscale models are relatively rare, particular those using LES (Toparlar et al., 2017). The most common application is to realistic case studies, where simulations are often compared against observations in order to evaluate model accuracy (e.g. Qu et al., 2011; Maggiotto et al., 2014; Toparlar et al., 2015; Acero and Arrizabalaga, 2018; Resler et al., 2020; Mughal et al., 2021). Another common application is to investigate UHI, heat stress mitigation strategies, or other thermal comfort related topics (e.g. Salata et al., 2017; Imbert et al., 2018; Fabbri et al., 2017, 2020; Mughal et al., 2021; Geletič et al., 2021; Anders et al., 2023), as well as air quality (Liu et al., 2012). Idealised geometries have been used to conduct parameter space investigations with respect to morphology and/or materiality into thermal processes (e.g. Nazarian and Kleissl, 2015; Chen et al., 2021*b*) as well as ventilation (e.g. Chen et al., 2021*a*) and pollutant dispersion (e.g. Saxena and Yaghoobian, 2022). This thesis incorporates many of these aspects, with the motivation being to understand the impact of thermal processes on urban microclimate and UBL development.

1.5 Thesis scope

The aim of this work is to develop and use a microscale numerical model capable of simulating the UBL over a diurnal cycle, which involves addressing the challenges discussed in Sect. 1.4. Specifically, in addition to including an SEB scheme, an appropriate microscale modelling tool should explicitly resolve atmospheric flows around realistic urban geometries at high resolution, and LES has been shown to achieve this with greater accuracy than RANS, as discussed in Sect. 1.4 (Blocken, 2018). The computational performance should be practically sufficient to run relatively long simulations over multiple days, which for LES is achieved by using a Cartesian grid with an IBM. Finally, the surface treatment should be high fidelity with respect to the SEB, meaning that the geometry representation should not be dependent on the underlying grid. As previously discussed, there are currently no Cartesian LES models that meet this final criterion, since all of them currently use an IBM which can only admit facets that align with the grid (see Table 1.2). After covering relevant background material to this thesis in Chapter 2, the initial part

of this thesis involves describing and validating the development of such a model, using uDALES v1.0 as a starting point (Suter et al., 2022).

Several features of uDALES v1.0 require upgrading in order for the model to address the aims of this thesis. Firstly, the fact that geometry specification is dependent on the grid hinders its ability to faithfully represent realistic urban morphologies. Secondly, the performance is practically limited by the way in which the code is parallelised (to run on multiple computer cores). Also, the pressure solver is not capable of using the FFT algorithm with all lateral boundary condition configurations. These limitations are addressed in a new version: uDALES v2.0, which has a geometry representation that is independent of the grid, enabling any morphology to be specified precisely. The code also has an improved parallelisation, which substantially decreases the runtime of large simulations in practice (by leveraging more computer cores). Also, the pressure solver always uses the FFT algorithm, which increases the performance of any individual simulation. These upgraded features of uDALES v2.0 are described in Chapter 3 and validated in Chapter 4 using a number of canonical urban case studies, which are ultimately designed to demonstrate the ability of the novel surface treatment to capture surface heat exchanges in situations where facets are not aligned with the grid.

Subsequently, uDALES v2.0 is used to simulate a diurnal cycle for two case studies. The first case study, presented in Chapter 5, is based on a realistic masterplan of a coastal urban environment in a hot, arid climate. The objective is to understand the development of the microclimate in terms of factors influencing thermal comfort. This involves investigating both the evolution of the SEB and its effect on the atmosphere aloft. The marine ABL is assumed to be neutral and only the prevailing wind direction is considered in order to simplify the structure of the oncoming flow. This case is also used to quantify the difference in the microclimate when running a dynamic simulation over a diurnal cycle in comparison to steady-state simulations at fixed time(s) of day. The results of this investigation are presented in Chapter 6.

The second case study, presented in Chapter 7, involves simulating the UBL in central London. The atmospheric stability is non-neutral, and mesoscale model output from the Met Office Unified Model (MetUM; Walters et al., 2019) is used to force the uDALES simulations. This involves comparing uDALES with MetUM while using several geometrical configurations in order to investigate the effect of morphology on the atmospheric flow

and SEB. The UCM used by MetUM (MORUSES; Porson et al., 2010a) represents the geometry using infinite canyons; the uDALES geometries include this configuration, as well as a staggered cubic array and a realistic geometry based on high resolution building data. The parameters for the idealised geometries are based on the surface parameters supplied to MORUSES, namely the plan and frontal area fractions.

Finally, in Chapter 8, the thesis is concluded with a discussion of the state of uDALES as a tool in light of the development carried out for this thesis, then a reflection on the diurnal cycle studies presented in relation to the outlook for urban microscale modelling.

1.6 Publications

1. Lead author of ‘A conservative immersed boundary method for the multi-physics urban large-eddy simulation model uDALES v2.0’, published in Geoscientific Model Development (Owens et al., 2024). This forms the basis of Chapters 3 and 4.
2. Lead author of ‘Large-eddy simulation of a diurnal cycle in a coastal urban environment’, published in Building and Environment (Owens et al., 2025). This forms the basis of Chapter 5.
3. Lead author of ‘Large-eddy simulation of a diurnal cycle of the urban boundary layer over London’, in preparation for submission to the Quarterly Journal of the Royal Meteorological Society. This forms the basis of Chapter 7.
4. Co-author of ‘uDALES 1.0: a large-eddy simulation model for urban environments’, published in Geoscientific Model Development (Suter et al., 2022).
5. Co-author of ‘uDALES: large-eddy simulation software for urban flow, dispersion, and microclimate modelling’ published in SoftwareX (Grylls et al., 2021).⁴

⁴Contributions to the uDALES master branch on Github include approximately 35,000 additions and 15,000 deletions.

Chapter 2

Background

This chapter provides a description of concepts that are relevant to the microscale modelling of the urban boundary layer (UBL) over a diurnal cycle, in particular the flow within the atmospheric boundary layer (ABL) and the surface energy balance (SEB), as well as the approach taken in uDALES to parameterise and simulate these processes.¹

2.1 Atmospheric flow

2.1.1 Governing equations

Mass conservation is expressed by the continuity equation, which in Cartesian coordinates (x_i), assuming incompressible flow and using Einstein notation, is given by

$$\frac{\partial u_j}{\partial x_j} = 0, \quad (2.1)$$

where u_i is the velocity component in the x_i direction (Garratt, 1994).

Momentum conservation is expressed by the incompressible Navier-Stokes equations within the Boussinesq approximation (Garratt, 1994):

$$\frac{\partial u_i}{\partial t} = -\frac{\partial u_j u_i}{\partial x_j} - \frac{\partial p}{\partial x_i} + \frac{\theta'_v}{\langle \theta_v \rangle} g \delta_{13} + \nu \frac{\partial^2 u_i}{\partial x_j^2} - 2\Omega \varepsilon_{ijk} \eta_j u_k. \quad (2.2)$$

¹The assumptions mentioned in this section, i.e. incompressibility and Boussinesq, are well-justified given the low velocities and density gradients present in the ABL, and are therefore widely used by microscale models. However, mesoscale models may use less strict assumptions in parts of the atmosphere, i.e. modelling anelastic or compressible flow.

The terms on the r.h.s of Eq. (2.2) correspond to tendencies of advection, pressure, buoyancy, diffusion, and the Coriolis effect respectively. In these terms, g is Earth's gravitational acceleration, ν is the kinematic viscosity, Ω is the angular frequency of the Earth's rotation ($\Omega \approx 2\pi/86400 \text{ rad s}^{-1}$), and $\boldsymbol{\eta} = (0, \sin \Phi, \cos \Phi)$, where Φ is the latitude. The Boussinesq approximation affects the pressure and buoyancy terms; fluctuations ($\cdot'$) of density (ρ) with respect to some reference level ($\langle \cdot \rangle$) are assumed to be negligible apart except where they influence the buoyancy force, where they can be expressed in terms of fluctuations of other thermodynamic quantities (Wyngaard, 2010), in particular the virtual potential temperature ($\theta_v \approx \theta(1 + 0.61q)$; see Eqs. (2.3) and (2.4) for the definitions of θ and q). In this formulation, p corresponds to the deviatoric kinematic pressure.

Energy conservation, or more precisely enthalpy/sensible heat conservation, is expressed in terms of the potential temperature (θ), which is the temperature that an air parcel would have if adiabatically brought to a reference pressure level at the ground.

$$\frac{\partial \theta}{\partial t} = -\frac{\partial u_j \theta}{\partial x_j} + \kappa_h \frac{\partial^2 \theta}{\partial x_j^2} + \frac{1}{\rho c_p} \frac{\partial R_j}{\partial x_j}, \quad (2.3)$$

where κ_h is the air thermal diffusivity and $\boldsymbol{R}$ is the radiative heat flux due to absorption and emission of radiation by the gases making up the atmosphere (Garratt, 1994). Note that the specific heat capacity of the air (c_p) is assumed to be constant.

Moisture conservation is expressed in terms of the specific humidity (q) (Garratt, 1994):

$$\frac{\partial q}{\partial t} = -\frac{\partial u_j q}{\partial x_j} + \kappa_w \frac{\partial^2 q}{\partial x_j^2}, \quad (2.4)$$

where κ_w is the diffusivity of water vapour (note that phase changes have been neglected).

2.1.2 Averaged quantities

Reynolds decomposition can be used to provide insight into the quantities and equations in Sect. 2.1.1. This involves expressing a quantity (e.g. φ) as the sum of a time-averaged ($\bar{\cdot}$) and fluctuating ($\cdot'$) components, i.e. $\varphi(x, y, z, t) = \bar{\varphi}(x, y, z) + \varphi'(x, y, z, t)$.

Turbulent fluxes of a quantity (φ) are equivalent to covariances with the velocity, i.e. $\overline{u_i' \varphi'}$, and are so-called because they act as transport terms in the governing equations

for the mean quantity $\langle \bar{\varphi} \rangle$.² Strictly speaking, these covariances are kinematic fluxes. Substituting the Reynolds decomposition of u_i into Eq. (2.2) yields

$$\frac{\partial \bar{u}_i}{\partial t} = -\frac{\partial \bar{u}_j \bar{u}_i}{\partial x_j} - \frac{\partial p}{\partial x_i} + \frac{\theta'_v}{\langle \theta_v \rangle} g \delta_{13} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j^2} - \frac{\partial \overline{u'_j u'_i}}{\partial x_j} - 2\Omega \varepsilon_{ijk} \eta_j \bar{u}_k. \quad (2.5)$$

When multiplied by ρ , the kinematic momentum fluxes $\overline{u'_j u'_i}$ are called Reynolds stresses. Furthermore, substituting the Reynolds decomposition of u_i and θ into Eq. (2.3) yields (Garratt, 1994):

$$\frac{\partial \bar{\theta}}{\partial t} = -\frac{\partial \bar{u}_j \bar{\theta}}{\partial x_j} + \kappa_h \frac{\partial^2 \bar{\theta}}{\partial x_j^2} - \frac{\partial \overline{u'_j \theta'}}{\partial x_j} + \frac{1}{\rho c_p} \frac{\partial R_j}{\partial x_j}, \quad (2.6)$$

where $\rho c_p \overline{u'_j \theta'}$ is the turbulent sensible heat flux (Garratt, 1994). Similarly, a governing equation for $\bar{q}$ can be obtained using Eq. (2.4), which features the specific humidity flux $\overline{u'_j q'}$, corresponding to a latent heat flux $\rho \mathcal{L}_v \overline{u'_j q'}$, where $\mathcal{L}_v$ is the latent heat of vaporisation.

In the ABL, quantities tend to vary more significantly in the vertical direction (z) than the horizontal directions. Denoting the vertical velocity component as w and the horizontal (streamwise) velocity component as u , the kinematic horizontal momentum flux in the vertical direction is $\overline{w' u'}$, and the kinematic sensible heat flux and specific humidity fluxes in the vertical direction are $\overline{w' \theta'}$ and $\overline{w' q'}$ respectively.

Triple decomposition can be used when quantities are averaged in the horizontal directions (x and y) as well as in time. In this thesis, $\langle \cdot \rangle$ is used to denote the ‘intrinsic’ average over the fluid, which for a quantity $\varphi(x, y, z)$ averaged over both x and y is defined as

$$\langle \varphi \rangle(z) \equiv \frac{1}{A_{\text{fluid}}(z)} \int_{A_{\text{fluid}}} \varphi \, dA_{\text{fluid}}, \quad (2.7)$$

where A_{fluid} is the horizontal area occupied by the fluid within the domain. It is then possible to express φ as the sum of a time- and horizontally-averaged component ($\langle \bar{\cdot} \rangle$), a purely time-averaged component ($\bar{\cdot}$), and a fluctuating component ($\cdot'$), i.e. $\varphi(x, y, z, t) = \langle \bar{\varphi} \rangle(z) + \bar{\varphi}''(x, y, z) + \varphi'(x, y, z, t)$. The total vertical flux is given by $\langle \overline{w \varphi} \rangle = \langle \bar{w} \rangle \langle \bar{\varphi} \rangle + \langle \bar{w}'' \bar{\varphi}'' \rangle + \langle \overline{w' \varphi'} \rangle$ (Sutzi, 2021). Here $\langle \bar{w}'' \bar{\varphi}'' \rangle$ is known as the dispersive flux, which is associated with heterogeneity of the surface. Further detail on this is available in Appendix A.

²Microscale CFD tools based on the RANS approach numerically solve Eq. (2.5).

Surface fluxes are the boundary conditions at the surface-atmosphere interface (_s) to the governing equations for mean quantities (Eqs. 2.5 and 2.6), and can be related to a characteristic velocity (u_τ), temperature (θ_τ), and specific humidity (q_τ) (Garratt, 1994):

$$u_\tau^2 = \overline{w'u'}|_s \quad u_\tau \theta_\tau = \overline{w'\theta'}|_s \quad u_\tau q_\tau = \overline{w'q'}|_s \quad (2.8)$$

In a meteorological context, these boundary layer quantities refers to the local- or meso-scales (as in Sect. 1.3.1), with the interface corresponding to ground level. However, when considering microscale flows, for the boundary layer attached to individual facets, the ‘vertical’ direction corresponds to the facet-normal direction, and indeed this is the usage adopted in Sect. 2.3.2.

The surface shear stress ($\tau_s = \rho u_\tau^2$) and sensible heat flux ($H = \rho c_p u_\tau \theta_\tau$) can be parameterised using a bulk transfer approach, relating them to atmospheric quantities via the drag coefficient C_m and heat transfer coefficient C_h (Garratt, 1994):

$$\tau_s = \rho C_m u_a^2, \quad H = \rho c_p C_h u_a \Delta T. \quad (2.9)$$

Here u_a is the streamwise velocity component adjacent to the surface, and $\Delta T = T_s - \theta_a$ is the difference between the surface temperature (T_s) and the air temperature (θ_a). Note that C_m and C_h are dependent on the properties of the surface (at the relevant scale).

Turbulent kinetic energy (TKE), denoted by k , is equal to the sum of the velocity components’ variances, i.e. $k = \frac{1}{2}(\overline{u'^2} + \overline{v'^2} + \overline{w'^2})$, where v denotes the spanwise component, and **stability** can be expressed by quantities such as the buoyancy frequency (N) and the Richardson number (Ri_f , Ri_g , and Ri_b for flux, gradient, and bulk definitions respectively), which are defined in Table 2.1 (Garratt, 1994).

Table 2.1: Definition and interpretation of buoyancy frequency (N) as well as flux, gradient, and bulk Richardson numbers (Ri_f , Ri_g , and Ri_b respectively). Here $\theta_0 \equiv \theta|_{z=z_0}$, where z_0 is the momentum roughness length, and κ is the von Kármán constant.

Quantity	Definition	Unit	Stable	Neutral	Unstable
N	$(\frac{g}{\theta} \frac{\partial \theta}{\partial z})^{1/2}$	s^{-1}	$N^2 > 0$	$N^2 \approx 0$	$N^2 < 0$
Ri_f	$\frac{\frac{g}{\theta} \overline{w'\theta'}}{(\overline{w'u'} \frac{\partial \bar{u}}{\partial z} + \overline{w'v'} \frac{\partial \bar{v}}{\partial z})}$	-	$Ri_f > 0$	$Ri_f \approx 0$	$Ri_f < 0$
Ri_g	$\frac{\frac{g}{\theta} \frac{\partial \theta}{\partial z}}{(\frac{\partial \bar{u}^2}{\partial z} + \frac{\partial \bar{v}^2}{\partial z})}$	-	$Ri_g > 0$	$Ri_g \approx 0$	$Ri_g < 0$
Ri_b	$\frac{g}{\theta_0} (\theta - \theta_0) z / (\bar{u}^2 + \bar{v}^2)$	-	$Ri_b > 0$	$Ri_b \approx 0$	$Ri_b < 0$

2.2 Surface energy balance

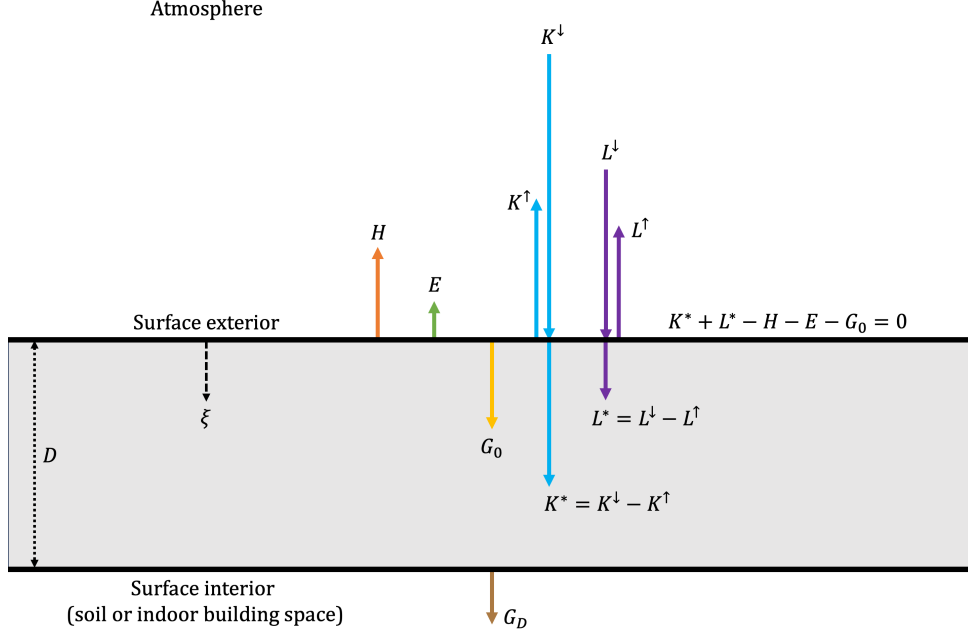


Figure 2.1: Surface energy balance fluxes for a single facet: incoming/outgoing/net short-wave radiation and longwave radiation ($K^\downarrow/K^\uparrow/K^*$ and $L^\downarrow/L^\uparrow/L^*$ respectively), sensible heat flux (H), latent heat flux (E), exterior conduction (G_0), and interior conduction (G_D). Here D is the facet depth and ξ is a coordinate from the exterior to the interior.

In this thesis, the SEB refers to energy conservation solely for the urban surface itself (rather than the surface combined with the adjacent air volume; Oke, 1988*b*). As discussed in Sect. 1.2, the smallest unit that the surface can be conceptually divided into are known as facets. In this thesis, in the context of microscale modelling, this name is therefore used to refer to the individual surfaces whose SEB is modelled.³ Each facet has a certain thickness (D) and material properties that vary only in the surface-normal direction, denoted here by ξ , which goes from the surface exterior to the interior. The SEB for a single facet is depicted in Fig. 2.1.

The facet temperature (T) is governed by enthalpy conservation:

$$C \frac{\partial T}{\partial t} = \frac{\partial}{\partial \xi} \left(\lambda \frac{\partial T}{\partial \xi} \right), \quad (2.10)$$

where C and λ are the volumetric heat capacity and conductivity of the facet respectively.

³In mesoscale models, the basic units in the SEB scheme tend to be referred to as tiles, and while this section refers to them as facets, the SEB formulation is scale-independent (not microscale-specific).

Equation (2.10) can be integrated from $\xi = 0$ to $\xi = D$ to give

$$\frac{d}{dt} \left(\int CT \, d\xi \right) \equiv Q = G_0 - G_D, \quad (2.11)$$

where $G_0 = -\lambda \frac{\partial T}{\partial \xi} \big|_{\xi=0}$ and $G_D = -\lambda \frac{\partial T}{\partial \xi} \big|_{\xi=D}$ are the conductive heat fluxes at the interior and exterior respectively, and Q denotes heat storage (total enthalpy) (Garratt, 1994).

At the surface-atmosphere interface ($\xi = 0$), the conduction (G_0) is balanced by the net shortwave radiation (K^*) and net longwave radiation (L^*), as well as the sensible and latent heat fluxes (H and E respectively) (Garratt, 1994):

$$K^* + L^* = H + E + G_0. \quad (2.12)$$

Note that conventionally, radiative fluxes are positive if energy is transferred into the surface, while turbulent and conductive fluxes are positive if it is transferred away (to the atmosphere or into the soil/building interior). The net radiative fluxes are given by the difference between incoming and outgoing contributions, denoted by $\cdot^\downarrow$ and $\cdot^\uparrow$ respectively, with $K^* = K^\downarrow - K^\uparrow$ for the shortwave contributions, and similarly $L^* = L^\downarrow - L^\uparrow$ for the longwave contributions. By modelling the radiative and turbulent fluxes, Eq. (2.12) acts as the exterior boundary condition for Eq. 2.11 (via G_0). Combined with the interior boundary condition (G_D), this can be used to ‘solve’ the SEB and evolve T in time.

Bulk surface energy balance quantities are calculated using the area-weighted average $\langle \cdot \rangle_s$ over a set of N_f facets. For a quantity X defined on each facet f , this is defined as

$$\langle X \rangle_s = \frac{\sum_{f=1}^{N_f} X_f A_f}{\sum_{f=1}^{N_f} A_f}, \quad (2.13)$$

where A_f is the area of facet f . To consider the SEB fluxes of a three-dimensional urban surface as if it were flat, the complete average $\langle X \rangle_c = \lambda_c \langle X \rangle_s$ can be used, where λ_c is the complete aspect ratio (see Sect. 1.2). This is relevant when evaluating the larger-scale effect on the atmosphere (Oke et al., 2017).

Penetration depth (δ) is the length scale associated with temperature oscillations in the surface. For a periodic forcing of angular frequency ω , Eq. (2.10) has a solution of the form

$T(\xi, t) = T_s + \Re(\hat{T} \exp(i\omega t - \gamma\xi))$, for some exterior value T_s and amplitude $\hat{T}$, where γ is a complex constant describing the decay and phase shift with depth. Assuming the material properties do not vary with ξ , it can be shown that $\gamma = \frac{1}{\delta}(1+i)$, where $\delta = \sqrt{\frac{2\lambda}{\omega C}}$ (Carslaw et al., 1962). Note that $T(\delta) = \frac{1}{e}T_s$, though the oscillations can only be considered to be negligible, e.g. below 5% of the surface value, when $\xi \approx 3\delta$.

Mean radiant temperature (MRT; see Sect. 1.3.2)) is determined by estimating the mean radiant flux on a human body (R_b):

$$R_b = \sum_{p=1}^6 \varrho_p ((1 - \alpha_b) \mathcal{K}_p^\downarrow + \epsilon_b \mathcal{L}_p^\downarrow), \quad (2.14)$$

where the sum is over the four cardinal directions (north, east, south, west) and the two vertical directions (up and down). Here $\mathcal{K}_p^\downarrow$ and $\mathcal{L}_p^\downarrow$ are the incoming shortwave and longwave radiation respectively from direction p , α_b and ϵ_b are the albedo and absorptivity of the human body respectively (with the latter assumed to be equal to the emissivity), and ϱ_p depends on the body's orientation and position. Following Thorsson et al. (2007), $\alpha_b = 0.3$, $\epsilon_b = 0.97$, and $\varrho_p = 0.22$ for the four vertical faces and $\varrho_p = 0.06$ for the two horizontal faces (assuming a rotationally symmetric body). Finally, the MRT is given by

$$\text{MRT} = \left(\frac{R_b}{\sigma \epsilon_b} \right)^{1/4}. \quad (2.15)$$

2.3 uDALES overview

uDALES is a large-eddy simulation (LES) model designed to simulate air flow, heat transfer, and pollutant dispersion in urban environments (Suter et al., 2022). The LES solver is based on DALES (Heus et al., 2010), with the governing equations for the fluid discretised using the finite-difference method on a Cartesian grid. On top of this, an immersed boundary method (IBM) is used to set appropriate boundary conditions for non-porous, stationary features that make up the urban surface, and wall functions are used to parameterise surface shear stress and sensible and latent heat fluxes at fluid cells with solid neighbours. The surface is divided into facets, each with user-defined material properties, and whose SEB can be modelled in a two-way-coupled manner with the flow. There is also the ability to model trees in terms of drag, deposition of pollutants, and

heat transfer (Grylls and van Reeuwijk, 2021). As discussed in Sect. 1.4, the only other LES-based model with this range of modelling features is PALM (Maronga et al., 2020). uDALES v1.0 has been used for studies concerning fundamental atmospheric boundary layer processes (Grylls et al., 2020; Wilson et al., 2025), air quality (Grylls et al., 2019; Lim et al., 2022), trees (Grylls and van Reeuwijk, 2022; Majumdar et al., 2024), and parameterisations for mesoscale models (Sützl et al., 2021a,b). This section summarises the modelling approaches for the atmospheric flow and SEB in order to provide context for the development of uDALES presented in Chapter 3.

2.3.1 Large-eddy simulation

The approach in uDALES involves applying an LES filter, which corresponds to spatial discretisation on a Cartesian grid, to Eq. (2.2) (Heus et al., 2010; Ferziger et al., 2019):⁴

$$\frac{\partial u_i}{\partial t} = -\frac{\partial u_j u_i}{\partial x_j} - \frac{\partial p}{\partial x_i} + \frac{\theta'}{\langle \theta_v \rangle} g \delta_{i3} + \frac{\partial}{\partial x_j} \left(K_m \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right) + F_i + S_{u_i}. \quad (2.16)$$

Note that the r.h.s terms have been modified in comparison to Eq. (2.2). For the diffusive term, a sub-grid scheme (Vreman, 2004) is used to calculate the turbulent eddy viscosity K_m .⁵ The Coriolis forcing may be included within F_i , though this term can also be defined in other ways to force the flow at larger scales. Finally, S_{u_i} represents a local sink of momentum due to surface shear stress for fluid cells with solid neighbours, calculated by a wall function. The IBM also modifies the governing equations in solid regions in order to set no-slip and no-penetration boundary conditions (which will be discussed in Sect. 3.4.1). The pressure term is calculated in a two-step procedure in order to enforce incompressibility (Eq. 2.1). This involves solving a Poisson equation for the pressure correction (the pressure difference between successive time steps; discussed in Sect. 3.3).

Scalar quantities (ϕ), such as the potential temperature (θ), specific humidity (q), and aerosol concentrations evolve according to:

$$\frac{\partial \phi}{\partial t} = -\frac{\partial u_i \phi}{\partial x_j} + \frac{\partial}{\partial x_j} \left(K_h \frac{\partial \phi}{\partial x_j} \right) + S_\phi, \quad (2.17)$$

⁴Due to filtering, the notation in Eqs. (2.16) and (2.17) is not strictly consistent with Sect. 2.1 — in the rest of the thesis, fields output by uDALES are denoted without diacritics for clarity.

⁵Like other common subgrid schemes (e.g. Smagorinsky (1963)), this assumes sub-grid-scale turbulence is isotropic, which may not be case in real turbulent flows (e.g. near walls).

where $K_h = K_m/Pr_t$ is the eddy diffusivity, Pr_t is the turbulent Prandtl number (a model parameter), and S_ϕ represents local scalar sources and sinks due to surface heat and moisture fluxes or chemical reactions. The IBM modifies the governing equations to ensure that scalars are conserved in the fluid (discussed in Sect. 3.4.1).

The equations are discretised in space on an Arakawa-C grid (Arakawa and Lamb, 1977), which entails defining pressure and scalars at cell centres, and defining the three velocity components (u_x , u_y , and u_z) at the lower cell face in each direction (x , y , and z) in a staggered manner.⁶ Second-order central difference schemes are used for all fields except aerosol concentrations, for which a flux-limited advection scheme is employed to ensure monotonicity (Hundsdoerfer et al., 1995). Time integration is carried out by a third-order Runge-Kutta scheme (Wicker and Skamarock, 2002), and the code is equipped with adaptive time stepping that ensures the Courant–Friedrichs–Lewy (CFL) condition holds (Heus et al., 2010). The y grid is always equidistant, whilst the z grid may be stretched. In uDALES v1.0, it is also possible to have a stretched grid in the x direction, though this is rarely used in practice due to considerations with the pressure solver (discussed in Sect. 3.3). The solver is parallelised using MPI by decomposing the domain into smaller chunks that are each operated on by a single processor (discussed in Sect. 3.2).

2.3.2 Wall functions

Wall functions use the atmospheric conditions at the cells closest to facets and the state and properties of the facets themselves to predict the surface shear stress (τ_s), sensible heat flux (H), and latent heat flux (E) (following Louis, 1979; Uno et al., 1995; Jarvis, 1976; Stewart, 1988). For a given fluid cell adjacent to a facet, the streamwise velocity, potential temperature, specific humidity, surface temperature, and distance to the facet are denoted as u_a , θ_a , q_a , T_s , and d respectively, as illustrated in Fig. 2.2. The kinematic momentum flux is given by

$$u_\tau^2 = \frac{\kappa^2 u_a^2}{(\log(d/z_0))^2} \mathcal{F}_m\left(\frac{d}{z_0}, \frac{d}{z_{0,h}}, Ri_{b0}\right), \quad (2.18)$$

where κ is the von Kármán constant, z_0 is the momentum roughness length, $z_{0,h}$ is the heat roughness length, $\mathcal{F}_m$ is the momentum stability function, and $Ri_{b0} = -gd\Delta\theta_0/(u_a^2\theta_0)$

⁶The velocity components are also referred to as u , v , and w as per convention, though u is also used to refer to the velocity in the *streamwise* direction, which is typically the x direction but not always.

is the bulk Richardson number associated with the difference between $\theta(d) \equiv \theta_a$ and $\theta(z_0) \equiv \theta_0$, i.e. $\Delta\theta_0 = \theta_0 - \theta_a$. Here $\Delta\theta_0$ and Ri_{b0} are determined using a one-step iterative method that uses the temperature at the heat roughness length $\theta(z_{0,h})$, which is assumed to be equal to T_s (Uno et al., 1995; Suter, 2018).⁷ Note that in neutral conditions, $\mathcal{F}_m = 1$, and the expression simplifies to the log-law of the wall (Pope, 2001).⁸ According to the bulk transfer approach (see Sect. 2.1.2), the drag coefficient $C_m = u_\tau^2/u_a^2$. The surface shear stress is considered for each velocity component; for a horizontal facet, $\tau_x = \rho C_m u_a u_x$ and $\tau_y = \rho C_m u_a u_y$ are used to determine the volumetric sinks S_{u_x} and S_{u_y} . In a similar manner, denoting the heat stability function by $\mathcal{F}_h$, the kinematic sensible heat flux is given by

$$u_\tau \theta_\tau = \frac{1}{Pr_t} \frac{\kappa^2 u_a \Delta\theta_0}{(\log(d/z_0))^2} \mathcal{F}_h \left(\frac{d}{z_0}, \frac{d}{z_{0,h}}, Ri_{b0} \right), \quad (2.19)$$

The heat transfer coefficient is defined by $C_h = u_\tau \theta_\tau / u_a \Delta\theta_s$, where $\Delta\theta_s = T_s - \theta_a$. The value of $u_\tau \theta_\tau$ is then used to determine the volumetric heat source/sink S_θ . Finally, the specific humidity flux is given by

$$u_\tau q_\tau = \frac{q_a - q_{sat}}{r_{air} + r_{can}} + \frac{q_a - q_{sat} RH}{r_{air} + r_{soil}}, \quad (2.20)$$

where q_{sat} is the air saturation specific humidity (which is dependent on T_s), RH is the relative humidity, $r_{air} = 1/(u_a C_h)$ is the aerodynamic resistance, and r_{can} and r_{soil} are the canopy and soil resistances respectively, which are model parameters. The value of $u_\tau q_\tau$ is then used to determine the moisture sink S_q (though note that moisture is neglected in the remainder of this thesis).

The fluxes of momentum, heat, and moisture are converted to volumetric source or sink terms by multiplying by the surface area and dividing by the volume over which they act, with the relevant area being the fraction of the adjacent facet that is within the fluid cell of interest, and the volume is that of the cell itself. In Fig. 2.2, the outlined fluid cell experiences fluxes from facet 3. In this 2D representation, half of facet 3 is inside the cell,

⁷Let $Ri_{bs} = -gd\Delta\theta_s/(u_a^2 T_s)$, then calculate $\mathcal{F}_m$ and $\mathcal{F}_h$. Let $M = Pr_t \log(d/z_0) \sqrt{\mathcal{F}_m}/\mathcal{F}_h$, and finally:

$$Ri_{b0} = Ri_{bs} - \frac{Ri_{bs} Pr_t \log(z_0/z_{0,h})}{Pr_t \log(z_0/z_{0,h}) + M}, \quad \Delta\theta_0 = \Delta\theta_s (Pr_t \log(z_0/z_{0,h})/M + 1).$$

⁸Note that wall functions assume that the wall boundary layer is in equilibrium, which is generally not the case for flows that in reality are unsteady and/or separated.

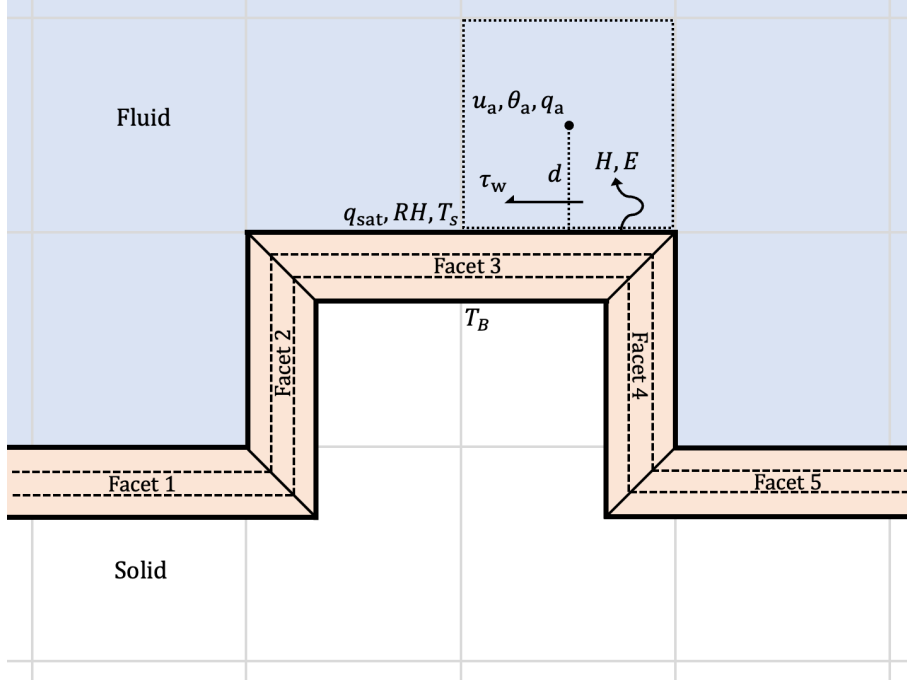


Figure 2.2: Two-way coupled wall functions and SEB in uDALES. Fluid cells adjacent to the boundary experience a surface shear stress (τ_s) and fluxes of sensible and latent heat (H and E), which are determined by wall functions. These fluxes act as volumetric sources or sinks in the fluid governing equations and simultaneously contribute to the SEB for the corresponding facet. For other nomenclature, refer to Sects 2.3.2 and 2.2.

so this is the area used in determining the source and sink terms. Note that this must be considered according to which staggered grid the relevant flow variable is defined on. The application of surface fluxes to the fluid is clearly strongly linked to the geometry specification, and is discussed further in Sect. 3.4.2.

2.3.3 Surface energy balance scheme

In the SEB scheme, the sensible and latent heat fluxes (H and E) for each facet are the average of the fluxes at neighbouring fluid cells calculated by the wall functions, with opposite sign to that experienced by the fluid. Note that these are calculated at every LES time step, but the SEB is generally evolved using a larger time step than the LES, meaning they are time averaged over the SEB time step before use in the SEB calculation.

The radiative fluxes are calculated using the radiosity approach, which assumes that the radiative transfer between facets is Lambertian, i.e. all reflection are diffuse and therefore view factors can be used (Oke et al., 2017).⁹ The view factor $\psi_{f,g}$ is a purely geo-

⁹The assumption of Lambertian radiative transfer fails to capture specular reflection from materials such as glass and lustrous metals.

metrical quantity defined as the fraction of diffuse radiation leaving facet f that impinges on facet g . This can be used to calculate the sky view factor $\psi_{f,\text{sky}}$, which is defined as the fraction of diffuse radiation that leaves facet f and does not impinge on any other facet, i.e. $\psi_{f,\text{sky}} = 1 - \sum_{g=1}^{N_f} \psi_{f,g}$, where N_f is the number of facets. The albedo (α) and emissivity (ϵ ; assumed to be equal to the absorptivity¹⁰) are specified for each facet.

For the shortwave radiation, the incoming and outgoing fluxes are related by $K_f^\uparrow = \alpha_f K_f^\downarrow$. This means that only $K_f^\downarrow$ needs to be modelled, and is done so by considering contributions from direct solar radiation, diffuse radiation scattered by the sky, and diffuse radiation reflected from other surfaces (this is described in further detail in Sect. 3.5). The incoming and outgoing longwave radiation contributions are given by $L_f^\downarrow = \psi_{f,\text{sky}} L_{\text{sky}} + \sum_{g=1}^{N_f} \psi_{f,g} L_g^\uparrow$ and $L_f^\uparrow = (1 - \epsilon_f) L_f^\downarrow + \epsilon_f \sigma T_{s,f}^4$ respectively, where L_{sky} is a model parameter quantifying the longwave radiation from the sky and $\sigma = 5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$ is the Stefan-Boltzmann constant. Note that unlike for shortwave radiation, multiple reflections are not considered for longwave radiation (due to the typically high value of ϵ), which simplifies the calculation.

The SEB is solved by discretising each facet into N_l layers along the depth (shown using dashed lines in Fig. 2.2). The layer edges are denoted by $\xi_0, \xi_1, \dots, \xi_{N_l}$, with $\xi_0 = 0$ and $\xi_{N_l} = D$, where D is the facet thickness. Conservation of enthalpy (see Eq. 2.11) within layer l can be expressed as

$$\frac{d}{dt} \int_{\xi_l}^{\xi_{l+1}} CT \, d\xi = \lambda(\xi_{l+1}) \left. \frac{\partial T}{\partial \xi} \right|_{\xi_{l+1}} - \lambda(\xi_l) \left. \frac{\partial T}{\partial \xi} \right|_{\xi_l}. \quad (2.21)$$

The solution for the temperature $T(\xi)$ is assumed to be a piecewise continuous quadratic polynomial (Suter et al., 2022). Denoting $T_l \equiv T(\xi_l)$ and $T'_l \equiv \left. \frac{\partial T}{\partial \xi} \right|_{\xi_l}$, and the layer thickness by $\Delta\xi_{l+1} = \xi_{l+1} - \xi_l$, it can be shown that

$$\frac{1}{2}(T'_l + T'_{l+1}) = \frac{T_{l+1} - T_l}{\Delta\xi_{l+1}}, \quad (2.22)$$

and that the mean temperature within each layer is given by

$$\frac{1}{\Delta\xi_{l+1}} \int_{\xi_l}^{\xi_{l+1}} T \, d\xi = \frac{1}{2}(T_l + T_{l+1}) + \frac{\Delta\xi_{l+1}}{12}(T'_l + T'_{l+1}). \quad (2.23)$$

¹⁰The assumption that the emissivity is equal to the absorptivity across the entire longwave radiation spectrum is strictly limited to surfaces in thermal equilibrium, and neglects directional effects and other factors such as roughness and low-emissivity coatings.

Combining Eqs. (2.21) and (2.23) while assuming the heat capacity in each layer (denoted by $C_{l+\frac{1}{2}}$) is constant yields

$$\frac{d}{dt} \left(\frac{\Delta \xi_{l+1}}{2} (T_l + T_{l+1}) + \frac{\Delta \xi_{l+1}^2}{12} (T'_l + T'_{l+1}) \right) = \frac{\lambda_{l+1}}{C_{l+\frac{1}{2}}} T'_{l+1} - \frac{\lambda_l}{C_{l+\frac{1}{2}}} T'_l. \quad (2.24)$$

where $\lambda_l \equiv \lambda(\xi_l)$.¹¹ Equations (2.22) and (2.24) represent a system of equations for the unknowns T_l and T'_l for $l = 0, 1, \dots, N_l$. The exterior boundary condition is the enforced closure of the SEB (Eq. (2.12)), i.e. $T'_0 = \frac{-1}{\lambda_0} (K^* + L^* - H - E)$. The interior boundary condition is isothermal, i.e. $\frac{dT'_{N_l}}{dt} = 0$ and $T_{N_l} \equiv T_D$; a model parameter that can be specified separately for the ground and buildings (the building temperature is denoted T_B in Fig. 2.2). By eliminating the gradient terms (T'_l), the equations can be simplified to:

$$\mathbf{A} \frac{d\mathbf{T}}{dt} = \mathbf{B}\mathbf{T} + \mathbf{c}, \quad (2.25)$$

where $\mathbf{T} = (T_0, T_1, \dots, T_{N_l})$ (Suter et al., 2022). The matrices $\mathbf{A}$ and $\mathbf{B}$ and the vector $\mathbf{c}$ depend on the material properties as well as $T_0 \equiv T_s$ due to the non-linearity of the Stefan-Boltzmann law, so T_0 is technically assumed to be constant in Eq. (2.25) (in $\mathbf{c}$). Time integration is performed using an implicit Euler scheme with a time step of $\mathcal{O}(10 \text{ s})$.

To calculate the mean radiant temperature (MRT; see Sect. 2.2), which is given by

$$MRT = \left(\frac{1}{\sigma \epsilon_b} \sum_{p=1}^6 \varrho_p ((1 - \alpha_b) \mathcal{K}_p^\downarrow + \epsilon_b \mathcal{L}_p^\downarrow) \right)^{\frac{1}{4}}, \quad (2.26)$$

the uDALES post-processing considers a cube, typically the size of a single computational cell, and calculates the incoming shortwave and longwave radiation for each face ($\mathcal{K}_p^\downarrow$ and $\mathcal{L}_p^\downarrow$ respectively). The sources of shortwave radiation are direct solar radiation $\mathcal{S}_p$ (calculated using the same algorithm as for the facets), diffuse sky radiation $\mathcal{D}_p$, and the outgoing shortwave and longwave radiative fluxes for all N_f facets, which for facet f are denoted $K_f^\uparrow$ and $L_f^\uparrow$ respectively. The total incoming shortwave radiation is given by

$$\mathcal{K}_p^\downarrow = \mathcal{S}_p + \mathcal{D}_p + \sum_f^{N_f} \psi_{p,f} K_f^\uparrow = \mathcal{S}_p + \psi_{p,\text{sky}} \mathcal{D}_{\text{sky}} + \sum_f^{N_f} \psi_{p,f} \frac{\alpha_f}{1 - \alpha_f} K_f^*, \quad (2.27)$$

¹¹Note that in Eq. (2.24), λ is defined on layer edges, whereas the model input is layer-wise. To ensure enthalpy conservation, $\lambda_l = \frac{1}{2}(\lambda_{l-\frac{1}{2}} + \lambda_{l+\frac{1}{2}})$ is used, with $\lambda_0 = \lambda_{\frac{1}{2}}$ and $\lambda_{N_l+1} = \lambda_{N_l+\frac{1}{2}}$.

where $\psi_{p,f}$ is the view factor from cube face p to facet f , $\psi_{p,\text{sky}}$ is the sky view factor for cube face p , and D_{sky} is the diffuse shortwave radiation from the sky. Note that uDALES outputs $K_f^* = K_f^\downarrow - K_f^\uparrow$, and so $K_f^\uparrow = \alpha_f K_f^\downarrow$ is used to obtain $K_f^\uparrow$.

For the longwave radiation, the outgoing radiation from the facets $L_f^\uparrow$ is more involved. The model outputs the *absorbed* longwave $L_{\text{abs},f} = \epsilon_f L_f^\downarrow$ and the *emitted* longwave $L_{\text{emit},f} = \sigma \epsilon_f T_{\text{s},f}^4$. The outgoing longwave is given by $L_f^\uparrow = (1 - \epsilon_f) L_f^\downarrow + L_{\text{emit},f}$, therefore

$$\mathcal{L}_p^\downarrow = \psi_{p,\text{sky}} L_{\text{sky}} + \sum_f^{N_f} \psi_{p,f} L_f^\uparrow = \psi_{p,\text{sky}} L_{\text{sky}} + \sum_f^{N_f} \psi_{p,f} \left(\frac{1 - \epsilon_f}{\epsilon_f} L_{\text{abs},f} + L_{\text{emit},f} \right). \quad (2.28)$$

Chapter 3

Development of uDALES v2.0

Based on journal article: ‘A conservative immersed boundary method for the multi-physics urban large-eddy simulation model uDALES v2.0’, published in Geoscientific Model Development (Owens et al., 2024).

3.1 Introduction

The chapter presents a new version of uDALES that is designed to address the limitations in surface fidelity and computational performance outlined in Sect. 1.5. In particular, objects in uDALES v1.0 must be aligned with the Cartesian computational grid, which means that building walls that do not meet this requirement are approximated as doing so. To illustrate, Fig. 3.1 shows a case that was used to demonstrate the capabilities of uDALES v1.0 (presented in Suter et al., 2022). The geometry was generated using a raster of a surface elevation map, and the shape of the buildings that are not aligned with the grid is distorted. Also, the code is parallelised with a one-dimensional (1D) domain decomposition implemented with bespoke routines using the message passing interface (MPI) library, which means it cannot effectively utilise the large number of processors available on high-performance computing (HPC) systems. The final limitation is that it is not possible to use the fast Fourier transform (FFT) algorithm to solve for the pressure with inflow-outflow boundary conditions (though it is possible for periodic conditions).

In uDALES v2.0, the geometry is specified as an unstructured triangulated surface that is given independently of the grid using the STL file format, and a novel technique for applying surface fluxes given this non-grid-aligned approach has been implemented

Table 3.1: Comparison of upgraded features between uDALES v1.0 and v2.0.

Feature	uDALES v1.0	uDALES v2.0
Domain decomposition	One-dimensional	Two-dimensional
Pressure solver	Only entirely FFT-based for periodic cases	Entirely FFT-based for both periodic and inflow-outflow cases
Geometry representation/IBM	Blocks (voxels) — grid-aligned	Triangulated surface — grid-independent
Shortwave radiation algorithm	Inaccurate shading	Accurate shading
Periodic (precursor) simulations	No method to avoid permanent streamwise super-structures	Method to avoid permanent streamwise super-structures

within the existing immersed boundary method (IBM) (described in Sect. 3.4). The code is parallelised with a two-dimensional (2D) domain decomposition, implemented using the 2DECOMP&FFT library (Li and Laizet, 2010; Rolfo et al., 2023), thus enabling it to run on many more processors than uDALES v1.0 (demonstrated in Sect. 3.2). Finally, it is capable of using an FFT-based method to solve for the pressure when using inflow-outflow boundary conditions, thereby enhancing the performance of simulations employing these conditions (discussed in Sect. 3.3). In addition to these major changes, uDALES v2.0 also has an improved algorithm for calculating shortwave radiation (presented in Sect. 3.5), as well as a novel method to prevent the formation of artificial flow features in periodic simulations (presented in Sect. 3.6). A summary of the upgrades is given in Table 3.1.

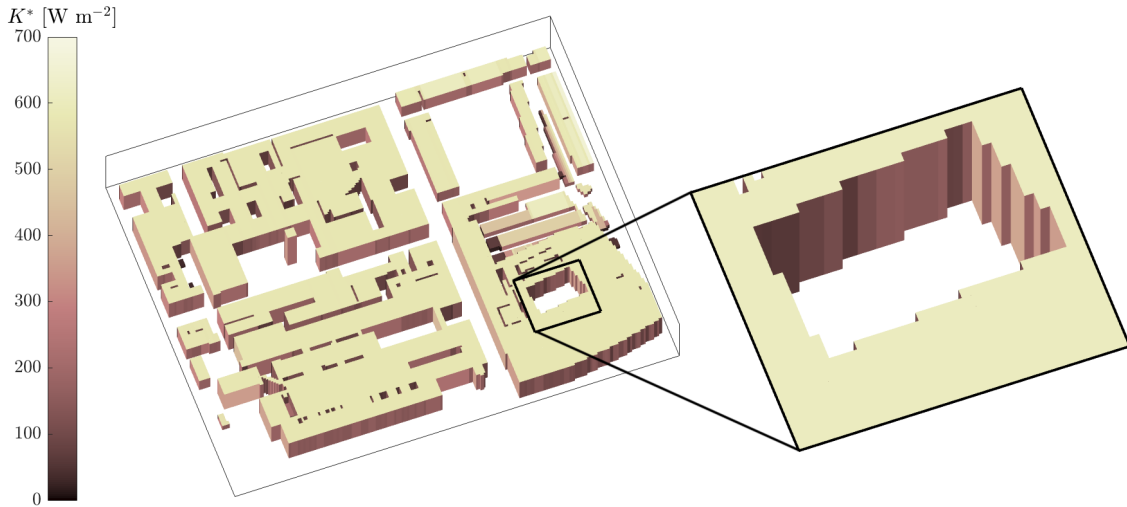


Figure 3.1: Net shortwave radiation (K^*) for the case presented in Suter et al. (2022).

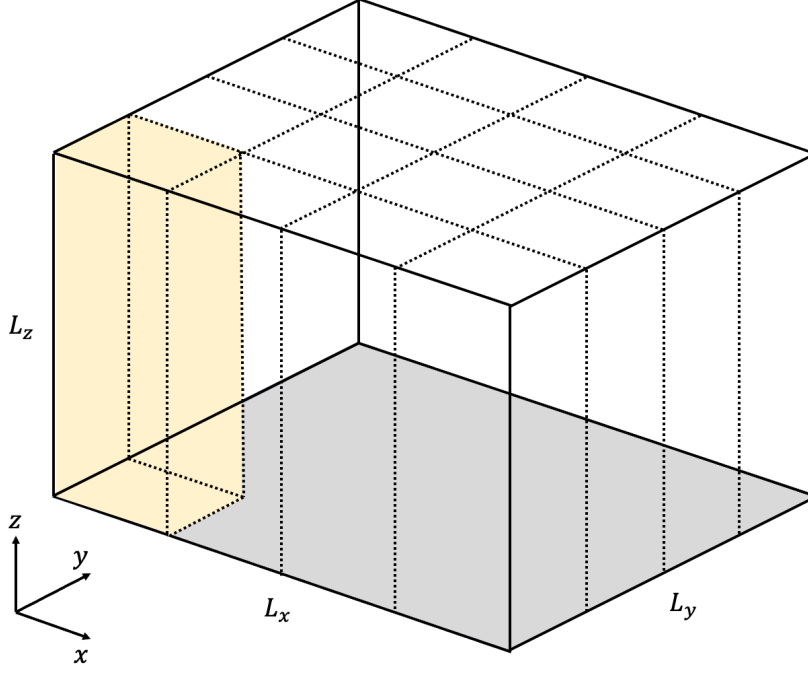


Figure 3.2: A two-dimensional domain decomposition. In this case, the x and y directions are decomposed across 4 processors, so there are 16 in total. The pencil operated on by a single processor is highlighted in yellow.

3.2 Two-dimensional domain decomposition

The 1D domain decomposition in uDALES v1.0 involves dividing the computational domain into ‘slabs’ along a single direction — primarily y . Each processor (also referred to as a ‘core’) generally stores and manipulates information regarding cells located within a single slab. This means the maximum number of cores that can be used is limited to the number of grid cells in the y direction (N_y). Given that typical use cases have N_y equal to 256-1024, and a single node on ARCHER2 (the UK National Supercomputing Service; EPCC, 2022, which is used for the simulations in this thesis) has 128 cores available, simulations with uDALES v1.0 can only use 8 nodes at most of the thousands available.

A 2D decomposition means the domain is divided into ‘pencils’, which is achieved in uDALES v2.0 using the 2DECOMP&FFT library (Li and Laizet, 2010; Rolfo et al., 2023). 2DECOMP&FFT was originally designed for use by Xcompact3d (then Incompact3d; Laizet and Li, 2011; Bartholomew et al., 2020), a direct numerical simulation (DNS) (and later large-eddy simulation (LES)) framework for turbulent flow simulation based on a Cartesian mesh discretised using the finite-difference method (similar to uDALES). 2DECOMP&FFT has been shown to scale efficiently using many cores on HPC

systems including ARCHER2 (EPCC, 2022), and has since been successfully adopted by other codes (e.g. Costa, 2018). The library has been developed for cross-platform usage and has been tested on all major HPC architectures, ensuring portability of uDALES.

In uDALES, the default pencil orientation is in the z direction, meaning the x and y directions are parallelised, as shown in Fig. 3.2. The extra dimension of parallelisation compared to uDALES v1.0 means that it is possible to run simulations with many more cores. The maximum number of cores that it is possible to use is equal to $N_x \times N_y$, where N_x is the number of cells in the x direction. In addition to the computational cells within the pencil, each core also stores the so-called ‘halo’ cells just outside it because they are part of the finite-difference stencil for cells at the edge of the pencil (stencil referring to the neighbouring cells that appear in the numerical scheme of a given cell). In order for the halo cells to store the correct values, MPI communication is required between cores corresponding to adjacent pencils for each time step.¹ Due to the use of halo cells, the only time when data is transposed from the z pencil to the x and y pencils is while solving for the pressure, because the full extent of the data is required for the FFT.²

Figure 3.3 shows the strong scaling (the speed-up achieved by increasing the number of cores used for a given number of cells) for cases of various sizes and boundary conditions run on ARCHER2 using 128 cores per node. To test the lower-level routines without any novel features, cases without any geometry using periodic boundary conditions were run using grid sizes of $N_x = N_y = N_z = 1024$ and $N_x = N_y = N_z = 2048$. The domain size is $L_x = L_y = L_z = 2048$ m, meaning these problem sizes are representative of use cases that involve modelling a convective atmospheric boundary layer at $\mathcal{O}(1$ m) resolution. The speed-up for each case is shown in Fig. 3.3a and b, respectively. The smaller case requires at least 8 nodes (in terms of memory usage), and a good parallel efficiency is observed up to 128 nodes. The larger case requires at least 64 nodes and achieves reasonable efficiency, though less so than the smaller case. Note that all but one (the 1024^3 case run with 1024 processors) are impossible to run using uDALES v1.0 due to the number of processors exceeding the number of cells in a single direction. An explicit comparison of uDALES v2.0 against v1.0 using $256^2 \times 128$ cells is shown in Fig. 3.4. This case uses the IBM, with a geometry similar to the validation case that is presented below in Sect. 4.2. The two

¹Excessive compute time dedicated to communication due to relatively few cells per MPI rank is a potential performance issue that is discussed later in this section.

²This is in contrast to Xcompact3d for example, which employs high-order finite difference schemes and uses transpositions to access cells in the stencil beyond the edge of the pencil.

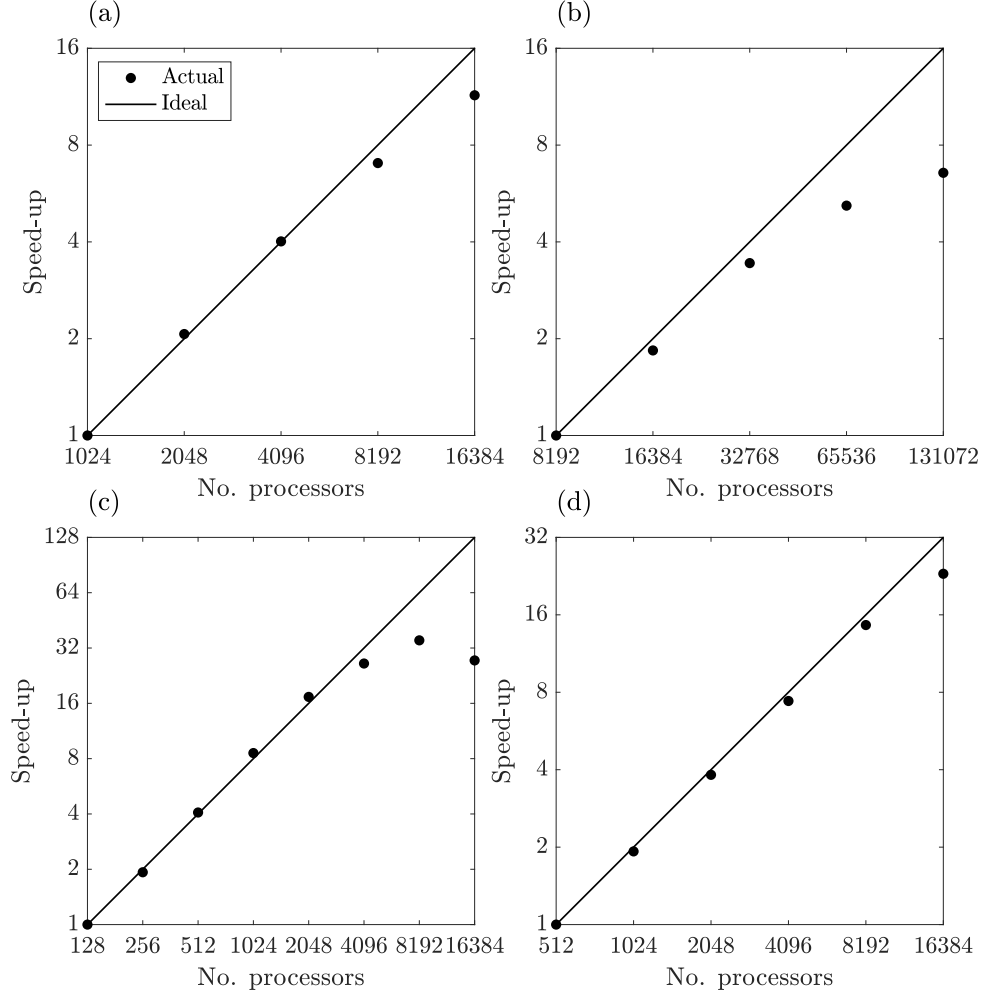


Figure 3.3: Strong scaling for cases: without IBM and periodic boundary conditions using (a) 1024^3 cells and (b) 2048^3 cells; with IBM and inflow-outflow boundary conditions using (c) $640 \times 384 \times 384$ cells and (d) $1280 \times 768 \times 768$ cells.

codes both scale well up to 128 cores, though only uDALES v2.0 is able to exceed 256 cores, and still scales reasonably up to 2048 cores.³

To test all the key features of uDALES v2.0, i.e. the IBM and the fully FFT-based pressure solver for inflow-outflow boundary conditions, cases similar to the validation case that is presented below in Sect. 4.4 were run. For practical purposes the resolution is higher, but temperature is not solved for, and the domain width is smaller (the domain size is $L_x \times L_y \times L_z = 190 \text{ m} \times 114 \text{ m} \times 114 \text{ m}$). The smaller case has a grid size of $N_x \times N_y \times N_z = 640 \times 384 \times 384$, and the larger case has a grid size of $N_x \times N_y \times N_z = 1280 \times 768 \times 768$. The speed-up for each case is shown in Fig. 3.3c and d respectively. It is possible to run the smaller case on a single node, and good parallel efficiency is

³Though results for solution time are not shown here, uDALES v2.0 and v1.0 exhibit similar performance for periodic simulations, and v2.0 is approximately 50% faster for inflow-outflow simulations due to the improved pressure solver (see Sect. 3.3).

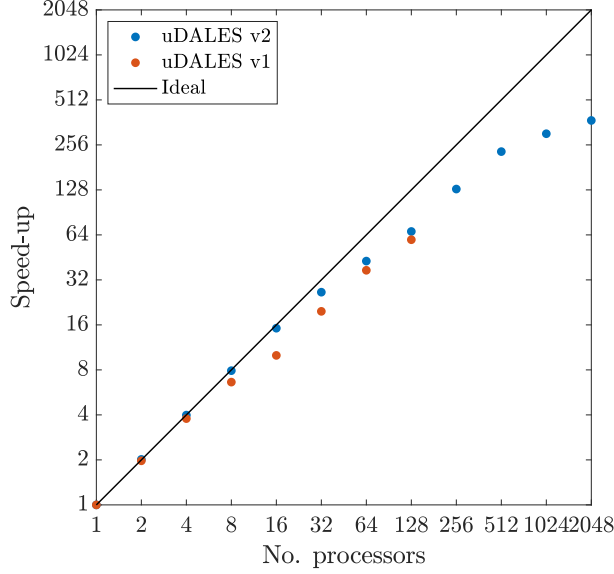


Figure 3.4: Strong scaling for uDALES v2.0 compared with v1.0 for a case using the IBM with periodic boundary conditions, with $256^2 \times 128$ cells.

observed until 8,192 cores are reached, beyond which extra parallelisation in fact becomes detrimental. The larger case required 4 nodes minimum and demonstrated good scaling up to 16,384 cores. These results demonstrate that the limit of parallelisation of uDALES has been increased substantially, including for simulations using the upgraded features.

While the weak scaling, i.e. the variation in performance while increasing the number of cells in proportion with the number of cores, was not explicitly determined, the strong scaling results reveal practical insights into the efficient use of uDALES v2.0. Namely, parallelising the x and y directions such that the number of cells spanning the pencil is less than 8 in each direction is unlikely to offer significant speed-up, and as low as 4 is likely to be detrimental (depending on the number of points in the z -direction).

3.3 Pressure solver

The Poisson equation that is satisfied by the pressure can be solved most efficiently using the FFT algorithm in the x and y directions and Gaussian elimination (GE) in the z direction (Swarztrauber, 1977). The reason for not using the FFT in the z direction as well is because GE supports a non-equidistant grid (unlike the FFT), and there is not likely to be a performance gain using the FFT rather than Gaussian elimination due to their algorithmic complexity ($\mathcal{O}(N_z \log N_z)$ versus $\mathcal{O}(N_z)$ respectively for a tridiagonal system). The velocity boundary conditions in the x and y directions determine the specific type of

transform performed. If the velocity is periodic, then the pressure is also periodic and the regular discrete Fourier transform (DFT) is used. If the velocity is inflow-outflow, then the pressure has a Neumann boundary condition and a discrete cosine transform (DCT) for a staggered grid is used (Schumann and Sweet, 1988). A detailed derivation of the Poisson equation and its solution using the DFT/DCT is available in Appendix B.

uDALES v1.0 uses the implementation of the DFT from the FFTPACK library (Swarztrauber, 1984), which does not include the staggered DCT. Note that uDALES v1.0 does not use the DCT for inflow-outflow situations; instead the cyclic reduction (CR) algorithm is used to solve the x and z directions, while the FFT is used in the y direction (meaning the y direction is always periodic). A non-equidistant grid can be used with CR, hence there is the ability to use a stretched x grid in uDALES v1.0. However, the CR-based solver is slower than the fully FFT-based solver, and is only practical to use with a 1D domain decomposition because CR requires the full extent of the data in both the x and z directions in order for it to be more efficient than GE.

uDALES v2.0 uses the DCT for inflow-outflow simulations, using the implementation from the FFTW library (Frigo and Johnson, 1998), specifically the type-II and type-III transforms, which are appropriate for a staggered grid (Swarztrauber, 1984). To solve for each direction requires transposing data between the three pencil orientations, which is achieved using routines from the 2DECOMP&FFT library. As the name suggests, the 2DECOMP&FFT library contains extensive auxiliary FFT functionality, but this was not used for uDALES v2.0. This is because the library is primarily designed for performing 3D FFTs, i.e. using the FFT to solve the z direction as well as x and y in the case of uDALES. For the reasons already discussed, this was not implemented in uDALES v2.0.

When using inflow-outflow lateral boundary conditions, the boundary condition at the top of the domain must be treated with care. In periodic simulations, there is a no-penetration boundary condition at the top, but with inflow-outflow lateral boundaries, fluid must be allowed to pass through, which is equivalent to setting a non-zero vertical velocity (u_z). The physical reasoning for this is that the incoming flow responds to the geometry, which may result in net motion in the z direction. Numerically, this is determined by the plane-averaged pressure gradient at the top, and is necessary for the flow satisfy incompressibility (mass conservation; Eq. 2.1).⁴

⁴In uDALES v1.0, u_z was set to zero even in inflow-outflow situations, but the flow was incompressible due to the nature of the cyclic reduction based pressure solver.

3.4 Geometry representation

The geometry in uDALES v1.0 is specified as a set of cuboid blocks with a given size in each Cartesian direction, and the faces of the blocks correspond to the facets. This approach is fundamentally limited as it requires the facets to align with the edges of computational cells, which is problematic when the geometry of interest does not in fact do so, as is frequently the case for realistic urban environments (see Fig. 3.1). Also, the block format is bespoke, which makes it impossible to import geometries directly from other software packages. Instead, custom scripts and workflows must be relied upon to perform the necessary voxelisation (from a 3D model) or rasterisation and extrusion (from a 2D surface elevation map).

The geometry in uDALES v2.0 is specified as a triangulated surface using an STL file, which consists of a list of triangles in terms of their three vertices in 3D Cartesian space, as well as their surface normals. This formatting is clearly independent of any grid specification, and is widely supported by other software packages. By treating each triangle as a facet in uDALES, the model can use this representation to capture non-grid-aligned geometries more faithfully in comparison to a voxel representation, and to leverage the tools available to manipulate them. Note that trees are not specified using facets, therefore the description in this section does not apply to them.

How exactly to divide a particular geometry into facets (i.e. choosing the size and shape of the triangles) in order to achieve accurate results depends on the interaction of the physical processes with the morphology. Assuming the surface energy balance (SEB) scheme is used, this should be done bearing in mind the assumption that each facet has constant properties. This includes the incident solar radiation, hence the shading across the surface should appear reasonable by visual inspection. However, there are constraints on this, including the effect of the grid resolution on the surface fluxes, and the increased computational resources required to perform the radiation calculations with a large number of facets (due to a large domain size for example); both of which are discussed later in this section. For simple, grid-aligned cases such as in Chapter 4, it may be that it may be that more triangles are needed to represent the geometry than it would do if using rectangles. However, this is not a performance concern because the performance of the IBM does not directly scale with the number of facets, and the performance of the algorithms that do has been upgraded, namely the calculation of shortwave radiation.

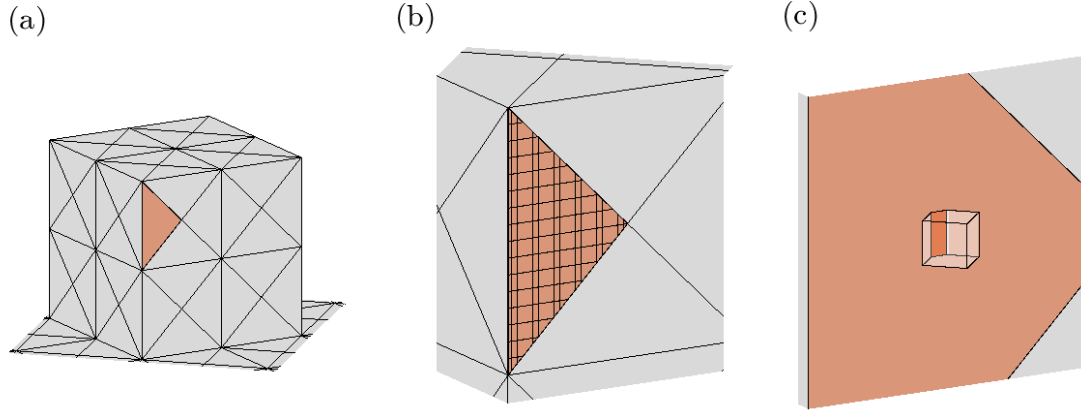


Figure 3.5: Surface treatment in uDALES v2.0: (a) triangular facets with one coloured orange, (b) a facet divided into sections according to grid cells, (c) a facet section and fluid boundary cell.

3.4.1 Conservative immersed boundary method

uDALES models the presence of the geometry using no-slip and no-penetration boundary conditions, and the fluxes of momentum and scalars across boundaries are prescribed by wall functions, rather than being determined by the advection and diffusion terms in the governing equations (Eqs. 2.16 and 2.17). This condition, i.e. zero flux other than what is prescribed by the wall functions, is particularly important for scalars; the IBM must be conservative, meaning there is no net transfer of heat, moisture, or pollutant concentration between the fluid and solid regions due to advection and diffusion terms.

In uDALES v2.0, each grid cell (for each of the staggered grids) is categorised as either fluid or solid depending on whether the cell centre is, respectively, outside or inside the triangulated surface that defines the geometry. This is achieved using the ray-casting method (Borazjani et al., 2008). Note that in this section, ‘point’ is often used to refer to a cell centre. In non-grid-aligned situations, a tolerance is used, meaning points that are in the fluid region but very close to the surface are classified as solid. This is in part for numerical reasons that are discussed in Sect. 3.4.2 and Appendix C. In addition to this, it is physically reasonable to classify as solid the points for which the distance to the surface is approximately equal to the size of protrusions on facets. Boundary points for both types are identified as those with at least one neighbour of the other type.

At the solid points on each velocity grid, the corresponding velocity component is set to zero. At the fluid boundary points on the velocity and scalar grids, the corresponding

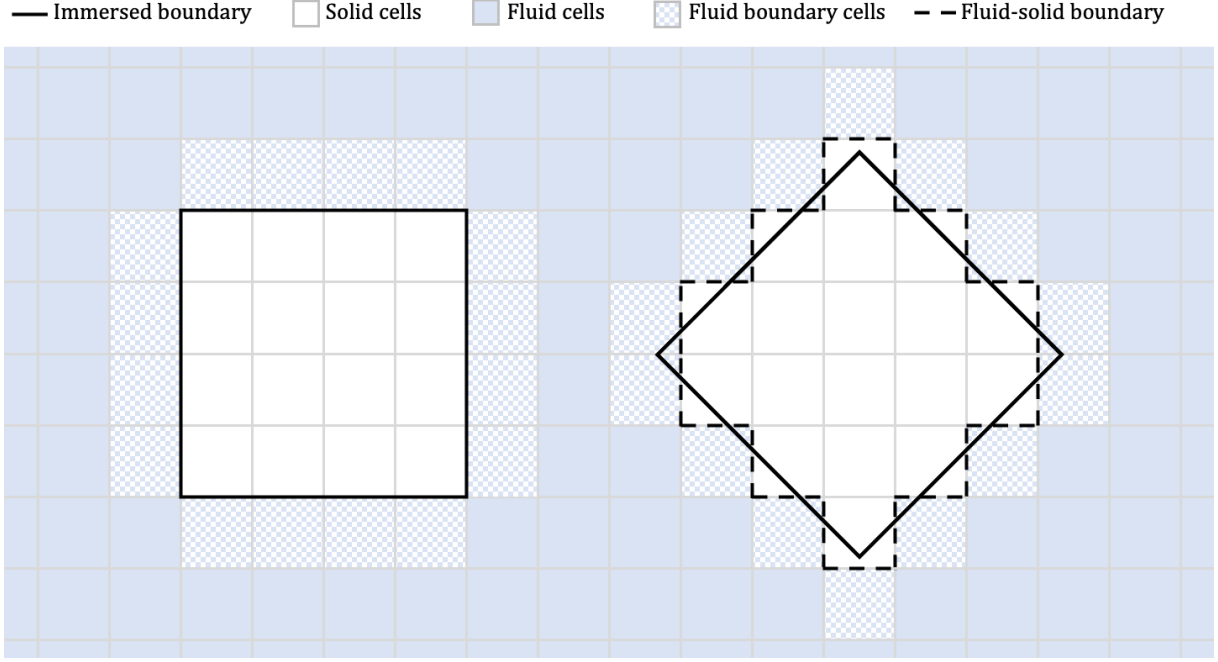


Figure 3.6: A 2D geometry depicted for grid-aligned (left) and non-grid-aligned (right) situations.

governing equations are modified such that any flux contribution due to advection and diffusion from neighbouring solid points is negated. This means that when the facets are aligned with the cell edges, the desired boundary conditions are satisfied exactly. If not, they must be interpreted as follows; the no-slip and no-penetration conditions mean the velocity at solid points is zero, and the zero flux condition (due to advection and diffusion) applies locally between each pair of fluid-solid neighbours. Therefore, according to these conditions, the boundary is located literally at the interface of the fluid and solid cells, aligned with the cell edges, as shown in Fig. 3.6. This aspect of the IBM is conceptually unchanged from v1.0, though was implemented from scratch in v2.0 to accommodate the 2D domain decomposition and the triangulated surface geometry representation.

An alternative approach would be to enforce that the value of a variable on the boundary, as determined by interpolating the values at nearby points, satisfies the boundary condition exactly. For example, one method would be to set the values at solid boundary points such that when interpolated across the boundary in the facet normal direction to an image point inside the fluid region, the value or flux on the boundary itself satisfies the desired flow condition (e.g. Majumdar et al., 2020). This approach is often used with DNS since the flow is fully resolved, hence the variation of quantities across near-surface cells is assumed to be linear, though this is generally not the case for LES. Another in-

herent challenge with this approach is that it is harder to ensure global conservation. For the approach described here, global conservation is guaranteed since local conservation is ensured by enforcing zero flux (due to advection and diffusion) between each fluid-solid pair. In alternative approaches, the zero flux condition would be at the boundary itself in an interpolated sense, so local conservation would no longer necessarily hold between fluid-solid pairs, but global conservation would still need to be enforced.

3.4.2 Surface fluxes

The IBM in uDALES uses wall functions to determine surface fluxes of momentum, sensible heat, and specific humidity at the fluid boundary points (see Sect. 2.3.2). Given the IBM is conservative, these parameterised fluxes are the only mechanism by which the surface exerts skin friction and exchanges heat and moisture with the fluid. The novelty of uDALES v2.0 is in the treatment of these fluxes given that the surface is not aligned with the grid. Another conservation principle that motivates the approach is that for the SEB scheme, the total heat flux into the fluid is equal to the total heat flux out of the surface. Whilst this principle is not relevant for momentum flux (drag), the same method is also applied for that calculation.

While many IBMs with parameterised fluxes effectively operate from the perspective of the fluid boundary points (Ma and Liu, 2017; Bao et al., 2018), the approach described here is based on considering the effect of each and every part of the surface on the fluid. As depicted in Fig. 3.5, the surface is divided cell-wise (for each grid) into facet sections such that each section lies in only one cell. Note that this cell can be fluid or solid — in either case, the flux it imparts to the fluid must be accounted for. In this approach, each section imparts flux to a single fluid boundary point, which means it is necessary to identify the fluid boundary point that is most appropriate to experience the flux. This process is illustrated in Figure 3.7. Note that the wall functions are defined in a wall-normal direction, and in this approach, the relevant ‘wall’ is the facet section. Therefore, in many cases, the chosen fluid boundary point for each facet section is the one for which there exists a vector from the facet section to the fluid boundary point in the direction of the facet normal. However, there may be some facet sections that do not have a fluid boundary point lying in the direction of the facet normal. For such facet sections, the appropriate fluid boundary point (to impart the flux to) is chosen to be the point which

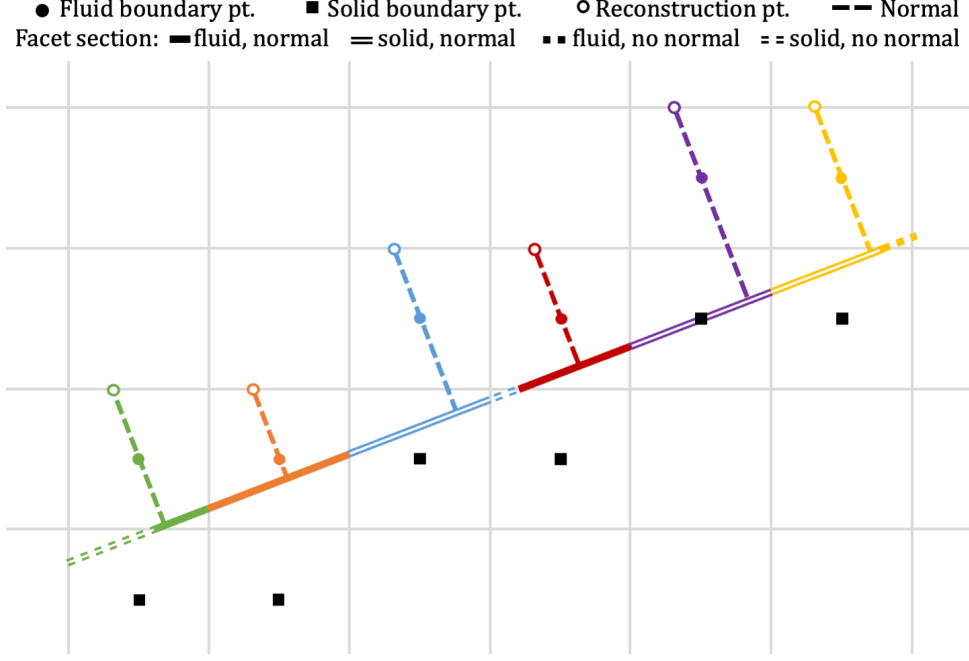


Figure 3.7: A 2D facet divided into sections. Fluid boundary points (and reconstruction points) are coloured uniquely. Facet sections are coloured by their corresponding fluid boundary point, and distinguished by whether they are in a fluid or solid cell, and whether a normal vector exists between the section and fluid boundary point.

maximises $\cos \psi/d$, where ψ is the angle between the facet normal and the surface-point vector, and d is the minimum distance between the facet section and the point. This minimises the angle between the surface normal and the surface-point vector, as well as the distance to the point.

For each facet section, the flux imparted to the appropriate fluid boundary point is calculated according to the wall functions using the properties of the facet that the section makes up, as well as the velocity and scalar fields, as discussed in Sect. 2.3.2. If d is sufficiently large, the fields are evaluated at the fluid boundary point itself, whereas if d is small then they are evaluated at a reconstruction point further from the surface, located at the boundary with the adjacent cell in the normal direction (Ma and Liu, 2017). This is because the wall functions are not valid when d is small. The reconstruction approach is discussed in further detail in Appendix C.

A local orthonormal coordinate system is defined (at the location where the field is evaluated) using the facet normal $\hat{\mathbf{n}}$, the spanwise direction $\hat{\mathbf{p}} = (\hat{\mathbf{n}} \times \mathbf{u})/||\hat{\mathbf{n}} \times \mathbf{u}||$, where $\mathbf{u}$ is the velocity, and the streamwise direction $\hat{\mathbf{t}} = \hat{\mathbf{p}} \times \hat{\mathbf{n}}$. The streamwise velocity component $\mathbf{u} \cdot \hat{\mathbf{t}}$ corresponds to the streamwise velocity u_a used in the wall functions. The surface stress (calculated using Eq. (2.18)) is in fact the component of a tensor that must

be transformed back to the corresponding Cartesian direction. This transformation is simplified because in the local basis, the stress is entirely parallel to $\hat{\mathbf{t}}$ and perpendicular to $\hat{\mathbf{n}}$. The global basis is denoted by $\mathbf{e}_i$, where $i = 1, 2$, and 3 corresponds to $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ respectively, and the local basis by $\mathbf{e}'_i$, where $i = 1, 2$, and 3 corresponds to $\hat{\mathbf{t}}$, $\hat{\mathbf{p}}$, and $\hat{\mathbf{n}}$ respectively. The local stress tensor $\boldsymbol{\tau}'$ is therefore defined by $\tau'_{13} = \tau_s$ and $\tau'_{ij} = 0$ otherwise. The transformation to the global basis is given by

$$\tau_{ij} = \sum_l \sum_m (\mathbf{e}_i \cdot \mathbf{e}'_l)(\mathbf{e}_j \cdot \mathbf{e}'_m) \tau'_{lm}. \quad (3.1)$$

The total stress in direction i is equal to $\|\boldsymbol{\tau} \cdot \mathbf{e}_i\|$, and the volumetric sink of momentum at the fluid boundary point $S_{u_i} = -\|\boldsymbol{\tau} \cdot \mathbf{e}_i\|a/(\rho V)$, where a is the facet section area, ρ is the air density, and V is the cell volume. To illustrate, consider the stress in the x direction:

$$\tau_{11} = (\hat{\mathbf{x}} \cdot \hat{\mathbf{t}})(\hat{\mathbf{x}} \cdot \hat{\mathbf{n}})\tau_s, \quad \tau_{12} = (\hat{\mathbf{x}} \cdot \hat{\mathbf{t}})(\hat{\mathbf{y}} \cdot \hat{\mathbf{n}})\tau_s, \quad \tau_{13} = (\hat{\mathbf{x}} \cdot \hat{\mathbf{t}})(\hat{\mathbf{z}} \cdot \hat{\mathbf{n}})\tau_s.$$

The total stress is then $\tau_x = \sqrt{(\tau_{11})^2 + (\tau_{12})^2 + (\tau_{13})^2}$. Note that when the facet is aligned with the grid, i.e. when $\hat{\mathbf{n}}$ is equal to $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, or $\hat{\mathbf{z}}$, then the total stress (for the x direction) further simplifies to the familiar expression $\tau_x = (\hat{\mathbf{x}} \cdot \hat{\mathbf{t}})\tau_s = \rho C_m u_a u_x$.

The kinematic sensible heat flux and specific humidity flux ($u_\tau \theta_\tau$ and $u_\tau q_\tau$) are calculated using Eqs. (2.19) and (2.20) respectively, and correspond to source and sink terms $S_\theta = u_\tau \theta_\tau a/V$ and $S_q = u_\tau q_\tau a/V$. If the SEB scheme is in use, the sensible and latent heat fluxes for facet f are given by

$$H_f = \frac{\rho c_p}{A_f} \sum_{n \in C_f} a_n (u_\tau \theta_\tau)_n, \quad E_f = \frac{\rho \mathcal{L}_v}{A_f} \sum_{n \in C_f} a_n (u_\tau q_\tau)_n. \quad (3.2)$$

Here, C_f is the set of facet sections comprising facet f , $A_f = \sum_{n \in C_f} a_n$ is the facet area, c_p is the air specific heat capacity, and $\mathcal{L}_v$ is the latent heat of vaporisation. Given this formulation, global conservation with the SEB scheme is guaranteed. This is because each section is accounted for exactly once (and the sum of their area equals the total surface area), and for each section the fluid cell and the facet experience an equivalent flux determined by the section area. A detailed depiction of the surface scheme in uDALES v2.0 is given in Appendix D.

Note that the computational performance of the IBM scales linearly with the total number of facet *sections*, rather than the number of facets, and the number of sections depends on the total surface area of the geometry and the grid resolution. Also, the IBM is parallelised in accordance with the 2D domain decomposition — each core only stores geometry data structures, i.e. solid cells, fluid boundary cells, and facet sections, that are contained within the corresponding pencil (as well as the halo cells). However, the size of the facets should be appropriate for the grid resolution (and vice versa). For excessively small facets, the issues relating to distance to the wall (d) tend to be more pronounced, which may cause problems with the accuracy of the IBM. It is therefore advised that the facets span several (at least two) grid cells.

3.5 Shortwave radiation

According to the radiosity assumption, the net shortwave radiation on a single facet f is given by $K_f^* = K_f^\downarrow - K_f^\uparrow = (1 - \alpha_f)K_f^\downarrow$ (see Sect. 2.3.3). The incoming shortwave radiation $K_f^\downarrow = \mathcal{S}_f + \mathcal{D}_f + \mathcal{R}_f$, where $\mathcal{S}_f$ is the direct solar radiation, $\mathcal{D}_f$ is the diffuse sky radiation, and $\mathcal{R}_f$ is the reflected radiation from other facets. The direct solar radiation depends on the position of the sun, which is specified using the solar azimuth (Φ_{sun}) and zenith (Θ). For a coordinate system defined such that the x direction is at an angle $\Phi_{\text{N} \rightarrow x}$ clockwise from north, letting $\Phi' = \Phi_{\text{sun}} - \Phi_{\text{N} \rightarrow x}$, the vector to the sun $\hat{\mathbf{s}}$ in the simulation reference frame is given by

$$\hat{\mathbf{s}} = \begin{bmatrix} \sin \Theta \cos \Phi' \\ -\sin \Theta \sin \Phi' \\ \cos \Theta \end{bmatrix} \quad (3.3)$$

In uDALES v1.0, $\mathcal{S}_f$ is calculated according to $\mathcal{S}_f = I \hat{\mathbf{n}}_f \cdot \hat{\mathbf{s}}$, where I is the direct normal irradiance (a model parameter) and $\hat{\mathbf{n}}_f$ is the facet normal. To account for shading, rays are projected from the facet corners and centre in the direction of the sun vector to check for intersection with any other facet. If so, then shading occurs, and $\mathcal{S}_f$ is reduced by a fraction for each of these points for which there is an intersection. This is a crude approximation for quantifying the radiation on shaded facets, and scales poorly; as $\mathcal{O}(N_f^2)$, where N_f is the number of facets.

The method used to calculate direct solar radiation in uDALES v2.0 is designed to address these limitations. It involves projecting the facets onto a plane whose normal is parallel to the sun vector. To define a point on this plane $\mathbf{p}_{\text{plane}}$, take the centre of the geometry $\mathbf{p}_{\text{geom}} = (L_x/2, L_y/2, 0)$ and project some reasonably large distance Γ in the direction of the sun vector: $\mathbf{p}_{\text{plane}} = \mathbf{p}_{\text{geom}} + \Gamma \hat{\mathbf{s}}$. To define an orthonormal pair of vectors spanning the plane, let $\hat{\mathbf{q}} = (-\hat{s}_2, \hat{s}_1, 0)$ and $\hat{\mathbf{r}} = \hat{\mathbf{q}} \times \hat{\mathbf{s}}$. Given a point $\mathbf{p}$, its projected position onto the plane is equal to $\mathbf{p} - v\hat{\mathbf{s}}$ for some unknown v , the distance between the point and the plane. The projected position can also be written as $\mathbf{p}_{\text{plane}} + \zeta\hat{\mathbf{q}} + \eta\hat{\mathbf{r}}$ for some unknown ζ and η , which can be thought of local coordinates with respect to the plane origin $\mathbf{p}_{\text{plane}}$. Equating these yields the system of equations for the unknowns:

$$\mathbf{p} - \mathbf{p}_{\text{plane}} = \begin{bmatrix} \hat{\mathbf{q}} & \hat{\mathbf{r}} & \hat{\mathbf{s}} \end{bmatrix} \begin{bmatrix} \zeta \\ \eta \\ v \end{bmatrix} \quad (3.4)$$

Solving this system for all the vertices making up the triangulated surface yields the projected position of all the facets in terms of ζ and η . The projected facets potentially overlap, which correspond to one blocking the path of radiation to the other, i.e. shading. The cell centres are therefore also projected so that they can be used to sort the facets by their distance from the plane (v). The plane is discretised into pixels, which are classified according to whether they are inside or outside a projected facet using a modified version of the MATLAB function `poly2mask` (which has also been ported to Fortran for improved performance). This classification is carried out sequentially for all the facets in order of decreasing distance to the plane, so that in the case of overlaps the pixels are recorded as belonging to the closer facet. The result is effectively an image of the facets from the sun's point of view, with pixels labelled according to which facet they correspond to. The unshaded projected area of a facet (A_f') is calculated by summing the pixels labelled by it and scaling the result by the discretisation resolution. Finally, denoting the true facet area by A_f , then $\mathcal{S}_f = IA_f'/A_f$, which is equal to $I\hat{\mathbf{n}}_f \cdot \hat{\mathbf{s}}$ for unshaded facets. This formulation accurately captures the radiation on shaded facets, and scales as $\mathcal{O}(N_f)$ because there are no pairwise facet calculations. However, note that obtaining an accurate result is dependent on discretising the plane at a sufficiently high resolution with respect to the size of the facets.

Once the direct solar radiation on each facet has been obtained, the net shortwave radiation is calculated via the same conceptual procedure as in uDALES v1.0, because it is not dependent on the geometry representation. The diffuse sky radiation on each facet is given by $\mathcal{D}_f = \psi_{f,\text{sky}} D_{\text{sky}}$, where D_{sky} is a model parameter quantifying the diffuse shortwave radiation from the sky, and $\psi_{f,\text{sky}}$ is the sky view factor for facet f . The reflected component on facet f is given by

$$\begin{aligned} \mathcal{R}_f &= \sum_{g=1}^N \psi_{f,g} K_g^\uparrow = \sum_{g=1}^N \psi_{f,g} \alpha_g K_g^\downarrow \\ &= \sum_{g=1}^N \psi_{f,g} \alpha_g (\mathcal{S}_g + \mathcal{D}_g + \mathcal{R}_g), \end{aligned} \tag{3.5}$$

where $\psi_{f,g}$ is the view factor between facet f and facet g . Equation (3.5) shows that the reflected component on each facet depends on that of all the other facets. This linear system of equations is solved iteratively to avoid the inversion of a large matrix (Suter et al., 2022). This physically corresponds to the initial radiation, i.e. the direct solar and diffuse sky components, being repeatedly reflected until all (up to a specified threshold) is either absorbed or is reflected to the sky.

In uDALES v1.0, the view factors are calculated using a bespoke algorithm implemented in MATLAB (Suter, 2018), which was designed for rectangular facets. In uDALES v2.0, view factors are calculated using the open source program View3D (which has been validated extensively and has been adopted by the widely-used software package EnergyPlus; Crawley et al., 2001; DeGraw and Walton, 2018), which is written in the C programming language and supports triangular facets. This offers better performance due to the optimisation techniques it employs, and the fact that C tends to have a faster runtime than MATLAB. Also, note that the shortwave radiation calculation occurs as a pre-processing step, meaning it does not affect the performance of simulations in the sense that was discussed in Sect. 3.2.

Despite the improvement of the shortwave radiation calculation in uDALES v2.0 compared to v1.0, there are still fundamental limitations. Unlike with the IBM (as discussed in Sect. 3.4.2), there is no reason why decreasing the size of the facets should not improve the accuracy so long as the plane discretisation resolution is increased as well. However, View3D is not parallelised, and can be a significant bottleneck when using a

large number of facets. To address this, a ‘range’ parameter has been added to View3D that causes calculations for facets that are greater than a certain distance apart to be skipped. Another constraint is storing the view factor matrix in computer memory, which has been partially addressed by using sparse matrix storage techniques in the uDALES pre-processing, however View3D itself does not use these techniques.⁵

3.6 Periodic precursor simulations

As discussed in Sect. 1.4, precursor simulations can be used to provide the time-dependent boundary conditions for inflow-outflow simulations (Suter et al., 2022; Grylls et al., 2019; Lim et al., 2022). They use periodic boundary conditions, and their streamwise and spanwise extent is typically limited, which can lead to the development of streamwise structures that span the entire domain and become permanent features of the average flow-field. These so-called superstructures are observed in reality (Hutchins and Marusic, 2007) but are exacerbated by the limited domain size used in precursor simulations. This is undesirable because it results in spanwise variations of mean quantities.

uDALES v1.0 simulations have been observed to suffer from these artificial superstructures, as there is no functionality for counteracting their formation. In contrast, uDALES v2.0 has a technique designed to avoid them by applying an advection forcing term $F_i = v_{\text{shift}} \frac{\partial u_i}{\partial y}$. Assuming mean flow in the x direction only, the effect of $v_{\text{shift}}(x, z)$ is to shift the flow by a spanwise displacement Δ_y over a streamwise distance Δ_x :

$$\Delta_y = \frac{1}{\langle u \rangle} \int_0^{\Delta_x} v_{\text{shift}}(x, z) dx, \quad (3.6)$$

where $\langle u \rangle(z)$ is the horizontally averaged streamwise velocity (in the x direction). The velocity v_{shift} can be chosen arbitrarily, but in order to avoid discontinuities in the forcing field, we require that $v_{\text{shift}} = 0$ at $x = 0$ and $x = \Delta_x$. Assuming a sinusoidal x -dependence that satisfies these conditions, i.e. $v_{\text{shift}}(x, z) = \hat{v}(z) \sin(\frac{\pi x}{\Delta_x})$ for some $\hat{v}(z)$ to be determined, the integral above can be evaluated to give

$$\Delta_y = \frac{2\Delta_x}{\pi} \frac{\hat{v}}{\langle u \rangle}. \quad (3.7)$$

⁵Due to these constraints, for a computer with 128 GB memory, the maximum number of facets is practically around 200,000.

Therefore, $\hat{v} = \frac{\pi\Delta_y}{2\Delta_x}\langle u \rangle$ which implies that the momentum forcing is given by

$$F_i = \frac{\pi\Delta_y}{2\Delta_x}\langle u \rangle \sin\left(\frac{\pi x}{\Delta_x}\right) \frac{\partial u_i}{\partial y}. \quad (3.8)$$

The parameters Δ_x and Δ_y are to be chosen on the basis of their effectiveness for disrupting the formation of the artificial flow features. For the simulations in this thesis that use this method, the output plane is at $x = 0$ with $\Delta_x = L_x/2$ and $\Delta_y = L_y/4$, which is found to work effectively in practice (see below in Sect. 4.4).

3.7 Conclusion

This chapter has presented uDALES v2.0, which is designed to address several key limitations of v1.0. The limit of parallelisation of the code has been increased by implementing a two-dimensional domain decomposition using the external library 2DECOMP&FFT (demonstrated in Sect. 3.2), which practically increases the scaling capabilities of the code. The pressure solver now makes use of the FFT algorithm for inflow-outflow boundary conditions (discussed in Sect. 3.3), which means that simulations using these conditions can be performed just as quickly as those using periodic ones. Finally, the geometry representation has been improved in that it can be specified independently of the computational grid (using the widely-used STL file format), and the IBM has been developed significantly to accommodate this (described in Sect. 3.4). In particular, the novel approach taken to apply parametrised surface fluxes ensures that heat and moisture are conserved with the SEB scheme. Chapter 4 aims to validate this development and demonstrate the utility of uDALES v2.0 for several urban use cases. A discussion of remaining limitations and potential future development of uDALES is given in the conclusion of this thesis (Chapter 8).

Chapter 4

Evaluation of uDALES v2.0

Based on journal article: ‘A conservative immersed boundary method for the multi-physics urban large-eddy simulation model uDALES v2.0’, published in Geoscientific Model Development (Owens et al., 2024).

4.1 Introduction

This chapter compares simulations of idealised urban cases using uDALES v2.0 with those using v1.0, as well as experimental and numerical studies from literature. The purpose of this is to firstly ensure that v2.0 produces similar results to v1.0 in situations where the case set-up is conceptually identical, and secondly to demonstrate that v2.0 exhibits greater accuracy when simulating non-grid-aligned geometries and explain the differences in results. The cases are chosen to isolate the various upgraded features of the model. Section 4.2 presents a case designed to test the novel immersed boundary method (IBM) approach solely with respect to momentum while keeping other settings constant. Section 4.3 presents a different case involving facets at constant temperature, which tests the IBM with respect to heat. Section 4.4 also involves heated facets and tests the novel inflow-outflow boundary conditions, as well as non-grid-aligned facets. Finally, Sect. 4.5 uses the same geometry and incoming flow as Sect. 4.4 while using the surface energy balance (SEB) scheme to evolve the facet temperature. All simulations were carried out using uDALES v2.0.0 (Grylls et al., 2024).

4.2 Neutral flow over a staggered array of cubes

This case is based on LES (Xie et al., 2008) and experiments (Cheng and Castro, 2002) of neutral flow over a staggered array of cubes with their width and mean height $h = 10$ m (see Fig. 4.1a). Note that the uDALES simulations are full scale, i.e. the dimensions are

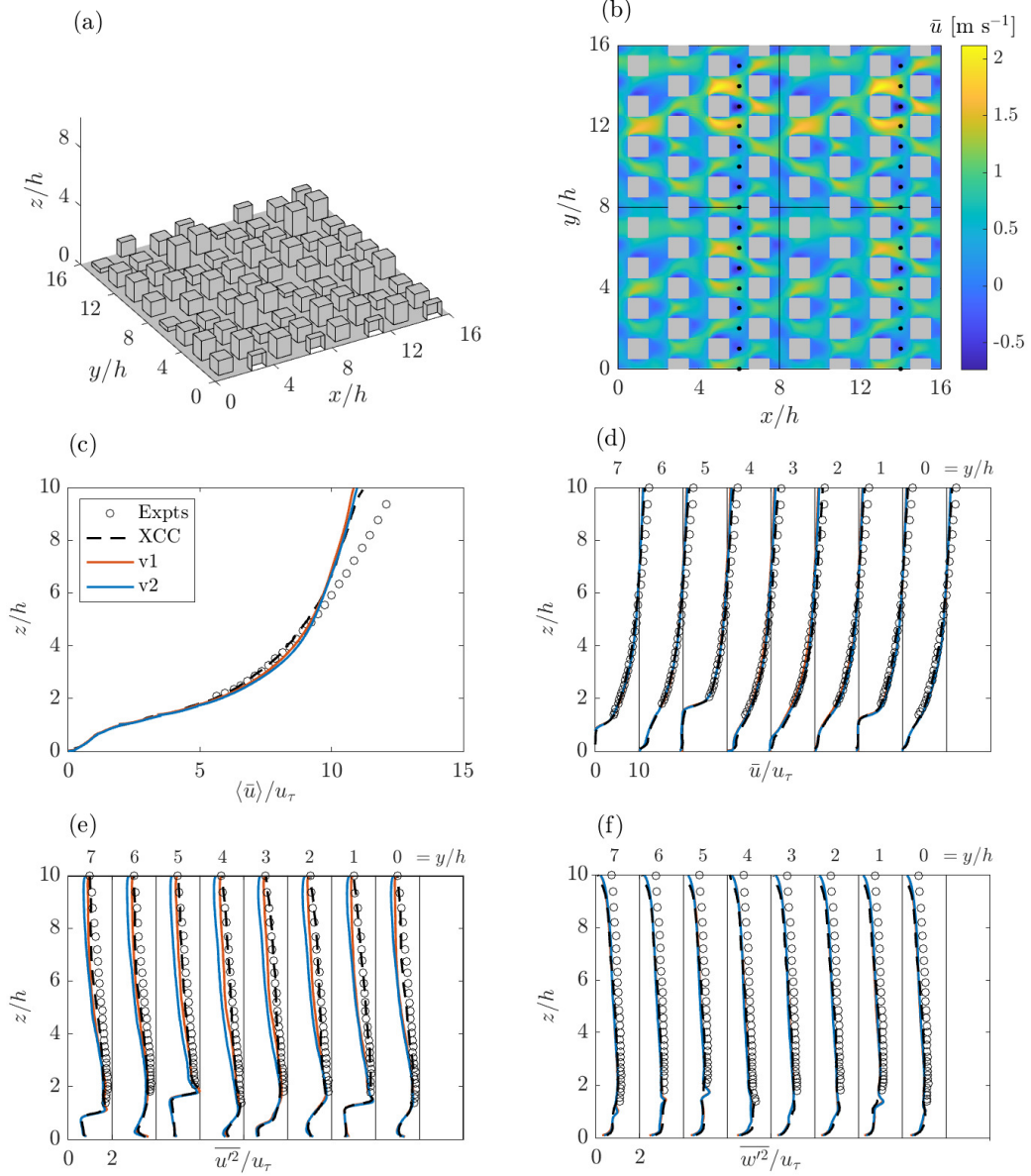


Figure 4.1: Staggered-cubes case: (a) computational domain and geometry, (b) mean x -velocity ($\bar{u}$) at $z = h/2$ with sampling locations and subdomains used in panels d-f indicated, (c) mean horizontally averaged x -velocity ($\langle \bar{u} \rangle$), (d) mean ($\bar{u}$) and (e) root mean square ($\overline{u'^2}$) x -velocity normalised by friction velocity (u_τ), and (f) normalised root mean square z -velocity ($\overline{w'^2}/u_\tau$) at locations shown in (b). The legend shown in (c) also applies for (d-f); ‘Expts’ refers to Cheng and Castro (2002), ‘XCC’ refers to Xie et al. (2008), and the others refer to uDALES.

1000 times larger than the experiment and numerical simulations from the literature.

Periodic lateral boundary conditions are used, with free slip at the top, and the flow is forced by a constant term $F_x = 4.1912 \times 10^{-3} \text{ m s}^{-2}$ (see Eq. (2.16)). The domain size is $L_x \times L_y \times L_z = 16h \times 16h \times 10h$ and the number of grid cells is $N_x \times N_y \times N_z = 256 \times 256 \times 256$. This yields a horizontal resolution of 0.625 m and a vertical resolution of 0.390625 m. The initial velocity profile is uniform; the value is equal to the vertically averaged profile of Xie et al. (2008), which was estimated to be 5.15 m s^{-1} . Since the geometry is aligned with the grid and the lateral boundaries are periodic, the IBM and pressure solver used in both versions of uDALES are conceptually identical.

The spatially averaged mean x velocity component (u) is shown in Fig. 4.1c. By visual inspection, uDALES v2.0 and v1.0 are both sufficiently close to the literature data considering the uncertainties involved (discussed in Xie et al., 2008).¹ Additionally, profiles of the mean and root mean square of u at different spanwise locations ($y/h = 0, 1, 2, \dots, 7$) along the centre line between the third and the fourth row of buildings ($x/h = 6$) are shown in Fig. 4.1d-f. Note that the geometry consists of four copies of a smaller unit, and each profile shown is an average of the four profiles within each subdomain. There is close agreement with the data of Xie et al. (2008) but the agreement with the experiment is less good, particularly higher up in the domain.² These differences are most likely for the same reasons discussed in Xie et al. (2008), namely that the experimental and numerical studies each use a different domain height. The result suggests that uDALES v2.0 can accurately simulate neutral flows over idealised, grid-aligned geometries with periodic boundary conditions, which is important because such cases are often used as precursor simulations (see Sect. 3.6).

4.3 Non-neutral flow in an infinite canyon with facets at constant temperature

This case is based on a numerical study by Cai (2012) consisting of non-neutral flow over a canyon that is $h = 18 \text{ m}$ tall and $c = 18 \text{ m}$ wide. This was used as to evaluate the

¹The comparison is purely qualitative, as no quantitative metrics are provided in Xie et al. (2008).

²uDALES v2.0 in fact appears to under-estimate $\overline{u'^2}$ for reasons that are unclear. However, given that this occurs higher in the domain, it is unlikely to be due to a problem with the surface representation, and is therefore not concerning.

wall function implementation in uDALES v1.0 (Suter et al., 2022), though the case was re-run with v1.0 for this study. Note that as in the case presented in Sect. 4.2, no modified features are used (non-grid-aligned facets and inflow-outflow boundary conditions). There are two different physical situations considered here, corresponding to the effect of buoyancy (due to surface heating) on the flow: assisting, where the upstream wall and roof are heated; and opposing, where the downstream wall and roof are heated. The roofs and heated wall have a fixed temperature $T_s = 302$ K and the initial air temperature $\theta_\infty = 293$ K. The domain size is $L_x \times L_y \times L_z = 24 \text{ m} \times 40 \text{ m} \times 90 \text{ m}$, and the grid size is $N_x \times N_y \times N_z = 80 \times 40 \times 92$. This yields a resolution of 0.3 m and 1 m in the x and y directions respectively. The z grid is stretched so as to obtain a vertical resolution of

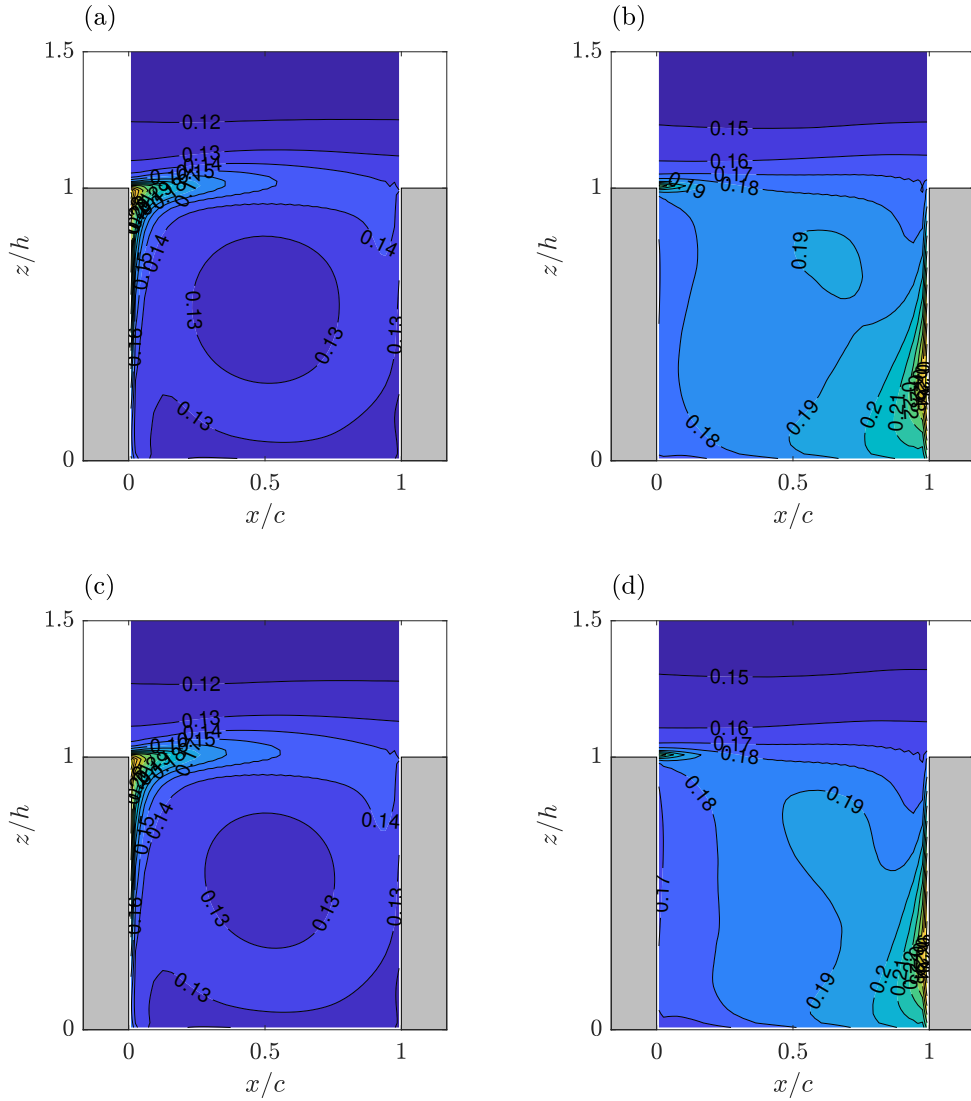


Figure 4.2: Infinite canyon with constant facet temperature case: mean normalised y averaged potential temperature $(\bar{\theta} - \theta_\infty)/(T_s - \theta_\infty)$ predicted by uDALES: (a) v1.0 assisting, (b) v1.0 opposing, (c) v2.0 assisting, and (d) v2.0 opposing.

0.3 m inside the canyon. The free-stream velocity $u_\infty = 2.5 \text{ m s}^{-1}$, which is achieved by the forcing $F_x = (u_\infty - \langle u \rangle_{z=L_z})/\Delta t$. The top boundary condition is free slip, and periodic lateral boundary conditions are used. For the wall functions, the momentum roughness length $z_0 = 0.01 \text{ m}$ and the heat roughness length is defined by $\ln(z_0/z_{0,h}) = 5$. It is not clear what values were used in Cai (2012) for the turbulent Prandtl number (Pr_t); here it is set to 1. The simulation is first run for 1800 s with all facet temperatures set to θ_∞ , and then run for 3600 s with increased facet temperatures. For the time-averaged data presented, fields are averaged every second and the last 1800 s is used as the averaging window.

Figure 4.2 compares the mean spanwise averaged normalised potential temperature for uDALES v1.0 and v2.0, and shows good agreement in terms of the flow structure and magnitude. The results demonstrate that the temperature surface treatment in uDALES v2.0 produces comparable results to that of v1.0 in grid-aligned situations. However, this is not a physically realistic situation because the use of periodic boundary conditions results in the spatially averaged temperature in the domain rising as the simulation progresses (and as a result the unheated facets have a cooling effect). In uDALES v2.0, it is possible to use a heat sink to counter-act this (though this was not used here). Alternatively, one can use inflow-outflow boundary conditions, which allows heat to exit the domain.

4.4 Non-neutral flow over a single cube with facets at constant temperature

This case is based on a numerical study by Boppana et al. (2013) and an experimental study by Richards et al. (2006). The uDALES simulations are run at full scale, i.e. 100 times larger than in the literature. The geometry consists of a single cube with a side length of $h = 19 \text{ m}$, and a subset of the facets are heated to a constant temperature, hence the results are compared to a non-neutral case presented in Boppana et al. (2013). In the original case, the cube is grid-aligned (see Fig. 4.3a,b), but this study also includes simulations in which the cube is rotated with respect to the grid (see Fig. 4.3c,d). The intention is to maintain the same flow over the cube for each simulation, as the physics should not depend on the reference frame. Figure 4.3c shows the effect of using a voxel representation for the geometry in uDALES v1.0 — many small facets are required for

Table 4.1: Single-cube case with constant surface temperature (Sect. 4.4): temperature difference between facets and the inlet ($\Delta T = T_s - \theta_\infty$).

	Leeward	Roof	Side	Floor 1	Floor 2	Floor 3
ΔT [K]	1.52	0.26	0.14	0.28	0.14	0.07

the rotated case in places where the actual geometry does not align with the grid.³

In the original (non-rotated) case, the domain size is $L_x \times L_y \times L_z = 10h \times 8h \times 6h$; the domain width has been increased from that used by Boppana et al. (2013) so that it matches that of the rotated case, therefore the two cases can use the same precursor simulation (see below). The centre of the cube is located at $x_c = 4.5h$, $y_c = 4h$. For the rotated case, the flow is rotated by an angle of 45° , and the domain size is $L'_x = L'_y = 8h$. The cube is positioned such that the distance from the origin to the cube centre is $4.5h$, i.e. the centre is at $x'_c = 4.5h/\sqrt{2}$, $y'_c = 4.5h/\sqrt{2}$. This means that the distance from the cube centre to the outlet is at least $5.5h$, thus making it possible to compare the wake with the original case. The grid sizes of the original and rotated cases are $N_x \times N_y \times N_z = 320 \times 256 \times 192$ and $N'_x \times N'_y \times N'_z = 256 \times 256 \times 192$ respectively, meaning the resolution is 0.59375 m in each direction.

The temperature of the facets is set to match the bulk Richardson number (Ri_b ; see Table 2.1) of Boppana et al. (2013), which requires the temperature difference between the facets and the air to be 100 times smaller. The inlet potential temperature (θ_∞) is equal to 293 K, and the temperature differences between the facets and the air are shown in Table 4.1. This corresponds to the case with $Ri_b = -0.66$ presented in Boppana et al. (2013). The Reynolds number (Re) for urban flows is typically sufficiently large for the viscous stresses to be negligible compared to the turbulent stresses and pressure, i.e. the flow is essentially independent of Re . This means the geometry scale can be changed while keeping the velocity constant (and thus changing Re) and obtain similar results, as in Sect. 4.2. However, Ri_b is a measure of the relative strength of buoyancy and shear forces, and this ratio must stay the same otherwise the character of the flow will change. It is not clear what values to set for the momentum and heat roughness lengths, as a different wall model is used in Boppana et al. (2013). Here $z_0 = 0.01$ m is used, with $z_{0,h} = z_0$ following Cai et al. (2008).

³The size of the facets also differs for the non-rotated cases, with uDALES v2.0 using four triangles for each rectangle used by v1.0, though this is unlikely to influence the results (compared to using two for example).

Regarding boundary conditions, the y direction is periodic and the vertical velocity at the top is allowed to vary (as discussed in Sect. 3.3). The x direction is inflow-outflow with the inlet velocity provided by a precursor simulation (in contrast, synthetic turbulence generation is used in Boppana et al. (2013)). The geometry in the precursor consists of staggered cubes of side length $h/8$ and plan area fraction $\lambda_p = 0.25$. The domain length is $12h$, with the same width, height, and resolution as the main simulation, as is required. The aim of the precursor is to generate mean x velocity and turbulent kinetic energy (TKE) profiles that match that of Richards et al. (2006) and Boppana et al. (2013). In the experiment, the flow is characterised by a power-law profile with exponent $\alpha = 0.52$:

$$u_{\text{exp}}(z) = u_{\text{ref}} \left(\frac{z}{z_{\text{ref}}} \right)^\alpha. \quad (4.1)$$

The reference height z_{ref} was taken to be 10 m and the reference velocity u_{ref} was estimated to be 0.33 ms^{-1} . The initial velocity is set to this profile, and during the simulation the plane-averaged velocity is forced towards it by using a nudging term $F_x = (u_{\text{exp}} - \langle u \rangle)/t_{\text{nudge}}$, with $t_{\text{nudge}} = 60 \text{ s}$. In order to avoid the formation of artificial superstructures, the shifting method described in Sect. 3.6 is used.

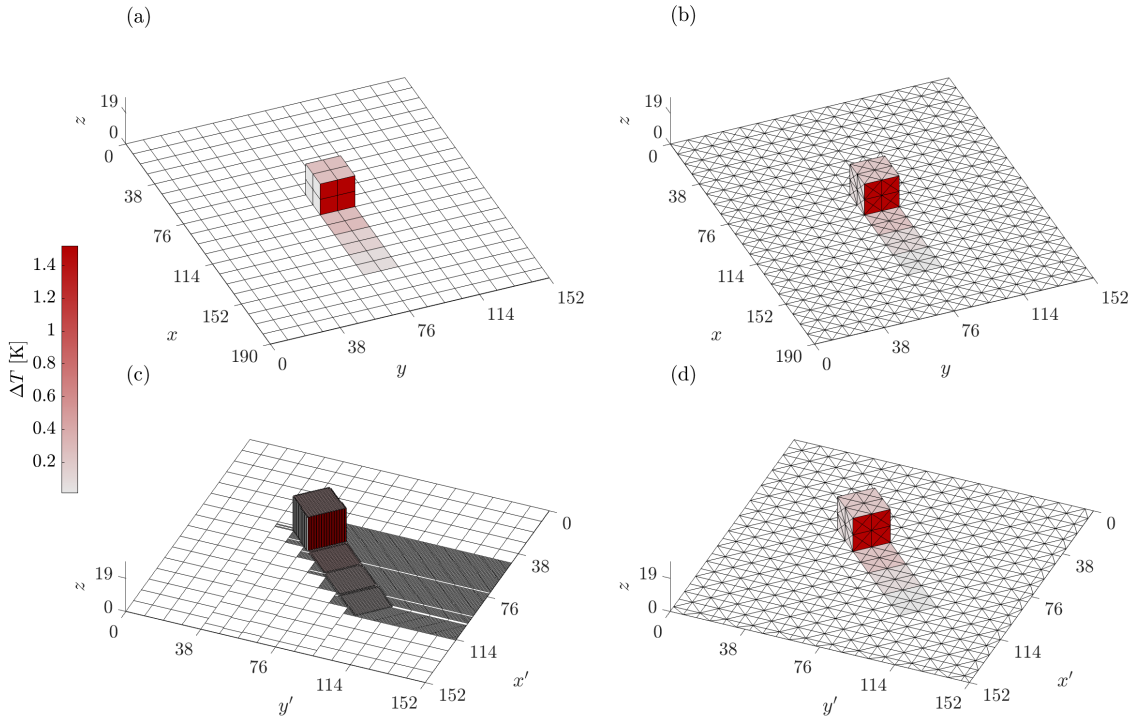


Figure 4.3: Single-cube case with constant surface temperature: facets coloured according to temperature difference ΔT for (a) v1.0 original, (b) v2.0 original, (c) v1.0 rotated, and (d) v2.0 rotated.

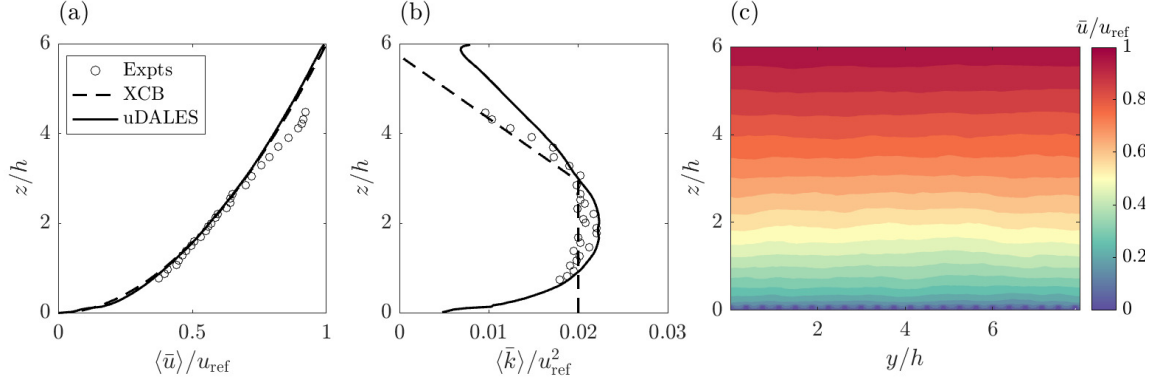


Figure 4.4: Single-cube case with constant surface temperature: spanwise-averaged inflow profiles of (a) streamwise velocity (u) and (b) turbulent kinetic energy (k), and (c) spanwise dependence of streamwise velocity. In the legend, ‘Expts’ refers to Richards et al. (2006) and ‘XCB’ refers to Boppana et al. (2013).

Figure 4.4c shows the time-averaged inflow plane velocity; it is reasonably uniform in the y direction, indicating that the shifting method is successful. Averaging this plane in the y direction results in the velocity profile shown in Fig. 4.4a, which matches the power-law profile almost exactly. The TKE is shown in Fig. 4.4b; the profile broadly agrees with the experimental and numerical values, in that the peak is at around 0.02 between $z/h = 1$ and $z/h = 3$ and decreases above this height.

For the main simulation, Figs. 4.5c-f shows slices of mean scaled potential temperature halfway up the cube. From this it appears that the v2.0 rotated case agrees better with the original v2.0 case, and indeed the original v1.0 case, than the v1.0 rotated case does. The slight asymmetry in the wake in the rotated cases is most likely due to the boundary conditions. The y/y' direction is periodic so that the turbulent inflow boundary condition in the x/x' direction can eventually reach both lateral sides of the cube, but the effective distance from the inlet to each of the sides is not the same. Figures 4.5a and b show profiles of mean normalised streamwise velocity and potential temperature downstream of the cube on the wake centre line. The velocity profiles are all generally in agreement, with greater discrepancy below cube height as the distance from the wall increases. This shows that the models capture the wake similarly in the near field. The temperature profile at a streamwise distance of $\chi/h = 0.55$ is very close to the leeward face, so the temperature gradient in the streamwise direction is large, making the comparison at this point less reliable. Other than at this location, uDALES generally agrees well with the simulations of Boppana et al. (2013), with v2.0 matching more closely than v1.0 in the

rotated case. Note that there is not good agreement with the experiments; this is discussed in detail in Boppana et al. (2013), and relates to the difficulty in determining the true boundary condition for heat on the leeward face. The results demonstrate that there is

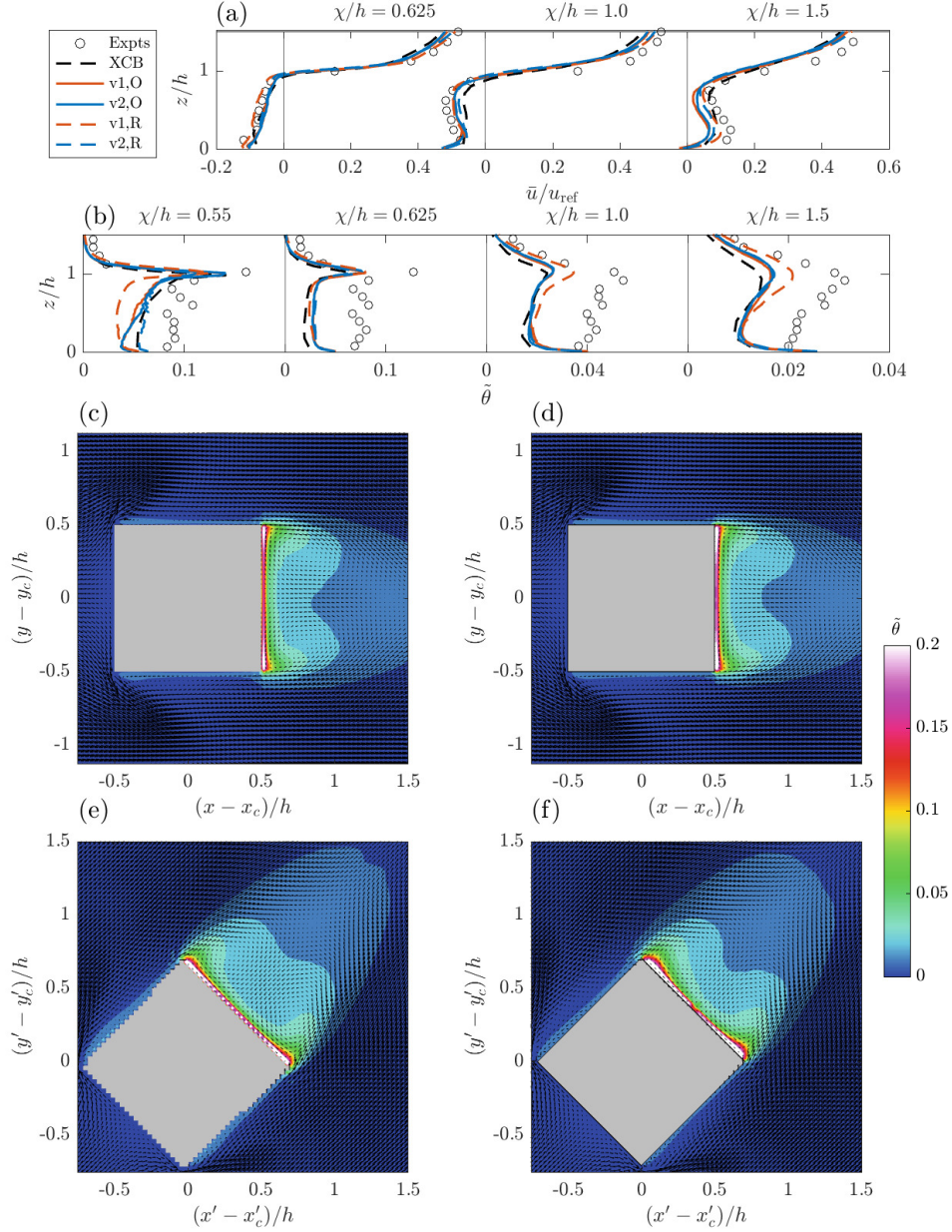


Figure 4.5: Single-cube case with constant surface temperature: normalised mean profiles of (a) streamwise velocity $\bar{u}/u_{\text{ref}}$ and (b) potential temperature $\bar{\theta} = (\bar{\theta} - \theta_{\infty})/(T_{\text{s,lee}} - \theta_{\infty})$, where $T_{\text{s,lee}}$ is the surface temperature of the leeward face, at downstream locations in the cube wake with streamwise distance from cube centre denoted by χ . In the legend, ‘Expts’ refers to Richards et al. (2006), ‘XCB’ refers to Boppana et al. (2013), and ‘O’ denotes original and ‘R’ denotes rotated cases for uDALES v1.0 and v2.0. Below: contours of $\bar{\theta}$ with mean velocity vectors at $z/h = 0.5$ for (c) v1.0 original, (d) v2.0 original, (e) v1.0 rotated, and (f) v2.0 rotated.

some advantage in terms of accuracy when using v2.0 in situations with constant surface temperature compared to v1.0, though the difference is not large. Also, the choice of rotation angle (45°) is in practice the most favourable for obtaining a symmetrical wake, most likely due to the effect of the lateral boundary conditions. It is expected that walls at arbitrary angles with respect to the grid would perform equally well in cases where the lateral boundary conditions have a weaker influence.

4.5 Non-neutral flow over a single cube using the surface energy balance model

Similarly to Sect. 4.4, this case involves simulating the flow around the original (non-rotated) and rotated geometries using uDALES v1.0 and v2.0, though here the facet temperatures evolve according to the SEB scheme. This is in order to both evaluate the implementation in uDALES v2.0 against v1.0 in the situations where the two models should agree, and to evaluate the rotated cases against the original cases.

The boundary conditions, including the precursor-defined inflow, are the same as in Sect. 4.4. The initial conditions are also unchanged apart from the facet temperatures. The simulation parameters pertaining to the SEB are given in Table 4.2. Note the relatively low facet volumetric heat capacity used, which allows the simulations to reach a steady-state faster. The steady-state reached does not depend on the volumetric heat capacity⁴, and it is only the steady-state (and not transient behaviour) that is of interest here. The solar position is chosen such that of the cube faces, only the leeward and roof (should) receive direct solar radiation. This means these faces should be heated more than the others, so the flow is expected to be qualitatively similar to Sect. 4.4.

Figure 4.6 shows the steady-state sensible heat flux (H) on the facets. It is clear that the v1.0 rotated case differs both qualitatively and quantitatively. For example on the leeward face, H does not reach as high a value, and the shaded region (with low H) is not captured accurately. This latter observation relates to the fact that how exactly the geometry is discretised into facets is significant, which is clearly non-physical. In the shaded region, the facets are fairly large in both dimensions, so the result would likely be improved by using much smaller facets. The facets making up the ground

⁴The heat capacity does not feature in Eq. (2.10) if $\frac{\partial T}{\partial t} = 0$.

Table 4.2: Parameters used in single-cube case with SEB, including radiation-related parameters: solar azimuth angle (Φ_{sun}), solar zenith angle (Θ), direct normal radiation (I), diffuse sky shortwave radiation (D_{sky}), sky longwave radiation (L_{sky}); and facet properties: albedo (α), emissivity (ϵ), volumetric heat capacity (C), thermal conductivity (λ), thickness (D), number of facet layers (N_l), interior temperature (T_D), and initial exterior temperature (T_s).

Parameter	Units	Value
Φ_{sun}	$^\circ$	90
Θ	$^\circ$	45
I	W m^{-2}	800
D_{sky}	W m^{-2}	80
L_{sky}	W m^{-2}	336
α	-	0.5
ϵ	-	0.85
C	$\text{MJ m}^{-3} \text{K}^{-1}$	0.1
λ	$\text{W m}^{-1} \text{K}^{-1}$	1
D	m	0.4
N_l	-	5
T_D	K	293
T_s (initial)	K	293

just downstream of the leeward face are very thin in the x' direction, but large in the y' direction, meaning the structure (namely H decreasing away from the cube) is not symmetric along the cube centre line like the other cases. This discussion indicates that the geometry specification for v1.0 is important, and this is ultimately because it is dependent on the underlying computational grid.⁵ Although the v2.0 rotated case is better, there is still some discrepancy, chiefly that the structure is not as symmetric along the cube centre line when compared to the original case. As discussed in Sect. 4.4, it is most likely that this discrepancy is due to the boundary conditions — the x' direction is inflow-outflow and the y' direction is periodic, which allows the turbulent inflow to reach both sides of the cube but having effectively travelled different distances to each. Another factor in this study is that the incoming flow (with uniform temperature) will be affected by the warmer ground facets, causing thermal inlet effects and variation in the x/x' direction. This is unavoidable when using the precursor simulation, but it seems from Fig. 4.6 that this effect has diminished sufficiently before reaching the cube so that the four cases are comparable.

⁵The rationale for using four triangles (in uDALES v2.0) per rectangle (in v1.0) is to achieve a symmetrical overall structure (along the centreline) — something that cannot be done using two triangles per rectangle.

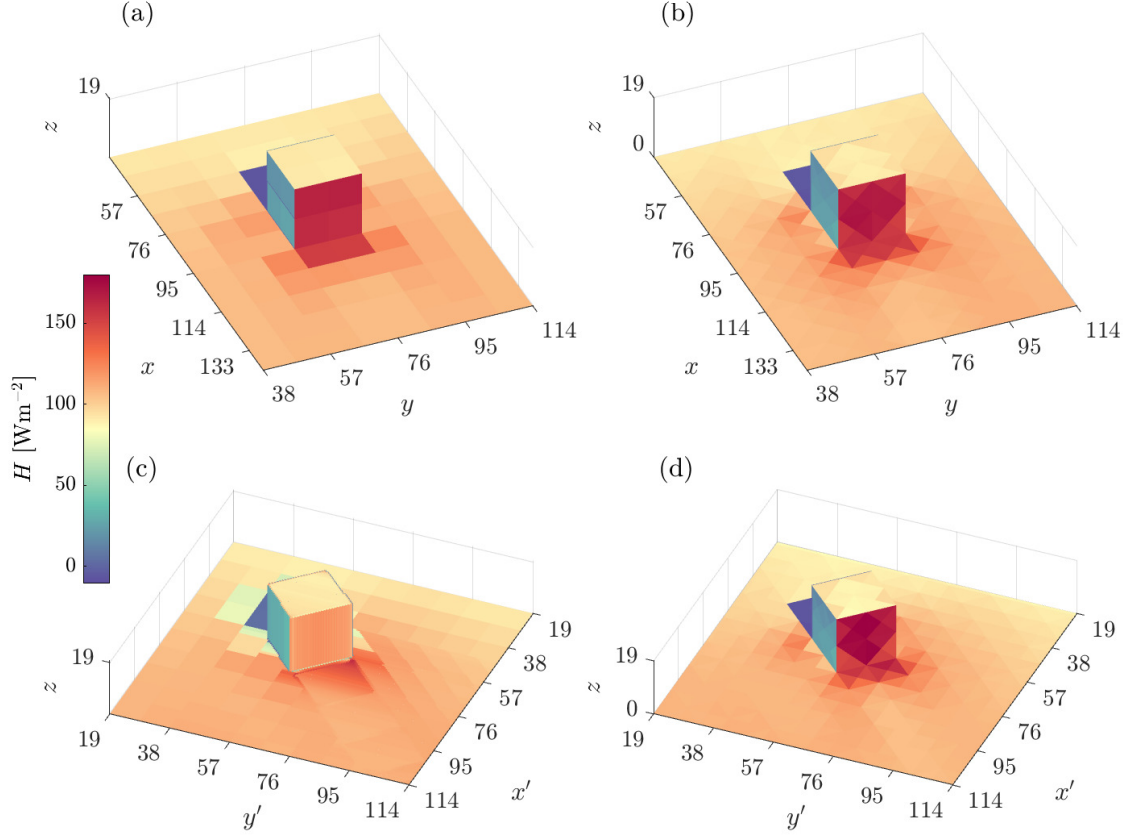


Figure 4.6: Single-cube case with surface energy balance: facets coloured according to sensible heat flux (H) for (a) v1.0 original, (b) v2.0 original, (c) v1.0 rotated, and (d) v2.0 rotated.

Figure 4.7 show the steady-state surface heat fluxes and internal temperatures for the roof, leeward, and lateral faces of the cube. The temperature difference between the surface of the leeward face and the inlet is approximately 16 times higher than in Sect. 4.4, thus yielding $Ri_b \approx -10$. This indicates that buoyancy is more significant for this case. For the roof, all cases agree, as the effect of the rotation is negligible. For the leeward and lateral sides, the v1.0 rotated case differs from the non-rotated cases to a much greater extent than the v2.0 rotated case; for the leeward side, the shortwave flux is around 20% less. These differences are primarily caused by errors in the radiation, which is directly affected by the rotation.

While the breakdown of net radiation by direct, reflected, and sky contributions is not shown here, their influence can be deduced as follows. The error is not due to the direct shortwave contribution, as the average of this quantity over the leeward face is correct in the v1.0 rotated case. This is because although each facet receives less than the other

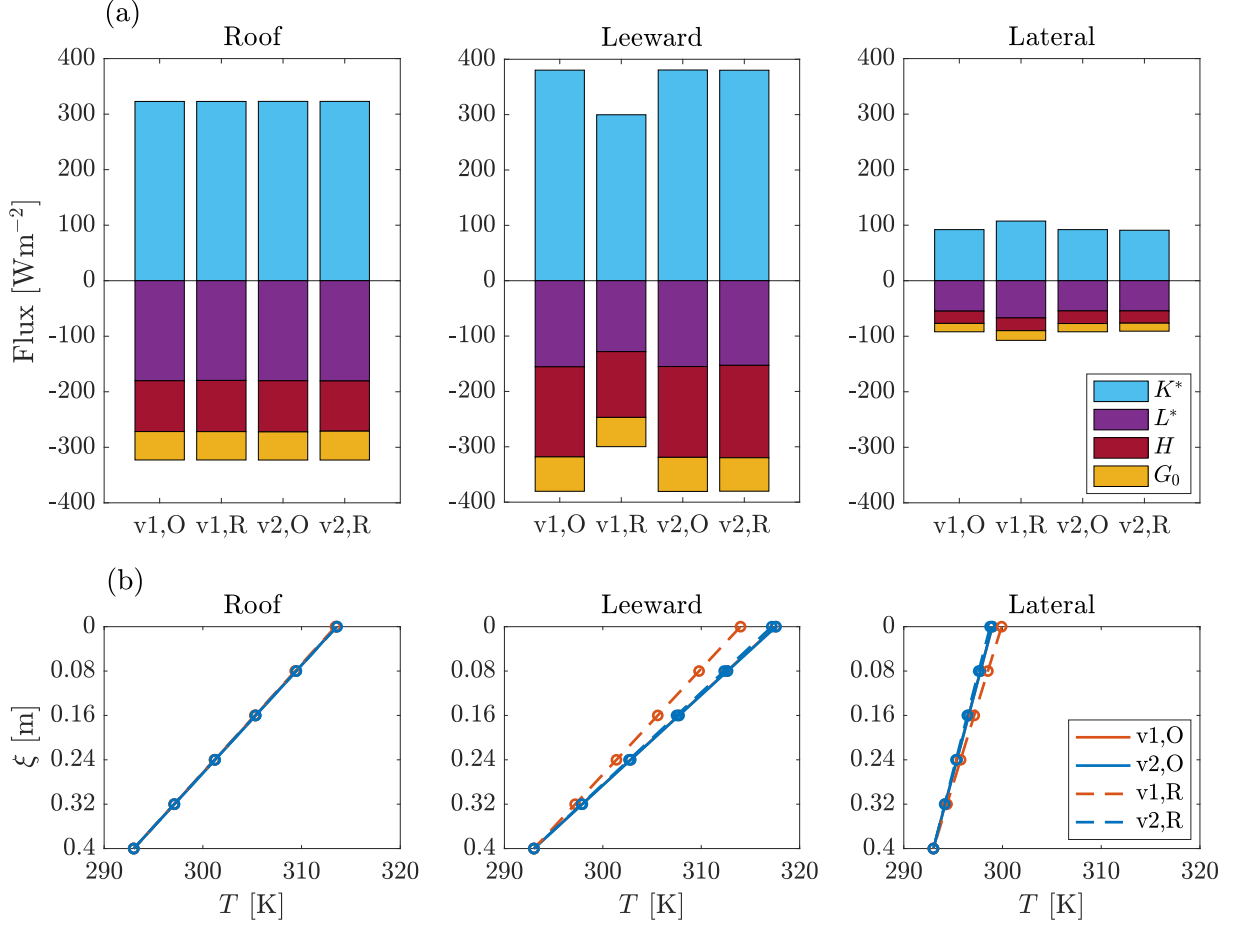


Figure 4.7: Single-cube case with surface energy balance: steady-state (a) surface energy balance fluxes (including net shortwave radiation K^* , net longwave radiation L^* , sensible heat flux H , and surface conduction G_0); and (b) temperature (T) as a function of depth (ξ) for the roof, leeward, and lateral faces.

cases (due to their normal being not aligned with the vector to the sun), the whole face's surface area is larger by the same factor (equal to $\sqrt{2}$ for this choice of solar position and rotation angle of 45°). This result would also hold for other angles so long as there is no internal shading on the face, which would introduce errors in the direct contribution. The error is therefore due to the other contributions to the net shortwave radiation. The reflected contribution caused by neighbouring facets facing each other is incorrect because it obviously should be zero for a flat surface. However, the net shortwave on the leeward face is in fact less than expected, so this error must be outweighed by the error in the diffuse sky radiation. If neighbouring facets can 'see' each other, their sky view factor is reduced, hence reducing this contribution. This discussion concerning contributions due to neighbour reflections and from the sky also holds for the lateral sides, though unlike the leeward face, the net shortwave on these sides is larger than expected. This is because

the sides should not have a direct contribution as they are not visible to the sun, but this is not in fact true for the v1.0 rotated case. Around half of the facets are actually oriented such that they are visible to the sun, and these are not completely shaded by the neighbour that they face. In fact, in uDALES v1.0 this contribution is much larger than it should be, because of the crude manner in which the shading is handled.

Regarding the other terms in the SEB, the leeward and side faces have reduced incoming longwave radiation for the same reasons given for the shortwave. This is consistent with the fact that the net longwave is less negative, and the outgoing longwave is directly determined by surface temperature, which is lower in the v1.0 rotated case. The temperature of the leeward face is lower because it has less available energy due to the reduced shortwave, which also acts to reduce the sensible heat and conductive fluxes. The side faces have more available energy due to the increased shortwave (despite the reduced longwave), and so the temperature is higher, which acts to increase the other fluxes, though the effects are small. These results demonstrate that uDALES v2.0 is better able to capture the radiative terms in the SEB than v1.0 when the geometry not aligned with the grid, because it does not susceptible to errors caused by voxelisation. This improvement in the modelling of shortwave radiation means that similar improvements are observed in the other SEB fluxes and surface temperature. In this case, the errors associated with voxelisation using uDALES v1.0 are due to the grid-aligned representation of each face of the cube individually, and the non-physical radiative transfer that occurs as a result. For cases with more radiative interaction between facets, e.g. in street canyons, these errors would likely be compounded.

4.6 Conclusion

Overall, the results presented in this chapter demonstrate that the development of uDALES v2.0 described in Chapter 3 is a success. In Sects. 4.2 and 4.3, the model was tested in neutral and non-neutral situations for periodic, grid-aligned cases, and it was proved that uDALES v2.0 is consistent with v1.0 in situations where the upgraded features are not in use. Furthermore, in Sects. 4.4 and 4.5 it was demonstrated that uDALES v2.0 is consistent with v1.0 when using inflow-outflow boundary conditions, and that it offers superior accuracy for non-grid-aligned geometries, including when using the SEB scheme.

This suggests that uDALES v2.0 is suitable for use in more realistic urban settings, which is the focus of the remainder of this thesis.

It is intentional that the test cases used in this chapter are simple, as using more complex cases that are not focused on isolating a particular aspect of the model would make explaining differences between uDALES v2.0 and v1.0 more challenging, and potentially mask conceptual and implementation errors. However, a limitation of them is that they do not include moisture, primarily because suitable validation studies in the literature are rare. Practically, this is not an issue for this thesis because moisture is neglected throughout. Moreover, latent heat transfer is conceptually handled in the same manner as sensible heat in the IBM approach, meaning it is expected that uDALES v2.0 would exhibit greater accuracy with respect to moisture than v1.0. Nonetheless, including moisture would strengthen the validity of the approach. A discussion of future validation and evaluation of uDALES is given in the conclusion of this thesis (Chapter 8).

Chapter 5

A diurnal cycle in a coastal urban environment

Based on journal article: ‘Large-Eddy Simulation of a Diurnal Cycle in a Coastal Urban Environment’, published in Building and Environment (Owens et al., 2025).

5.1 Introduction

The microscale variation of environmental conditions within the urban canopy layer (UCL) can affect the human experience in terms of thermal comfort. Standard indices for quantifying thermal comfort are in part dependent on the flow, namely the wind speed, air temperature, and humidity. They also depend on additional factors such as the mean radiant temperature (MRT) (see Sects. 2.2 and 2.3.3), which is determined by the incident radiation, and thus the surface temperature (Coccolo et al., 2016; Potchter et al., 2018). While using thermal comfort indices is common in the context of urban design (Lai et al., 2019; Aghamolaei et al., 2023), the fact that the multiple fundamental factors influencing thermal comfort can have a competing effect means that underlying physics may be obscured. For a deeper understanding, it is insightful to consider the factors themselves.

Many diurnal cycle simulations of realistic urban environments that use computational fluid dynamics (CFD) opt for the Reynolds-averaged Navier-Stokes (RANS) approach, for which the atmospheric stability is usually assumed to be neutral. A popular modelling tool is ENVI-met (e.g. Maggiotto et al., 2014; Salata et al., 2017; Acero and Arrizabalaga, 2018; Fabbri et al., 2020), though these studies suffer from limitations of the model,

in particular that the geometry is represented using voxels, which inherently limits the accuracy with respect to radiative transfer for realistic geometries. Other studies have represented the geometry in a more realistic manner (e.g. Toparlar et al., 2015; Imbert et al., 2018). Due to the fact that commonly-used RANS turbulence closures do not tend to perform well in non-neutral situations (Hanjalić, 2002), studies involving convective or stable atmospheric boundary layers are rarer (e.g. Qu et al., 2011; Kaoru et al., 2011).

Alternatively, large-eddy simulation (LES) can be used, though studies of realistic urban areas over a diurnal cycle that use LES are less common than those using RANS due to the increased computational cost and the complexity of applying turbulent boundary conditions. Many studies use PALM (Resler et al., 2017; Maronga et al., 2020; Krč et al., 2021), and are primarily focused on comparing the model against observations by coupling with mesoscale model data (e.g. Resler et al., 2020; Geletič et al., 2021; Anders et al., 2023). While these simulations are sophisticated, they do not provide insight into how the fundamental processes affecting thermal comfort evolve over the diurnal cycle. Also, like ENVI-met, PALM uses a voxel-based geometry representation, which as previously mentioned is likely to cause errors with radiation.

Most cases studies involve large cities with a temperate climate, while studies of hot, arid urban environments over a diurnal cycle are less common (Setaih et al., 2013; Kumar and Sharma, 2020). Urban environments are expected to store more heat during the day than rural surroundings, and to have greater thermal inertia, contributing particularly to higher temperatures at night (Oke, 1982; Roth et al., 1989). Also, the increased use of non-vegetative materials leads to less water being stored, and to a greater fraction of available energy being used to increase air temperature and less to evaporating water (Spronken-Smith and Oke, 1998; Coutts et al., 2007). However, these processes are counter-acted by the fact that buildings provide shade from the sun, which tends to reduce surface temperature (Lin et al., 2010; Lan and Zhan, 2017). Also, the drier and less vegetative the surrounding area, the less pronounced the previously mentioned cooling effect. This is compounded by the fact there is minimal shading from trees, which also has a cooling effect (Akbari et al., 2001; Gomez-Muñoz et al., 2010; Upreti et al., 2017).

The aim of this study is to model an urban environment with a hot, arid climate in order to provide insight into the microclimatic processes contributing to thermal comfort. The case, which comprises a set of buildings that are located on an island in Saudi Arabia,

is described in Sect. 5.2.1. Section 5.3.1 involves analysing the bulk thermal response of the whole surface in terms of the temperature and the surface energy balance (SEB), for both the buildings and the surrounding terrain. The resulting heat storage is analysed in terms of its dependence on the radiative forcing and used to quantify thermal inertia. Then, Sect. 5.3.2 investigates the evolution of the net radiation, the surface temperature, and the sensible heat flux for the various surface facets (roofs, walls, streets, and terrain). Finally, Sect. 5.3.3 aims to understand the behaviour of atmospheric quantities, including the pedestrian-level air temperature and MRT, considering these key SEB quantities and the flow behaviour. This also includes analysing the development of the thermal boundary layer over the buildings and the surrounding terrain in terms of air temperature, as well as the sensible heat flux, at streamwise locations in the domain.

5.2 Methodology

5.2.1 Case description

The site is located on a small island in the Saudi Arabian Red Sea, at the southern tip of the Sinai Peninsula. According to the Köppen–Geiger climate classification system, Saudi Arabia corresponds to the BWh category, defined by a hot, arid desert climate (Oke et al., 2017). The morphology, shown in Fig. 5.1, was designed as part of an architectural

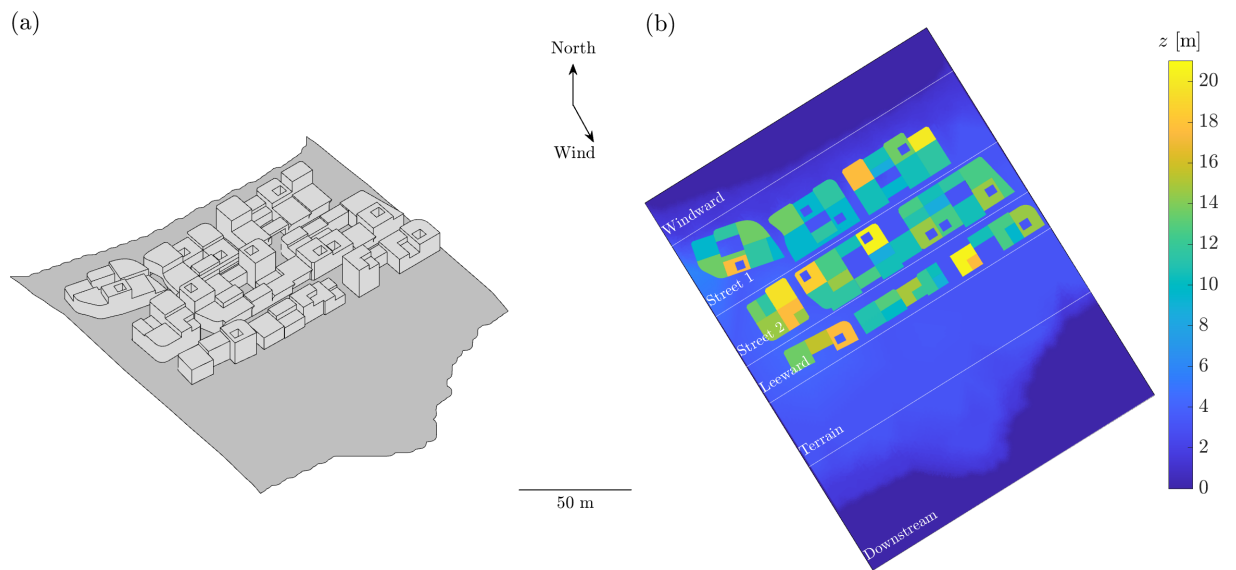


Figure 5.1: Built environment and underlying terrain: (a) 3D geometry visualisation, (b) height above sea-level (z) including streamwise locations used for analysis in Sect. 5.3.3.

competition, and contains features to improve thermal comfort, including narrow streets, courtyards, and overhangs to encourage shading. There is a substantial section of terrain where there are no buildings, which enables the thermal response to be compared to the built environment. At the site, the prevailing wind direction is north-north-west (NNW). The incoming flow is a marine boundary layer, which can be approximated as neutral in terms of atmospheric stability as there is relatively little heating or cooling at the surface compared to over land (Garratt, 1994). As the flow passes from ocean to land, the slope of the terrain will modify the flow. Given the small and gradual elevation change (≈ 5 m), this is unlikely to be a substantial effect compared to that of the buildings.

5.2.2 Precursor simulation

A precursor simulation is used to generate an inflow boundary condition that is characteristic of the marine boundary layer at the site. It is assumed that the surface upstream has a roughness length of $z_0 = 0.05$ m and that $u_{\text{ref}} = 5$ m s⁻¹ at $z_{\text{ref}} = 10$ m. Modelling the incoming velocity profile as a log-law suggests that $u_\tau = \kappa u_{\text{ref}} / \log(\frac{z_{\text{ref}} + z_0}{z_0}) \approx 0.387$ m s⁻¹, where κ is the von Kármán constant. The precursor domain size is $L_x \times L_y \times L_z = 320 \text{ m} \times 160 \text{ m} \times 120 \text{ m}$, and the grid resolution used is 0.625 m in each direction. The flow forcing is defined such that the horizontally-averaged velocity components in the x and y directions ($\langle u \rangle$ and $\langle v \rangle$ respectively) have a flow rate equal to the vertical-average of the log-law profile $u_{\text{in}} = \frac{u_\tau}{\kappa} \log(\frac{z + z_0}{z_0})$ over the domain height. Specifically, letting $U \equiv \frac{1}{L_z} \int_0^{L_z} u_{\text{in}} dz$, then over any given time step Δt :

$$F_x = \frac{1}{\Delta t} \left(U \cos \Phi_{x \rightarrow U} - \frac{1}{L_z} \int_0^{L_z} \langle u \rangle dz \right), F_y = \frac{1}{\Delta t} \left(-U \sin \Phi_{x \rightarrow U} - \frac{1}{L_z} \int_0^{L_z} \langle v \rangle dz \right), \quad (5.1)$$

where F_i denotes the momentum forcing in the x_i direction (see Eq. (2.16)), and $\Phi_{x \rightarrow U}$ is the angle between the x direction and the prevailing wind (given below in Sect. 5.2.3). The domain height $L_z = 120$ m, giving $U \approx 6.4$ m s⁻¹. The negative sign before U in the definition of F_y is because $\Phi_{x \rightarrow U}$ is a clockwise rotation.¹ The lateral boundary conditions are periodic, the top is free-slip, and the roughness length at the surface used in the wall functions is $z_0 = 0.05$ m, matching that of the desired log-law. The precursor is run for 73 hours, with a plane normal to the x direction output every second after one hour.²

¹Since the mean flow is at an angle to the x , the shifting method described in Sect. 3.6 is not required.

²Approximately one hour is required to reach a statistically steady state.

Figure 5.2a shows the time- and horizontally-averaged velocity magnitude, with the averaging period being the final 72 hours of the simulation. The velocity matches the log-law profile (u_{in}), which suggests that the volume flow rate forcing is successful and that the desired log-law is physically consistent with the surface boundary condition. Figure 5.2b shows the total vertical momentum flux, which has a linear profile, indicating that the flow is in a steady state (Sützl et al., 2021b). Finally, Fig. 5.2c shows the turbulent kinetic energy, which is reasonable for a marine boundary layer, peaking at the surface and decreasing with height (Tjernström and Smedman, 1993).

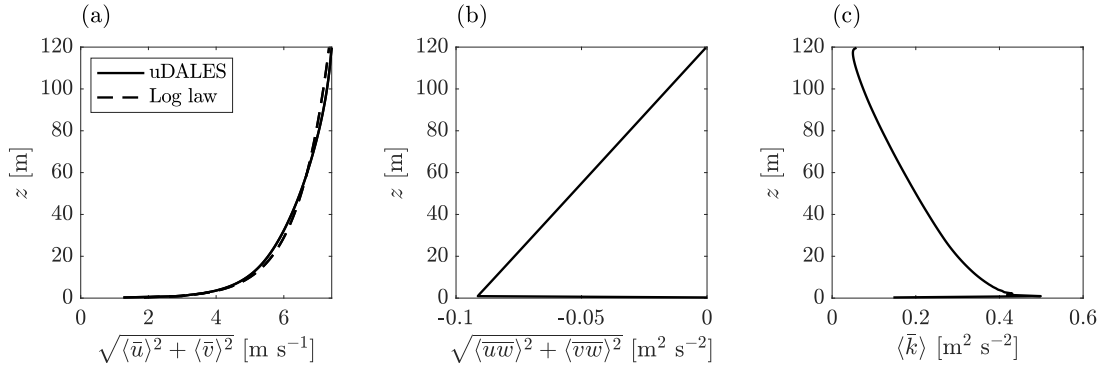


Figure 5.2: Precursor simulation: time- and horizontally-averaged profiles of: (a) wind speed $\sqrt{\langle \bar{u} \rangle^2 + \langle \bar{v} \rangle^2}$, (b) total kinematic vertical momentum flux $\sqrt{\langle \bar{u}\bar{w} \rangle^2 + \langle \bar{v}\bar{w} \rangle^2}$, and (c) turbulent kinetic energy $\langle \bar{k} \rangle = \frac{1}{2} \left(\langle \bar{u}'^2 \rangle + \langle \bar{v}'^2 \rangle + \langle \bar{w}'^2 \rangle \right)$.

5.2.3 Main simulation

The geometry is specified in uDALES v2.0 as an STL that was generated from a Rhino3D model using a maximum edge length of 2 m, resulting in 37,789 triangular facets (see Sect. 3.4). The facet size is relatively small in order to capture shading at high resolution. The STL was manually modified to remove defects, with overlapping facets being particularly problematic for uDALES. Since the facets are not necessarily grid-aligned, when classifying computational grid points as fluid or solid, a tolerance is used such that points outside the geometry that are a sufficiently small distance away are classified as solid. This avoids non-physical behaviour in situations where facets are very close to (but not actually coincident with) the edges of computational cells. The tolerance chosen is the length scale associated with protrusions on the buildings that act as roughness elements to the flow but are not modelled explicitly. This is assumed to be approximately $10z_0 = 0.1$ m (Oke et al., 2017), since $z_0 = 0.01$ m. Following Cai (2012), the heat rough-

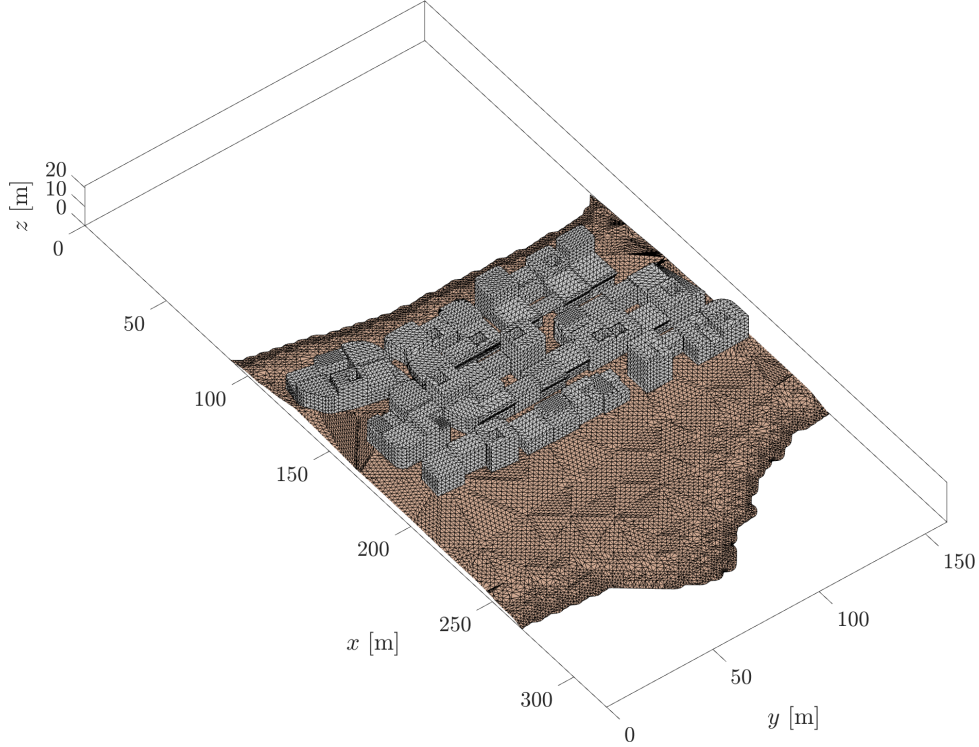


Figure 5.3: Facets and computational domain used for the main simulation. The facets are colour-coded by material: the ground is brown, and the buildings are grey. Note that the vertical extent has been cropped; the domain height is 120 m.

ness length ($z_{0,h}$) is assumed to satisfy $\log(z_0/z_{0,h}) = 5$, yielding $z_{0,h} = 6.7 \times 10^{-5}$ m. The final geometry, shown in Fig. 5.3, is rotated such that the x direction is at an angle of 141° with respect to north so that the buildings more closely align with the computational grid.³ Since the direction of the prevailing (NNW) wind with respect to north is 157.5° , this results in an effective rotation angle with respect to the wind of $\Phi_{x \rightarrow U} = 16.5^\circ$.

The computational domain size and resolution used for the main simulation is equal to that of the precursor ($L_x \times L_y \times L_z = 320 \text{ m} \times 160 \text{ m} \times 120 \text{ m}$, with a resolution of 0.625 m in each direction). The region containing the buildings and streets is referred to as the built environment in the present study, and is approximately in the middle of the domain (see Fig. 5.3). The distance between the buildings and the domain inlet, outlet, and top is approximately $6h$, where $h \approx 20$ m is the maximum building height.⁴ This ensures that there is sufficient space for the flow to develop and be unaffected by the presence of the boundaries to a sufficient extent (Tominaga et al., 2008; Abu-Zidan et al., 2021). The boundary condition in the x direction is inflow-outflow, with the instantaneous velocity at the inlet provided by the precursor simulation (see Fig. 4.4a), and the temperature given

³This is expected to offer better accuracy for the flow (which is still voxel-based — see Sect. 3.4.1)

⁴The mean building height is approximately 13 m.

Table 5.1: Parameters used in the SEB scheme for ground and buildings (including exterior and interior layers): albedo (α), emissivity (ϵ), density (ρ), specific heat capacity (c_p), volumetric heat capacity (C), thermal conductivity (λ), thickness (D), number of facet layers (N_l), and internal temperature (T_D). Material properties are based on representative values from Chartered Institution of Building Services Engineers (CIBSE) (2015).

Parameter	Units	Ground	Building (exterior)	Building (interior)
α	-	0.25	0.35	
ϵ	-	0.9	0.9	
ρ	kg m ⁻³	1500	2200	12
c_p	J K ⁻¹ kg ⁻¹	1840	880	1030
$C = \rho c_p$	MJ K ⁻¹ m ⁻³	2.76	1.936	0.01236
λ	W m ⁻¹ K ⁻¹	1.0	1.28	0.042
D	m	1.0	0.25	0.25
N_l	-	20	10	10
T_D	°C	33.91		24

by local weather data (discussed below; see Fig. 5.4f). The boundary condition in the y direction is periodic, which captures the effect of buildings that are within the masterplan of the urban environment that are not included in this study. At the top, a zero flux condition is used for temperature, and the vertical velocity is non-zero (see Sect. 3.3).

The material properties and boundary conditions for the SEB scheme are shown in Table 5.1. The buildings are modelled using an exterior layer of concrete and an interior layer of insulation.⁵ The number of layers ($N_l = 20$) is relatively high in order for the SEB discretisation scheme to accurately capture transient behaviour, as well as the large difference in material properties of the walls. Note that on the ground, there is no distinction for paved and unpaved surfaces in the masterplan, which is a reasonable assumption in this case, because the terrain at the site is expected to have similar material properties to common street surfaces.⁶ The temperature of the ground (33.91 °C) is based on previous analysis using a simplified SEB model; taking the value at the depth at which the temperature oscillation is negligible over a diurnal cycle (see Sect. 2.2). Finally, the indoor air temperature (24 °C) is based on a likely comfortable value for the given climate.

In addition to the division of facets into ground and building types according to materiality, for purposes of analysis they are further grouped into streets, surrounding terrain, walls, and roofs. Walls are defined as building facets with a surface normal in either the x or y direction (approximately), while roof facets are those with their surface

⁵The relatively thick insulation layer accounts for the fact that the interior wall temperature is assumed to be equal to the indoor air temperature. In reality, they may be different, yielding additional resistance.

⁶As in the rest of this thesis, the ground facets are modelled as dry — no water is stored.

normal in the z direction (and are above ground level). The ground facets also have their surface normal in the z direction, and the streets are defined as those within the region $100 < x < 220$, which corresponds roughly to those that are shaded by the buildings at some point during the diurnal cycle, and excludes the surrounding terrain. The terrain consists of any other ground facets, which are almost entirely unshaded.

The simulations use climate data from a weather station in the nearby city of Sharm El Sheikh for a typical meteorological year, which is then ‘banded’ to produce a representative cyclic day in June (Chartered Institution of Building Services Engineers (CIBSE), 2015). The data, which is available hourly, includes the (inlet) air temperature (θ_{in}), direct normal shortwave radiation (I), diffuse sky shortwave radiation (D_{sky}), solar azimuth (Φ_{sun}), solar zenith (Θ), and sky longwave radiation (L_{sky}). These quantities, shown in Fig. 5.4, are interpolated prior to the simulation; those relevant to the shortwave radiation vary more rapidly and are interpolated to every 6 minutes, while the sky longwave radiation and air temperature vary more slowly and are interpolated to every 15 minutes. The time step used for the SEB scheme is 60 s. The simulation is run for 72 hours, and the final 24 hours are used for the results presented in Sect. 5.3.

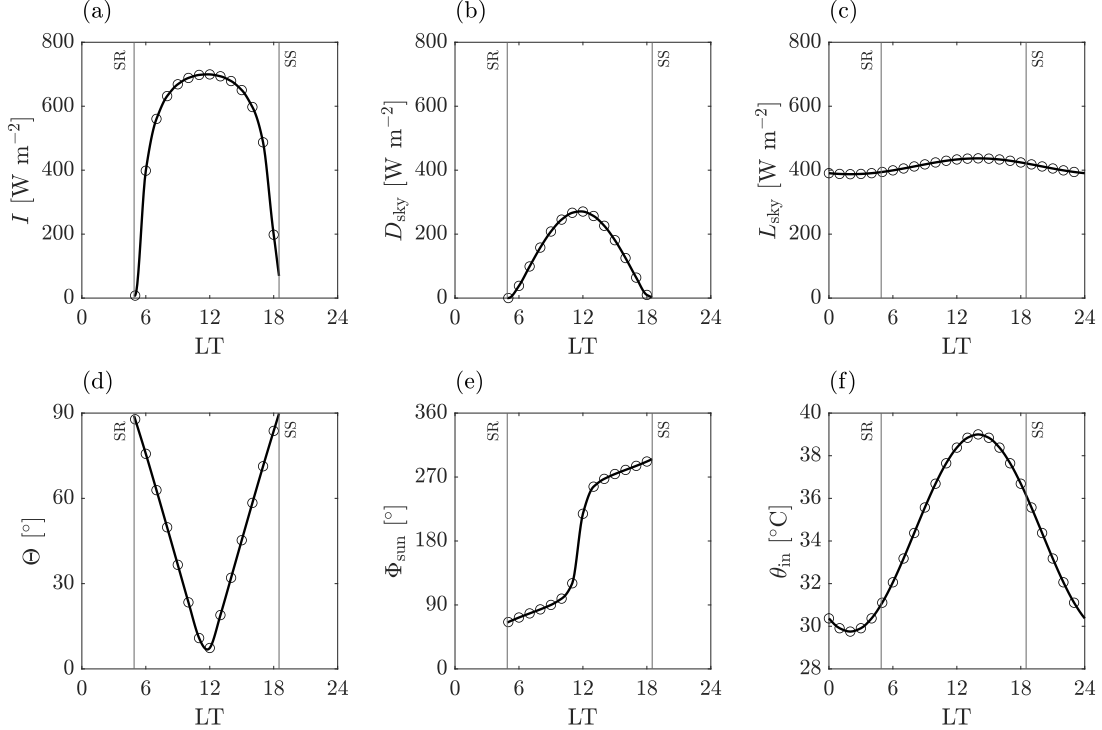


Figure 5.4: Simulation parameters obtained from local weather data, with sunrise (SR) and sunset (SS) indicated: (a) direct normal shortwave radiation (I), (b) sky shortwave radiation (D_{sky}), (c) sky longwave radiation (L_{sky}), (d) solar zenith (Θ), (e) solar azimuth (Φ_{sun}), and (f) incoming air temperature (θ_{in}). Note solar noon occurs just before 12 LT.

5.3 Results

5.3.1 Bulk surface energy balance

Figure 5.5a shows the complete average SEB fluxes for the entire built environment, including the streets and buildings. Note that the complete average, defined by Eq. (2.13), involves multiplication by the complete aspect ratio ($\lambda_c = 1.98$), which is appropriate when comparing the SEB of the 3D built environment to the relatively flat terrain.

As expected, net shortwave radiation is the dominant process, and drives the evolution during the day, while the net longwave radiation is relatively large (and negative) at night. The daytime behaviour of the sensible heat flux is typical of a system with thermal

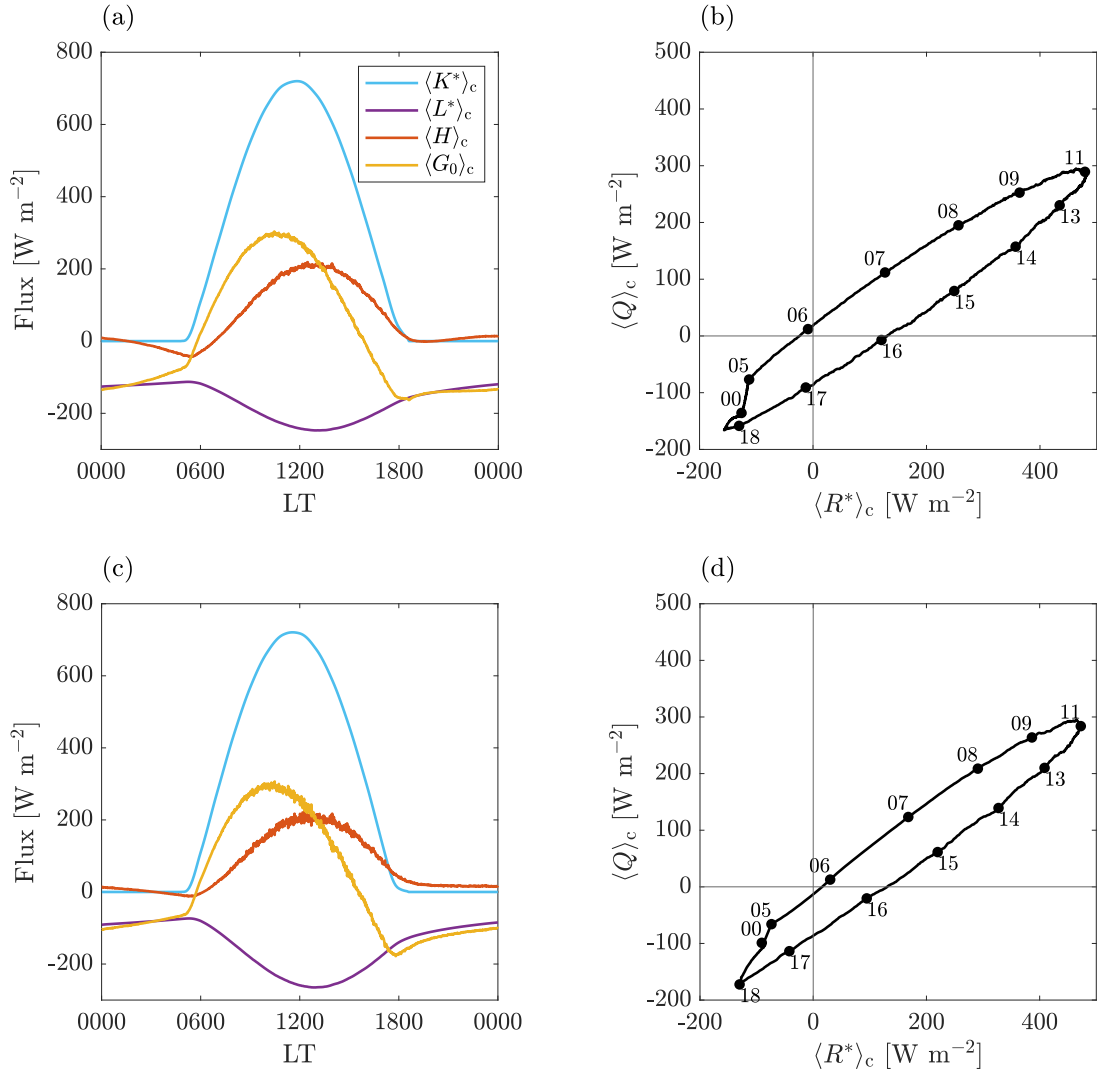


Figure 5.5: Evolution of bulk SEB for the built environment (a,b) and the terrain (c,d): complete average fluxes (denoted by $\langle \cdot \rangle_c$; see Eq. (2.13)) of net shortwave radiation (K^*), net longwave radiation (L^*), sensible heat flux (H), and conduction (G_0) against time; and storage ($Q = G_0 - G_D$) against net radiation ($R^* = K^* + L^*$) as a Lissajous figure.

inertia, with the peak occurring after that of the net shortwave radiation (Garratt, 1994). This is due to its dependence on surface temperature, which is discussed in more detail below. The nocturnal behaviour of the sensible heat flux is influenced by the fact that it is also dependent on air temperature. Immediately after sunset it is slightly negative, then becomes positive again, likely due to the air cooling while the facets remain warm (due to thermal inertia). Eventually, they cool to below air temperature and the sensible heat flux turns negative again until well after sunrise. Finally, conduction acts to transfer the remaining thermal energy away from the surface (exterior) during the day and towards it at night, peaking before the net shortwave does (again due to thermal inertia). The time lag associated with the response of the surface is approximately 1.5 hours. Figure 5.5c shows the same quantities for the surrounding terrain, which are overall quite similar to that of the built environment. This is likely because the complete average net shortwave happens to be approximately equal for the two environments, despite their differing morphological and material properties. However, at night, the sensible heat flux appears to always stay positive over the terrain; in contrast to the common assumption that the sensible heat flux is positive at night in urban areas and negative in rural ones (though the high thermal and lack of moisture means that this is not a typical ‘rural’ environment).

The thermal inertia can be visualised in Fig. 5.5b and d, which show the dependence of the complete average heat storage $\langle Q \rangle_c = \langle G_0 \rangle_c - \langle G_D \rangle_c$, where G_D is the interior conduction), on the complete average net radiation $\langle R^* \rangle_c = \langle K^* \rangle_c + \langle L^* \rangle_c$, forming a Lissajous curve. During the day, the relationship between $\langle Q \rangle_c$ and $\langle R^* \rangle_c$ is a hysteresis cycle, demonstrating the dependence of the system on its history. The built environment and terrain behave similarly during the day, both peaking around 1100 LT. At night, the differences visible between them are related to the behaviour of $\langle H \rangle_c$ previously discussed: the times when $\langle H \rangle_c > 0$, appears to correspond to when $\langle Q \rangle_c < 0$, and vice versa.

The relationship between $\langle Q \rangle_c$ and $\langle R^* \rangle_c$ can be parameterised using a hysteresis model: (Grimmond et al., 1991)

$$\langle Q \rangle_c = a_1 \langle R^* \rangle_c + a_2 \frac{\partial \langle R^* \rangle_c}{\partial t} + a_3 \quad (5.2)$$

Regression analysis of the cycles in Fig. 5.5b and d to find the coefficients a_1 , a_2 , and a_3 is shown in Table 5.2. As expected from the qualitative similarity of the cycles of the built environment and terrain, the difference between these coefficients is relatively small in

Table 5.2: Hysteresis model coefficients (see Eq. (5.2)).

	a_1 [-]	a_2 [h]	a_3 [W m ⁻²]
Built environment	0.69	0.42	-40.60
Terrain	0.70	0.36	-45.39

comparison to that typically observed between urban and rural environments (Grimmond and Oke, 1999b). The slope of the cycle (a_1) represents the strength of the dependence of Q on R^* , with very similar values for the built environment and the terrain. The width of the cycle (a_2) is related to the phase or time lag; the built environment has a slightly larger value than the terrain, hence by this metric exhibits greater thermal inertia. The final coefficient (a_3) relates to when Q becomes negative in relation to R^* , which occurs later for the built environment than the terrain, again suggesting greater thermal inertia.⁷

Figure 5.6 shows the average SEB fluxes and internal facet temperature for each type of facet (streets, roofs, walls, and terrain). In general, as the depth (ξ) increases, $\langle T(\xi) \rangle_s$ peaks later in the day, with an initial surface lag of around 1–2 hours for the streets, roofs, and terrain, and around 3 hours for the walls. The two major factors that explain the evolution of each type are shading and materiality. The streets and terrain have the same albedo, but unlike the streets, the terrain is practically unshaded throughout the day (by definition), which means $\langle K^* \rangle_s$ is always larger for the terrain. This results in a larger peak of surface temperature $\langle T_s \rangle_s \equiv \langle T(\xi = 0) \rangle_s$, and consequently $\langle L^* \rangle_s$ is more negative. However, $\langle H \rangle_s$ has a similar amplitude, which must be caused by flow conditions counter-acting the differing $\langle T_s \rangle_s$. The building walls and roofs have a higher albedo than the streets and terrain, meaning the maximum possible value of $\langle K^* \rangle_s$ is lower. It is expected that the roofs tend to be unshaded, while the walls are often shaded and oriented horizontally, so a significantly lower peak of $\langle K^* \rangle_s$ is to be expected for the walls. There are in fact two maxima of $\langle K^* \rangle_s$, likely corresponding to the times when the two major sets of walls, oriented roughly in the $+y$ and $-y$ directions, are aligned with the direct solar radiation in the morning and afternoon respectively. Other studies of hot, arid regions have explored the substantial effect of building morphology on shading and local surface and atmospheric conditions (e.g. Bourbia and Awbi, 2004; Shareef and Abu-Hijleh, 2020), and this will be discussed in further detail in Sect. 5.3.2.

⁷These coefficients are relevant to the objective hysteresis model (OHM) approach, in which empirically or analytically (AnOHM; Sun et al., 2017) determined values are used to predict Q using known time series of R^* using Eq. (5.2).

For the streets and terrain, which have uniform material properties, there is a depth ($\xi \approx 0.6$ m) beyond which the heating and cooling of the surface over the diurnal cycle does not penetrate (see Sect. 2.2), and so $\langle T \rangle_s$ does not vary in time, instead remaining

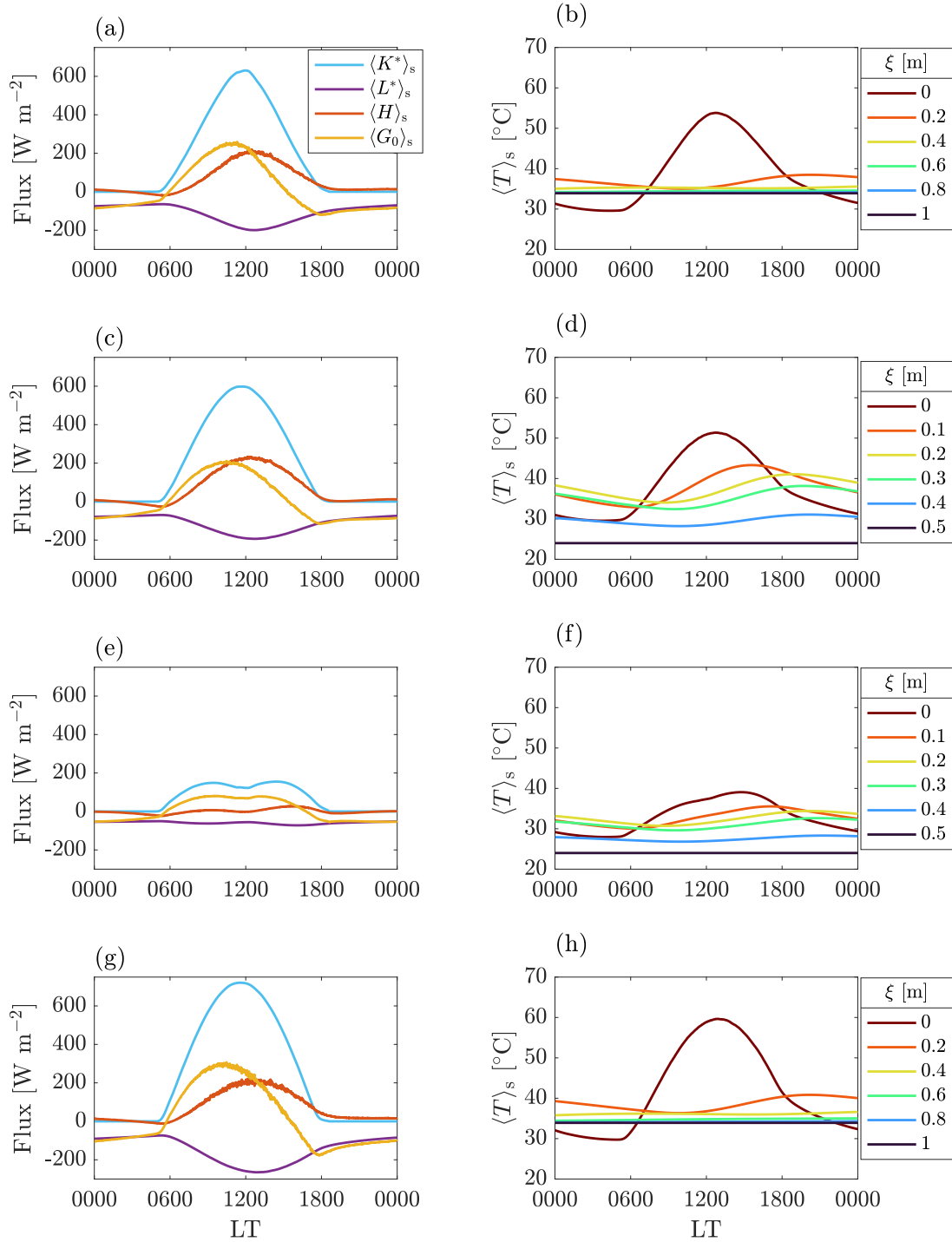


Figure 5.6: Evolution of bulk SEB quantities for (a,b) streets, (c,d) roofs, (e,f) walls, and (g,h) terrain: average (denoted by $\langle \cdot \rangle_s$; see Eq. (2.13)) fluxes of net shortwave radiation (K^*), net longwave radiation (L^*), sensible heat (H), and conduction (G_0); and average facet temperature (T) as a function of depth (ξ).

equal to the prescribed ground temperature (T_D). While $\langle T_s \rangle_s$ becomes less than T_D at night, at just a small depth ($\xi \approx 0.2$ m) the temperature remains above T_D and peaks remarkably late (well after sunset). The fact that the building walls and roofs are a composite of two layers results in markedly different behaviour to the streets and terrain. The high-conductivity outer layer tends to have a small temperature gradient, whereas the low-conductivity inner layer tends to have a large one. At night, there is an inflection point as the temperature near the surface falls below that of deeper layers. This is likely a result of the insulation, which acts to further dampen and delay temperature oscillations.

5.3.2 Spatial variation of surface energy balance

The quantities R^* , T_s , and H for each facet at four instances are shown in Fig. 5.7, and probability densities (P) for these quantities are shown in Fig. 5.8. These quantities are most relevant because R^* is the source of energy and drives the evolution (as discussed in Sect. 5.3.1), while T_s represents the state of the surface (and affects MRT via longwave radiation), and H directly influences air temperature.

Before sunrise (0400 LT; see Figs. 5.7a-c and 5.8a-c), R^* is small and negative, since the net shortwave contribution is zero and so is composed only of the net longwave contribution. The negative value reveals that the outgoing longwave radiation is greater than the incoming, though the building walls and streets have a slightly less negative value because they have higher values of incoming radiation as a result of being more visible by other facets. At this time, both T_s and H are relatively uniform, with T_s being approximately equal to air temperature (see Fig. 5.4f) and H being approximately zero.

Just before midday (1000 LT; see Figs. 5.7d-f and 5.8d-f), solar radiation and thus R^* is high on facets that are unshaded, and roughly speaking the higher R^* , the higher T_s . While to some extent this is also true for H , this quantity is also strongly influenced by the turbulent flow, with significant variation across facets with similar R^* . At this time, the terrain facets generally have the highest temperature because they are unshaded. On the other hand, the walls generally have the lowest temperature, as many of these are shaded. The surface temperature distribution of street facets is bimodal, with the two groups likely corresponding to facets that are shaded or not. The street and roof facets generally have a lower temperature than the terrain facets (as shown in Fig. 5.6). However, they do not generally have a lower sensible heat flux. This indicates that, due to the flow conditions

over the street and roof facets, the rate of heat transfer from these facets to the air is generally larger than for the terrain, despite the terrain's higher temperature.

As the day progresses and the sun's position changes, the wall and street facets (and to some extent roof facets) that are shaded changes, while the terrain facets are almost always unshaded in the daytime. By late afternoon (1600 LT; see Figs. 5.7g-i and 5.8g-i), R^* is generally smaller than at 1000 LT due to a decrease in K^* . However, T_s is

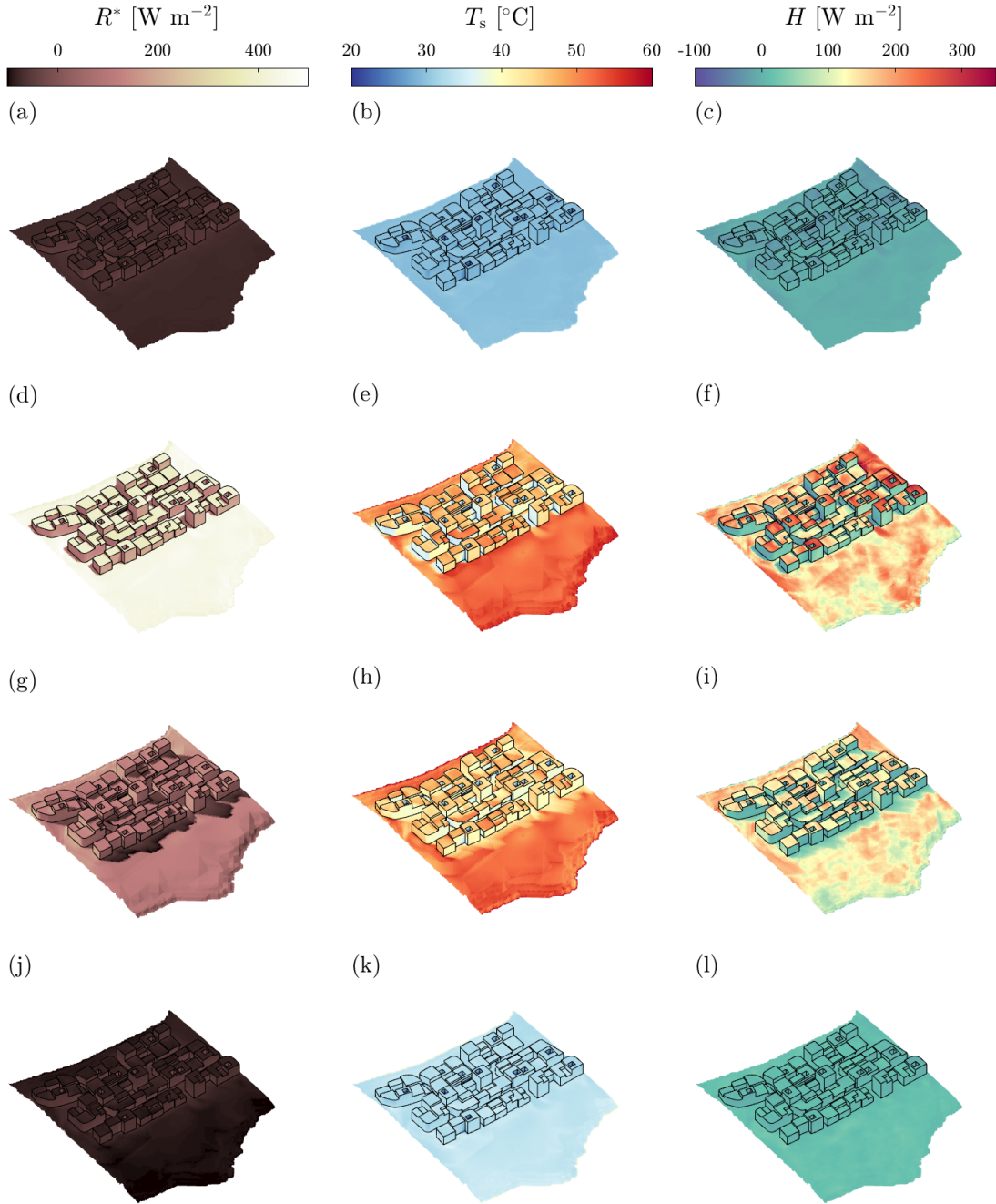


Figure 5.7: Visualisation of facet net radiative flux (R^*), surface temperature (T_s) and sensible heat flux (H) at 0400 LT (a-c), 1000 LT (d-f), 1600 LT (g-i), and 2200 LT (j-l). The topography, orientation, and prevailing wind direction are visible in Fig. 5.1a.

very similar, which is a clear demonstration of thermal inertia. Also, the temperature of the (unshaded) street facets are actually higher than at 1000 LT, and consequently their sensible heat flux appears to be the larger than many of the other facets. By the late evening (2200 LT; see Figs. 5.7j-l and 5.8j-l), the quantities have started to converge again, and eventually return to their initial state.

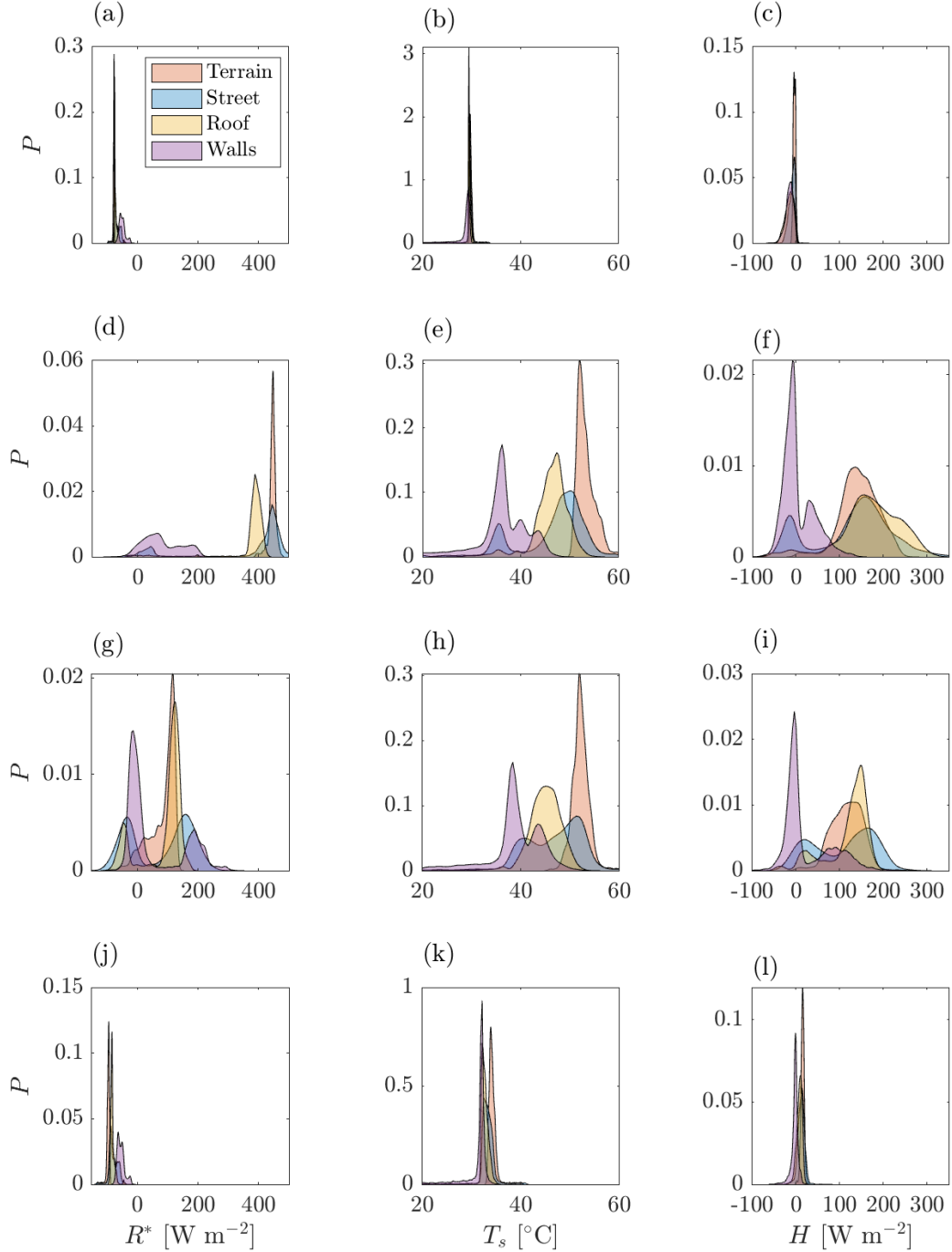


Figure 5.8: Probability density functions (P) for net radiative flux (R^*), surface temperature (T_s) and sensible heat flux (H) for facet types, respectively at 0400 LT (a-c), 1000 LT (d-f), 1600 LT (g-i), and 2200 LT (j-l). Note the change in vertical scale.

5.3.3 Atmospheric quantities

Figure 5.9 shows time-averaged pedestrian-level (1.5 m above the ground; approximately 6.5 m above sea-level ($z = 0$)) quantities including wind speed and direction, air potential temperature deviation with respect to the inlet (denoted $\tilde{\theta} = \bar{\theta} - \bar{\theta}_{\text{in}}$), and MRT at the same four times of day as in Sect. 5.3.2. The flow variables have been averaged over an interval of one hour⁸, while the MRT represents one SEB time step. In conjunction, time- and y -averaged vertical profiles of velocity, potential temperature deviation $\langle \tilde{\theta} \rangle_y$, and atmospheric sensible heat flux $\langle \overline{w'\theta'} \rangle_y$ are shown in Figs. 5.10b, 5.11, and 5.12 respectively. These are plotted at the windward side of the buildings, the first street canyon, the second street canyon, at the leeward side of the buildings, over the terrain, and finally downstream of the terrain. Note that in Fig. 5.9, the wind does not vary significantly in time, hence Fig. 5.10b shows the average over the entire diurnal cycle. Figure 5.10a also shows time-averaged streamlines at a fixed y location to illustrate the flow behaviour.

Throughout the diurnal cycle, the internal courtyards have significantly lower $\tilde{\theta}$. This is likely because in street canyons and courtyards (which are just ≈ 5 m across) there is limited exchange with the flow above, effectively trapping cool nighttime air inside (see Fig. 5.10a). The MRT is also lower in the courtyards than other shaded areas, which must be due to lower surface temperature and reduced outgoing longwave radiation. The surface sensible heat flux does not appear to be particularly low (negative) inside the courtyards despite low T_s (see Fig. 5.7), which is consistent with low wind speed. Similar results have been obtained in studies on courtyard microclimates (Zamani et al., 2018).

Before sunrise (see Figs. 5.9a-c, 5.11a, and 5.12a), the MRT is higher near the buildings due to the increased longwave radiation received from the walls. At this time, the flow cools as it passes over the buildings, with $\langle \tilde{\theta} \rangle_y$ reaching a minimum in the second street canyon, before increasing slightly over the terrain. The cooling is likely as result of H being generally negative at this time (see Figs. 5.7 and 5.8), which is reflected in the generally negative values of $\langle \overline{w'\theta'} \rangle_y$, corresponding to weakly stable atmospheric conditions. The relatively large value of $\langle \overline{w'\theta'} \rangle_y$ at the windward side of the buildings may be a result of updrafts caused by the interaction of the incoming flow with the bluff obstacle.

During the day (see Figs. 5.9d-f, 5.11b-c, and 5.12b-c), the MRT is strongly influenced by the direct solar radiation, with the shaded streets having a substantially lower MRT.

⁸A visualisation of the instantaneous flow fields is available in Sect. F.1

The flow is heated as it passes over the buildings due to H being generally positive aside from turbulent fluctuations (see Figs. 5.7 and 5.8). This results in positive values of $\langle w'\theta' \rangle_y$

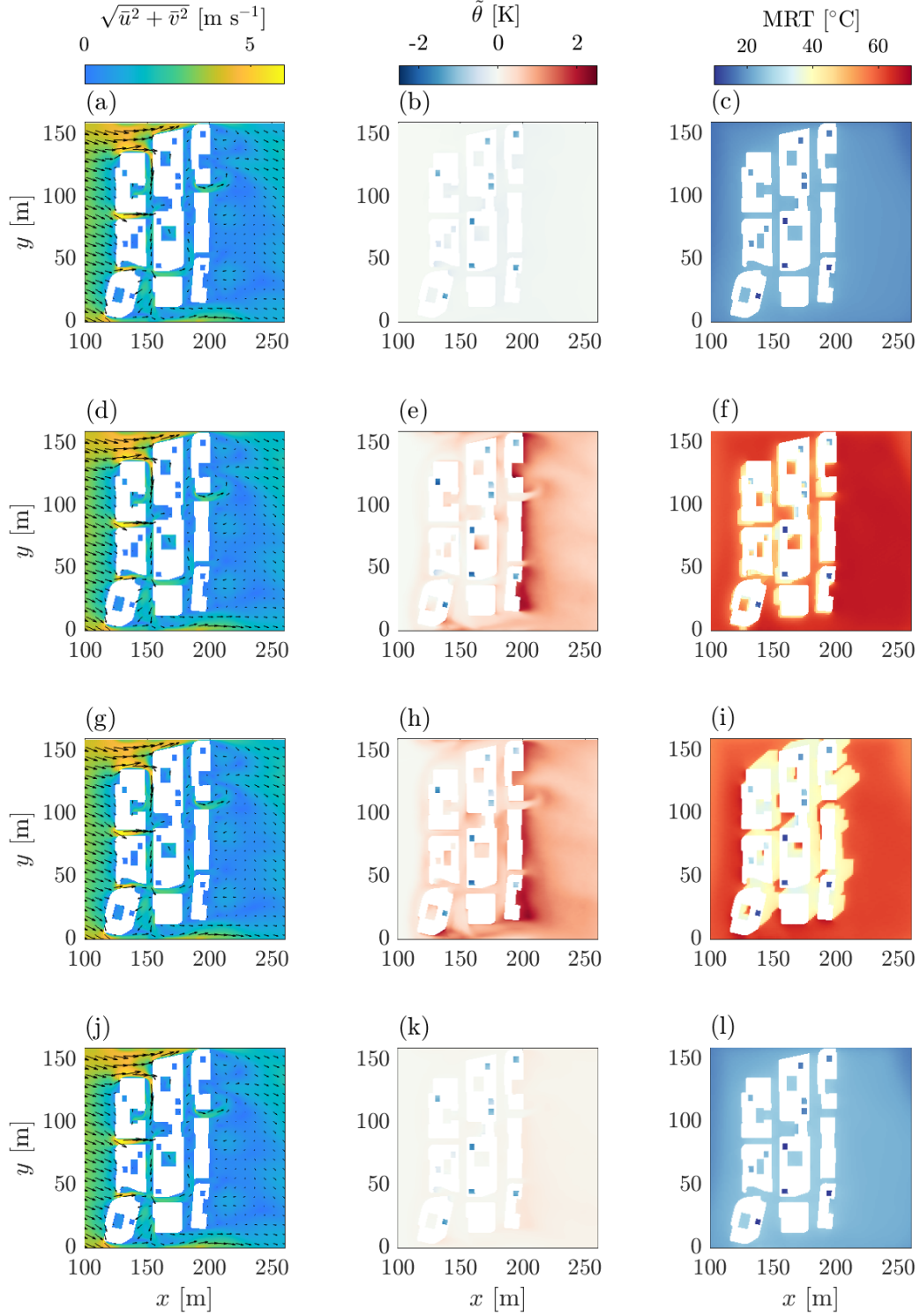


Figure 5.9: Evolution of: pedestrian-level wind speed $\sqrt{\bar{u}^2 + \bar{v}^2}$ with velocity vectors every 10 m, and air potential temperature deviation $\bar{\theta} = \bar{\theta} - \bar{\theta}_{\text{in}}$, both averaged during time interval: 0300-0400 LT (a,b), 0900-1000 LT (d-e), 1500-1600 LT (g,h), 2100-2200 LT (j-k); and MRT at 0400 LT (c), 1000 LT (f), 1600 LT (i), 2200 LT (l).

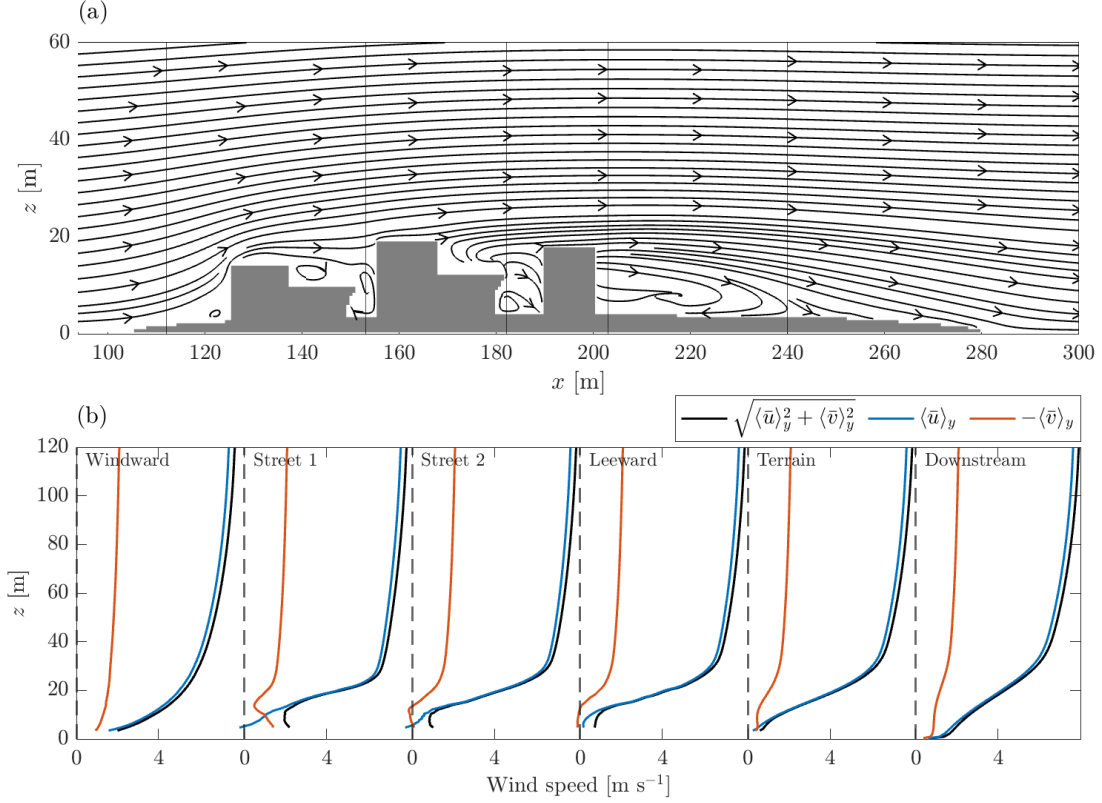


Figure 5.10: Velocity time-averaged over complete diurnal cycle: (a) streamlines at $y = 50$ m, with streamwise locations relevant to (b) indicated; (b) y -averaged magnitude $\sqrt{\langle \bar{u} \rangle_y^2 + \langle \bar{v} \rangle_y^2}$, x -component $\langle \bar{u} \rangle_y$, and y -component $\langle \bar{v} \rangle_y$ at the windward side of buildings ($x = 112$ m), in the first street canyon ($x = 153$ m), in the second street canyon ($x = 182$ m), at the leeward side of the buildings ($x = 203$ m), over the terrain ($x = 240$ m), and downstream of the terrain ($x = 300$ m).

beyond the first street canyon, suggesting unstable conditions. The value of $\langle \tilde{\theta} \rangle_y$ reaches a maximum at the leeward side of the buildings in both the morning and afternoon. Given that the leeward facets are shaded in the afternoon, and consequently have low T_s and H at this time (see Figs. 5.7 and 5.8), this suggests that this effect not due to shading, but due to advection.

Since heat is advected in the direction of the mean flow, it is expected that the leeward side has a higher temperature than the windward side. However, note that there are locations on the leeward side which have relatively low values of $\tilde{\theta}$, which occur in streets that are aligned with the mean flow, and so local conditions are clearly also important in determining this quantity. The wind speed tends to be relatively high in the streamwise-aligned streets, and on the entire windward side of the domain, so heat is advected away more quickly in these regions. Conversely, immediately in the lee of the buildings, the wind speed is low and so heat is transported away more slowly. In fact, the flow reverses in

some places at pedestrian level, which actually transports heat towards the leeward side of the buildings. This is due to a separation bubble that forms in the wake (see Fig. 5.10a), which is typical of flow around buildings (Peterka et al., 1985). Over the terrain, the flow recovers, i.e. the wind speed tend to increase with distance from the buildings (see 5.10b), which acts to reduce $\tilde{\theta}$ over the terrain despite H being higher. This is consistent with the fact that the peak of $\langle w'\theta' \rangle_y$ occurs at roof level in the street canyons and at ground level over the terrain during the day, reinforcing the fact that the heating at the leeward side of the buildings is not primarily due to the street or wall facets.

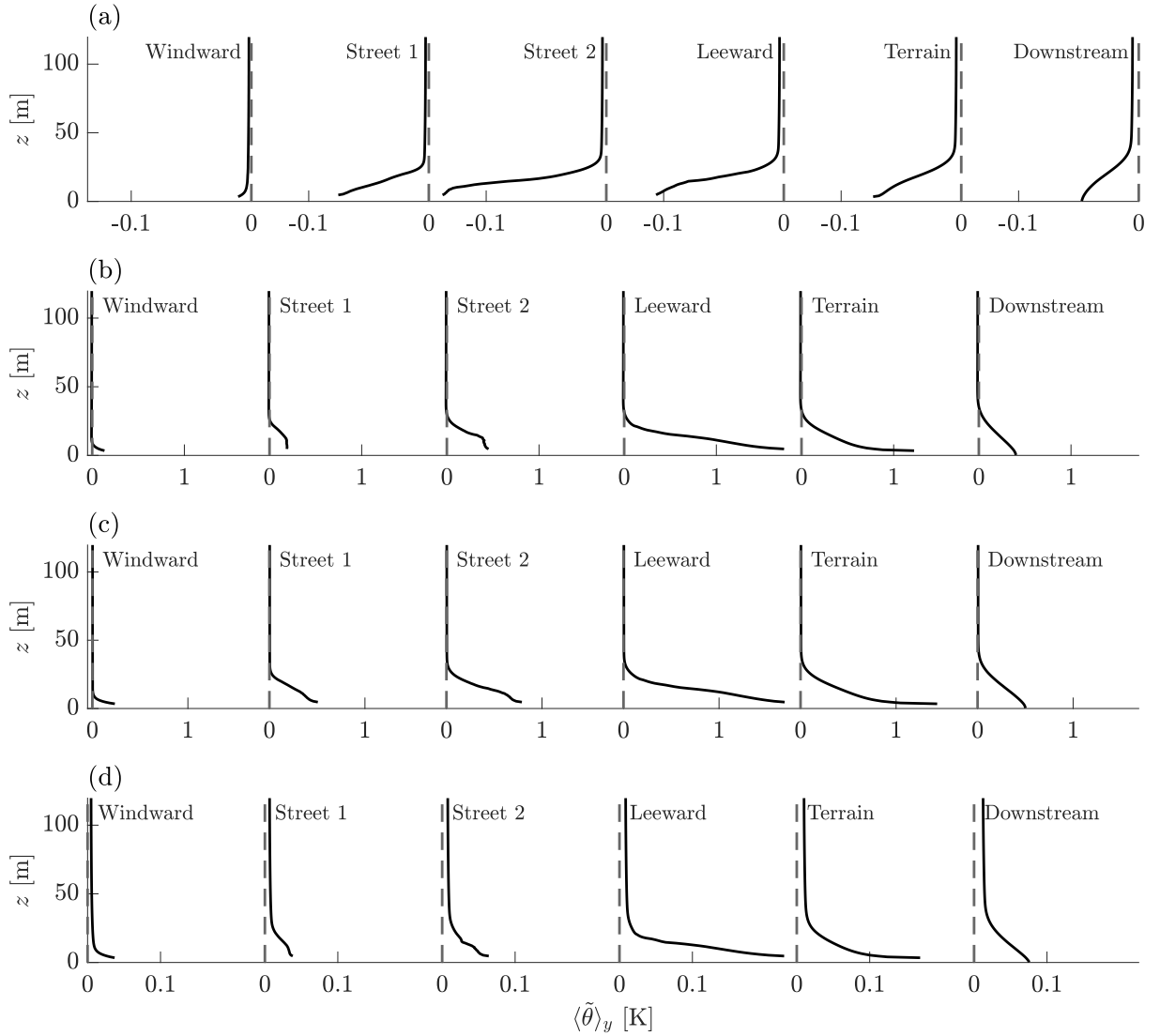


Figure 5.11: Evolution of y -averaged air potential temperature deviation $\langle \tilde{\theta} \rangle_y = \langle \bar{\theta} \rangle_y - \langle \bar{\theta}_{\text{in}} \rangle_y$ at the windward side of the buildings ($x = 112$ m), in the first street canyon ($x = 153$ m), in the second street canyon ($x = 182$ m), at the leeward side of the buildings ($x = 203$ m), over the terrain ($x = 240$ m), and downstream of the terrain ($x = 300$ m); averaged during: (a) 0300-0400 LT, (b) 0900-1000 LT, (c) 1500-1600 LT, and (d) 2100-2200 LT. Note the change in horizontal scale between sub-figures.

After sunset (see Figs. 5.9j-l, 5.11d, and 5.12d), the temperature tends to remain positive apart from in the courtyards, with the highest value of $\langle \tilde{\theta} \rangle_y$ located over the terrain. This is a result of H being slightly positive late in the day for much of the surface (see Fig. 5.7 and 5.8), which is reflected in the behaviour of $\langle \overline{w'\theta'} \rangle_y$, which suggests the atmosphere is still unstable at this time. This clearly illustrates how elevated surface temperature later in the day due to thermal inertia influences the evolution of the boundary layer over a diurnal cycle; a result which has been observed in other studies of hot, arid regions (e.g. Ait-Mesbah et al., 2015).

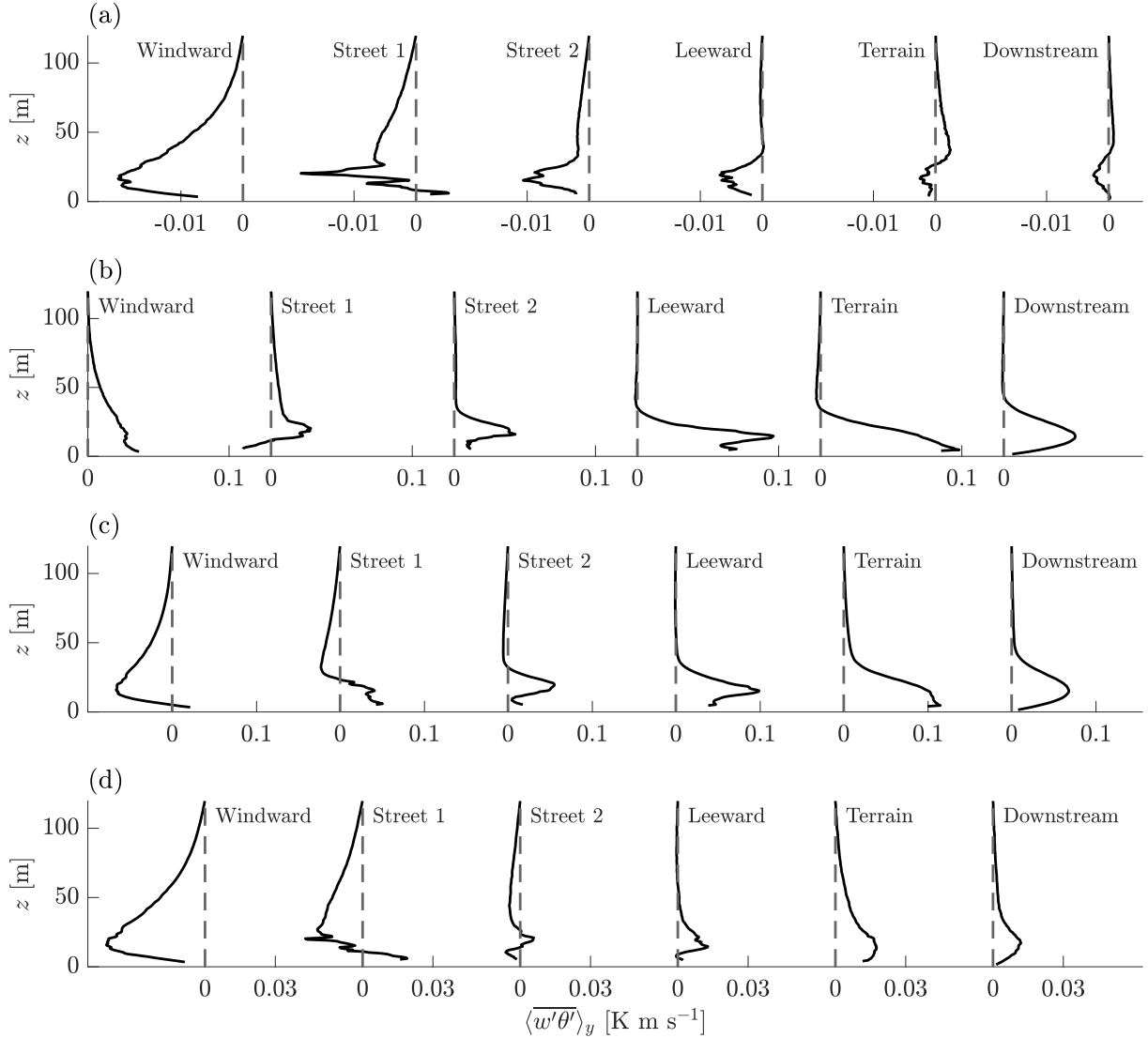


Figure 5.12: Evolution of y -averaged sensible heat flux $\langle \overline{w'\theta'} \rangle_y$ at the windward side of the buildings ($x = 112$ m), in the first street canyon ($x = 153$ m), in the second street canyon ($x = 182$ m), at the leeward side of the buildings ($x = 203$ m), over the terrain ($x = 240$ m), and downstream of the terrain ($x = 300$ m); averaged during: (a) 0300-0400 LT, (b) 0900-1000 LT, (c) 1500-1600 LT, and (d) 2100-2200 LT. Note the change in horizontal scale between sub-figures.

5.4 Conclusion

This study aimed to explore how microclimate evolves in a hot, arid coastal environment, focusing on thermal processes in the built environment and the surrounding terrain. Sect 5.3.1 showed that the bulk SEB, including the extent of thermal inertia, is similar for the buildings and the terrain, though the surface temperature of the former is lower than that of the latter. Sect 5.3.2 demonstrated the importance of solar radiation in predicting the surface temperature, in particular the effect of shading. However, thermal inertia is also influential, causing surface temperature to remain elevated late into the evening. Solar radiation is also crucial in determining the MRT, which exhibits large differences between shaded and unshaded areas. Finally, Sect. 5.3.3 discussed that as well as surface effects, the air temperature is influenced by the wind, to such an extent that there are high temperatures in regions with relatively low surface heating due to flow separation and recirculation.

In terms of implications for urban design, these results suggest that the built environment can provide thermal comfort in the context of the climatic conditions in this study, while highlighting the substantial impact that shading has on microclimate for sites exposed to high levels of solar irradiance. In addition, the timing of factors influencing thermal comfort is particularly important with respect to predicting and responding to heat stress for example. Finally, mitigation measures, e.g. a wind break, may be a useful design intervention for preventing heat transfer from hotter to cooler areas.

The results are of course dependent on the morphological and material properties used in the simulation. Changing the thermal properties will no doubt influence the behaviour of SEB quantities, and in particular the fact that the streets and surrounding terrain are made of the same material may be unrealistic in other cases. This is also true for the use of an insulating material for the interior of building facets. However, it is unlikely that the broad patterns in the bulk SEB observed in this study will be affected unless the radiative properties are changed in a significant manner, because the direct solar radiation (shading) and the flow behaviour were shown to be the key factors.

The flow in the wake of the buildings in this study is typical of bluff-body aerodynamics, and this behaviour is also likely to be observed for other morphologies. Nonetheless, the nature of the wake (and the resulting air temperature distribution) would be sensitive to the incoming flow conditions, particularly the wind direction. While in this case

only the prevailing wind direction was considered, for other cases it may be preferable to analyse multiple wind directions.

The results presented in Sect. 5.3.3 are also likely to be influenced by the fact that the incoming marine boundary layer is assumed to be neutral, which may not be applicable to other cases (and indeed is unlikely to be strictly true for this case in reality). To capture a more typical urban boundary layer, which generally have diurnally-varying atmospheric stability, it would be necessary to have a more sophisticated (height-dependent) temperature forcing. The incoming boundary layer would also be defined by greater surface roughness, which would likely require the use of explicit roughness elements upstream. Despite the additional complexity involved, further studies are needed in order to expand our understanding of physical processes within the built environment. This study demonstrates their value in understanding urban microclimate, and highlights the importance of using high-fidelity multi-physics microscale models to capture behaviour over a diurnal cycle.

Chapter 6

The importance of diurnal cycle simulations

6.1 Introduction

The thermal response of an urban (or rural) surface is dependent on the state history (Best and Grimmond, 2013, 2014; Lipson et al., 2022), i.e. the internal temperature, as well as the instantaneous surface energy balance (SEB), which tends to be dominated by shortwave radiation. This results in thermal inertia, in which the response is delayed and damped compared to the shortwave radiation. This behaviour is largely determined by materiality, with surfaces possessing higher thermal mass exhibiting higher thermal inertia. These phenomena were explored in Chapter 5. In addition, due to the more complex morphologies generally present in urban areas, there is greater visibility between the various facets making up the surface. This may result in greater absorption of the longwave radiation emitted by the facets, and greater absorption of shortwave radiation originating from the sun due to repeated scattering between facets (Oke et al., 2017). Furthermore, shading tends to occur within street canyons, which causes shaded facets to have a reduced instantaneous response to the solar forcing. These factors concerning radiative transfer act to increase the inter-dependence of the state of the facets, and hence may also increase the hysteresis of the surface as a whole (Grimmond and Oke, 1999b).

When using microscale modelling tools to simulate urban microclimate, some studies only simulate specific times of day (e.g. Nazarian and Kleissl, 2016; Nazarian et al., 2017; Gaspari and Fabbri, 2017; Gaspari et al., 2018). This saves computational cost,

but assumes the state is history-independent (unless there is some method to account for thermal inertia). To capture heat transfer accurately, it is necessary to simulate the entire diurnal cycle continuously (e.g. Nazarian and Kleissl, 2015; Fabbri et al., 2017). The simulation should ideally be carried out for multiple days until the results are independent of initial conditions (e.g. Toparlar et al., 2015; Salata et al., 2017; Acero and Arrizabalaga, 2018; Imbert et al., 2018; Fabbri et al., 2020; Chen et al., 2021*a,b*). The purpose of this chapter is to investigate the extent to which simulating urban microclimates at fixed time(s) of day captures the behaviour observed when simulating a complete diurnal cycle. The aim is to compare a diurnal cycle (DC) simulation, in which the solar position and air temperature vary continuously throughout the day, to a set of simulations which each have a fixed solar position and air temperature representing one hour of day, with the surface allowed to reach a statistically steady state (SS) given the thermal forcing.

The case set-up is identical to that of Chapter 5 (see Sect. 5.2.1), with the DC and SS simulations only differing conceptually in their thermal forcing (and runtime). The geometry is shown in Fig. 6.1 (with facets coloured according to sky view factor ψ_{sky} ; see Sect. 2.3.3). The exact morphology and materiality used in the study is not particularly salient, given that the focus is the comparison between the two modelling assumptions. Nonetheless, this is an advantageous case to use given the research objectives. Since the climate is hot and arid, thermal effects are significant, which is expected to make differences between the DC and SS modelling assumptions more apparent. Also, the fact that the oncoming flow is neutral means that the resulting boundary layer structure due to the built environment (and the terrain) is entirely dependent on the thermal processes at the surface, thus differences thereof between the DC and SS simulations can be identified more clearly. This also means it is more straightforward to ensure that the DC and SS simulations have identical incoming flow, though there are techniques for achieving steady-state simulations with non-neutral boundary layers (e.g. Grylls et al., 2020).

The investigation consists of three parts, which are similar to that of Chapter 5. Section 6.3.1 compares the SEB, primarily in terms of the facet types (streets, roofs, and walls). Then, Sect. 6.3.2 compares the microclimatic conditions, including the pedestrian-level wind speed, air temperature and mean radiant temperature (MRT). Finally, Sect. 6.3.3 compares the streamwise development of the thermal boundary layer over the built environment using vertical profiles of the air temperature and sensible heat flux.

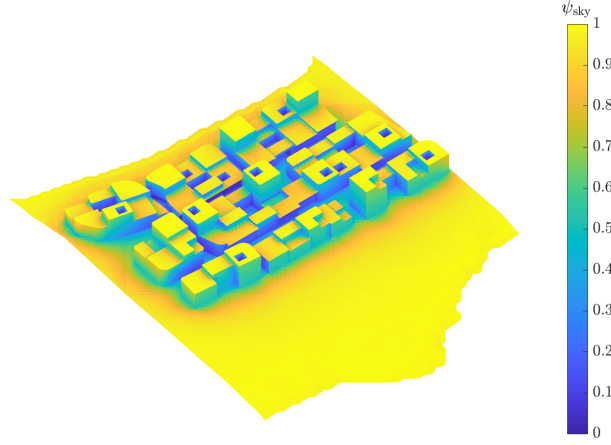


Figure 6.1: Facets coloured by sky view factor (ψ_{sky}); for scale and orientation see Fig. 5.1.

6.2 Methodology

The methodology for the DC simulation is unchanged from Chapter 5, and is described in detail in Sect. 5.2. The inflow boundary condition is generated by a precursor simulation (see Sect. 5.2.2), and given that the mean velocity profile is constant, this precursor can also be used for all the SS simulations. This assumes that the precursor turbulence is in a statistically steady state, and is therefore the same throughout the diurnal cycle. Each SS simulation corresponds to a single hour of the day, which involves using a constant value for the solar position, inlet temperature, and sky radiation (see Fig. 5.4). The simulations are run for four hours, and data for the final hour is time-averaged and used for the results in Sect. 6.3. Practically, this is sufficient time for the system to reach a statistically steady state based on the facet temperatures approaching a constant value.

Several changes were made for the SS simulations compared to the DC simulation for numerical reasons. The volumetric heat capacities (C) of the materials were reduced by a factor of 100 (in comparison to Table 5.1) for faster convergence to the steady state. Note that the steady state that the SEB reaches is not dependent on the value of the heat capacity; the only material property that affects this is the conductivity (λ), which was not changed. The atmospheric state, when time-averaged, is assumed to be unaffected by the fact that the lower C causes greater fluctuations around the steady state. The number of facet layers (N_l) was reduced from 20 to 10, as the lack of transience in the shortwave forcing for the SS simulations means that it is unnecessary to use as many layers. Finally, the SEB time step was reduced to 10 s as it was found to be unstable when using 60 s.¹

¹Likely due to the larger fluctuations around the steady state.

6.3 Results

6.3.1 Surface energy balance

Figure 6.2 shows the complete average SEB fluxes and the average surface temperature $\langle T_s \rangle_s$ of the facets making up the buildings and streets for the DC and SS simulations (see Sect. 2.2 for the definition of the averaging). The net shortwave radiation $\langle K^* \rangle_c$ is identical for the two sets of simulations at each hour of the day, as this is not dependent on the state of the surface (or the atmosphere). The largest discrepancy is with the conduction $\langle G_0 \rangle_c$, which is generally much smaller for the SS simulations than for the DC simulations. For the SS simulations, there is thermal equilibrium within each facet, i.e. the heat flux is constant throughout, and tends to be very small. In contrast, for the DC simulation the facets generally exhibit transient heat transfer, which results in larger heat fluxes, particularly at the surface where the forcing occurs.

As a result of the reduced conduction in the SS simulations, the peak of the surface temperature $\langle T_s \rangle_s$ is larger. Furthermore, the peak of $\langle T_s \rangle_{s,SS}$ occurs at the same time as that of $\langle K^* \rangle_c$, whereas $\langle T_s \rangle_{s,DC}$ peaks later, approximately 1.5 hours afterwards. As a result, $\langle T_s \rangle_{s,SS}$ tends to be greater than $\langle T_s \rangle_{s,DC}$ during the day and less than $\langle T_s \rangle_{s,DC}$ at night, except for a period during the late afternoon (1600-1800 LT) for which $\langle T_s \rangle_{s,DC}$ is greater than $\langle T_s \rangle_{s,SS}$. A similar pattern is visible in the sensible heat flux $\langle H \rangle_c$, though

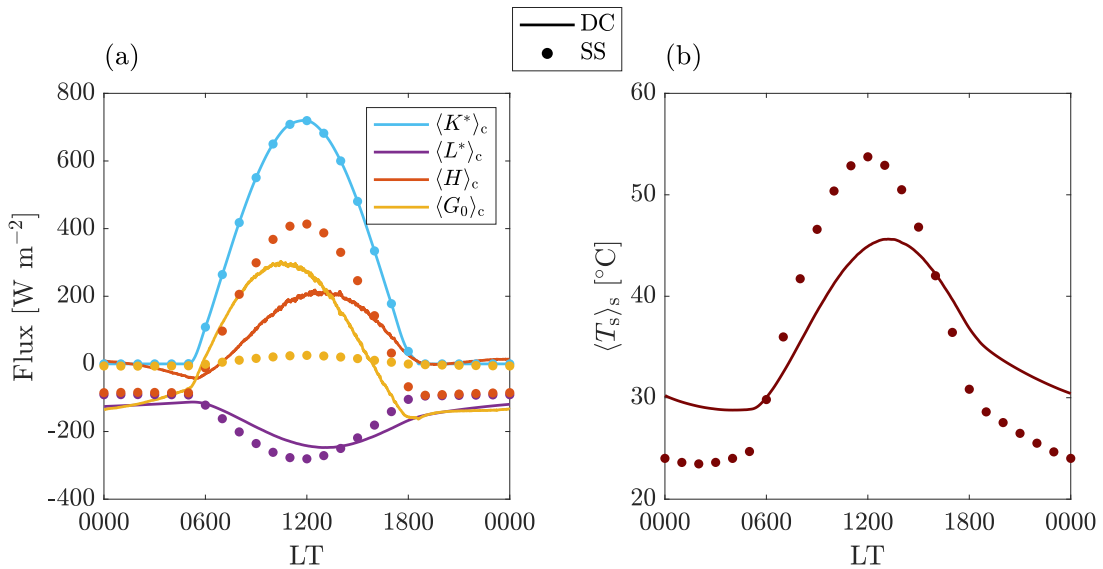


Figure 6.2: Evolution of bulk SEB quantities for the built environment: (a) complete average ($\langle \cdot \rangle_c$; see Eq. (2.13)) fluxes of net shortwave radiation (K^*), net longwave radiation (L^*), sensible heat (H), and conduction (G_0); (b) average ($\langle \cdot \rangle_s$) surface temperature (T_s).

the behaviour is more complex as this quantity is also affected by the air temperature. At night, $\langle H \rangle_{c,DC}$ is slightly negative initially, then becomes positive as a likely result of the air cooling and the surface remaining warmer due to thermal inertia. Then, as the surface cools to below air temperature, $\langle H \rangle_{c,DC}$ becomes negative again until after sunrise. This behaviour is not replicated with $\langle H \rangle_{c,SS}$, which is substantially over/under-estimated during the day/night in a similar manner to $\langle T_s \rangle_{s,SS}$ as a result of $\langle G_0 \rangle_{c,SS}$ being very small. The net longwave radiation $\langle L^* \rangle_c$ has a fairly similar magnitude for the two cases, though there is a time lag between the minima of $\langle L^* \rangle_{c,SS}$ and $\langle L^* \rangle_{c,DC}$ due to their dependence on surface temperature. Both the incoming and outgoing longwave radiation are likely to be affected by the differences between $\langle T_s \rangle_{s,SS}$ and $\langle T_s \rangle_{s,DC}$, with their effects on $\langle L^* \rangle_{c,SS}$ appearing to approximately cancel.

Figure 6.3 shows the average SEB fluxes and temperature as a function of depth (ξ) for each type of facet (streets, roofs, and walls). Much of the previous discussion of Fig. 6.2 regarding the difference in the behaviour of the fluxes in general also applies here. The internal temperature distribution of the DC and SS simulations differ substantially as this is directly affected by thermal inertia. In addition to the time lag between the peak of $\langle K^* \rangle_s$ and $\langle T_s \rangle_{s,DC}$, it is also visible that as ξ increases, $\langle T \rangle_{s,DC}$ peaks later in the day. In contrast, $\langle T \rangle_{s,SS}$ in each layer generally peaks at the same time that $\langle K^* \rangle_s$ peaks. The small magnitude of $\langle G_0 \rangle_{s,SS}$ is consistent with the fact that the temperature gradient at the surface for the SS simulations appears to be smaller than that for the DC simulation. The fact that there is constant conductive heat flux in each facet for the SS simulations has different implications for the various surface types. For the average street facet (see Fig. 6.3a,b), which are materially uniform, the constant heat flux results in a constant temperature gradient throughout for any given time (simulation). For the DC simulation there is a depth ($\xi \approx 0.6$ m) beyond which the surface forcing over the diurnal cycle is not felt (see Sect. 2.2), and so $\langle T \rangle_{s,DC}$ remains equal to the prescribed ground temperature (T_G); this is not the case for the SS simulations, because all the facet layers effectively have had time to respond to the surface forcing. At night, $\langle T \rangle_{s,SS}$ is less than T_G after sunset throughout the layer, in contrast to the more complex behaviour of $\langle T \rangle_{s,DC}$; only the surface temperature becomes less than T_G , and deeper layers ($\xi \geq 0.2$ m), $\langle T \rangle_{s,DC}$ remain greater than T_G . The building facets are a composite of two layers of different materials — a regular (concrete) exterior and an insulating interior. For the SS simulations, the

temperature gradient within the facets is constant within each layer of material; the high-conductivity outer layer has a small gradient, whereas the low-conductivity inner layer has a large gradient. The average roof facet remains above the internal building temperature (T_B) for both the DC and SS simulations (see Fig. 6.3c,d), whereas the for average wall facet, $\langle T \rangle_{s,SS}$ falls below T_B at night (see Fig 6.3e,f).

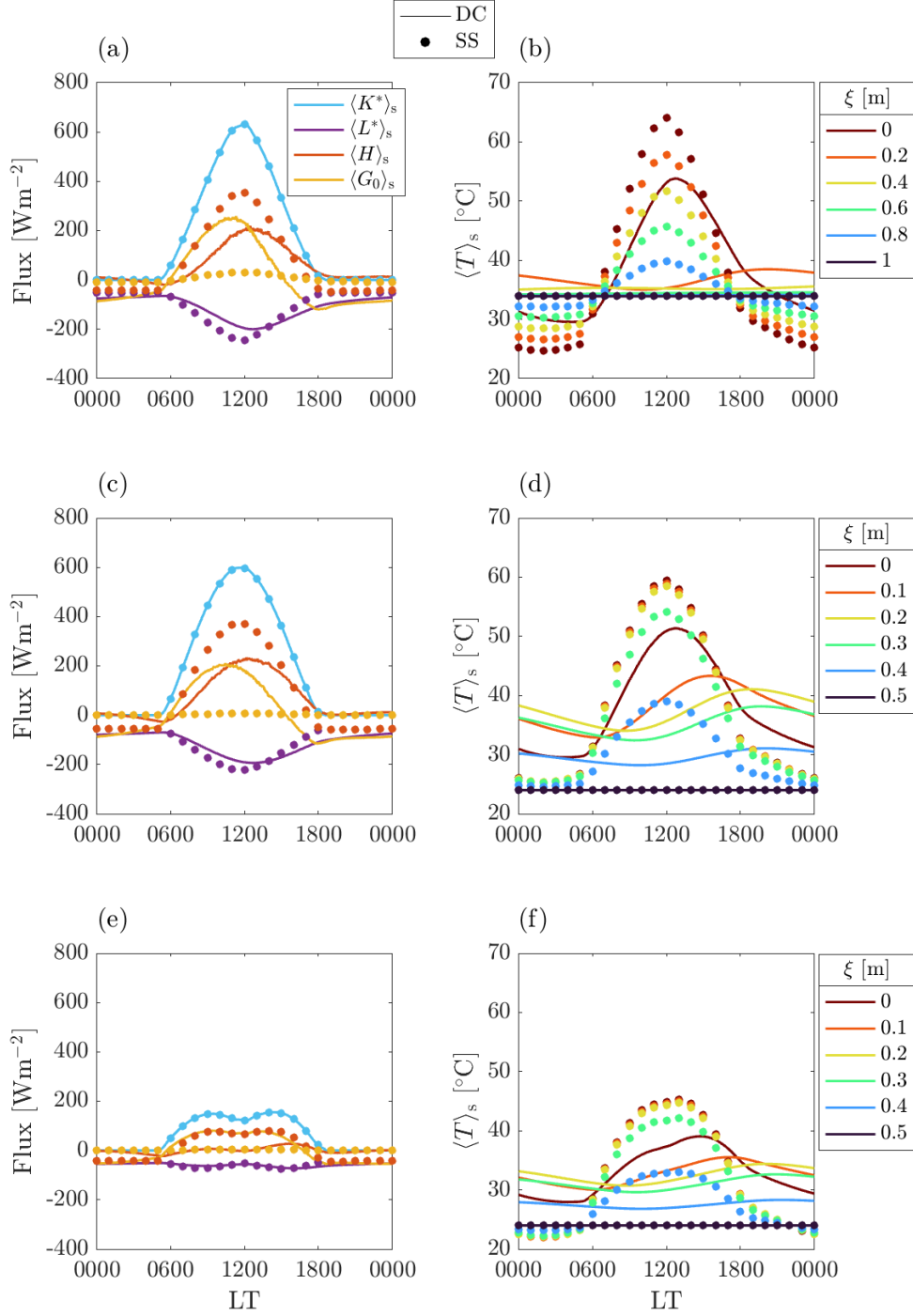


Figure 6.3: Evolution of bulk SEB quantities for streets (a,b), roofs (c,d), and walls (e,f): average ($\langle \cdot \rangle_s$; see Eq. (2.13)) fluxes of net shortwave radiation (K^*), net longwave radiation (L^*), sensible heat (H), and conduction (G_0); average temperature (T) with depth (ξ).

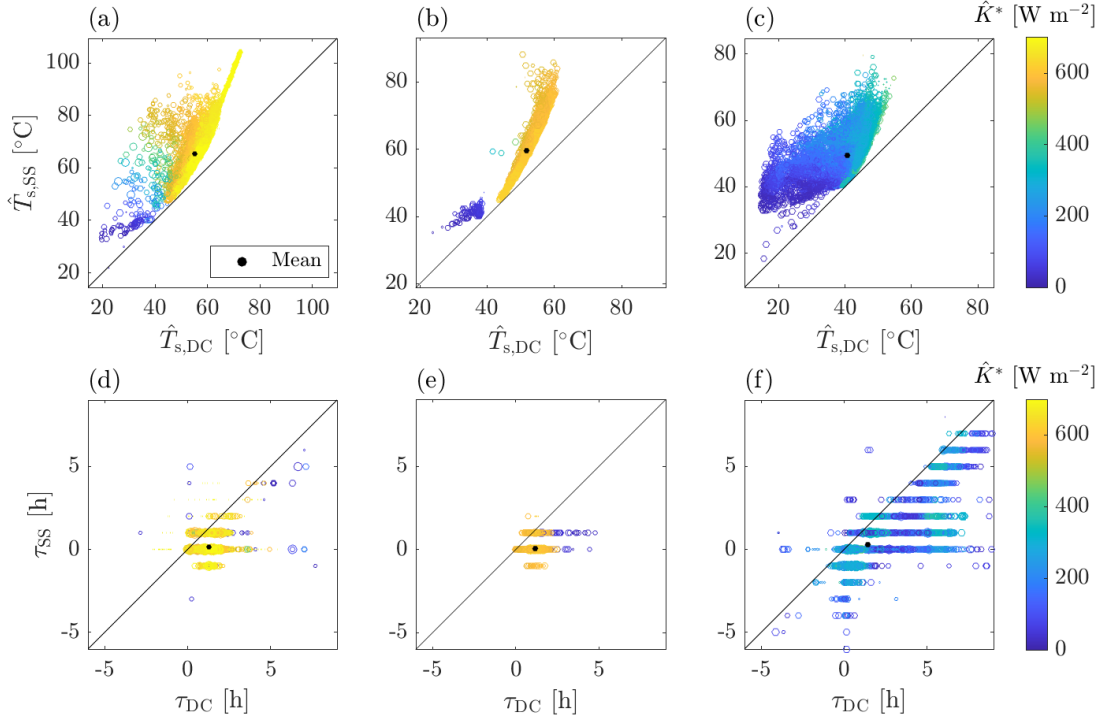


Figure 6.4: Surface temperature amplitude ($\hat{T}_s$) and time lag (τ) between the peaks of net shortwave radiation ($\hat{K}^*$) and surface temperature for the streets (a,d), roofs (b,e), and walls (c,f). Each facet is represented by a point with the horizontal/vertical position given by its value in the DC/SS simulation, which are coloured according to $\hat{K}^*$ and their size is proportional to the facet area, with the surface average $\langle \hat{T}_s \rangle_s$ also shown.

In order to quantify the behaviour of individual facets, Fig. 6.4 shows the surface temperature amplitude ($\hat{T}_s$) and the time lag (τ) between when the peak of net shortwave radiation ($\hat{K}^*$) occurs and when $\hat{T}_s$ occurs for the facets making up the streets, roofs, and walls. Each facet is represented by a point on the plane, allowing the values predicted by the DC and SS simulations to be compared directly. For the vast majority of facets, $\hat{T}_s$ is over-predicted by the SS simulations, and τ is under-predicted. This is consistent with the behaviour shown in Fig. 6.3, though Fig. 6.4 illuminates the fact that there is significant variation about the mean. The range of $\hat{K}^*$ values exhibited by the facets making up the streets appears to be fairly continuous (see Fig. 6.4a), which is due to the variation in the time of day that each is unshaded (if at all). It seems that generally, a higher value of $\hat{K}^*$ corresponds to a higher value of $\hat{T}_{s,DC}$. There is not a clear relationship between $\hat{T}_{s,DC}$ and $\hat{T}_{s,SS}$, though there are regions in the space of possible values which contains no points, which are both bounded in what seems to be a linear fashion. The values of τ are quite tightly clustered around the mean value (see Fig. 6.4d), to the extent that facets with intermediate $\hat{K}^*$ are not visible due to points representing facets with higher $\hat{K}^*$.

having been plotted on top. The distribution of $\hat{K}^*$ on the roof facets is almost entirely bimodal (see Fig. 6.4b); they are either unshaded, with a high value of $\hat{K}^*$ occurring at the same time as each other (around midday); or shaded throughout the entire day, and thus with low $\hat{K}^*$. The former corresponds to the facets on top of buildings (the actual roofs), and the latter to those overhanging the streets.² With respect to the relationship between $\hat{T}_{s,DC}$ and $\hat{T}_{s,SS}$, the unshaded facets all roughly sit on a straight line, and the shaded facets sit on another. These lines seem to be at a similar angle to the axes as those bounding the points corresponding to the street facets in Fig. 6.4a. The τ values are also clustered slightly more tightly around the mean than the streets (see Fig. 6.4e). The reduced spread of the points (for both $\hat{T}_s$ and τ) compared to the streets is expected; roof facets generally have a large sky view factor, and are less influenced by the state of the other facets compared to those of the other types. For wall facets, the opposite is true; they generally interact with the other facets to a greater extent, and have a low sky view factor. This is evidenced by the generally lower $\hat{K}^*$ values, and the fact that there is less clustering around the mean, particularly for τ (see Fig. 6.4c,f). Again, in a similar manner to the other types, there seems to be a region with high $\hat{T}_s$ that contains no points, and a region of low $\hat{T}_s$ that contains relatively few points. It is likely that the points in the latter region correspond to facets that are anomalous in some way, for example by being part of a very narrow gap, and so entirely obscured by other facets.

To investigate the evolution of individual facets over the diurnal cycle, Fig. 6.5 shows T_s using a similar format to Fig. 6.4, with the points representing the facets coloured according to K^* during the day and sky view factor ψ_{sky} (see Fig. 6.1) during the night, and the air temperature (θ_{in}) is also included. Meanwhile, Fig. 6.6 shows the difference in surface temperature ($\Delta T_s = T_{s,SS} - T_{s,DC}$) as a 3D visualisation of the geometry. Before sunrise (0400 LT), $T_{s,SS}$ is consistently less than $T_{s,DC}$, and $T_{s,DC}$ tends to be less than θ_{in} . The facets generally fall into two groups based on their sky view factor, particularly the facets making up the roofs (for the same reasons discussed previously with respect to Fig. 6.4). For those with $\psi_{sky} \approx 0$, it seems that the difference between $T_{s,DC}$ and $T_{s,SS}$ is approximately proportional to the difference between $T_{s,DC}$ and θ_{in} . For the rest (with $\psi_{sky} > 0$), it seems that $T_{s,DC} \approx \theta_{in}$, and the difference between $T_{s,DC}$ and $T_{s,SS}$ is approximately inversely proportional to ψ_{sky} . This is likely because the facets with higher

²Note that the definition of roof facets in Sect. 5.2 includes any overhangs; while these arguably could be classified as walls, it is useful to categorise them as roofs to contrast them with the rest.

ψ_{sky} are less influenced by the state of the other facets, which makes the value for the SS simulations more likely to match that for the DC simulations. Given that K^* peaks around midday, the behaviour at 1000 LT (Fig. 6.5d-f) is similar to that in Fig. 6.4.

In the afternoon, the facets tend to cool. Whether T_s is over- or under-estimated at any given time depends on competing effects: the fact that $\hat{T}_{s,\text{SS}}$ tends to be greater than $\hat{T}_{s,\text{DC}}$, and the fact that τ_{DC} tends to be greater than τ_{SS} (see Fig. 6.4). At around 1600

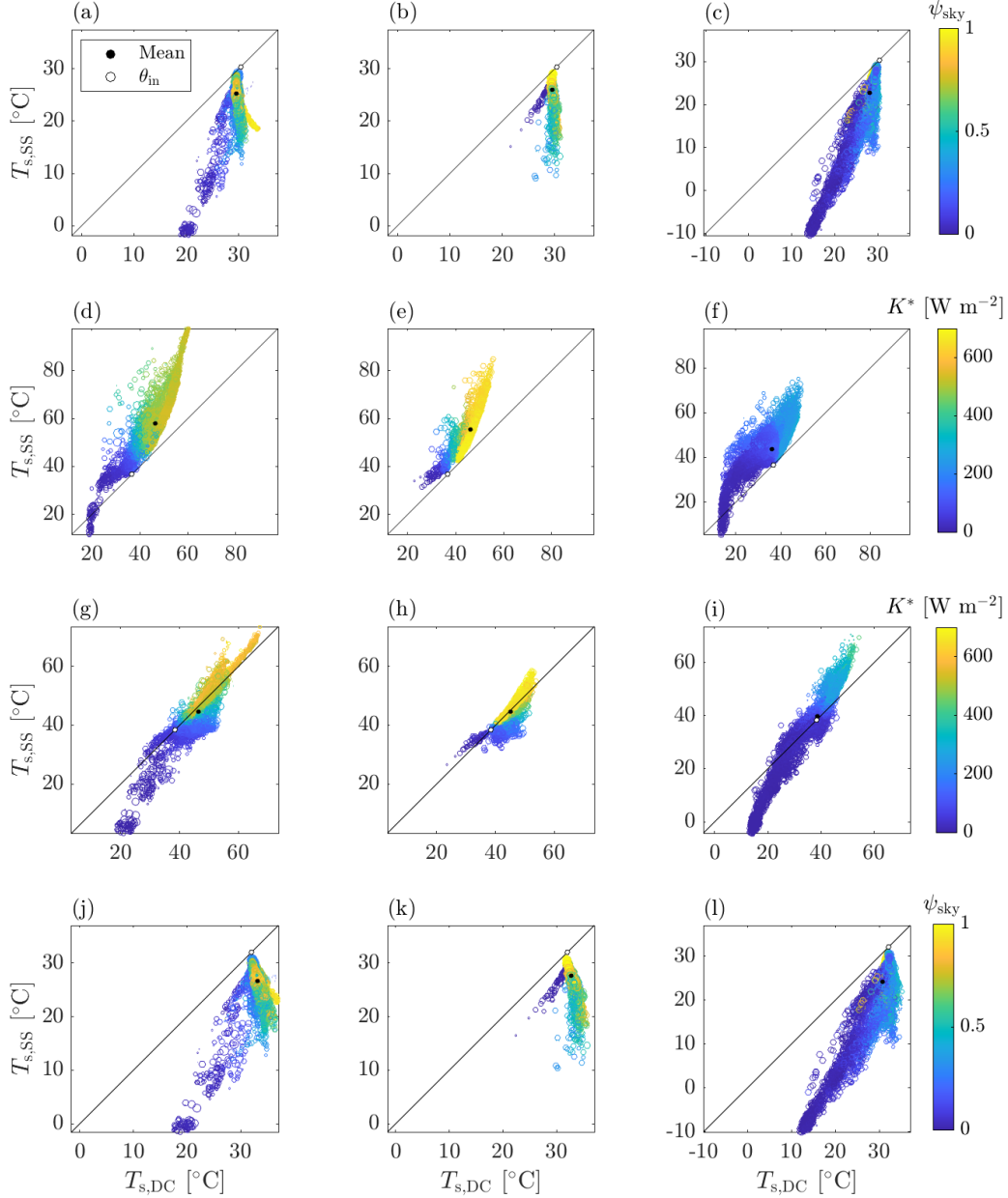


Figure 6.5: Surface temperature (T_s) of the streets, roofs, and walls at 0400 LT (a-c), 1000 LT (d-f), 1600 LT (g-i), 2200 LT (j-l) for DC and SS simulations. Each facet is represented by a point with the horizontal/vertical position given by its value in the DC/SS simulation, which are coloured according to sky view factor (ψ_{sky}) and their size is proportional to area, with the mean value and the inlet air temperature (θ_{in}) also shown.

LT, the mean value of $T_{s,ss}$ is well-predicted (this can also be seen from Fig. 6.3), however there are still many facets whose $T_{s,ss}$ are not well-predicted at this time (see Fig. 6.5h). It seems that it is unshaded facets that tend to be well-predicted at this time (see Fig. 6.6h), which is reflected in the mean because unshaded facets generally outnumber shaded facets during the day. In the late evening (2200 LT), the behaviour is similar to that discussed in the early morning (0400 LT), though it is noticeable that $T_{s,DC}$ is greater than θ_{in} for a substantial number of facets. This is likely because these facets have stored enough energy throughout the day for their surface to remain elevated above air temperature.

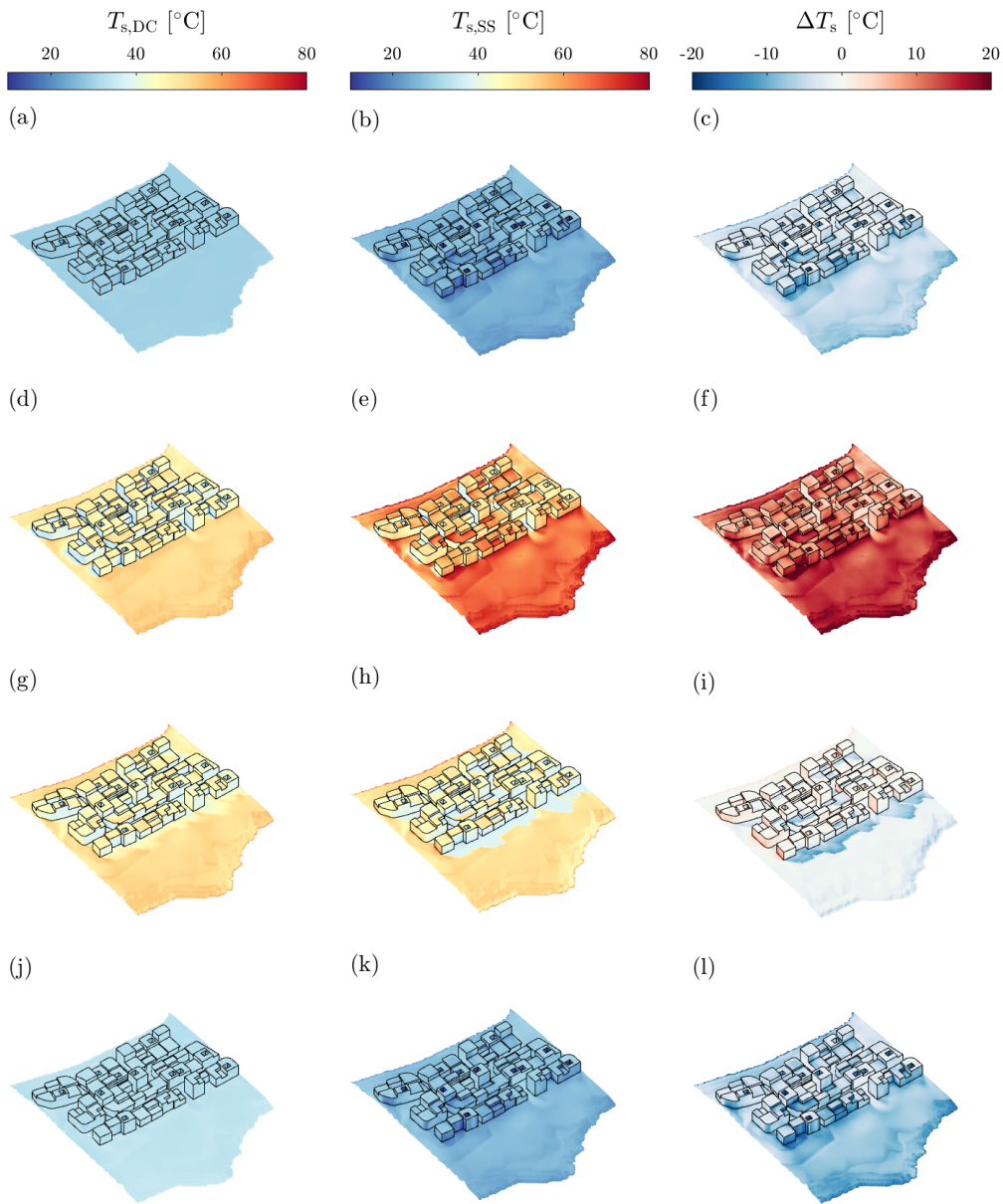


Figure 6.6: Visualisation of facets coloured by surface temperature in the DC simulation ($T_{s,DC}$) and SS simulations ($T_{s,ss}$), and difference between them ($\Delta T_s = T_{s,ss} - T_{s,DC}$) respectively at 0400 LT (a-c), 1000 LT (d-f), 1600 LT (g-i), and 2200 LT (j-l).

6.3.2 Pedestrian-level quantities

It is not straightforward to directly compare the state of the atmosphere at a given time of day between the DC and SS simulations because each SS simulation has fixed forcings (in particular the inlet temperature), whereas the forcings vary continuously in the DC simulation. Also, the flow is turbulent, and so must be time-averaged, and it is not clear which averaging window should be taken such that the comparison is ‘fair’. Given that there is one SS simulation for each hour of the day, the averaging window used is also an hour — each SS simulation is therefore mapped onto a (time-averaged) hour of the DC simulation. The bounds of each averaging window are chosen to be the times of the SS simulation, i.e. at 0000 LT, 0100 LT, etc, such that the SS inlet temperature matches the initial DC inlet temperature for each averaging window. By effectively sampling the DC simulation at the point after which the hourly forcing for the SS simulation occurs, the lag between forcing and response that is present in the DC simulation (and not present in the SS simulations) is accounted for to some extent (and not exacerbated). Given that the ambient (inlet) air potential temperature (θ_{in}) will not match in general, the difference in deviation from this temperature ($\tilde{\theta} = \overline{\theta} - \theta_{\text{in}}$) is used in order to make a comparison.

Figure 6.7 shows the differences between the SS and DC simulations with respect to wind speed, air potential temperature deviation ($\tilde{\theta}$), and MRT at pedestrian-level (1.5 m above the ground). The wind speed does vary slightly over the diurnal cycle, but there is no clear systematic pattern, which suggests that any differences are due to (unavoidable) turbulent fluctuations associated with the inflow boundary condition. Overall, the potential temperature and MRT differences vary in a similar manner to T_s as discussed in Sect. 6.3.1, as these quantities are affected by it. Namely, at 0400 LT (Fig. 6.7a-c), $\tilde{\theta}_{\text{DC}} > \tilde{\theta}_{\text{SS}}$ and $\text{MRT}_{\text{DC}} > \text{MRT}_{\text{SS}}$, while at 1000 LT (Fig. 6.7d-f), the reverse is true. At 1600 LT, the sign of the difference between the SS and DC simulations varies in space, because as discussed earlier, this happens to be the time when facets in the SS simulation are likely to ‘flip’ from overestimating to underestimating temperature. The spatial pattern is more pronounced for ΔMRT in comparison to $\Delta\tilde{\theta}$, likely because MRT is solely influenced by T_s , whereas $\tilde{\theta}$ is also influenced by the flow (which does not vary significantly between the SS and DC simulations). The difference in MRT within courtyards is particularly large, likely because of the inter-dependence (in terms of radiative transfer) of the facets that make them up. Finally, the differences at

2200 LT are similar to those observed at 0400 LT only larger, which is likely due to the thermal inertia of the facets for the DC simulation causing elevated surface temperature.

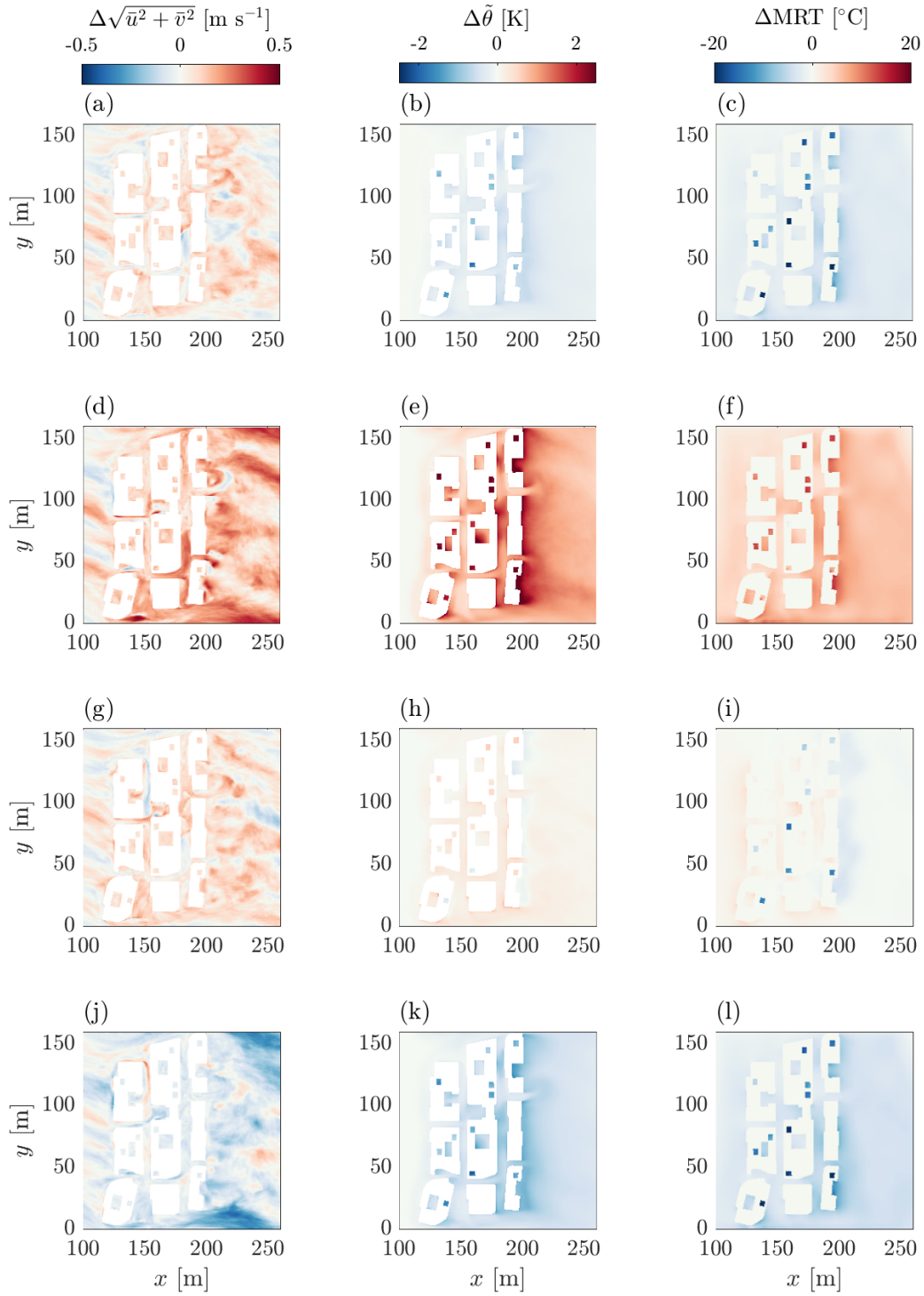


Figure 6.7: Differences between SS and DC simulations of pedestrian-level wind speed ($\Delta\sqrt{\bar{u}^2 + \bar{v}^2} = \sqrt{\bar{u}^2 + \bar{v}^2}_{\text{SS}} - \sqrt{\bar{u}^2 + \bar{v}^2}_{\text{DC}}$), air potential temperature deviation ($\Delta\tilde{\theta} = \tilde{\theta}_{\text{SS}} - \tilde{\theta}_{\text{DC}}$), and mean radiant temperature ($\Delta\text{MRT} = \text{MRT}_{\text{SS}} - \text{MRT}_{\text{DC}}$) respectively at 0400 LT (a-c), 1000 LT (d-f), 1600 LT (g-i), 2200 LT (j-l).

6.3.3 Thermal boundary layer development

Figures 6.8 and 6.9 respectively show profiles of y -averaged air potential temperature deviation $\langle \tilde{\theta} \rangle_y$ and kinematic sensible heat flux $\langle \overline{w'\theta'} \rangle_y$ against height above sea-level (z) at several streamwise locations over the diurnal cycle: at the windward side of the buildings, the first street canyon, the second street canyon, at the leeward side of the buildings, over the terrain, and finally downstream of the terrain.

At 0400 LT (see Figs. 6.8a and 6.9a), both $\langle \tilde{\theta} \rangle_{y,DC}$ and $\langle \tilde{\theta} \rangle_{y,SS}$ are less than zero, with

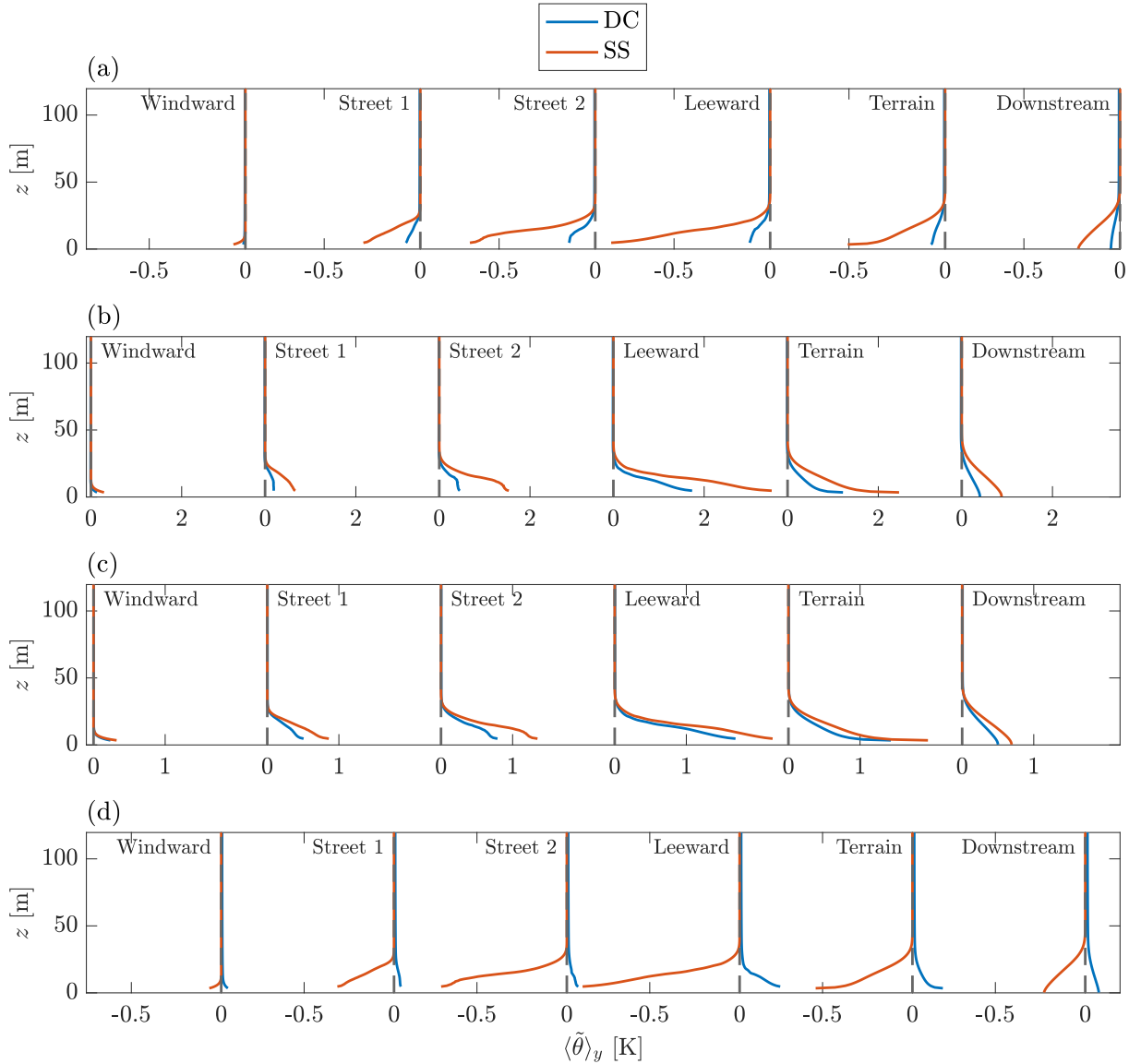


Figure 6.8: Evolution of y -averaged air potential temperature deviation $\langle \tilde{\theta} \rangle_y = \langle \bar{\theta} \rangle_y - \langle \bar{\theta}_{in} \rangle_y$ for the DC and SS simulations, at the windward side of buildings ($x = 112$ m), in the first street canyon ($x = 153$ m), in the second street canyon ($x = 182$ m), at the leeward side of the buildings ($x = 203$ m), over the terrain ($x = 240$ m), and downstream of the terrain ($x = 300$ m); at 0400 LT (a), 1000 LT (b), 1600 LT (c), and 2200 LT (d).

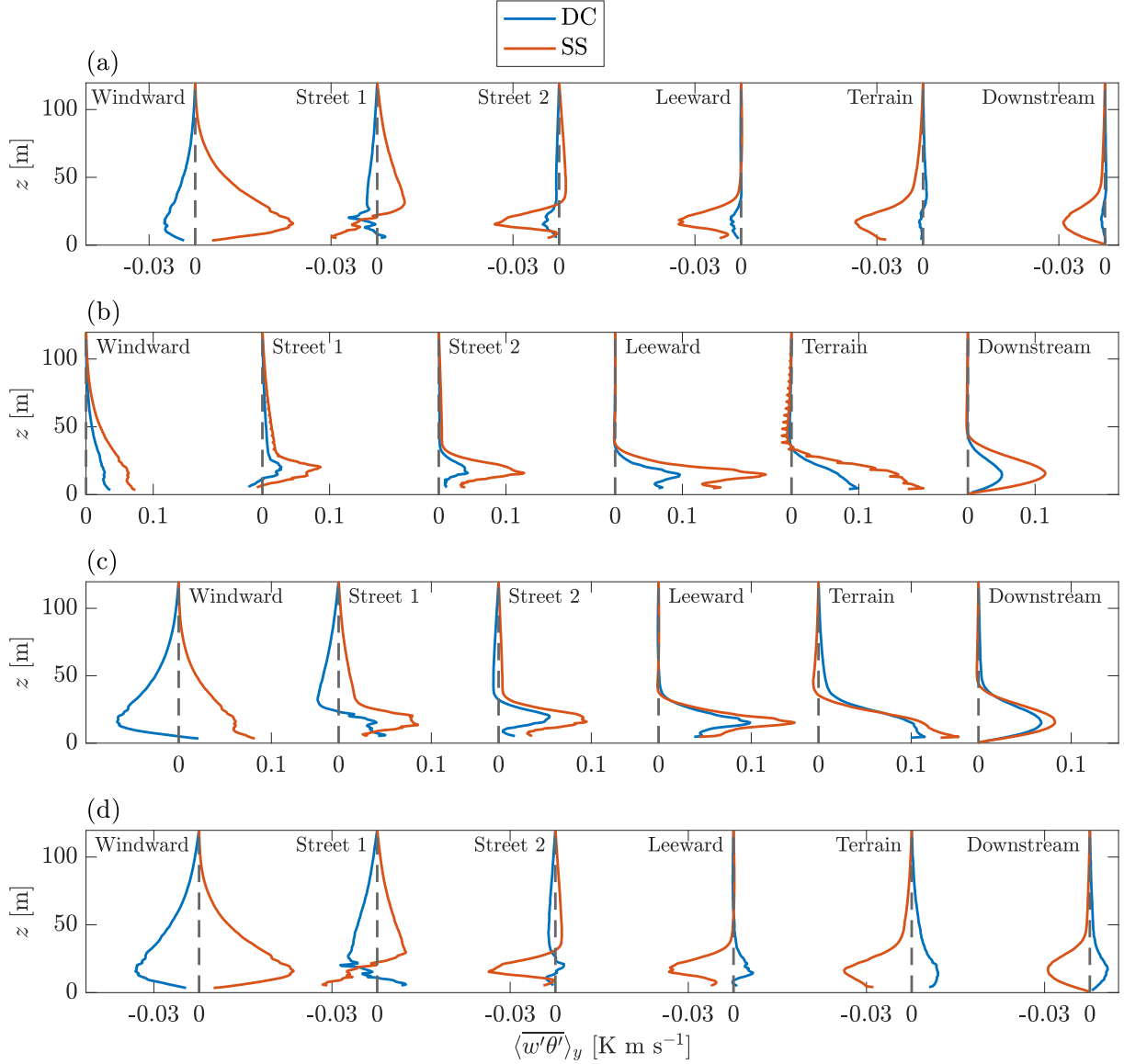


Figure 6.9: Evolution of y -averaged sensible heat flux $\langle \overline{w'\theta'} \rangle_y$ for the DC and SS simulations, at the windward side of buildings ($x = 112$ m), in the first street canyon ($x = 153$ m), in the second street canyon ($x = 182$ m), at the leeward side of the buildings ($x = 203$ m), over the terrain ($x = 240$ m), and downstream of the terrain ($x = 300$ m); at 0400 LT (a), 1000 LT (b), 1600 LT (c), and 2200 LT (d).

$\langle \tilde{\theta} \rangle_{y,SS}$ more negative than $\langle \tilde{\theta} \rangle_{y,DC}$ at each location. While $\langle \tilde{\theta} \rangle_{y,DC}$ takes its minimum value in the second street, $\langle \tilde{\theta} \rangle_{y,SS}$ does so at the leeward side of the buildings. At this time, $\langle \overline{w'\theta'} \rangle_{y,DC}$ and $\langle \overline{w'\theta'} \rangle_{y,SS}$ differ quite substantially, particularly at the windward side of the buildings and in the first street canyon, where they have opposite sign. The fact that there is generally poor agreement between $\langle \overline{w'\theta'} \rangle_{y,SS}$ and $\langle \overline{w'\theta'} \rangle_{y,DC}$ at the windward side of the buildings suggests that the stability is relatively variable at this location. This is likely because there is little surface heating, as evidenced by the small gradient of $\tilde{\theta}$,

while there is a large vertical velocity due to the flow first encountering the buildings.

At the other locations, where both $\langle \overline{w'\theta'} \rangle_{y,DC}$ and $\langle \overline{w'\theta'} \rangle_{y,SS}$ are negative near the surface, $\langle \overline{w'\theta'} \rangle_{y,SS}$ is larger in magnitude than $\langle \overline{w'\theta'} \rangle_{y,DC}$, which is almost zero over the terrain and further downstream. At both 1000 LT and 1600 LT (see Figs. 6.8b,c and 6.9b,c respectively), $\langle \tilde{\theta} \rangle_{y,DC}$ and $\langle \tilde{\theta} \rangle_{y,SS}$ are greater than zero, with $\langle \tilde{\theta} \rangle_{y,SS}$ greater than $\langle \tilde{\theta} \rangle_{y,DC}$ at each location. The similarity of $\langle \tilde{\theta} \rangle_{y,SS}$ to $\langle \tilde{\theta} \rangle_{y,DC}$ is closer at 1600 LT, which is consistent with previous results which found the mean temperature well-predicted. At 1600 LT, the signs of $\langle \overline{w'\theta'} \rangle_{y,SS}$ and $\langle \overline{w'\theta'} \rangle_{y,DC}$ are again opposite at the windward side of the buildings, whilst they are relatively similar at other locations. In contrast, at 1000 LT, $\langle \overline{w'\theta'} \rangle_{y,SS}$ and $\langle \overline{w'\theta'} \rangle_{y,DC}$ are positive, and while $\langle \overline{w'\theta'} \rangle_{y,SS}$ is greater than $\langle \overline{w'\theta'} \rangle_{y,DC}$, the profiles look similar at each location up to a scale factor. At 2200 LT (see Figs. 6.8d and 6.9d), the difference in $\langle \tilde{\theta} \rangle_y$ is dramatic at each location: $\langle \tilde{\theta} \rangle_{y,SS}$ is less than zero, while $\langle \tilde{\theta} \rangle_{y,DC}$ is greater than zero. Furthermore, the profiles of $\overline{w'\theta'}$ also have opposite signs, and both change sign as x increases. The SS simulations therefore completely fail to capture the stability of the urban canopy layer according to the DC simulation at this time. This result highlights the significance of surface processes, particularly thermal inertia, on the atmosphere aloft.

6.4 Conclusion

This study quantifies the differences in urban microclimate between a diurnal cycle (DC) simulation that include thermal inertia, with a set of simulations that assume the system is in a steady state (SS) at each hour of the day. Sect. 6.3.1 shows that the SS simulations have very little conduction occurring within the surface, which is associated with large differences in average surface temperature and sensible heat flux in particular compared to the DC simulation. Specifically, the SS simulations generally over-predict surface temperatures and sensible heat flux during the day, and under-predict these during the night. An analogous effect is visible (in Sect. 6.3.2) for the pedestrian-level air temperature and MRT, which has implications for urban design in that there may be large differences in modelled thermal comfort. During the transition between these two situations (in the morning and afternoon), it may be that quantities are quite well-predicted by the SS simulations on average, but there is spatial variation over the domain, as discussed in

Sects. 6.3.1 and 6.3.2. The variation can be partially explained by the net shortwave radiation and sky view factor. For unshaded facets, there appears to be a linear relationship between the surface temperature amplitude in the SS simulation and that in the DC simulation. Further work could be carried out in order to understand the reason for this relationship, and determining if/how it varies across the parameter space. As Sect. 6.3.3 shows, there are also substantial differences between the DC and SS simulations in terms of the vertical structure of the urban canopy layer, particularly after sunset, when thermal inertia is influential. This has implications for processes which are sensitive to atmospheric stability, such as pollutant dispersion (Grylls and van Reeuwijk, 2022). However, it is important to acknowledge that modelling the incoming flow as neutral likely influences the results in Sect. 6.3.3, so while this approach is justified for this case involving a marine boundary layer, the results may not be applicable to other cases involving diurnally-varying atmospheric stability.

The exact nature of the errors incurred by using SS simulations compared to a DC simulation will be case-dependent. Nonetheless, the results presented in this work are expected to be relevant to other cases, particularly those involving urban environments in hot, dry climates. Given that thermal effects are relatively significant in these climates, the differences between the DC and SS simulations are expected to be more apparent. In other climate zones in which the boundary layer evolution over a diurnal cycle is less strongly influenced by the surface energy balance, it is possible that the error would be reduced. The presence of moisture would likely have a strong influence on the thermal inertia and difference thereof between DC and SS simulations (Best and Grimmond, 2014).

It was shown in Chapter 5 that the difference in thermal inertia between the built environment and the surrounding terrain was relatively similar, therefore the terrain was not included in the study in this chapter. However, urban environments often generally exhibit greater thermal inertia than rural ones. If using a case that exhibited greater difference in thermal inertia between urban environment and surroundings, it would be possible to investigate the effect of this assumption with respect to urban-rural differences. Moreover, it may be possible to account for the lack of thermal inertia in the SS simulations by modifying the interior boundary condition in the SEB scheme. Practically, this could utilise the objective hysteresis model (OHM; see Sect. 5.3.1) to estimate the value of the heat storage based on the net shortwave radiation.

The overall conclusion of the results, i.e. that SS simulations do not yield similar predictions in comparison to DC simulation in general, is to be expected. Nonetheless, the results presented here illuminate why this is the case, and give an idea of the error as a function of space and time. In particular, the fact that the system transitions from being underestimated to being overestimated by the SS simulation in the morning, and vice versa in the afternoon, suggests that steady-state simulations may be used more reliably at these cross-over times. By systematic investigation of the parameter space associated with the built environment,³ future work could attempt to provide guidelines for how to correct for the errors incurred by using SS simulations. In any case, the unique methodology employed in this study demonstrates the necessity of considering the evolution of urban microclimate over a complete diurnal cycle in order to reliably capture surface heat transfer, so the work serves something of a reality check. Any numerical study has little relevance without accounting for thermal inertia, and therefore this study motivates further research exploring how to achieve this.

³In particular, varying the materiality so as to modify the bulk thermal response of the surface.

Chapter 7

A diurnal cycle in London

7.1 Introduction

Physical processes within the urban boundary layer (UBL) can be simulated using mesoscale and microscale models, depending on the phenomena of interest (see Sect. 1.4). Mesoscale models are often used to study the characteristic diurnal cycle of the UBL (see Sect. 1.3.3) because they include most of the relevant physical processes, and the use of nesting means that the domain size used is generally large enough to encompass the largest length scales that are present in the UBL. However, turbulence in the atmosphere may be poorly represented by mesoscale models when the associated length scale is at or below the scale of the grid resolution, as small-scale flow behaviour must be parameterised (Dudhia, 2014, 2022). Furthermore, an urban canopy model (UCM) is used to model surface exchanges, which do not explicitly resolve the surface and often assume a simplified morphology (Lipson et al., 2024). Due to the low spatial resolution and assumptions regarding the geometry, UCMs can struggle to accurately capture processes relevant to the urban canopy layer (UCL) and surface energy balance (SEB). In particular, there are challenges surrounding radiative transfer (Schoetter et al., 2023), the distribution of surface shear stress and heat fluxes, (Schoetter et al., 2020; Sützl et al., 2021a,b), and parameterisation of turbulent and dispersive fluxes (Blunn et al., 2022; Nagel et al., 2023), which become particularly relevant as the resolution increases (Hertwig et al., 2021; Lean et al., 2024).

By resolving air flow at high resolution and explicitly modelling radiative transfer between buildings and other features, microscale models are expected to capture atmospheric turbulence and surface exchanges more accurately than mesoscale models. As a

result, microscale models are often used (with simplified, idealised geometries) to inform surface parameterisations for mesoscale models (Martilli et al., 2015; Nazarian et al., 2020; Buccolieri et al., 2021). Some studies consider the evolution over a diurnal cycle (Nazarian and Kleissl, 2015; Chen et al., 2021*a,b*; Saxena and Yaghoobian, 2022), but the representation of the atmosphere is typically simplified as resolving the entire (characteristically non-neutral) UBL is expensive, and microscale models may lack physical processes that are important to the development. To address this, mesoscale model output can be used to force the flow (e.g. Kaoru et al., 2011; Resler et al., 2020; Geletič et al., 2021; Anders et al., 2023). However, these studies use realistic geometries and are conducted for the purposes of model evaluation, rather than to explore how the surface influences the UBL and SEB in bulk (from a mesoscale perspective). Comparing mesoscale and microscale models (over a diurnal cycle) is vital for their improvement, though this is relatively rare.

This study investigates the influence of morphology on atmospheric and surface conditions predicted by uDALES v2.0 over a diurnal cycle while coupling with and comparing to a mesoscale model (MetUM; Walters et al., 2019). MetUM and uDALES v2.0 are set up in an equivalent manner and used to simulate an area of central London, UK (described in Sects. 7.3 and 7.4 respectively), and are compared to observations from two measurement sites at different heights within the UBL (described in Sect. 7.2). The atmospheric state in uDALES is nudged towards MetUM output above a certain height using time-height profile assimilation in order for the mean flow predicted by the models to approximately match. In terms of the drag exerted by the surface, the UCM used by MetUM uses parameterisations based on staggered cubic arrays, whereas the SEB scheme assumes the geometry consists of infinite canyons. Therefore, uDALES is run with these two idealised configurations, as well as a realistic geometry generated using a high resolution building dataset. The idealised geometries used in uDALES are set up to match the morphometric indicators that are supplied as parameters to the surface scheme in the MetUM, namely the plan area fraction (λ_p), frontal area fraction (λ_f), and mean building height (h). Section 7.5.1 presents the mean flow quantities in uDALES that are nudged towards MetUM data to check the efficacy of the forcing technique over the vertical extent of the atmospheric boundary layer and to analyse any differences in near-surface behaviour (below nudging height). Section 7.5.2 investigates the turbulence statistics predicted by the two models, in particular the shear stress and sensible heat

flux, to assess whether the models capture turbulence in a similar manner despite their different spatial resolution. Section 7.5.3 compares the mean and turbulent flow quantities to observations at the measurement sites; one of which is just above average roof height, while the other is approximately 200 m above the ground. Finally, Sect. 7.5.4 focuses on the SEB, namely the bulk SEB of the two models and the breakdown of the SEB for the uDALES simulations by facet type (streets, walls, roofs).

7.2 Case description

During the ACTUAL campaign (Barlow et al., 2015), two measurement sites recorded observations of the UBL over London; one located at the top of the BT Tower (latitude, longitude = 51.5216, -0.1390) at a height of 191 m, and the other on the rooftop of Westminster City Council (WCC) (latitude, longitude = 51.5212, -0.1606) at a height of 18 m. The date for this study is 30/09/2011, as the measurements taken between 28/09/2011 and 01/10/2011 suggest this was an unusually cloudless, low wind, high pressure period. As described in Sect. 1.3.3, under these conditions local effects (due to the surface) are more pronounced and are significant in determining the evolution.

The observations suggest that from sunrise at 0600 UTC¹ to around midday, a convective boundary layer (CBL) develops, with the height increasing during this time. This is characterised by a mixed layer bounded by an unstable surface layer below and a stable capping inversion above. From 1300 to 1600 UTC, the CBL is fully developed, with the height approximately constant. The mixing height reaches a maximum of approximately 1.4 km (Barlow et al., 2015; Lean et al., 2019). Above the CBL lies the free atmosphere, which is largely unaffected by the surface and is weakly stable. From 1700 to 2000 UTC, the CBL decays, forming a stable residual layer. From 2100 to 0000 UTC there is a stable boundary layer, though the surface layer remains slightly unstable. Finally, from 0100 to 0600 UTC the surface layer eventually becomes stable as well, or at least neutral. The evolution is visible in Fig. 7.1, which shows the square of the buoyancy frequency (N) predicted by MetUM, calculated using instantaneous data at the grid cell containing the BT tower. Note that the evolution is approximately cyclic, meaning the description of the UBL development applies to both the first day and the second day of the study period.

¹Note that the local time is British Summer Time (BST = UTC + 1).

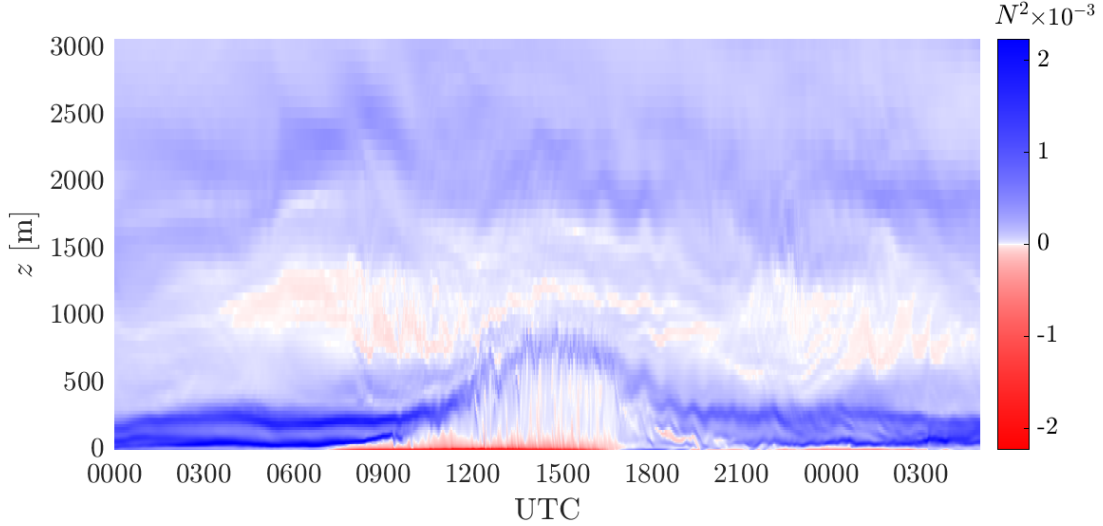


Figure 7.1: Evolution of the square of the buoyancy frequency (N ; see Table 2.1) calculated using instantaneous UM output for the BT tower grid cell.

7.3 MetUM

For the current work, Met Office Unified Model (known as MetUM or ‘the UM’; Walters et al., 2019) was set up as in the same manner as in Lean et al. (2019). A nested set of model configurations (shown in Fig. 7.2) were run with MetUM v11.4, with the largest being the 1.5 km resolution model used for operational forecasting (the ‘UKV’; Tang et al., 2013), which covers the UK, Ireland, and northern France and includes data assimilation from observations. A 500 m model with a domain size of $300 \text{ km} \times 300 \text{ km}$ covering southern and central England is one-way coupled to the UKV, and finally within the 500 m model is a 100 m model with an $80 \text{ km} \times 80 \text{ km}$ domain that is centred on London. The higher-resolution models use a 140-level set in the vertical direction, which consists of the standard 70-level set used for the UKV doubled all the way up to the domain top at 40 km. The orography and land use data are based on 100 and 25 m datasets respectively, with the latter based on the Institute of Terrestrial Ecology dataset (ITE; Bunce et al., 1996). In the land-surface model (LSM) used by the UM (JULES; Best et al., 2011), each grid box contains a percentage land use of each cover type (or ‘tile’). There are ten tiles; five vegetative and five non-vegetative, including two urban (built) types; the total urban fraction is visible in Figs. 7.2 and 7.3a. The surface exchanges are calculated separately for each tile and the results are averaged, accounting for the fractional area of each tile. This is justified by the concept of a blending height (conceptually related to the inertial sub-layer; Essery et al., 2003). Note however that in standard MetUM versions, the fluxes

are applied at the first atmospheric level rather than at the blending height. The ability to ‘distribute’ the fluxes in the vertical direction in order to faithfully capture the effect of building height is an active research area (e.g. Sützl et al., 2021a,b). The surface shear stress (τ_s) and sensible heat flux (H) are calculated according to the bulk transfer approach (similar to Eq. (2.9)).

The UCM used in JULES (MORUSES; Porson et al., 2010a) assumes the urban morphology consists of a 2D street canyon for the SEB scheme; one tile corresponds to the roofs and the other to the canyon walls and streets combined. This two-tile scheme was shown to be as accurate as a four-tile scheme (a roof, two walls, and a street) when compared with idealised observations of surface fluxes (Porson et al., 2010b). The material properties, including the albedo (α), emissivity (ϵ), volumetric heat capacity (C), and thermal diffusivity (κ) are specified for the streets, walls, and roof separately. The morphological parameters describing the urban tiles are the street canyon width (c), the building width (b), and the building height (h), which are derived from the urban land cover fraction using empirical relationships (established in Bohnenstengel et al., 2011).

The morphological parameters can be used to calculate morphometric indicators, in-

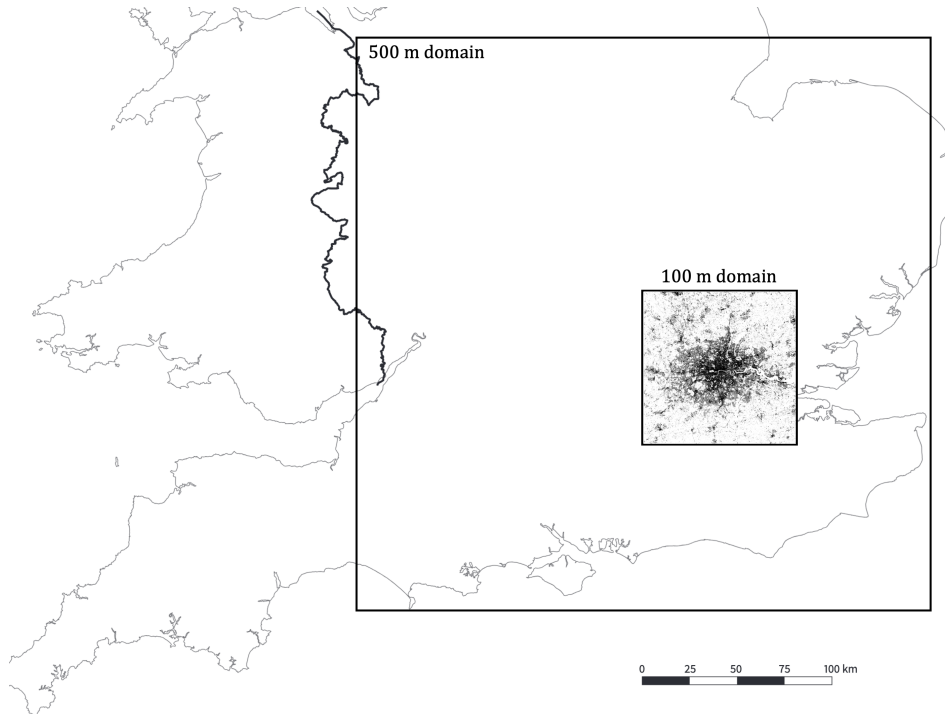


Figure 7.2: Nested domain configurations used by the Met Office Unified Model overlaid on an outline map of the UK (Ordnance Survey, 2016). The image of Greater London visible within the 100 m domain is determined by the urban land use fraction parameter used in the land-surface scheme, with darker being higher (Lean et al., 2019)

cluding the plan area fraction $\lambda_p = b/(b + c)$ and the direction-averaged frontal area fraction $\lambda_f = \frac{2}{\pi}h/(b + c)$ (the factor of $\frac{2}{\pi}$ accounts for the averaging over all wind directions). Morphometric indicators (h , λ_p , and λ_f) for a $10 \text{ km} \times 10 \text{ km}$ area in the centre of London are shown in Fig. 7.3b-d. The city appears heterogeneous at the neighbourhood scale ($\mathcal{O}(100 \text{ m} - 1 \text{ km})$), with features including large parks and the River Thames visible. For the urban tiles, the roughness length (z_0) is calculated using an empirical formula for staggered cubic arrays using the value of λ_p (Macdonald et al., 1998, see Appendix E).

For the SEB, each tile is modelled as a single layer that is coupled to the soil via the ground heat flux (G) and to the air via the sensible heat flux (H). The SEB scheme in MORUSES is discussed in further detail in Appendix E. The thickness (D) of the layer is set to $(2\kappa/\Omega)^{\frac{1}{2}}$ where Ω is the angular frequency of the Earth’s rotation, corresponding to the penetration depth (δ) defined in Sect. 2.2. The material properties are based on a previous study of London (Bohnenstengel et al., 2011), which are used to define the parameters set in uDALES given in Table 7.3.

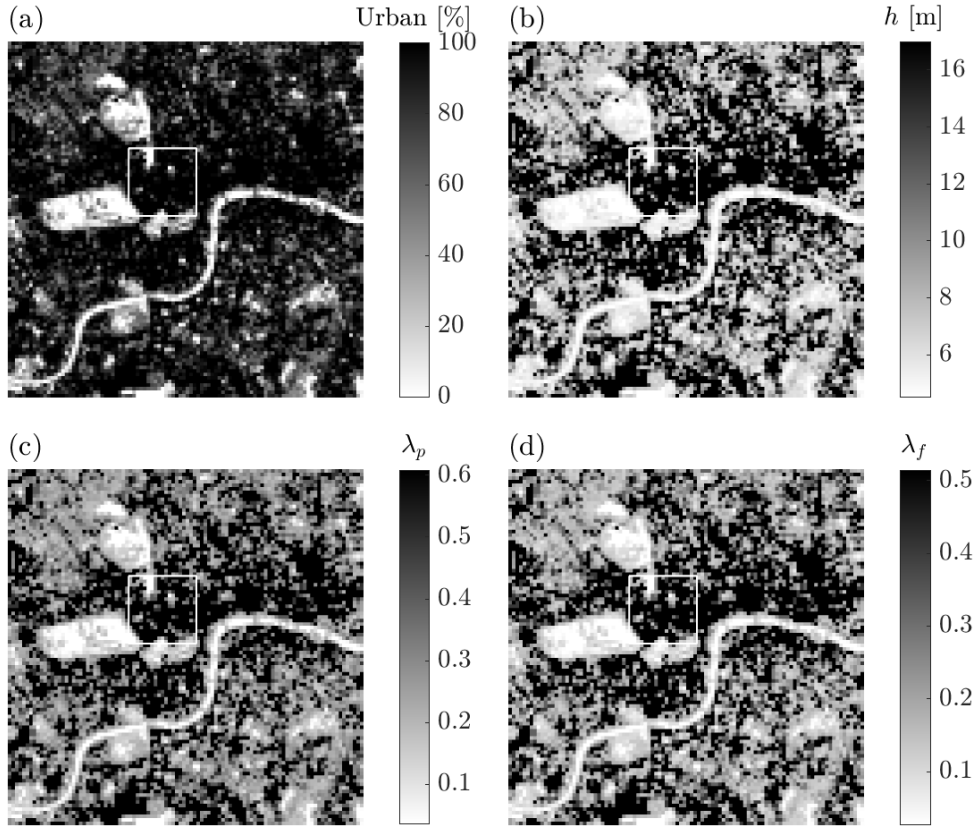


Figure 7.3: The morphology of a 100 km^2 area of central London according to MORUSES at 100 m resolution: (a) urban (built) fraction (sum of canyon and roof tiles), mean building height (h), plan area fraction (λ_p), and frontal area fraction (λ_f) (Bunce et al., 1996; Bohnenstengel et al., 2011). White squares indicate the uDALES area of interest.

7.3.1 Coupling data

The UM was run for 36 hours from 1800 UTC on 29/09/2011 to 0600 UTC on 01/10/2011, with the first 6 hours consisting of spin-up time, and the remaining 30 hours used to compare with uDALES output. To generate the data to force the uDALES simulations, several quantities in the UM output are horizontally averaged over the $2 \text{ km} \times 2 \text{ km}$ area indicated in Fig. 7.3 (this choice of area is justified below in Sect. 7.4). The atmospheric quantities that are used are the mean vertical profiles of wind speed ($\mathbf{u}$) and potential temperature (θ), with the period for the time averaging being 15 minutes.² The instantaneous surface variables that are used are the sensible heat flux (H) and incoming longwave flux ($L^\downarrow$), which are available every 15 minutes and hourly respectively.³

To generate cyclic forcing data from the available UM output so as to be able to run multiple days in succession with uDALES, the variables are ‘blended’. During the blending period, which is 0000 to 0600 UTC on 01/10/2011, the output from the same period on 30/09/2011 is linearly assimilated with the output on 01/10/2011 so that the forcing data at the end of the blending period matches the output at 0600 UTC on 30/09/2011. Denoting output from days 1 and 2 by φ_1 and φ_2 respectively and time-shifting one of the signals by 24 hours such that $t = 0$ corresponds to 0000 UTC on both days, the ‘blended’ forcing data is given by:

$$\varphi(t) = \frac{t}{t_b} \varphi_1 + (1 - \frac{t}{t_b}) \varphi_2, \quad 0 \leq t \leq t_b. \quad (7.1)$$

Here the blending period $t_b = 21600 \text{ s}$. The result of interpolating the non-blended and blended profiles onto the uDALES vertical grid are shown in Fig. 7.5. The surface sensible heat flux is shown in Fig. 7.4 and the longwave flux is shown in Fig. 7.9b.

The wind in the UM is defined in the easterly (zonal) and northerly (meridional) directions, denoted by u_E and u_N respectively. To determine the nudging velocity components with respect to the uDALES domain coordinates, denoted u_x and u_y , a rotation is applied by an angle $\Phi_{E \rightarrow x}$:

$$\begin{bmatrix} u_x \\ u_y \end{bmatrix} = \begin{bmatrix} \cos \Phi_{E \rightarrow x} & -\sin \Phi_{E \rightarrow x} \\ \sin \Phi_{E \rightarrow x} & \cos \Phi_{E \rightarrow x} \end{bmatrix} \begin{bmatrix} u_E \\ u_N \end{bmatrix} \quad (7.2)$$

²The timestamps for the time-averaged data correspond to the midpoint of each averaging window.

³All forcing data (time-averaged or instantaneous) is interpolated onto the uDALES flow time steps to ensure consistency.

Since the wind is initially south-easterly according to observations (Barlow et al., 2015), $\Phi_{E \rightarrow x}$ should be in this quadrant, i.e. $90 \leq \Phi_{E \rightarrow x} \leq 180$. The exact value is given and justified in Sect. 7.4 by taking into consideration the street layout of central London.

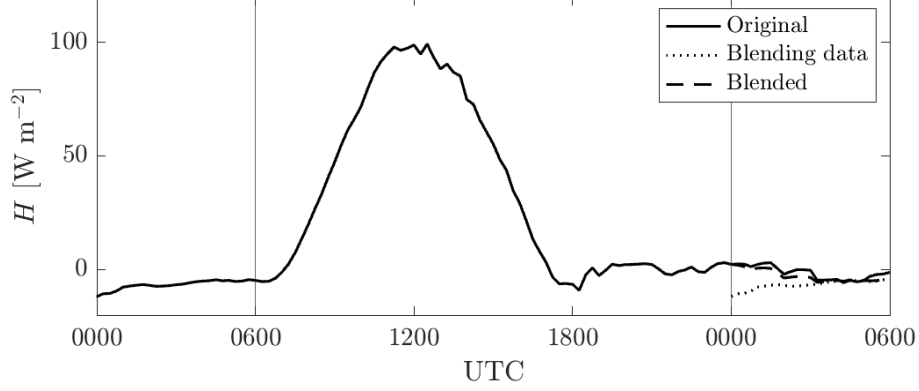


Figure 7.4: Surface sensible heat flux (H) from MetUM (averaged over area of interest shown in Fig. 7.3), prescribed in the uDALES precursor simulation (SC0), including an illustration of the blending procedure: between 0000 and 0600 UTC on the second day, data from the first day is blended (linearly assimilated) such that the final signal is cyclic.

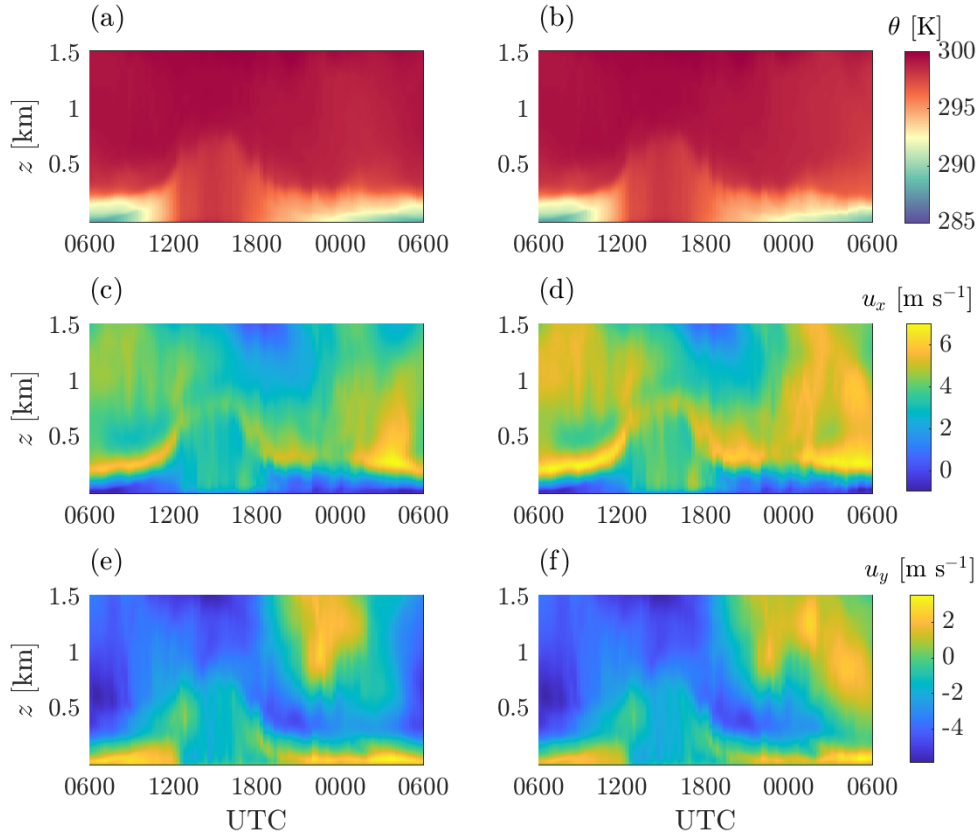


Figure 7.5: Atmospheric quantities from MetUM (averaged over the area of interest shown in Fig. 7.3) against height above ground level (z), used to force the uDALES simulations (via nudging), blended and non-blended respectively: (a,b) potential temperature (θ), (c,d) x component of velocity (u_x), and (e,f) y component of velocity (u_y).

Table 7.1: uDALES simulation nomenclature and set-up including domain size, grid size, and boundary conditions (BC).

	SC0	SC1	IC1	IC2	R
L_x [m]	1920	1920	1920	1920	960
L_y [m]	1920	1920	1920	1920	1920
L_z [m]	960	1536	1536	1536	960
N_x	960	960	960	960	480
N_y	960	960	960	960	960
N_z	320	480	480	480	320
BC (surf.)	Prescribed H	SEB	SEB	SEB	SEB
BC (x)	Periodic	Periodic	Periodic	Periodic	Inflow-outflow
Notes	Precursor for R		Canyons $\parallel y$	Canyons $\parallel x$	Inflow from SC0

7.4 uDALES

A summary of the uDALES simulations is given in Table 7.1. They include case SC0, which consists of staggered cubes with the surface sensible heat flux prescribed (using UM output — see Fig. 7.4), and is used as a precursor simulation for case R, which has realistic buildings and uses the SEB scheme. Several other simulations use the SEB scheme, including case SC1, which has staggered cubes (like SC0), and cases IC1 and IC2, which both have infinite canyons. In the former, the canyons are perpendicular to the streamwise direction, while in the latter they are parallel. The simulations with idealised geometries (SC0, SC1, IC1, IC2) use periodic lateral boundary conditions, while the realistic geometry simulation (R) uses inflow-outflow conditions.

The morphologies are based on a $2 \text{ km} \times 2 \text{ km}$ area at the centre of London that is indicated in Figs. 7.3 and 7.6. This area of interest (AOI) is intended to be representative of the observations as it contains the BT tower and the WCC rooftop is only slightly outside it.⁴ The buildings within the AOI tend to lie on a grid that is at an angle of approximately 17° anticlockwise from north (see Fig. 7.6), and this is chosen to be the x direction (corresponding to $\Phi_{E \rightarrow x} = 107^\circ$). According to the UM surface morphological properties (see Fig. 7.3), the ‘urban’ tile fraction in the AOI is relatively high ($\approx 80\%$) and the morphometric indicators are fairly uniform. This means that vegetation is neglected in uDALES and that it is reasonable to represent the area using idealised geometries that are homogeneous at the street canyon scale. The UM surface properties for the grid boxes within the AOI are $h \approx 16 \text{ m}$, $\lambda_p \approx 0.55$, and $\lambda_f \approx 0.45$.⁵

⁴Yu et al. (2023) divided London into 1 km^2 zones; the four central ones are used as the AOI.

⁵These parameters yield $z_d \approx 13 \text{ m}$ and $z_0 \approx 0.5 \text{ m}$ using the formulae in Appendix E



Figure 7.6: Plan view of buildings in central London (Ordnance Survey, 2019) with the area of interest (AOI) and realistic geometry domain for uDALES indicated.

For the idealised geometries, shown in Fig. 7.7, it is not possible in general to obtain any arbitrary combination of morphometric indicators exactly. The configurations used for this study, shown in Table 7.2, were chosen to match the mean building height (h) in the UM, with the building width (b) and canyon width (c) chosen to obtain similar λ_p and λ_f (while also having a repeating unit whose dimensions divide the computational domain size). As previously mentioned, two possible orientations for the canyon geometry are included in this study; one aligned with the x direction (as in Fig. 7.7) and the other with the y . Given that MORUSES considers a canyon with no particular orientation (averaged over all directions), a comprehensive comparison would include more orientations than these two, but this would be prohibitively computationally expensive, and in this case it is apparent which orientations are likely to be more similar to the real urban area.

For the realistic geometry, a domain based on the AOI (shown in Fig. 7.6) was selected such that it contains the measurement sites and accounts for the lateral boundary conditions. The presence of large parks surrounding the AOI makes this challenging. The y direction is periodic, which is reasonable in this case since the two sides of the domain are fairly similar in terms of street layout. The x direction is inflow-outflow, and the upwind side is likely to be representative of the AOI since the flow is broadly south-easterly. The

Table 7.2: Morphometric indicators for staggered cubes (SC), infinite canyons (IC), and realistic (R) geometries in uDALES: building width (b), canyon width (c), building height (h), plan area fraction (λ_p), frontal area fraction (λ_f), and complete area fraction (λ_c). The average building width for case R is given by $b = \Gamma / (N_b \pi)$, where Γ is the perimeter of the buildings at ground level and N_b is the number of buildings (Sutzi, 2021), while h is defined as the area-weighted average height of the roofs. The direction-averaged λ_f for R is approximated here by bh/A_t , where A_t is the total plan area of the domain.

Geometry	b [m]	c [m]	h [m]	λ_p [-]	λ_f (x wind) [-]	λ_f (avg. wind) [-]	λ_c [-]
SC	16	8	16	0.44	0.44	0.57	2.78
IC	12	12	16	0.5	0.42	0.66	2.33
R	18.0	-	15.5	0.43	0.26	0.64	2.09

terrain is assumed to be flat for all cases, and so z denotes height above ground level.

The geometry includes buildings (from Ordnance Survey, 2019)⁶ that are entirely within the chosen domain, and each is initially represented as a polygon with an associated height, which is vertically extruded to form a prism. The base is removed, while the roof and walls are divided into facets (see Sect. 3.4), forming a triangulated surface. The next step is to remove non-manifold features, i.e. overlapping walls, as this would introduce errors in the SEB scheme. Therefore, the coinciding walls are subtracted, e.g. the overlapping area is removed, and new facets are formed from the resulting polygons. Finally, ground facets are constructed using a quadrilateral mesh with an edge length of 8 m, which is then triangulated to form facets. Note that the ground facets are similar in size to that of the idealised geometries, and are relatively small compared to the roof facets in order to capture shading with greater accuracy. The final geometry has similar values of h , b , λ_p , and direction-averaged λ_f to the idealised geometries (see Table 7.2).

The horizontal domain size for the periodic (idealised) simulations is $L_x \times L_y = 1920 \text{ m} \times 1920 \text{ m}$, which is roughly equal to the area of the AOI and is large enough to avoid self-interaction of streamwise structures due to circulation in the convective boundary layer (CBL) at $\mathcal{O}(1 \text{ km})$ scale. The inflow-outflow (realistic) simulation has $L_x \times L_y = 960 \text{ m} \times 1920 \text{ m}$; due to computational constraints (associated with the more complex geometry), L_x is smaller than for the periodic simulations, though this is acceptable as the flow does not self-interact in the x direction unlike them. The idealised simulations using the SEB scheme (SC1, IC1, and IC2) have $L_z = 1536 \text{ m}$, which is larger

⁶The Ordnance Survey (2019) building data is more recent than the dataset used by the UM, though the AOI has seen comparatively little development (compared to other areas of London) during this period that would significantly alter the morphometric indicators (Sutzi, 2021).

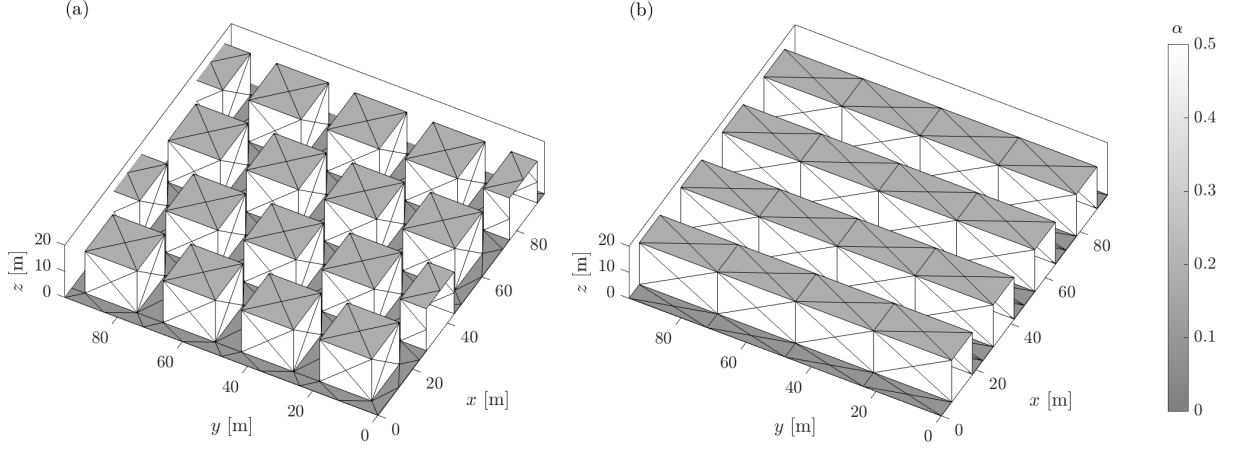


Figure 7.7: Several repeating units of the idealised geometries used in uDALES: (a) staggered cubes and (b) infinite canyons, with facets coloured by albedo (α ; see Table 7.3).

than the mixing height of approximately 1.4 km (Barlow et al., 2015; Lean et al., 2019). The precursor and corresponding inflow-outflow simulations (SC0 and R respectively) have $L_z = 960$ m, which is likely to be sufficient to resolve the full vertical extent of the CBL (see Fig. 7.5 for example), though does not capture as much flow above the CBL. In both cases, the largest structures (on the scale of the CBL depth) are contained within the domain. At the top boundary, a zero flux condition is used for the potential temperature for all simulations, and a free-slip condition is used for the periodic simulations, while the inflow-outflow simulation has a non-zero vertical velocity component (see Sect. 3.3).

The flow in the periodic simulations is nudged towards the profiles from the UM above a certain height that theoretically should correspond to the top of the roughness sub-layer (RSL). This is approximately $2-5h$ over urban areas so is accordingly set to $3h = 48$ m (Barlow, 2014). Blended data is used for the first day, while for the second day the true data is used, with the results presented in Sect. 7.5 corresponding to the second day. The nudging is given by the term (see Eqs. 2.16 and 2.17):

$$F_\varphi = \frac{\varphi_{\text{UM}} - \langle \varphi_{\text{uDALES}} \rangle}{t_{\text{nudge}}}, \quad (7.3)$$

for $\varphi = \{u_x, u_y, \theta\}$ and $t_{\text{nudge}} = 900$ s. For the precursor simulation, a plane normal to the x direction is written every 10 s. This is relatively large in comparison to the LES time step of $\mathcal{O}(0.1$ s) due to practical constraints on disk space, meaning the smallest scales of the turbulence are unlikely to be captured. However, it is sufficient to resolve wind gusts and convective motion, and smaller-scale motion develops quickly after flow enters

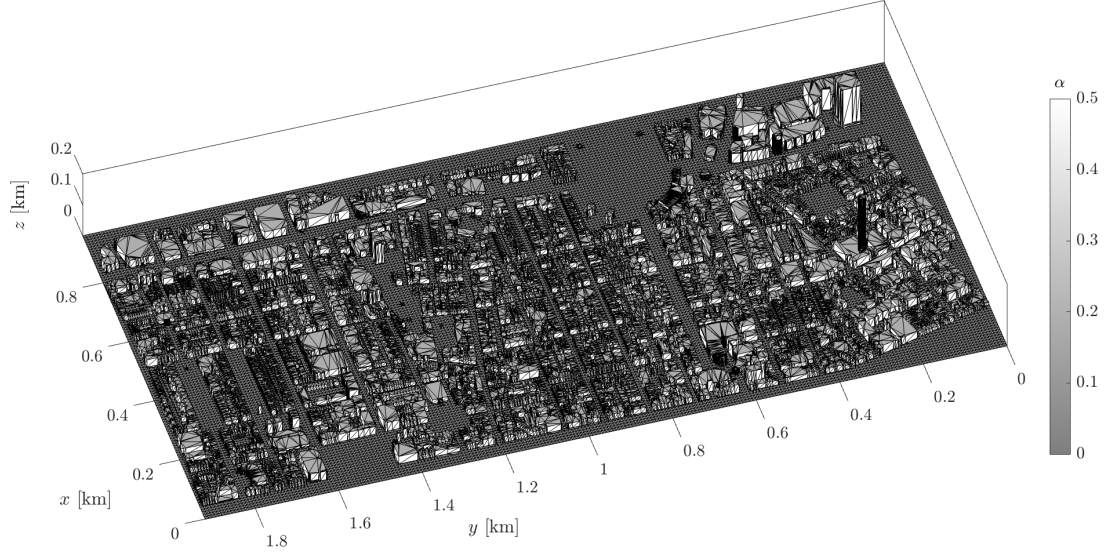


Figure 7.8: Realistic geometry used in uDALES, with facets coloured by albedo (α ; see Table 7.3). Note that the vertical extent has been cropped; the domain height is 960 m.

the domain (in the inflow-outflow simulation) from these larger-scale processes.

The grid resolution used is 2 m in the x and y directions, as well as the z direction up to 196 m (greater than the height of the BT tower), with a non-equidistant grid above.⁷ For the precursor simulation (SC0), the UM sensible heat flux (see Fig. 7.4) is prescribed on roof and ground facets. The hourly data is interpolated to the LES time steps during the simulation. For the others, the flux varies according to the SEB. In contrast to JULES, in uDALES the momentum and heat roughness lengths (z_0 and $z_{0,h}$) are user-defined parameters (and refer to facets rather than tiles — see Sect. 7.3). In this study, $z_0 = 0.05$ m and $z_{0,h} = 0.00035$ m (following Cai (2012); $\log(z_0/z_{0,h}) \approx 5$ for rough walls).

The facet properties used for the SEB scheme are intended to match those used for MORUSES (see Table 7.3). The thermal conductivity (λ) is calculated using the values of volumetric heat capacity (C) and thermal diffusivity (κ) provided in Bohnenstengel et al. (2011) (according to $\lambda = \kappa C$). The method for calculating tile thickness (D) in MORUSES based on the thermal penetration depth yields relatively small values ($D \approx 0.1$ m). In uDALES, the facet thickness is set to more realistic, larger values. In particular, the ground facets are many times thicker than the penetration depth in order for the temperature oscillations, and therefore the heat flux, to be negligible at the interior.

The ASHRAE (2011) solar radiation model is used to provide values of direct solar irradiance (I) and diffuse sky irradiance (D_{sky}), which are shown in Fig. 7.9a. According

⁷With just 4-6 grid cells within each street canyon, this resolves the flow at a minimal level of detail, which is acceptable given that this is not the focus of this study.

Table 7.3: Facet properties used in the uDALES SEB scheme: albedo (α), emissivity (ϵ), volumetric heat capacity (C), and thermal conductivity (λ) (based on MORUSES; Bohnenstengel et al., 2011), as well as thickness (D) and number of layers (N_l).

Parameter	Units	Streets	Walls	Roofs
α	-	0.08	0.5	0.18
ϵ	-	0.95	0.9	0.92
C	$\text{MJ m}^{-3} \text{K}^{-1}$	1.94	1.37	1.77
λ	$\text{W m}^{-1} \text{K}^{-1}$	0.74	0.84	0.83
D	m	0.8	0.4	0.4
N_l	-	10	10	10

to this model, for clear skies $I = \mathcal{A} \exp(-\mathcal{B}/\cos \Theta)$ and $D_{\text{sky}} = \mathcal{C}I$, where the parameters are set to the September values: $\mathcal{A} = 1152 \text{ W m}^{-2}$, $\mathcal{B} = 0.177$, and $\mathcal{C} = 0.092$. This formulation depends on the solar zenith angle (Θ), which is determined using the National Oceanic & Atmospheric Administration (NOAA) (2024) algorithm. The sky longwave radiation (L_{sky}) is set to the incoming longwave radiation output from the UM, which was estimated using the net longwave radiation at the surface and the average surface temperature, and is shown in Fig. 7.9b. The SEB time step is set to 60 s in uDALES, meaning K^* and L_{sky} are interpolated during the simulation. The facets are discretised into 10 layers, and the initial surface temperature of each is set to 288 K, which is approximately equal to the air temperature at the lowest atmospheric level in the UM at 0600 UTC. The initial room and soil temperatures are set to 293 K. The simulations start at 0600 UTC, just before sunrise, and are run for one day as spin-up (using blended forcing data) in order to ensure the facet temperatures are in an approximately cyclic state (independent of the initial conditions). The simulations were run on ARCHER2 (EPCC, 2022) using 6,400 processors (50 nodes), which results in a runtime of approximately 24 hours each.

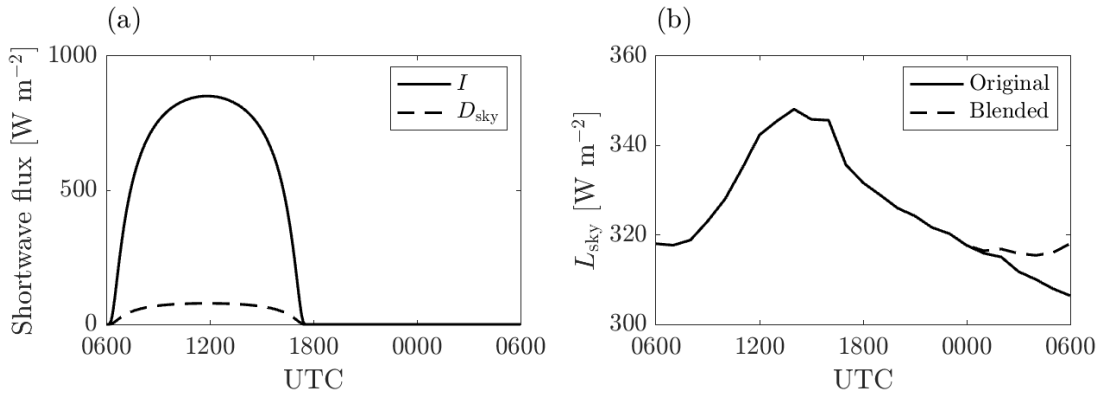


Figure 7.9: Radiative forcing used in the uDALES SEB scheme: (a) direct normal (I) and diffuse sky (D_{sky}) shortwave radiation, and (b) sky longwave radiation (L_{sky}).

7.5 Results

7.5.1 Mean flow

The nudging method (see Eq. 7.3) is designed to force the horizontally-averaged vertical profiles of potential temperature and velocity components towards those of the UM within the AOI. These mean quantities, shown in Fig. 7.10 at several times of day, show good agreement in the upper UBL, indicating that the forcing method works as expected. To investigate the behaviour below nudging height (48 m), Fig. 7.11 shows only the lowest 96 m. The potential temperature for all uDALES simulations agree fairly well with the UM in the late morning (1000 UTC), afternoon (1400 UTC), and evening (1800 UTC) but at night (2200 UTC and 0200 UTC) and the early morning (0600 UTC) there is greater disagreement. By eye, the IC cases appear to underestimate the potential temperature compared to the UM, while the SC0 cases overestimates it, and the SC1 case is the closest.

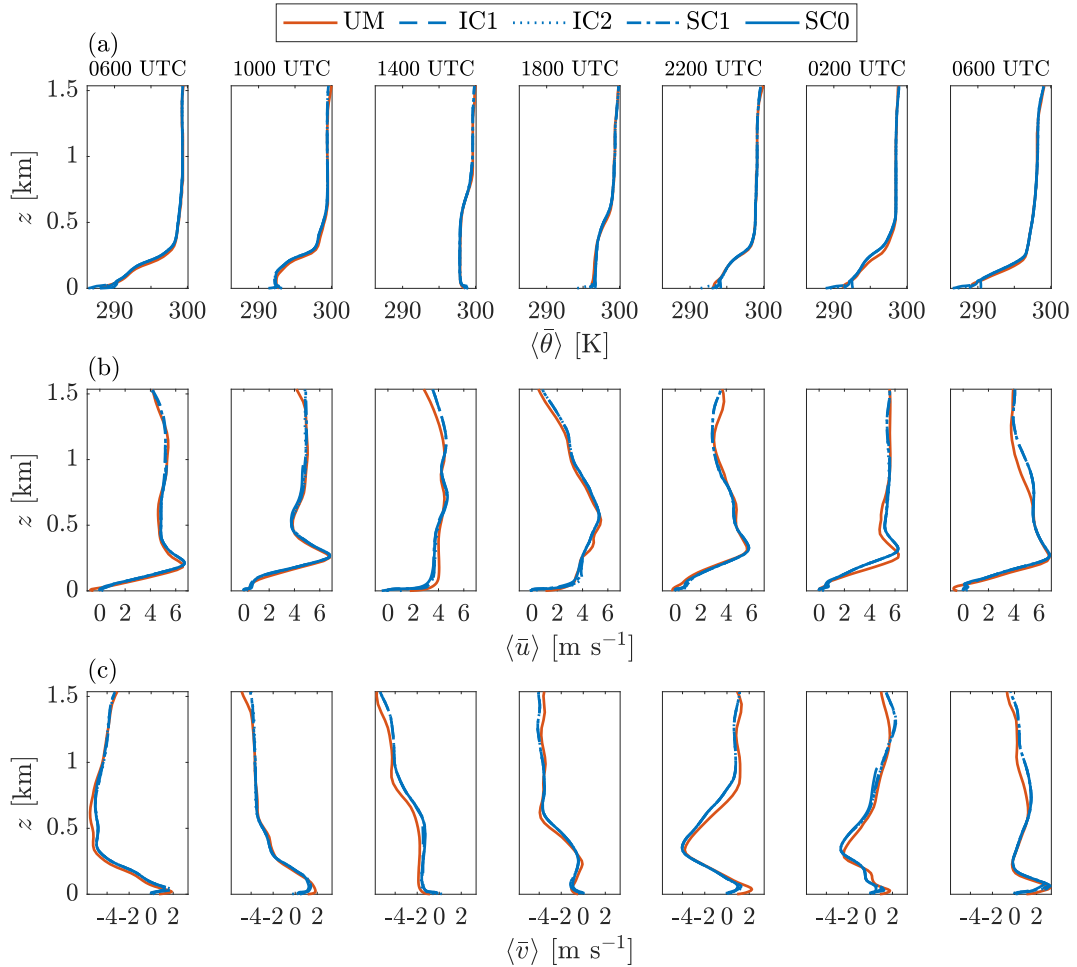


Figure 7.10: Vertical profiles of mean quantities: (a) potential temperature $\langle \bar{\theta} \rangle$, (b) x velocity component $\langle \bar{u} \rangle$, and (c) y velocity component $\langle \bar{v} \rangle$.

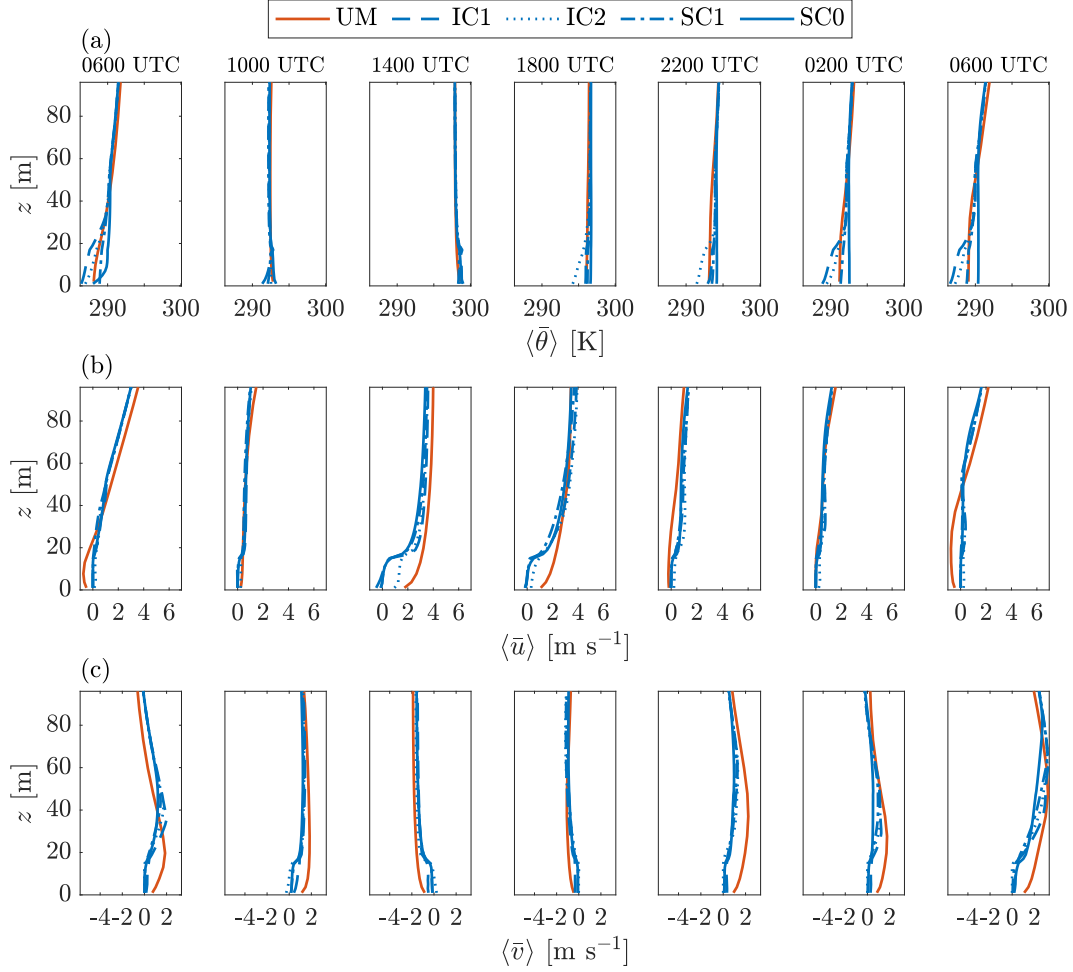


Figure 7.11: Vertical profiles of mean quantities below 96 m (twice nudging height): (a) potential temperature $\langle \bar{\theta} \rangle$, (b) x velocity component $\langle \bar{u} \rangle$, (c) y velocity component $\langle \bar{v} \rangle$.

On first impressions, this is somewhat surprising given that the sensible heat flux for SC0 is set directly by that of the UM, and is therefore intuitively expected to have the most similar effect on the near-surface temperature.

The velocity components for the uDALES simulations are generally lower than for the UM below the nudging height, which is expected given the explicit resolution of buildings in uDALES. There is a visible displacement height, and within the street canyon (up to 16 m), the mean of each velocity component is expected to be low due to flow recirculation in the canyon, though the wind speed evaluated at any particular location in space may be higher. In contrast, the UM does not exhibit any actual displacement of the flow, since the value of z_d used in the surface scheme is merely used to parameterise the flux that is exerted at ground level, and the model is not able to resolve canyon circulation. The fact that SC1 exhibits higher velocity than the other uDALES simulations (e.g. at 1400 UTC) is because the canyons are parallel to the x direction, so there is less flow obstruction.

7.5.2 Turbulence statistics

The total vertical fluxes for the uDALES simulations using idealised geometries is defined as the horizontal average over the entire domain, and accounts for the dispersive fluxes as well as turbulent fluxes (see Sect. 2.1.2 and Appendix A).⁸ For the UM, the total vertical flux is the sum of a parameterised and a resolved component, which are generally similar in magnitude in relatively high-resolution (100 m) configurations like the one here (Lean et al., 2019). While the parameterised flux is available as model output, the resolved flux must be calculated manually. This is achieved using a spatial average over a large area (5 km $\times$ 5 km) with the same centre as the AOI, with the resolved vertical flux of a quantity φ given by $\langle w\varphi \rangle - \langle w \rangle \langle \varphi \rangle$. Following Lean et al. (2019), this is interpreted as the flux at the central grid cell within this larger area, which is assumed to be representative of the AOI. Unlike for uDALES, the data is not time-averaged, which potentially reduces the accuracy of the statistics.

Figure 7.12 show the total sensible heat flux and the shear stress in the x and y directions for the uDALES periodic simulations and the UM. The sensible heat flux shows good agreement in the day (1000 UTC and 1400 UTC), with the profiles characteristic of a developing CBL (Garratt, 1994). At night (2200 UTC and 0200 UTC), both models exhibit values close to zero, indicating the decay of turbulence into a neutral residual layer. By the early morning (0600 UTC) the UM behaviour near the surface is characteristic of a stable boundary layer, though this is not reproduced by uDALES. It is possible that this behaviour is due to radiative transfer in the atmosphere, which is not modelled by uDALES. The stresses in the uDALES simulations show fair agreement with each other and with the UM within the boundary layer (up to approximately 750 m), with the x component matching more closely than the y component. Above it, uDALES exhibits large values, which may be due to the nudging compensating for the lack of Coriolis forcing (which is present in the UM).

Figure 7.13 show the sensible heat flux and shear stresses in the lowest 96 m only. For all quantities, the nighttime values are very low in magnitude for all model configurations, though note that the UM has larger (more negative) values of sensible heat flux above building height than uDALES, which suggests that the sensible heat flux is not due to surface cooling. In the daytime, the sensible heat flux for the SC0 case matches the

⁸In this case, the dispersive fluxes tend to be relatively small, especially far from the surface.

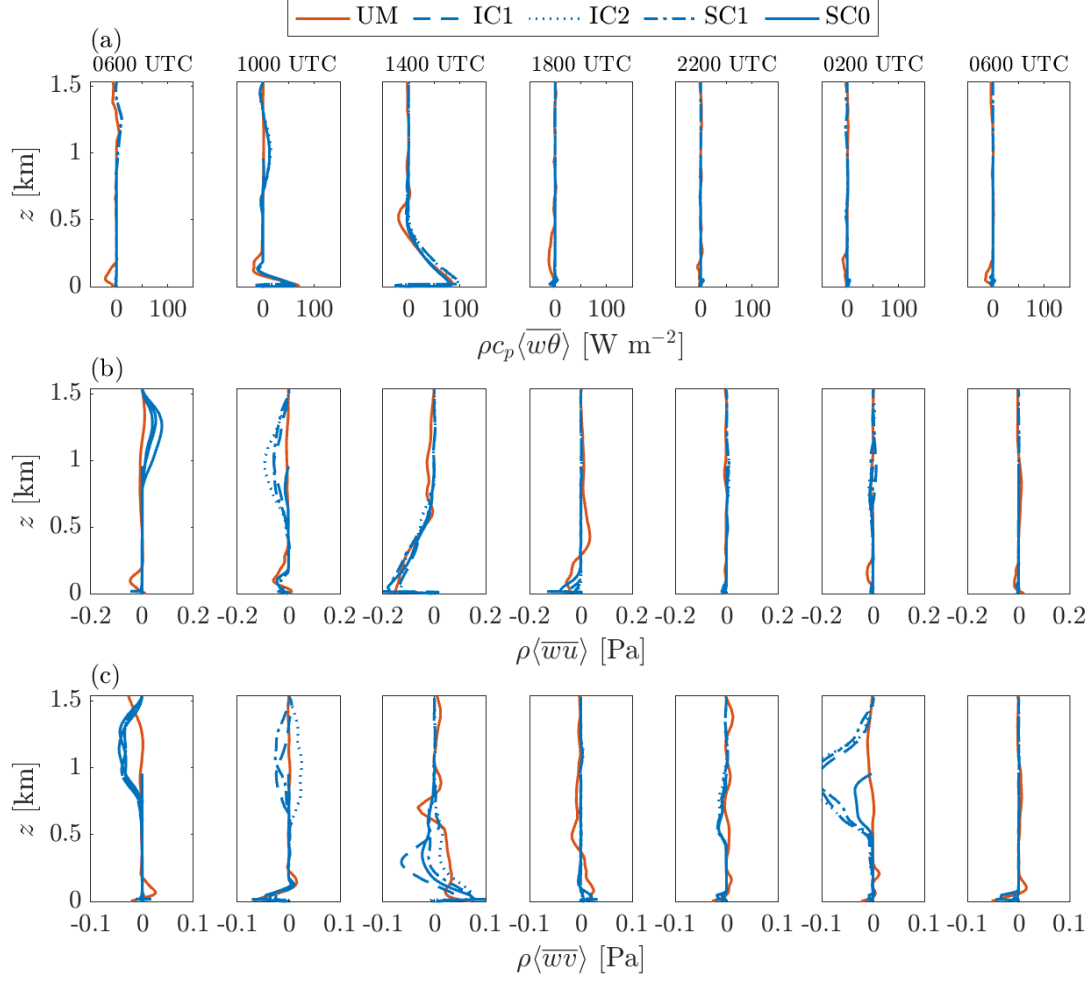


Figure 7.12: Vertical profiles of turbulence statistics: (a) sensible heat flux $\rho c_p \langle w\theta \rangle$, (b) shear stress in x direction $\rho \langle w\bar{u} \rangle$, and (c) shear stress in y direction $\rho \langle w\bar{v} \rangle$.

UM closely, which is expected given that this case uses the UM output directly for the boundary condition (on building roofs and the streets). The SC0 case exhibits much higher values below building height than the other cases, which may explain why the potential temperature is higher (see Fig. 7.11).⁹ The fact that the cases using the SEB scheme (SC1, IC1, and IC2) have low sensible heat flux below building height is due to the relatively low sensible heat flux on the walls and streets compared to that on the roof, which is discussed in further detail in Sect. 7.5.4. For the shear stresses, the SC0 and SC1 exhibit extremely similar behaviour, which is expected seeing as the geometry is identical. The IC cases generally exhibit lower values, indicating that there is less vigorous turbulent mixing due to these geometries.

⁹Note that the behaviour of SC0 below building height is not particularly important in its own right for this study, because it is used as a precursor simulation for the realistic geometry case (R), where the flow in the UCL will be dominated by the surface in that simulation.

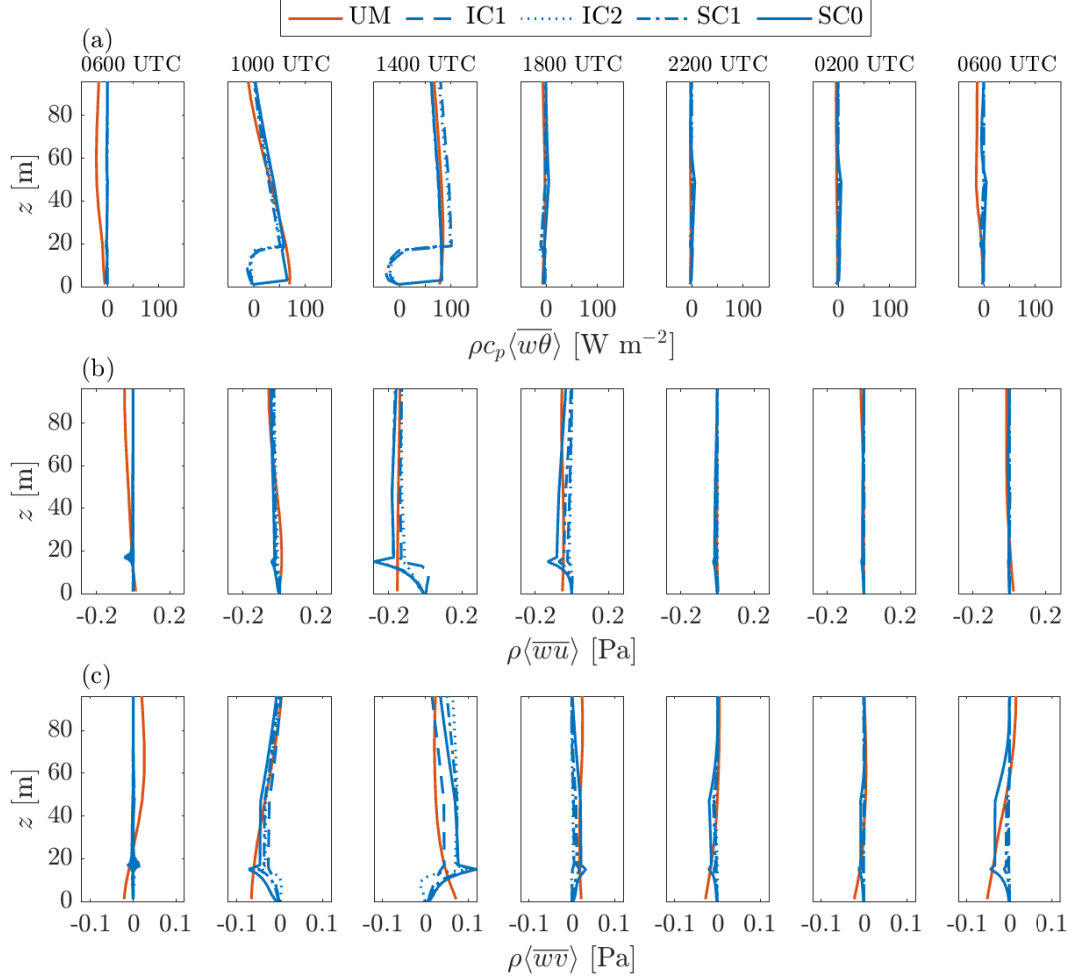


Figure 7.13: Vertical profiles of turbulence statistics below 96 m (twice nudging height): (a) sensible heat flux $\rho c_p \langle w\theta \rangle$, (b) shear stress in x direction $\rho \langle w\bar{u} \rangle$, (c) shear stress in y direction $\rho \langle w\bar{v} \rangle$.

7.5.3 Observations

Horizontally-averaged mean flow quantities and turbulence statistics from uDALES and the UM (as in Sects. 7.5.1 and 7.5.2) linearly interpolated to the height of the WCC rooftop ($z = 18$ m) and BT tower ($z = 191$ m) are shown in Fig. 7.14, as well as observations from those measurement sites. The WCC rooftop is just above building height in the RSL and is thus expected to be strongly driven by the surface, whereas the BT tower is comfortably above nudging height, possibly in the inertial sub-layer (ISL) or mixed layer, offering two different perspectives on the UBL (Barlow et al., 2015).

In general, the models agree more closely with each other than any one of them does with observations, which is perhaps unsurprising given that uDALES is forced with UM output. The potential temperature in the models is slightly underestimated during the

day and overestimated at night compared to both sites. The UM generally overestimates the wind speed at the WCC rooftop, particularly at night, whereas uDALES shows better agreement. The nighttime wind speed is particularly low, which likely contributes towards the low values of shear stress and sensible heat flux (see Fig. 7.12).

At the BT tower, the wind speed is substantially overestimated by the UM (and therefore uDALES too), again particularly at night. The sensible heat flux for the two models shows good agreement at the WCC rooftop, suggesting that the surface schemes

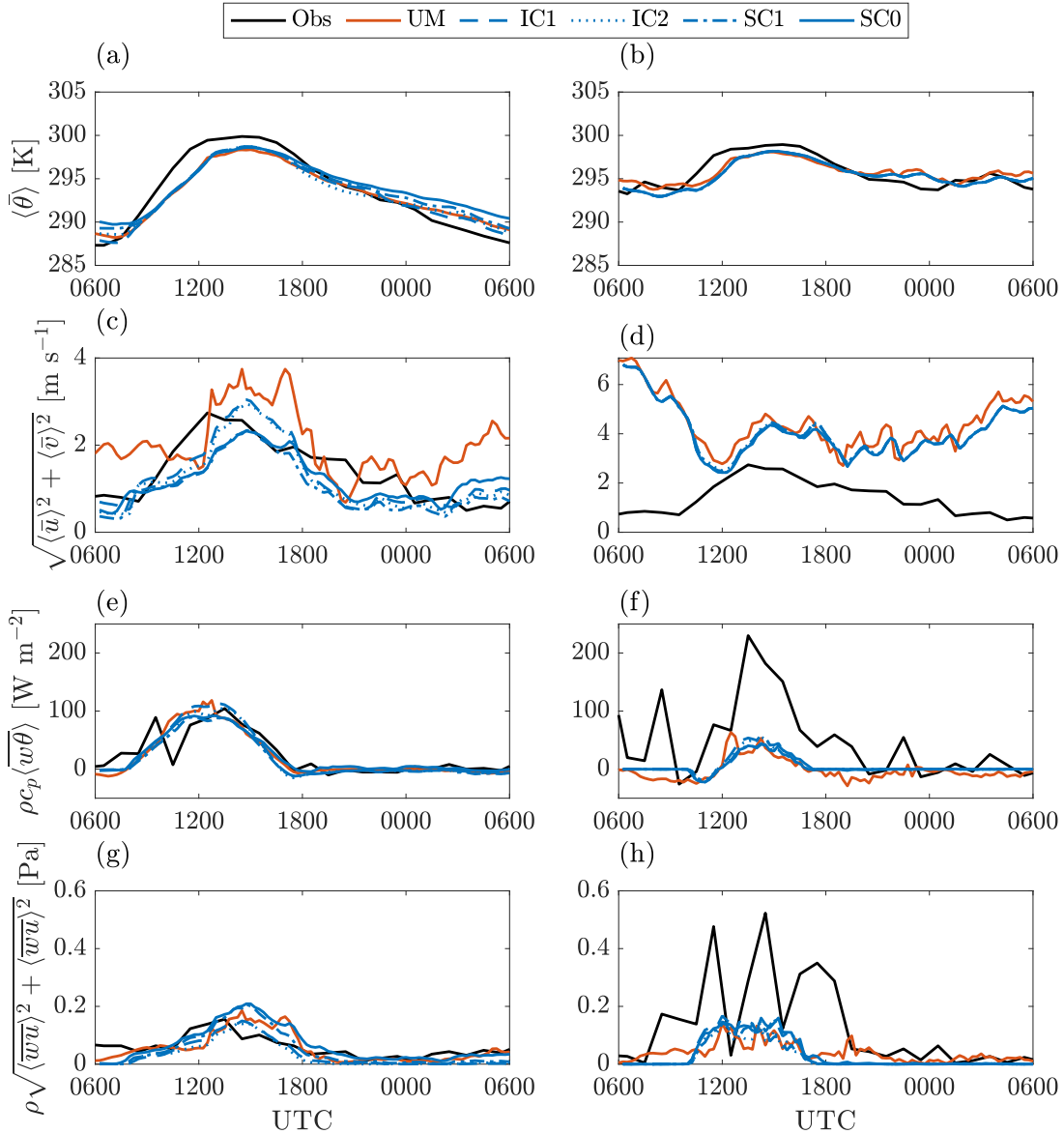


Figure 7.14: Comparison of UM and uDALES simulations with observations (Obs) at the WCC rooftop and the BT tower respectively: (a,b) potential temperature $\langle \bar{\theta} \rangle$, (c,d) velocity magnitude $\sqrt{\langle \bar{u} \rangle^2 + \langle \bar{v} \rangle^2}$, (e,f) sensible heat flux $\rho c_p \langle w\bar{\theta} \rangle$, and (g,h) shear stress magnitude $\rho \sqrt{\langle \overline{wu} \rangle^2 + \langle \overline{wv} \rangle^2}$. Note that the UM and uDALES values are the domain averaged value at the height of the corresponding measurement site.

in the models are able to capture the real urban environment in this case. However, there is poor agreement at the BT tower, with the observations exhibiting much larger values in the day. Similarly, the total shear stress is well-predicted by the two models at the WCC rooftop, whereas both exhibit lower values than those observed at the BT tower, though uDALES is slightly closer. The discrepancy may be due to the influence of the BT tower itself on the observations, which is likely to cause significant vertical flow deflection, and thus a dispersive flux (Barlow et al., 2011). This effect is not present in the simulations because the data has been spatially-averaged. There are also questions concerning the source area of the observed fluxes (Saunders et al., 2024). Given these issues, it is therefore not clear whether it is appropriate to compare the measurements with the simulations for the BT tower.

7.5.4 Surface energy balance

Figure 7.15 compares the bulk SEB fluxes and surface temperature (T_s) for the two models. For uDALES, the complete average (denoted by $\langle \cdot \rangle_c$) is used for the fluxes. This involves multiplication of the area-weighted average (denoted by $\langle \cdot \rangle_s$) with the complete aspect ratio (λ_c), and is appropriate to compare the 3D surfaces in uDALES to the flat surface in the UM (see Sect. 2.2). The latent heat flux for the UM is included to show that the value is much less than the other fluxes, justifying the omission of vegetation in uDALES. The anthropogenic heat flux (see Sect. 1.3.2), which is also omitted in uDALES, is also relatively low ($\mathcal{O}(10 \text{ W m}^{-2})$) for the UM in London; Iamarino et al., 2012; Bohnenstengel et al., 2014; Hertwig et al., 2020).

Overall, the uDALES simulations exhibit greater similarity with each other than with the UM. The magnitude of the sensible heat flux shows good agreement between the uDALES and the UM, which is consistent with the fact that this is also true for the atmosphere immediately aloft (at the height of the WCC rooftop) as discussed in Sect. 7.5.3, although that of the uDALES simulations tends to peak slightly later. The fact that MORUSES may struggle to capture the phase of the sensible heat flux is acknowledged in Porson et al. (2010b). The net shortwave radiation shows very good agreement. Since the sky is clear, the direct solar radiation is expected to be very similar, though this result also indicates that the radiative exchange between streets and walls is comparable. This is again is somewhat expected given the models have the same materiality and similar

morphometric indicators. However, it is also likely that these exchanges contribute relatively little to the net value in this case because λ_p and h are relatively high, meaning the behaviour of roof facets/tiles dominates due to substantial shading of walls and streets.

The conduction exhibits greater differences between uDALES and the UM. Note that the exterior conduction (G_0) for the UM is calculated as the residual of the radiative and turbulent fluxes (i.e. $G_0 = K^* + L^* - H - E$). There is reasonably good agreement for G_0

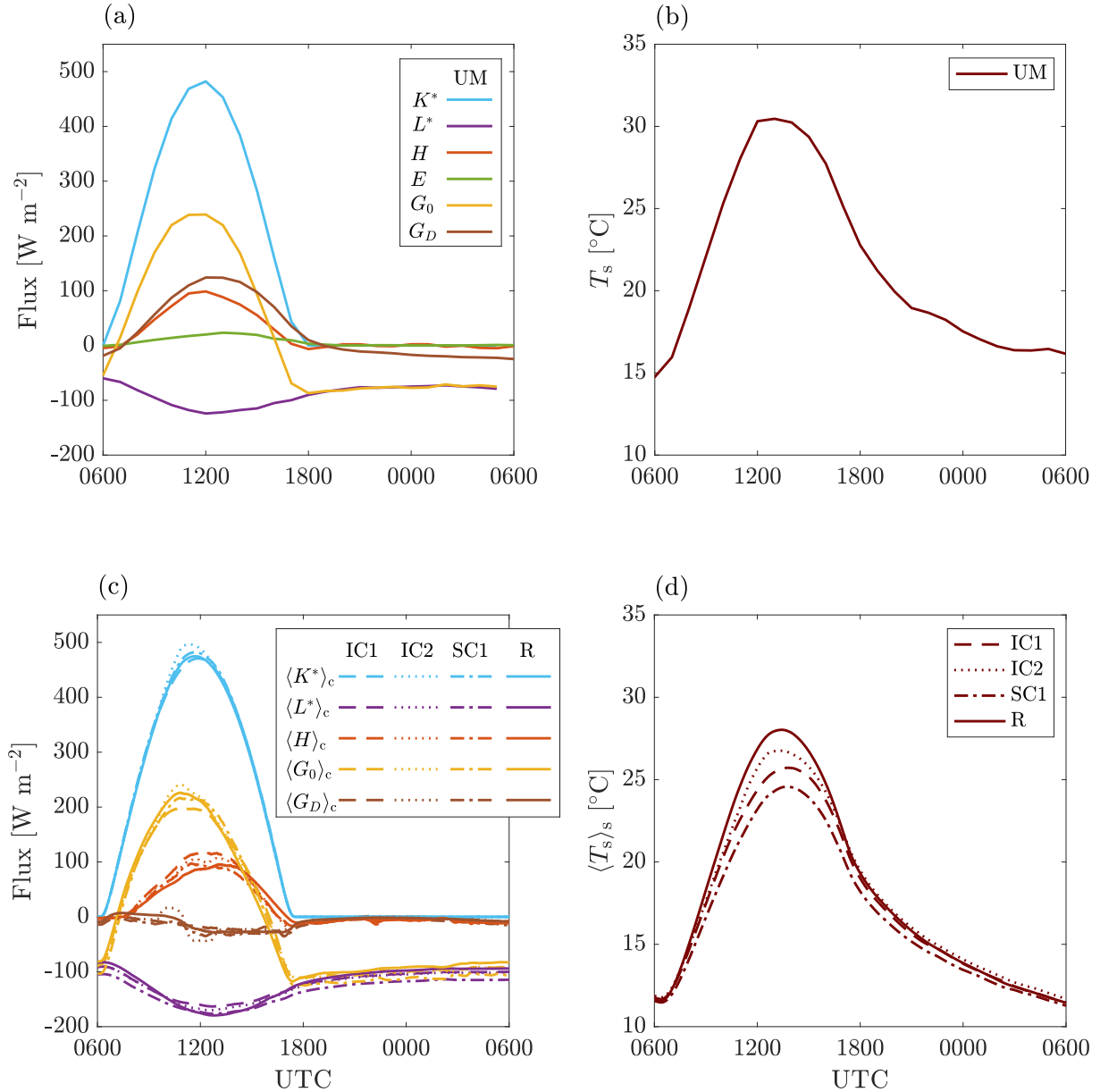


Figure 7.15: Bulk SEB fluxes and surface temperature (T_s) respectively for (a,b) the UM and (c,d) uDALES. The fluxes for both models include the net shortwave radiation (K^*), net longwave radiation (L^*), sensible heat flux (H), exterior conduction (G_0), and interior conduction (G_D); and the UM latent heat flux (E) is also shown. The uDALES fluxes are complete averages (denoted by $\langle \cdot \rangle_c$) and the surface temperature is the area-weighted average (denoted by $\langle \cdot \rangle_s$).

but very poor agreement for the interior conduction (G_D). The small negative daytime value of G_D for uDALES indicates that the soil and the interior of buildings together act as a net source of energy to the urban surface, whereas the relatively large positive value for the UM indicates that the surface transfers energy to the soil. This difference can be attributed to the fact that heat transfer within the surface is modelled in conceptually distinct ways. Since the uDALES facets are substantially thicker than UM facets, their interior is less strongly coupled to the forcing at their exterior, resulting in lower G_D .

The longwave radiation exhibits a consistent difference between the two models. However, the effect of scaling by λ_c when calculating the complete average may be somewhat inappropriate when comparing this quantity because the incoming longwave radiation in uDALES was set using the non-scaled value in the UM. More generally, while this scaling is insightful when considering the atmospheric fluxes relative to a flat surface, it is not relevant to any given facet. The result of the processes contributing towards the SEB is that the exterior surface temperature in the uDALES simulations is consistently lower than in the UM. Moreover, the UM temperature is closer to the air temperature (at night), which is similar for the two models (see Sect. 7.5.1). This is associated with a lower sensible heat flux, however the wind speed is higher for the UM at roof level, which is associated with a higher sensible heat flux. Given that the sensible heat flux is similar for the two models, it appears that these counter-acting effects approximately cancel out. The reason that uDALES predicts a lower surface temperature than the UM may be due to the fact that the net longwave radiation is lower (when scaled by λ_c), resulting in less available energy. There is also the influence of the interior temperature on T , which in uDALES is determined by the assigned (isothermal) boundary condition, but in the UM evolves according to separate processes (Best et al., 2011). In any case, since the treatment of temperature and heat storage within the two models is conceptually distinct, differences in this aspect are expected.

To further investigate the SEB for the uDALES simulations, Fig. 7.16 shows the SEB and internal temperatures averaged separately over the three facet types: streets, roofs, and walls. The roofs and walls exhibit a relatively high degree of similarity in these quantities; less so for the streets. The roofs (see Fig. 7.16c,d) in the idealised geometries are all at the same height, which means that they are unshaded and so have effectively identical $\langle K^* \rangle_s$. They also have similar wind speed over them, resulting in similar $\langle H \rangle_s$.

In contrast, for the realistic geometry, the roofs have varying height, meaning at any given time a proportion of them are shaded, resulting in decreased $\langle K^* \rangle_s$. Also, this is likely to result in decreased wind speeds, which may contribute towards the decreased $\langle H \rangle_s$, despite the fact that $\langle T_s \rangle_s$ is slightly higher than for the idealised simulations throughout the

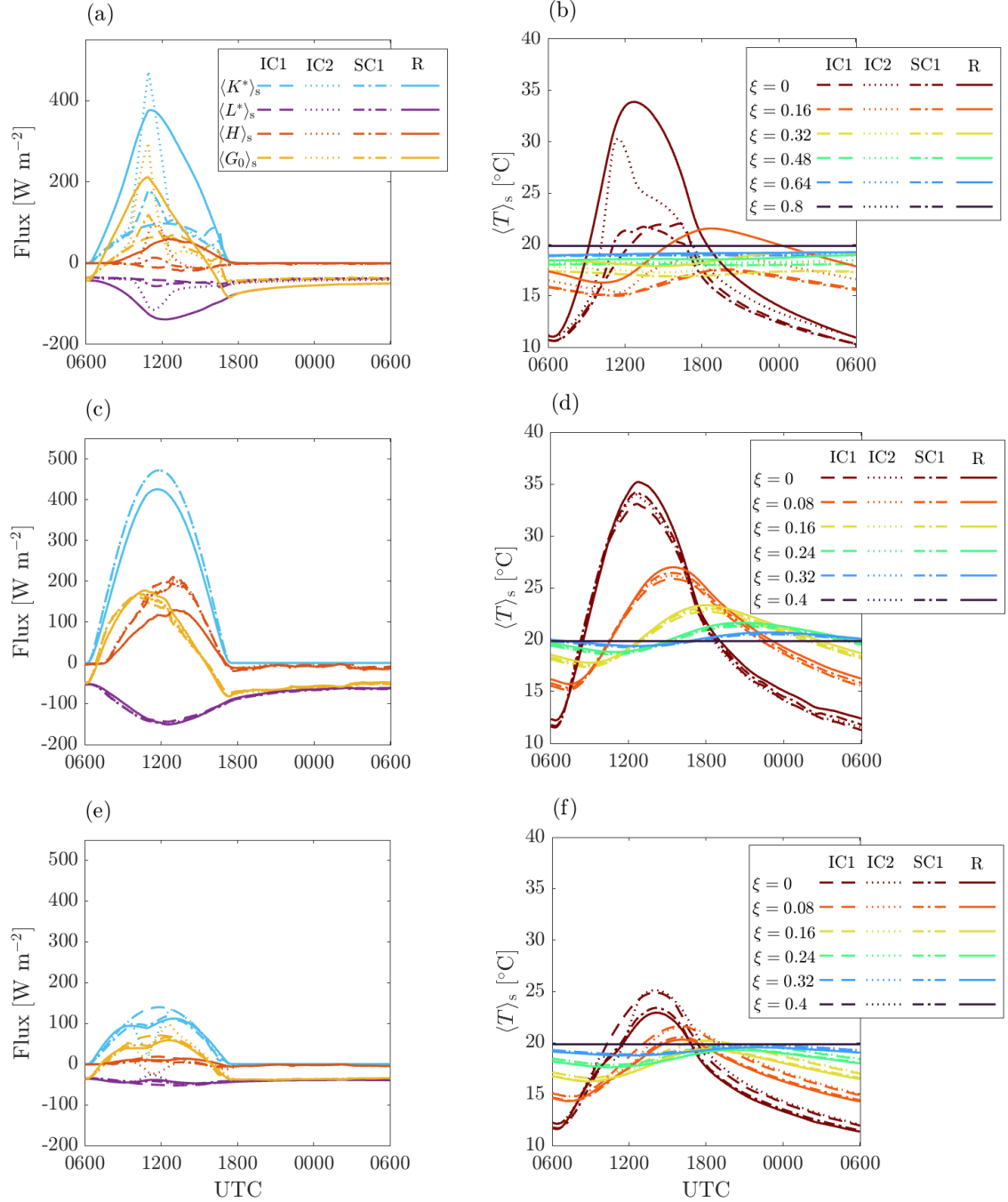


Figure 7.16: Average ($\langle \cdot \rangle_s$) SEB fluxes and temperature (T) as a function of depth (ξ) for the streets (a,b), roofs (c,d), and walls (e,f) in uDALES. The fluxes include the net shortwave radiation (K^*), net longwave radiation (L^*), sensible heat flux (H), and conduction (G_0). For the temperature, only every other layer has been plotted for clarity.

diurnal cycle. Roof facets reach the highest temperature of all the facets, with the value in each layer oscillating above and below the building temperature. The oscillations become increasingly delayed and damped as the depth into the facets increases. The fact that the roof temperature evolution for the different simulations is relatively similar is consistent with the similar $\langle G_0 \rangle_s$, as well as outgoing longwave radiation. The incoming longwave is similar due to no/little radiative transfer between roof facets in the idealised/realistic cases, hence $\langle L^* \rangle_s$ is similar.

For the walls (see Fig. 7.16e,f), the evolution of $\langle K^* \rangle_s$ is determined by their orientation with respect to the sun. For the IC1 case, there is one (infinitely long) wall visible to the sun for most of the day while the other is not, hence $\langle K^* \rangle_s$ follows a sinusoid-like curve with a single maximum. The other simulations have multiple maxima (at a lower value than that of IC1) as various groups of walls become visible to the sun over the course of the day. While IC2 generally has the lowest $\langle K^* \rangle_s$, it attains the highest $\langle T \rangle_s$, which is surprising. During the day, $\langle H \rangle_s$ is generally small and positive for all simulations other than IC2, which has a larger negative value, indicating that the surface is being heated by the air. This is unexpected, and suggests that this simulation may exhibit some unrealistic behaviour. The behaviour of the realistic case is closer to that of SC1, suggesting that staggered cubes may be more consistent with the true urban environment than infinite canyons. The evolution of $\langle T \rangle_s$ is nonetheless relatively similar across the simulations, resulting in similar $\langle G_0 \rangle_s$ and $\langle L^* \rangle_s$. However, in contrast to the roofs, only the outer layers ($\xi \leq 0.08$ m) attain a value of $\langle T \rangle_s$ above ground temperature, with the rest remaining below.

The streets (see Fig. 7.16a,b) exhibit the greatest differences between the different simulations because like the walls, they are strongly affected by shading, but unlike the walls they can absorb a large amount of shortwave radiation due to their average orientation being towards the sun to a greater extent, as well as their lower albedo. The SC1 and IC1 cases have comparatively low $\langle K^* \rangle_s$ owing to them being shaded for most of the day, with the principal contribution being reflected radiation from the walls. Both exhibit small peaks; that of SC1 at around midday corresponds to when the (approximately) north-south oriented streets are unshaded, and that of IC1 is just before sunset corresponds to when the (approximately) east-west streets are unshaded.¹⁰ Like SC1, the IC2 case also

¹⁰The lack of a peak in the morning for the IC1 case is due to the fact that the streets are at an angle of 17° from north, and so they are actually shaded by the north-facing walls.

has a peak around midday, and it is the highest of all the simulations because all the streets are in the same direction. The R case has a large and relatively broad peak, which indicates that the streets are less shaded than for the other cases. This is evident with the fact that many streets are visibly wider in the realistic geometry (see Fig. 7.8). This indicates a limitation of idealised geometries with the morphometric indicators used in this study, namely that the streets are assumed to be unrealistically narrow in order to achieve a relatively high λ_p . In fact, this is consistent with the findings of Schoetter et al. (2023), in which street canyon and cubic geometries generally are associated with systematic over/underestimation of the fraction of solar radiation absorbed by the walls/streets. However, it is also likely that $\langle K^* \rangle_s$ on the streets is overestimated here compared to the true urban environment because of the omission of vegetation. There are several large regions of ‘streets’ that are in fact small parks, which would likely absorb less shortwave radiation due to the comparatively higher albedo of grass than streets. In addition, the presence of trees would provide shade to streets (as well as walls). There are also areas at the edge of the domain that contain buildings in reality, but were not included in the geometry. As with the other facet types, the other fluxes evolve in a manner that is explained by $\langle K^* \rangle_s$, with the values for R being larger in magnitude. The value of $\langle H \rangle_s$ is substantially higher, indeed some of the others are negative, which is likely to result in higher air temperatures at street level. The temperature for the R case is also higher, with the evolution being comparable to the roof, while the IC1 and SC1 cases barely attain an exterior temperature above building temperature during the day. Due to their larger thickness, after a certain depth ($\xi \approx 0.64$ m) heat penetration is negligible for the streets, in contrast to the walls and roofs.

7.6 Conclusion

This study has focused on a direct comparison of a high-resolution version of a mesoscale model (MetUM) and a microscale model (uDALES) in the context of a diurnal cycle of the UBL over central London, with the mean flow in the uDALES simulations nudged towards MetUM output. Multiple geometrical configurations were used for uDALES in order to investigate the effect of the surface representation on the mean flow (Sect. 7.5.1), turbulence statistics (Sect. 7.5.2), and the SEB (Sect. 7.5.4). Observations of two sites at

different heights within the UBL were also included in the comparison (Sect. 7.5.3).

The results suggest that some quantities are predicted similarly by the two models, not least the mean flow (due to the nudging). The models agree on the bulk net shortwave radiation, which is important because this is the dominant process contributing towards the SEB and so strongly influences the other terms. In particular, the models predict similar daytime sensible heat flux both at the surface and in the atmosphere, which drives the convective boundary layer development. The models also tend to agree with respect to the shear stress, suggesting that despite the differences in spatial resolution, the turbulence is captured similarly during the day. The turbulence statistics are also fairly similar to observations near the surface.

However, other quantities do not show as good agreement. With the exception of potential temperature, both models do not match observations higher up in the atmosphere. Furthermore, the wind speed is consistently overestimated by MetUM compared to observations and uDALES (near the surface). This would likely be improved by using a distributed drag formulation that accounts for the vertical extent of buildings, though addressing solely this may also influence other processes that currently seem to be parameterised effectively in this case (such as sensible heat flux; Sützl et al., 2021a,b). In addition to the impact on surface exchanges and microclimate (including wind and thermal comfort), the over-estimation of wind speed has implications for the use of MetUM for weather forecasting, particularly in extreme weather events involving high-speed flow. In this study, the near-surface wind speed is particularly low during the nighttime, which contributes towards the fact that there is relatively little turbulence. The nighttime cooling predicted by MetUM may be due to atmosphere radiative transfer, which is not captured by uDALES, limiting the comparison during this period. It would be preferable to account for this process in future work involving modelling nocturnal boundary layers using uDALES.

The absence of any large-scale forcing term below nudging height in uDALES also likely lowers the wind speed. There is uncertainty in the effect of the nudging timescale on the flow, which should be large enough to allow turbulence to develop, but small enough for the mean flow to match the forcing data. It seems that the simple forcing applied in this study, namely constant nudging height and timescale throughout the diurnal cycle, results in reasonable results for the daytime convective boundary layer flow. However,

the reduced turbulence at nighttime may require a different forcing in order to better capture the nocturnal boundary layer. In addition, there was some evidence of non-physical behaviour above the convective boundary layer, further highlighting the need for a more sophisticated nudging strategy in flow regions where there are relatively low levels of turbulence (and are instead more influenced by large-scale processes). It may also be more physically reasonable to use a forcing that is continuous in the vertical direction.

MetUM consistently overestimates the surface temperature compared to uDALES, likely because there are fundamental differences in how the models treat heat storage, though there is also uncertainty involved in setting equivalent longwave radiation. This aspect was not investigated in detail in this study as it would require MetUM output that was not available, namely the SEB of the separate tiles and soil temperature. Also, the lack of observations for surface temperature for this case makes it impossible to say which model is closer to the truth. Evaluation of MetUM using land surface temperature observations suggest that there are city-scale observation-model differences, with MetUM exhibiting both substantial over- and under-estimation depending on location and time (Hall et al., 2024). Given that the cause of these differences are not fully understood, the application of these results to the present study is not straightforward. While the discrepancy in surface temperature does not seem to translate to the atmosphere in this study, further work on understanding the origin of the discrepancy and its relationship to the SEB would be valuable.

The various geometries used in uDALES were overall more similar to each other in their bulk SEB than any particular one is to that of MetUM. This result suggests that the bulk SEB for surfaces with the same materiality and morphometric indicators are not strongly affected by the exact morphology. The results also indicate that the current assumed geometry (infinite canyons) is likely to perform as well as a more complex simplified 3D geometry (e.g. a cubic array), though further work would be needed to demonstrate this convincingly. After all, a more sophisticated idealised representation is still a simplification, and may not necessarily be significantly closer to reality (Schoetter et al., 2023; Lipson et al., 2024). This is supported by the results of breaking down the SEB for the uDALES simulations by facet type, which reveals differences between the simulation using the realistic geometry and those using idealised geometries. The results suggest that it is difficult to replicate the radiative exchanges in urban environments with inhomogeneity at

the street canyon scale using idealised geometries. Future work could involve expanding the study to include idealised geometries with variable height, or buildings placed via a pseudo-random procedure while maintaining consistent morphometric indicators with those used in this study (e.g. Schoetter et al., 2023). The variation in the SEB across facet/tile types is only relevant for MetUM insofar as it influences the bulk SEB since the surface exchanges are blended after being calculated by JULES. However, the breakdown would become important if the fluxes were distributed in a more sophisticated manner (at multiple model levels). Another avenue of future work could be to compare the combined SEB of the walls and streets in uDALES with the canyon tile in MORUSES to evaluate the two-tile urban scheme in use in the latter, though as previously mentioned this is not possible with the current dataset.

The methodology employed in this study with uDALES could be used to address other research questions related to this case, particularly those focused on the microclimate within the realistic geometry. For example, investigating spatial variation of pedestrian-level quantities such as wind speed and air temperature, as well as quantities relating to the SEB, in a similar manner to Chapter 5.¹¹ However, to carry out more thorough analysis, it would be necessary to use a higher spatial resolution to enable the flow within the UCL to be captured in greater detail. Also, though the bulk effect of vegetation is not likely to be substantial in this case, it would also be preferable to include vegetation as this would likely influence local microclimatic conditions. The effect of specular reflection from glazing may also be significant in central London (Kotthaus and Grimmond, 2014), though this is currently not possible to model using uDALES. Also, the realistic geometry had a relatively low level of detail (LoD), consisting simply of extruded polygons. For microclimate studies, it would be advantageous to use a higher LoD, e.g. pitched roofs, overhangs, and protrusions on walls. In general, using geographic data to define buildings at an appropriate LoD is an important step in the microscale modelling of real urban environments. Tools such as City4CFD (Paden et al., 2022, 2024) or the PALM-based tool developed by Coburn and Xie (2024) are likely to prove valuable for standardising this often time-consuming and error-prone task. However, it is subject to practical constraints on data availability and quality, which vary by location (Masson et al., 2020b).

The methodology is also applicable to other cases provided that there is a clear pre-

¹¹Visualisation of the surface energy balance and instantaneous flow fields over the diurnal cycle are available in Sects. F.2.1 and F.2.2 respectively.

vailing wind direction that can be used to define the coordinate system used in uDALES (or alternative microscale model). If comparing microscale and mesoscale modelling approaches is not the focus of the study, the source of the forcing data obviously need not be a mesoscale model dataset for the entire urban region; any dataset with sufficiently high vertical resolution to capture the UBL development could be used, such as observations or single-column model output. This makes the strategy an appealing alternative to domain nesting, which can be unwieldy for addressing research questions for which large-scale horizontal processes are not particularly relevant. The methodology therefore furthers the capability to carry out high resolution modelling of the UBL over a diurnal cycle, which is vital for improving understanding of both microscale and mesoscale urban climate processes.

Chapter 8

Conclusion

This thesis has presented the development and use of an urban microscale modelling tool (uDALES v2.0) that is capable of simulating air flow and heat transfer in the built environment at high fidelity, resolution, and performance, in order to provide insight into microclimate and urban boundary layer (UBL) processes over a diurnal cycle. This chapter first summarises the contributions made, including the upgraded scaling and geometry representation of uDALES v2.0, and the methodologies employed for the use cases presented in this thesis (Sect. 8.1). Subsequently, the impact of the work, including the capabilities of uDALES v2.0 and the implications of the findings obtained are discussed (Sect. 8.2). Possible future work is also discussed, including further development and evaluation of uDALES, as well as further research based on the case studies (Sect. 8.3). Finally, more general considerations related to the topics explored in this thesis are discussed in the context of urban climate modelling (Sect. 8.4).

8.1 Contributions

The substantial upgrades made to uDALES under the tag of v2.0, described in Chapter 3, address the key limitations associated with previous versions. The scaling of the computational fluid dynamics (CFD) solver was upgraded by implementing a two-dimensional domain decomposition (using the external library 2DECOMP&FFT) and by enhancing the pressure solver so that the efficient fast Fourier transform (FFT) algorithm can always be used. In addition, the facets are specified as an unstructured triangulated surface using the STL file format, meaning the surface no longer has to be aligned with

the Cartesian computational grid. Aspects of the immersed boundary method (IBM) were developed in order to accommodate this geometry representation, and the approach that was implemented conserves heat and moisture with the surface energy balance (SEB) scheme. The upgraded features were validated for neutral and non-neutral flows in Chapter 4, which includes a novel test case designed to evaluate the SEB for non-grid-aligned facets. The fact that uDALES v2.0 uses large-eddy simulation (LES) with an IBM that can handle the surface not being aligned with the grid makes it unique among urban microscale models for atmospheric flows and the SEB.

Chapter 5 involved the application of uDALES v2.0 to studying microclimate in realistic urban environments over a diurnal cycle. The case study is based on a small, coastal masterplan in a hot, arid climate, which are relatively under-represented in urban climate studies. The case was well-suited for being studied with uDALES v2.0, not least because a high-quality 3D model for the geometry was available that could be used to generate the STL file. The incoming flow from the ocean was unobstructed by other urban (or rural) features, and so could be modelled in a relatively simple manner as a neutral marine boundary layer. The mean flow was assumed to be constant, with the incoming air temperature and solar position varying over the diurnal cycle. The evolution of the microclimate was investigated in terms of surface temperature and SEB fluxes (in bulk and across the domain), pedestrian-level quantities (including the mean radiant temperature (MRT)), and the thermal plume resulting from the urban environment in terms of the streamwise development of the mean flow and turbulence statistics. This simulation was also used in Chapter 6, in which it was compared to a set of simulations that each have a fixed solar position and air temperature that represent a particular hour of the day. In these simulations, the system was allowed to reach a statistically steady state. The effect of the two different modelling assumptions was investigated using similar quantities as in Chapter 5, with a greater focus on heat transfer within the buildings.

Finally, Chapter 7 presented a study of the UBL over London, comparing uDALES v2.0 with a mesoscale model (the Met Office Unified Model; MetUM). This was more ambitious than the case in Chapter 5 in almost every aspect. The entire vertical extent of the UBL was included within the domain, with time-varying mean wind speed and direction, and a non-neutral temperature profile. In order to ensure the models match with respect to the larger-scale UBL development, a one-way coupling was implemented to nudge the

mean flow in uDALES to MetUM output above a certain height. The primary aim was to investigate the effect of surface representation, so multiple morphological configurations were used for the uDALES simulations. In addition to realistic buildings from Ordnance Survey (2019) data, the geometry configurations included infinite canyons and staggered cubes, with the STL files generated by bespoke scripts. The comparison includes analysing the bulk SEB as well as the UBL in terms of the horizontally-averaged mean flow variables and turbulence statistics. The models were also compared with observations at two sites at different heights within the UBL.

8.2 Discussion of results

As a consequence of the upgrades described in Chapter 3, uDALES v2.0 is a far more practical tool than v1.0. The code scales well for realistic problem sizes up to a large number of processors on high-performance computing (HPC) systems, meaning simulations can be run far more quickly (with both periodic and inflow-outflow boundary conditions). This makes it possible to perform simulations at high resolution (as in Chapters 5 and 6) or with large domains (as in Chapter 7) over multiple diurnal cycles. Furthermore, the STL file format that is used to specify the facets is compatible with widely-used CAD tools (e.g. Rhino3D, used for the geometry in Chapter 5), as well as software based on geographic formats such as 2D surface elevation maps and 3D point cloud data, e.g. City4CFD (Paden et al., 2022, 2024), thus improving the versatility of the model. The validation case for the SEB presented in Chapter 4 shows that having a non-grid-aligned geometry representation is crucial for accurately modelling shortwave radiation. This result is particularly important in the context of diurnal cycle studies, as shortwave radiation tends to drive the other SEB terms during the day (see below). The ability of uDALES v2.0 to accurately model the SEB for non-grid-aligned facets means that it can be used reliably for the simulations involving realistic urban geometries (as in Chapters 5, 6, and 7).

The results of Chapter 5 show that the distribution of radiation across the environment strongly influences the SEB, and the buildings exhibit a lower temperature than the surrounding terrain due to shading. This is an important result given the climate in this case, in which a key design consideration is the ability of the built environment to provide

thermal comfort (relative to the surroundings). Moreover, flow structure was shown to be a crucial factor in determining pedestrian-level air temperature, with the highest values observed in locations that do not necessarily have the highest surface temperature. This result demonstrates the value in coupling wind and thermal processes in order to provide insight into the factors influencing thermal comfort.¹

The effect of thermal inertia is visible in the results of Chapter 5, and is quantified extensively in Chapter 6. In contrast to the diurnal cycle (DC) simulation, in which the thermal response is transient, each steady-state (SS) simulation exhibits thermal equilibrium, so the surface cannot store heat and responds instantaneously to the thermal forcing. In general, there are substantial differences between the DC and SS simulations, with a maximum error of 20 °C in the MRT for the SS cases during the day for example, and opposite stability in the urban canopy layer (UCL) predicted by the two modelling assumptions at night. However, the errors are somewhat predictable, with quantities such as surface temperature tending to be over-estimated by the SS cases during the day and under-estimated at night, resulting in two cross-over times (in the early morning and late afternoon) for which SS simulations may be more reliable. Nonetheless, the results reinforce how important thermal inertia is in determining the evolution of the SEB over a diurnal cycle and its effect on microclimate.

In Chapter 7, the coupling of uDALES to MetUM generally results in good agreement between the models with respect to the mean quantities throughout the diurnal cycle, and the daytime convective boundary layer is similar in terms of the sensible heat flux and shear stress. The near-surface wind speed for MetUM is over-estimated in comparison to uDALES and observations due to the model lacking vertical distribution of the drag. Bulk SEB terms including the net shortwave radiation and sensible heat flux are predicted similarly by the models, whereas the surface temperature is consistently over-estimated by MetUM, likely due to the difference in how the models treat heat transfer within the surface. This may contribute towards the differences observed in nocturnal boundary layer development, though the lack of atmospheric radiative transfer in uDALES may also have an impact at this time. The SEB of the various uDALES geometries exhibit greater similarity with each other than with MetUM, which has implications for urban canopy model (UCM) parameterisation using idealised geometries. Overall, the results suggest

¹Guidelines for wind and thermal comfort, for example in the City of London, often state that these can be modelled separately, or with a one-way coupling at most (RWDI, 2020*a,b*).

that morphology may be less influential than other aspects of the modelling approach (when matching morphometric indicators), particularly heat storage. In addition, the study serves to demonstrate the use of a widely applicable methodology for using LES to study realistic UBLs that is more straightforward to implement and requires a smaller dataset than domain nesting, for example.

The results of the case studies in this thesis consistently demonstrate the key role that solar radiation plays in driving the evolution of the SEB over a diurnal cycle. The case studies speak to the interaction of solar radiation with morphological variation, either within a single urban environment or when comparing different configurations. The surface orientation (with respect to the sun) and shading strongly affects local SEB quantities, including the MRT, as well as the breakdown of bulk SEB quantities by facet type. This implies that the influence of solar radiation on urban heat, in addition to merely the availability of daylight,² should be a key concern for urban design across scales. Furthermore, the studies explore the relationship between morphology and wind speed and direction, including the resulting effect on the atmospheric temperature and sensible heat flux. This demonstrates the value in using a microscale modelling approach capable of specifying the geometry in a high-fidelity manner, particularly for design applications below the neighbourhood-scale, such as masterplans. Finally, it was shown that thermal inertia is significant to the evolution of the SEB over a diurnal cycle, and that accurate modelling of heat storage within the urban surface is crucial for accurately modelling surface temperature — a key quantity in determining thermal comfort and building energy performance. Since heat storage is, in reality, strongly influenced by materiality, this demands that the thermal effects of building materials should be considered. These outcomes prove how multi-physics, microscale diurnal cycle studies can be used to provide insights into a wide range of urban climate processes and better inform urban design.

8.3 Future development and research

Inevitably, there are limitations of uDALES that remain. The test cases presented in Chapter 4 are simple by design, as the priority was to validate the fundamental aspects

²In UK law, the ‘Right to Light’ protects properties from significant obstruction from daylight by neighbouring buildings (Bickford-Smith et al., 2007). Currently no similar laws exist for other environmental aspects such as wind/ventilation and thermal conditions — perhaps as a result of these processes being more challenging to model and measure accurately.

of the development, in particular the novel features of the IBM. As such, the cases do not capture the full complexity of urban areas. In order to strengthen the robustness and applicability of the model, future work should involve evaluation of a more diverse and realistic range of urban morphology, materiality, and environmental conditions (e.g. Resler et al., 2021), comparing with other modelling tools if possible. Trees were not included in the validation studies because the way they are modelled (as voxels) was not changed from v1.0 to v2.0. In a future version, trees could be represented in the same way as facets (using a triangulated surface). This would require integrating trees into the 3D radiative transfer scheme, which is challenging for the current approach based on the radiosity assumption. There are also concerns regarding the applicability of the radiosity approach to urban environments that contain extensive use of non-Lambertian materials such as glass (Schoetter et al., 2023). Furthermore, uDALES v2.0 still only has the option to specify a time-varying inlet in the x direction (and not the y direction), and this is obtained from a precursor simulation with the same resolution as the main simulation. Other models have the ability to nest a high-resolution simulation within a lower-resolution, larger-scale one, with the option of using a separate (mesoscale) model for the latter (Lin et al., 2021; Kadasch et al., 2021); this requires all lateral boundaries to be time-varying inlets. Finally, despite the performance upgrade, it is not practical to carry out very high resolution (≤ 1 m) studies of larger (≥ 1 km) urban areas over a diurnal cycle (see Chapter 7).³

uDALES v2.0 provides a firm foundation for future work in these areas. Unlike in v1.0, the upgraded pressure solver for inflow-outflow simulations does not fundamentally treat the lateral directions differently, meaning that implementing a domain nesting technique would simply involve copying the current implementation for x for y as well. This would need to be combined with a synthetic turbulence generation technique, which has been implemented in the codebase (by others). Nesting could then be used as an alternative to the methodology employed in Chapter 7. Given the code now uses low-level routines from the 2DECOMP&FFT library, which is used by many other modelling tools (e.g. Xcompact3D; Bartholomew et al., 2023), any development thereof can potentially be adopted in uDALES in order to further enhance performance. For example, support for NVIDIA GPUs has recently been added to 2DECOMP&FFT with support for the other vendors

³PALM appears to be the only LES-based model capable of doing this (e.g. Anders et al., 2023).

planned (Rolfo et al., 2023), which would allow future efforts to port uDALES to GPUs to focus only on the uDALES-specific components. The use of GPUs would also suit a more advanced radiative transfer scheme that is based on ray tracing, which could capture specular reflection and transmission by non-Lambertian materials, and is an attractive approach for modelling trees. It would also be beneficial to implement a radiative transfer scheme for the atmosphere, as this likely impacts nocturnal boundary layer development. This could be ported from DALES (the model that uDALES was based on; Heus et al., 2010), which also includes more sophisticated cloud physics. In general, the improved low-level functionality of the codebase prepares uDALES for exascale HPC systems, meaning it will be increasingly feasible to perform higher resolution simulations for longer periods.

An aspect of the modelling approach that is particularly relevant for relatively high-resolution simulations (such as those in Chapters 5 and 6) is the use of wall functions to parameterise wall (facet) boundary layer flow. In general, wall functions are only assumed to be valid for cells in the log-law region of the boundary layer, which is typically $\mathcal{O}(10 \text{ cm} - 1 \text{ m})$ from the wall. The use of reconstruction in IBMs (see Appendix C) involves only using field values that are in this region, which means that refining the grid beyond a certain level will not resolve the wall boundary layers any higher. This is in contrast to the body-fitted mesh approach, in which it is possible in principle to resolve the viscous sub-layer beneath the log-layer (see Sect. 1.4). This offers greater accuracy as it is generally unlikely that the flow over urban facets is actually in the state of local equilibrium that would result in a logarithmic velocity profile due to the strong pressure gradients, separated and unsteady flow, and spatial variation in surface roughness that occur. Moreover, the stability-related correction to the log-law due is only justified for horizontal surfaces, thus the wall function approach is particularly questionable for vertical surfaces in non-neutral conditions. Due to the large number of computational cells required, and the lower performance of non-Cartesian solvers, near-surface grid refinement is currently only practical with LES for relatively simple geometries and/or short simulations. With greater computational resources it becomes more feasible for smaller cases such as in Chapter 5, though for studies of large urban areas such as in Chapter 7, particularly those using nested model configurations with variable resolution, wall functions seem practically impossible to avoid. Parameterising near-wall processes in real urban environments will therefore continue to be an important area of research. In light

of this, the novel IBM implemented in uDALES v2.0 is flexible (compared to v1.0) to modification of the wall functions.

For future research into microclimate using uDALES (similar to Chapter 5) it may be beneficial to implement post-processing tools for calculating standard thermal comfort indices. This would make the model more applicable to urban design, and able to address potential questions concerning strategies for improving comfort and mitigating heat stress. Calculating comfort indices would involve combining the MRT with atmospheric quantities, namely the wind speed, air temperature, and humidity (which would be necessary to consider for more humid climates than that of Chapter 5). It would also be worthwhile to evaluate the effect of assuming a neutral incoming flow on the results, as this simplifies the methodology hugely (compared to Chapter 7 for example), but inevitably introduces errors in atmospheric quantities. More generally, in principle any variation in simulation parameters will impact the outcome of a microclimate study, so quantifying the sensitivity of the results on the chosen parameters is important going forward. Indeed, in some sense the aim of Chapter 6 was to carry out such a study with respect to thermal inertia. For this study, a key question arising from the results is whether errors between diurnal cycle and steady-state simulations are somewhat predictable. If so, then it is possible that they could be accounted for when running a steady-state simulation, which would be beneficial as they are clearly more expedient than diurnal cycle simulations. In order to explore this, it may not be practical to use high-resolution LES, given the relevant process is heat transfer within the urban surface, and simpler models for the atmosphere may provide sufficient accuracy with a lower computational cost.

Regarding further research related to Chapter 7, the set of morphological configurations used in the study could be expanded in order to systematically explore the parameter space. For example, randomised, more realistic building layouts, with matching morphometric indicators (e.g. Schoetter et al., 2023), could be used to explore the variability of results. Alternatively, a single geometry could be used with varying morphometric indicators (which would involve using a different area within the MetUM domain). Research of this kind would enable the evaluation and development of the surface scheme in MetUM (or other mesoscale models), in particular how to vertically distribute fluxes (e.g. Sützl et al., 2021b), and may indeed be valuable for its own sake to better understand the effect of morphology on microscale urban processes. However, performing a large number of

simulations similar to those in Chapter 7 in order to carry out a reliable study of the parameter space would be extremely expensive with LES. Practically, it may therefore be necessary to assess whether resolving the entire UBL (using LES) is important given the study aims. While this study explored the effect of morphological properties, the results of this thesis suggest that research into other factors influencing the SEB, in particular thermal inertia (which is affected by the material properties), would be valuable as well.

Generally speaking, despite their neglect in this thesis, studies of microscale air flow and heat transfer would be enriched by the inclusion of vegetation (including trees) and moisture (including clouds). These features are likely to decrease the thermal response of the surface to solar radiation: trees and clouds contribute to shading, and vegetative surfaces use up energy for evaporation (in a way that is influenced by the humidity). Investigating these effects over a diurnal cycle, both in relation to microclimate studies and mesoscale model comparisons, is necessary to better understand the full range of urban environmental conditions that occur.

8.4 Outlook

By combining the advantages of using high-performance LES to model the flow with a high-fidelity geometry representation for the SEB, uDALES is positioned at the cutting-edge of microscale modelling techniques for urban environments. Given the extent of recent development of microscale models more generally, and the variation in approaches involved, there is a pressing need for these tools and methodologies to be evaluated against each other across the range of applications they are used for (Mirzaei, 2021; Tominaga et al., 2023). For example, this could be carried out in the same vein as the Urban-PLUMBER project, which compared UCMs (Lipson et al., 2024).⁴ This is supported by the fact that for some results in this thesis, the differences in values that were discussed are relatively small; potentially smaller than the systematic error that may exist between models. Moreover, despite the performance upgrade to uDALES, LES tools are likely to remain significantly more expensive than the Reynolds-averaged Navier-Stokes (RANS) approach. The comparison should include models with varying complexity and consider performance as well as accuracy, seeing as the holistic goal of modelling is to provide a so-

⁴Progress has been made by uDALES and PALM developers to organise this.

lution with acceptable accuracy given the time or computational resources available. This thesis motivates the comparison to include heat transfer and consider the evolution over a diurnal cycle, and to use cases relevant to key applications of the models: microclimate and mesoscale model parameterisation studies.

Microclimate studies are used to inform the design of the built environment, and so are highly relevant to the lives of urban residents. Studies of this kind are frequently used for validating models in realistic configurations, and as previously discussed, it would be beneficial to apply uDALES v2.0 in this context. Furthermore, it would be valuable to have guidelines (similar to RWDI, 2020*a,b*) for using microscale CFD models to predict wind and thermal comfort while accounting for the variability of the UBL and SEB over a diurnal cycle.⁵ In addition to covering techniques concerning geometry preparation, computational mesh generation, physical parameterisations, and numerical methods, this could include approaches for coupling with mesoscale models in order to capture larger-scale processes, and two-way coupling with thermal models.

This being said, there is an intrinsic limitation of using them to predict comfort for the purposes of urban design. If climate data for a particular day is used to define simulation parameters, for model validation and evaluation purposes for example, the results are clearly only truly representative of this day (which is in the past). Therefore, climate data is often averaged (like in Chapter 5) in an attempt to predict a typical day in a particular month or season. In order to predict average microclimate conditions while avoiding running a simulation using data from each day of the historical climate record, then averaging all the simulations, it is expedient to first average the climate data, then run a single simulation that is forced with the averaged data. The validity of this approach, given the inter-dependence of microscale processes and the hysteresis of the surface (shown in Chapters 5 and 6) is questionable. Alternatively, ‘extreme’ scenarios may be of interest, for example the hottest day in summer or coldest day in winter, in order to provide a conservative prediction — if the extreme scenario is deemed acceptable then it is assumed that other scenarios are too. However, it is not clear how to determine the extreme scenario a priori in terms of a comfort index that combines multiple factors (rather than only considering one factor, for example temperature). Given the challenges involved in using climate data to map results onto real-world scenarios, combined with

⁵Existing guidelines assume that the UBL is neutral (RWDI, 2020*b*), and accurately modelling thermal inertia is challenging, typically involving the use of Fourier analysis (Davies, 1994).

uncertainty in other parameters (e.g. material properties), as well as climate change, it seems that high-resolution, multi-physics studies are perhaps better suited for the purpose of understanding phenomena at a more fundamental level under the expectation that the results can be applied more generally, as Chapter 5 attempts to do.

Studying how urban surfaces behave in bulk (by comparing microscale and mesoscale models, as in Chapter 7) is important for weather forecasting and understanding mesoscale climate processes in general. An over-arching question that is relevant to studies of this kind is to what extent near-surface processes influence the larger-scale UBL development, and vice versa. For instance, from a microscale perspective, precisely how important is it to capture in detail the non-neutrality and full vertical extent of the UBL for studies where surface processes are the primary focus. Microscale modelling tools (notably PALM) are increasingly being scaled up in terms of using larger, nested domains, and including parameterisations for larger-scale processes such as atmospheric radiative transfer and cloud physics. Meanwhile, mesoscale models are being scaled down to have higher horizontal resolution, such as the 100 m version of MetUM used in Chapter 7 (Lean et al., 2024). However, neither were originally designed to be used in the ‘grey zone’ in which they overlap, and so care must be taken to ensure models are reliable therein. Since microscale models can specify the surface at an arbitrary level of detail, a key challenge is defining morphology and materiality with sufficient accuracy whilst not sacrificing ease-of-use or performance, as well as applying appropriate boundary conditions given that the entire urban region cannot be included within the domain (for which mesoscale models can be used). Mesoscale models must ensure that UCL processes such as radiative transfer between buildings and the distribution of surface fluxes are parametrised faithfully, and avoid double-counting of atmospheric fluxes, i.e. both resolving and parameterising the same process. Microscale models, particularly those based on LES, are likely to continue to be used to inform this (Lean et al., 2024). Eventually, it would be sensible for urban modelling tool inter-comparisons to span across scales, navigating the terra incognita between microscale and mesoscale models, and Chapter 7 is a step in this direction.

Bringing the thesis to a close, the aim of advancing microscale modelling capabilities to enable high-resolution studies of realistic urban environments over multiple days has been achieved, and the value of the tools and methodologies that have been established have been demonstrated for several applications. There is nonetheless a myriad of pos-

sibilities for future research and development, with research based on the principle that it is highly beneficial to couple microscale air flow and heat transfer over a diurnal cycle, and development driven by the goal of higher fidelity and performance. As the availability of computational resources increases, so does the ability of modelling tools to resolve processes at a wider range of scales with greater complexity. It would also be remiss not to mention that tools based on machine learning (rather than solely numerically solving the governing equations) are likely to play an increasingly significant role in urban climate modelling in the future, though their accuracy has not been proven sufficiently to be widely accepted by academia and industry (yet). Taking a step back, a key theme running through this section is a fundamental concern pertaining to modelling: the risk of finding a detailed answer to an ill-posed or practically irrelevant question. In general, it is possible that the sensitivity of results on uncertainty or inaccuracy in simulation parameters may in fact be more significant than the aspect of study, and it may therefore be more reliable and cheaper to use simpler tools to investigate multiple scenarios that capture this uncertainty. It therefore is vital to consolidate knowledge of how to accurately model processes at different levels of complexity across various scales, including the coupling between them, in order to address the problem at hand in a manner that is faithful to reality for the given application and is practical for the given time-frame. This involves evaluating various model configurations in realistic urban environments, with experiments and observations acting as an anchor to the comparison. Provided disparities are identified and rectified, this will give greater confidence in the tools used to understand and predict urban environmental processes and expand their use in decision-making. Efficient, versatile, and reliable modelling tools are vital to improving the cities and towns in which so many of us live, and this thesis is a contribution towards this ongoing goal.

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Appendix A

Flow averaging

The time average of a quantity $\varphi(t)$ in the interval $t_0 \leq t \leq t_1$ is given by

$$\bar{\varphi} = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} \varphi \, dt \quad (\text{A.1})$$

The intrinsic horizontal spatial average of a quantity $\varphi(x, y, z)$ is defined as

$$\langle \varphi \rangle(z) \equiv \frac{1}{A_{\text{fluid}}(z)} \int_{A_{\text{fluid}}} \varphi \, dA_{\text{fluid}}, \quad (\text{A.2})$$

where A_{fluid} is the horizontal area occupied by the fluid within the domain. Practically, this is calculated for a Cartesian domain with horizontal lengths L_x and L_y according to

$$\langle \varphi \rangle(z) \equiv \frac{\int_0^{L_y} \int_0^{L_x} \Pi \varphi \, dx \, dy}{\int_0^{L_y} \int_0^{L_x} \Pi \, dx \, dy}, \quad (\text{A.3})$$

where $\Pi(x, y, z)$ is a masking function that is equal to one inside the fluid and zero inside the solid. Note that if only averaging over a single direction, e.g. when determining $\langle \varphi \rangle_y(x, z)$, the definition is very similar to above, only the other direction (x) is not integrated over.

To determine the triple decomposition, let $\bar{\varphi}''(x, y, z) = \bar{\varphi}(x, y, z) - \langle \bar{\varphi} \rangle(z)$, then substitute this into the Reynolds decomposition, i.e. $\varphi(x, y, z, t) = \bar{\varphi}(x, y, z) + \varphi'(x, y, z, t)$ to obtain $\varphi(x, y, z, t) = \langle \bar{\varphi} \rangle(z) + \bar{\varphi}''(x, y, z) + \varphi'(x, y, z, t)$.

It can be shown that the total vertical flux is given by $\langle \bar{w} \bar{\varphi} \rangle = \langle \bar{w} \rangle \langle \bar{\varphi} \rangle + \langle \bar{w}'' \bar{\varphi}'' \rangle + \langle \bar{w}' \varphi' \rangle$ (Sutzi, 2021). When modelling the flow with periodic lateral boundary conditions and a free slip top boundary condition, $\langle \bar{w} \rangle = 0$. This can be seen from the time averaged

continuity equation ($\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} = 0$). Integrating over the x and y directions yields $\int_0^{L_y} [\bar{u}]_0^{L_x} dy + \int_0^{L_x} [\bar{v}]_0^{L_y} dy + L_x L_y \frac{\partial \langle \bar{w} \rangle}{\partial z} = \text{constant}$. The first two terms vanish by periodicity, so integrating in the z direction yields $\langle \bar{w} \rangle = mz + c$ for some constants m and c . Since $w(z = 0) = w(z = L_z) = 0$ with no penetration at the bottom and free slip boundary conditions at the top, $m = c = 0$, and thus $\langle \bar{w} \rangle = 0$, therefore the first term vanishes. The second and third terms are referred to as the dispersive and turbulent fluxes. The turbulent flux can be calculated using $\langle \overline{w'\varphi'} \rangle = \langle \overline{w\varphi} \rangle - \langle \bar{w}\bar{\varphi} \rangle$, and combining this with the expression for the total flux implies that the dispersive flux is given by $\langle \bar{w}''\bar{\varphi}'' \rangle = \langle \bar{w}\bar{\varphi} \rangle$. Note that there is also a contribution to the flux due from the sub-grid scheme, though this is often negligible compared to the turbulent and dispersive fluxes.

Appendix B

Pressure solver

Following Ferziger et al. (2019), the time evolution for velocity (discretised using an Euler time scheme for simplicity) can be expressed as

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = -\nabla p^{n+1} + \mathbf{r}^n. \quad (\text{B.1})$$

Here $\mathbf{r}^n$ includes all processes other than the kinematic deviatoric pressure (p^{n+1}). This is determined using a two-step scheme which involves introducing the pressure correction $\pi^n = p^{n+1} - p^n$ and a predicted velocity $\mathbf{u}^*$ defined according to

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} = -\nabla p^n + \mathbf{r}^n. \quad (\text{B.2})$$

Substitution into Eq. (B.1) yields

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} = -\nabla \pi^n \quad (\text{B.3})$$

Requiring incompressibility ($\nabla \cdot \mathbf{u}^{n+1} = 0$) results in a Poisson equation for the pressure correction:

$$\nabla^2 \pi^n = \frac{\nabla \cdot \mathbf{u}^*}{\Delta t} \quad (\text{B.4})$$

Discretising in space and denoting the right hand side of Eq. (B.4) as f :

$$\begin{aligned} & \frac{\pi_{i+1,j,k} - 2\pi_{i,j,k} + \pi_{i-1,j,k}}{\Delta x^2} + \frac{\pi_{i,j+1,k} - 2\pi_{i,j,k} + \pi_{i,j-1,k}}{\Delta x^2} + \\ & \frac{\frac{\pi_{i,j,k+1} - \pi_{i,j,k}}{\Delta z_{k+1/2}} - \frac{\pi_{i,j,k} - \pi_{i,j,k-1}}{\Delta z_{k-1/2}}}{\Delta z_k} = f_{i,j,k} \end{aligned} \quad (\text{B.5})$$

Next, take the discrete Fourier transform (DFT) of both sides with respect to x then y , using $\hat{\cdot}$ to denote a transformed quantity. The regular DFT, yielding a periodic function, in the x direction of a quantity φ is (according to the FFTW library; Frigo and Johnson, 1998):

$$\hat{\varphi}_n = \sum_{i=0}^{N_x-1} \varphi_i \exp\left(\frac{-2\pi J n i}{N_x}\right), \quad n = 0, \dots, N_x - 1, \quad (\text{B.6})$$

where $J = \sqrt{-1}$. The (unnormalised) inverse transform is identical with the n and i indices swapped, only with the opposite sign of the exponential.¹

The type-II discrete cosine transform (DCT) yielding an even function, thereby satisfying Neumann boundary conditions, is (Frigo and Johnson, 1998):

$$\hat{\varphi}_n = 2 \sum_{i=0}^{N_x-1} \varphi_i \cos\left(\frac{\pi n(i + \frac{1}{2})}{N_x}\right), \quad n = 0, \dots, N_x - 1. \quad (\text{B.7})$$

The inverse is the type-III transform, which is identical with the n and i indices swapped. The y direction is similar, with the modes denoted by m . It can be shown that performing the DFT/DCT on Eq. (B.5) yields:

$$a_k \hat{\pi}_{n,m,k-1} + b_{n,m,k} \hat{\pi}_{n,m,k} + c_k \hat{\pi}_{n,m,k+1} = \hat{f}_{n,m,k} \quad (\text{B.8})$$

Here $a_k = \frac{1}{\Delta z_k \Delta z_{k-1/2}}$, $c_k = \frac{1}{\Delta z_k \Delta z_{k+1/2}}$, and $b_{n,m,k} = -(a_k + c_k) + \lambda_n + \lambda_m$, where λ_n and λ_m are given by

$$\lambda_n = \begin{cases} \frac{2}{\Delta x^2} (\cos \frac{2\pi n}{N_x} - 1) & \text{DFT} \\ \frac{2}{\Delta x^2} (\cos \frac{\pi n}{N_x} - 1) & \text{DCT} \end{cases} \quad n = 0, \dots, N_x - 1, \quad (\text{B.9})$$

$$\lambda_m = \begin{cases} \frac{2}{\Delta y^2} (\cos \frac{2\pi m}{N_y} - 1) & \text{DFT} \\ \frac{2}{\Delta y^2} (\cos \frac{\pi m}{N_y} - 1) & \text{DCT} \end{cases} \quad m = 0, \dots, N_y - 1. \quad (\text{B.10})$$

For each mode, this is a tridiagonal system with $k = 0, \dots, N_z + 1$, which is solved using Gaussian elimination. In uDALES, boundary conditions are not inserted into $\hat{f}_0$ and

¹Care must be taken with the size and types of data arrays. The FFTW implementation of the DFT used in uDALES is defined for complex functions, and satisfies Hermitian symmetry, i.e. $\hat{\varphi}_n = \hat{\varphi}_{n-i}$. This means that for real functions, half of the output array is redundant (being the complex conjugate of the other half), and so the (real) output is actually of size $N_x/2 + 1$. Before using the inverse transform, this must be converted back to a complex array of size N_x .

$\hat{f}_{N_z+1}$ in order to explicitly solve for the ghost cells $\hat{\pi}_0$ and $\hat{\pi}_{N_z+1}$. Instead, the equations for $k = 1$ and $k = N_z$ are modified in light of the top and bottom boundary conditions, which is numerically equivalent. Specifically, the bottom boundary condition is Neumann for all modes, i.e. $\hat{\pi}_{n,m,0} = \hat{\pi}_{n,m,1} \ \forall \ n, m$. This means that the $k = 1$ equation becomes:

$$(a_1 + b_{n,m,1})\hat{\pi}_{n,m,1} + c_1\hat{\pi}_{n,m,2} = \hat{f}_{n,m,1}. \quad (\text{B.11})$$

The top is Neumann for all modes other than $n = m = 0$ (the zero mode) in which case it is Dirichlet, i.e. $\hat{\pi}_{N_z+1} = -\hat{\pi}_{N_z}$. Applying the Neumann condition results in:

$$a_{N_z-1}\hat{\pi}_{n,m,N_z-1} + (b_{n,m,N_z} + c_{N_z})\hat{\pi}_{n,m,N_z} = \hat{f}_{n,m,N_z}, \quad (\text{B.12})$$

and the Dirichlet condition for the zero mode:

$$a_{N_z-1}\hat{\pi}_{0,0,N_z-1} + (b_{0,0,N_z} - c_{N_z})\hat{\pi}_{0,0,N_z} = \hat{f}_{0,0,N_z}. \quad (\text{B.13})$$

Numerically, this avoids the problem being ill-posed: since $b_{0,0,k} = 0$, the matrix describing the system of equations (B.8) is singular if both the first and last rows are the same, which would be the case if both correspond to a Neumann condition. Setting a Dirichlet condition instead at the top is also a physically reasonable choice because the zero mode is equal to the plane-averaged pressure, which can reasonably expected to be zero at the top of the domain. For inflow-outflow simulations, the pressure gradient at the top is accounted for in the boundary condition for vertical velocity $w \equiv u_z$. Given that the Dirichlet boundary condition for plane-averaged pressure is $\langle \pi \rangle_{N_z+1} = -\langle \pi \rangle_{N_z}$, the vertical velocity satisfies

$$\frac{w_{i,j,N_z+1}^* - w_{i,j,N_z+1}^n}{\Delta t} = \frac{2\langle p^n \rangle_{N_z}}{\Delta z_{N_z+1}} \quad \forall i, j, \quad (\text{B.14})$$

$$\frac{w_{i,j,N_z+1}^{n+1} - w_{i,j,N_z+1}^*}{\Delta t} = \frac{2\langle \pi^n \rangle_{N_z}}{\Delta z_{N_z+1}} \quad \forall i, j. \quad (\text{B.15})$$

Appendix C

Flow reconstruction

If the distance between the facet and a fluid boundary point (d) is less than $z_0 e$, where z_0 is the momentum roughness length, the wall functions become non-physical because there is a factor of $\log(d/z_0)$ (see Sect. 2.3.2). In these cases, it is necessary to use reconstruction, in which the flux is calculated at a point further away in the facet normal direction. Once the flux has been calculated at this reconstruction point it can be applied to the fluid boundary point because by assumption the region in which the wall functions are valid (the log layer) has constant fluxes. The location is found by projecting a ray in the normal direction from the fluid boundary point until it hits one of the edges of the cell. A common approach is to project a fixed distance into the adjacent cell, but this would mean it is possible that the surrounding points are at least two indices away, which is problematic if the flux point is on the edge of a decomposition pencil. This approach guarantees that all the points used in the stencil are known to the current MPI rank (assuming that a single halo cell is used).

Trilinear interpolation is used to determine the value of flow variables at the reconstruction point. To calculate a variable φ at a point (x, y, z) somewhere in cell i, j, k of a given grid, i.e. $x_i \leq x \leq x_{i+1}$, $y_j \leq y \leq y_{j+1}$, and $z_k \leq z \leq z_{k+1}$, let

$\tilde{x} = (x - x_i)/(x_{i+1} - x_i) = (x - x_i)/\Delta x$, and similar for $\tilde{y}$ and $\tilde{z}$. The value is given by:

$$\begin{aligned}
\varphi(x, y, z) &= \varphi(x_i, y_j, z_k)(1 - \tilde{x})(1 - \tilde{y})(1 - \tilde{z}) \\
&+ \varphi(x_{i+1}, y_j, z_k)\tilde{x}(1 - \tilde{y})(1 - \tilde{z}) \\
&+ \varphi(x_i, y_{j+1}, z_k)(1 - \tilde{x})\tilde{y}(1 - \tilde{z}) \\
&+ \varphi(x_{i+1}, y_{j+1}, z_k)\tilde{x}\tilde{y}(1 - \tilde{z}) \\
&+ \varphi(x_i, y_j, z_{k+1})(1 - \tilde{x})(1 - \tilde{y})\tilde{z} \\
&+ \varphi(x_{i+1}, y_j, z_{k+1})\tilde{x}(1 - \tilde{y})\tilde{z} \\
&+ \varphi(x_i, y_{j+1}, z_{k+1})(1 - \tilde{x})\tilde{y}\tilde{z} \\
&+ \varphi(x_{i+1}, y_{j+1}, z_{k+1})\tilde{x}\tilde{y}\tilde{z}
\end{aligned}$$

Note that in this case, since the reconstruction point is at one of the cell edges, the scheme for variables defined on this edge reduces to a bilinear interpolation. A 2D example for a scalar variable is shown in Fig. C.1.

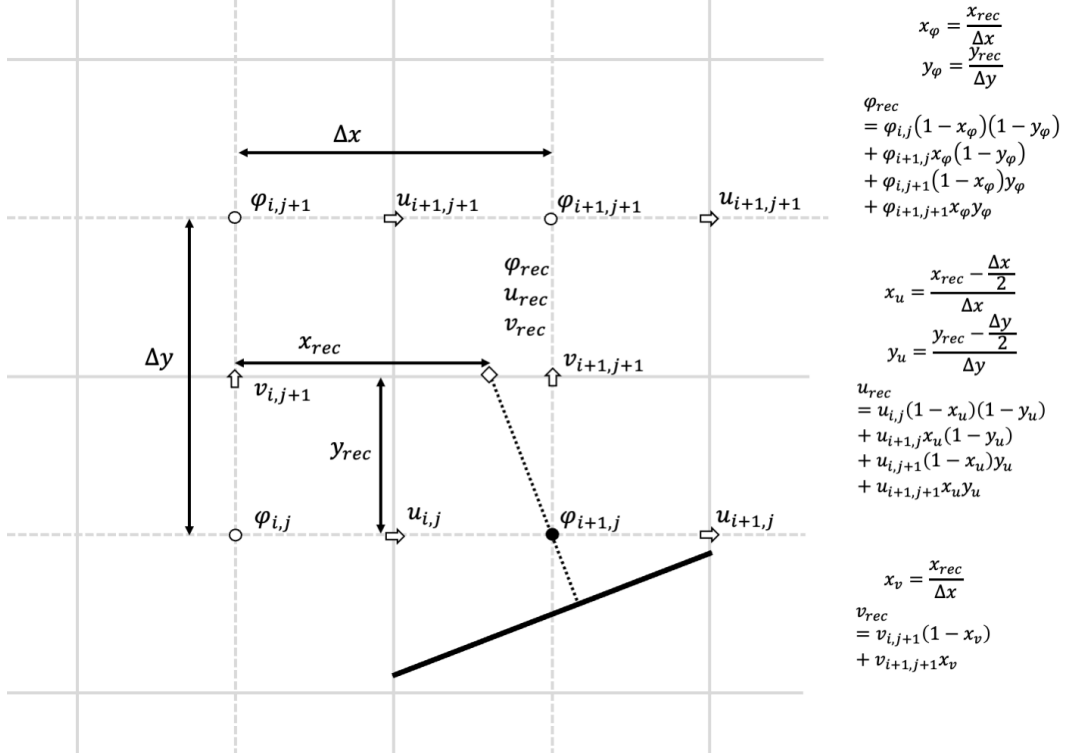


Figure C.1: Reconstruction of flow variables φ in 2D using a bilinear interpolation scheme. A facet section is shown in solid black, the scalar grid cell edges are solid grey, and the u and v grid cell edges are dotted grey (where they are staggered with respect to the scalar grid). Note that the bilinear interpolation reduces to a linear one for the v component.

Appendix D

Surface scheme in uDALES v2.0

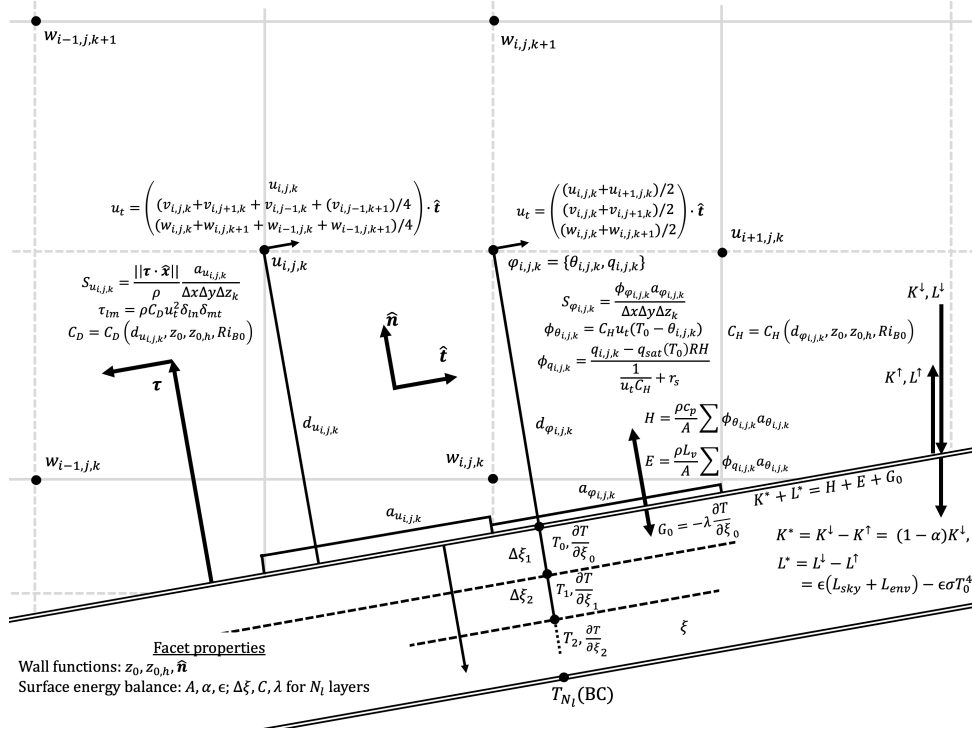


Figure D.1: Surface scheme in uDALES v2.0, including the surface energy balance and parameterised shear stress, sensible heat flux, and latent heat flux at fluid boundary points. For nomenclature, refer to Sects. 2.2, 2.3.2, and 3.4.2.

Appendix E

MORUSES

In JULES (Best et al., 2011), the drag coefficient is given by $C_m = \kappa^2 / \mathcal{F}_m^2$, where κ is the von Kármán constant, and in neutral conditions $\mathcal{F}_m = \log(\frac{z_1 + z_0}{z_0})$, where z_1 is the first atmospheric model level and z_0 is the momentum roughness length. In non-neutral conditions, $\mathcal{F}_m$ is a modification of this formulation. Similarly, the heat transfer coefficient is given by $C_h = \kappa^2 / (\mathcal{F}_m \mathcal{F}_h)$, where $\mathcal{F}_h = \log(\frac{z_1 + z_0}{z_{0,h}})$ in neutral conditions, with modifications for non-neutral conditions, where $z_{0,h}$ is the heat roughness length.

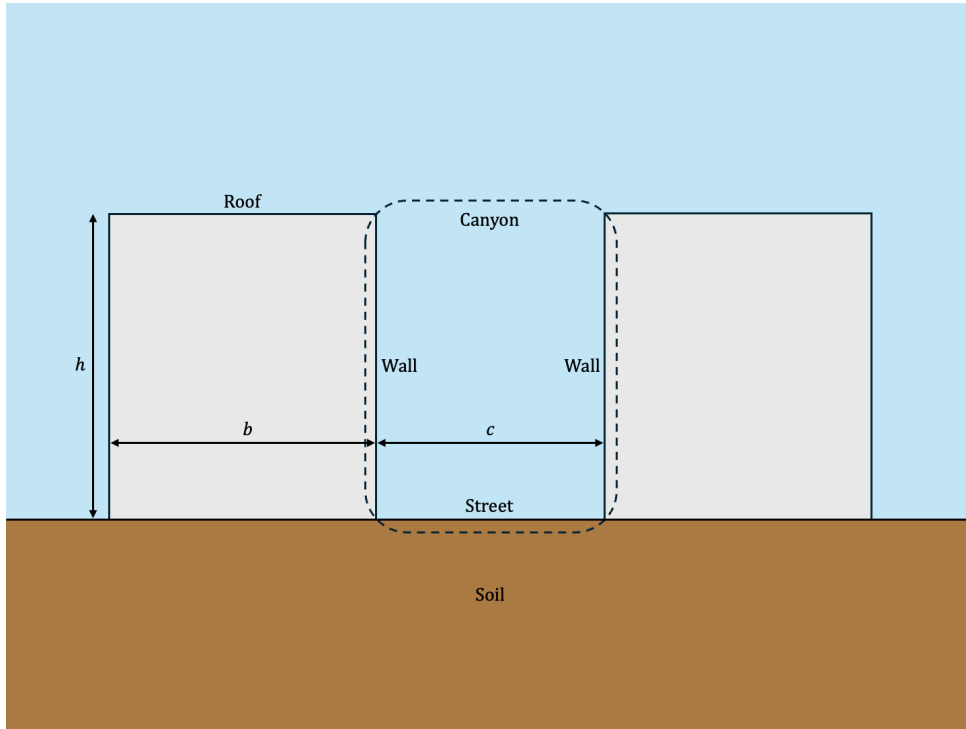


Figure E.1: Street canyon geometry representation in MORUSES, the UCM used by MetUM (Porson et al., 2010a). There are two urban tiles: roofs and canyons, with the latter consisting of the walls and streets combined.

For the urban tiles in MORUSES (Porson et al., 2010a), z_0 is calculated using an empirical formula for staggered cubic arrays (Macdonald et al., 1998). The displacement height (z_d) is given by

$$z_d = (1 + a_0^{-\lambda_p}(\lambda_p - 1))h, \quad (\text{E.1})$$

and z_0 is given by

$$z_0 = \left(\left(1 - \frac{z_d}{h} \right) \exp \left(- \left(\frac{1}{2} \beta \frac{C_{m,0}}{\kappa^2} \left(1 - \frac{z_d}{h} \lambda_f \right)^{-\frac{1}{2}} \right) \right) h, \quad (\text{E.2})$$

where $a_0 = 4.43$, $\beta = 1$, and $C_{m,0} = 1.2$.

Furthermore, $z_{0,h}$ is given by

$$z_{0,h} = h(z_1 + z_0) \left(h \exp \left(\frac{\kappa^2 r_{\text{bulk}}}{\log \left(\frac{z_1 + z_0}{z_0} \right)} \right) \right)^{-1}, \quad (\text{E.3})$$

where r_{bulk} is a resistance that depends on the tile and accounts for the flow regime over the canyon based on the ratio h/c (and thus cannot be calculated a priori).

Each urban tile is modelled as a single layer that is coupled to the soil (at temperature T_{soil}) via the ground heat flux (G) and to the air via the sensible heat flux (H). The SEB is given by

$$CD \frac{dT_{\text{tile}}}{dt} + G(T_{\text{tile}}, T_{\text{soil}}) = R^*(T_{\text{tile}}) - H(T_{\text{tile}}, \theta_a, u_a), \quad (\text{E.4})$$

where D is the thickness of the tile, set to $(2\pi/\Omega)^{\frac{1}{2}}$ where Ω is the angular frequency of the Earth's rotation ($\Omega = 2\pi/86400 \text{ s}^{-1}$). The volumetric heat capacity of the canyon tile (C_{canyon}) is given by

$$C_{\text{canyon}} = C_{\text{street}} + \frac{2h}{c} C_{\text{wall}}. \quad (\text{E.5})$$

The net radiation (R^*) is expressed in terms of shortwave (K^*) and longwave (L^*) contributions:

$$R^* = K^* + L^* = (1 - \alpha)K^\downarrow + \epsilon(L^\downarrow - \sigma T_{\text{tile}}^4). \quad (\text{E.6})$$

For the canyon tile, to account for scattering between the street and walls, an effective albedo (α_{canyon}) and emissivity (ϵ_{canyon}) are used. The former is given by

$$\alpha_{\text{canyon}} = \Psi_{\text{street}} + \Upsilon_{\text{street}} + \frac{2h}{c} (\Psi_{\text{wall}} + \Upsilon_{\text{wall}}), \quad (\text{E.7})$$

with a similar expression for ϵ_{canyon} . Here $\Psi(\Theta)$ represents the fraction of incoming solar radiation reaching the street/walls after sky diffusion and shading effects, and $\Upsilon(\Theta)$ represents the radiation reflected between the streets and walls (note the dependence on the solar zenith angle Θ).

When calculating G , the canyon is assumed to be conductively coupled with the soil, whereas the roof is radiatively coupled, i.e.

$$G_{\text{canyon}} = -\lambda_{\text{canyon-soil}} \frac{2(T_{\text{soil}} - T_{\text{canyon}})}{D_{\text{soil}}}, \quad G_{\text{roof}} = \sigma T_{\text{roof}}^4 - \sigma T_{\text{soil}}^4, \quad (\text{E.8})$$

where $\lambda_{\text{canyon-soil}}$ is the thermal conductivity of the canyon-soil interface. Note that G is therefore assumed to be constant in the layer.

Appendix F

Additional visualisations

F.1 Chapter 5

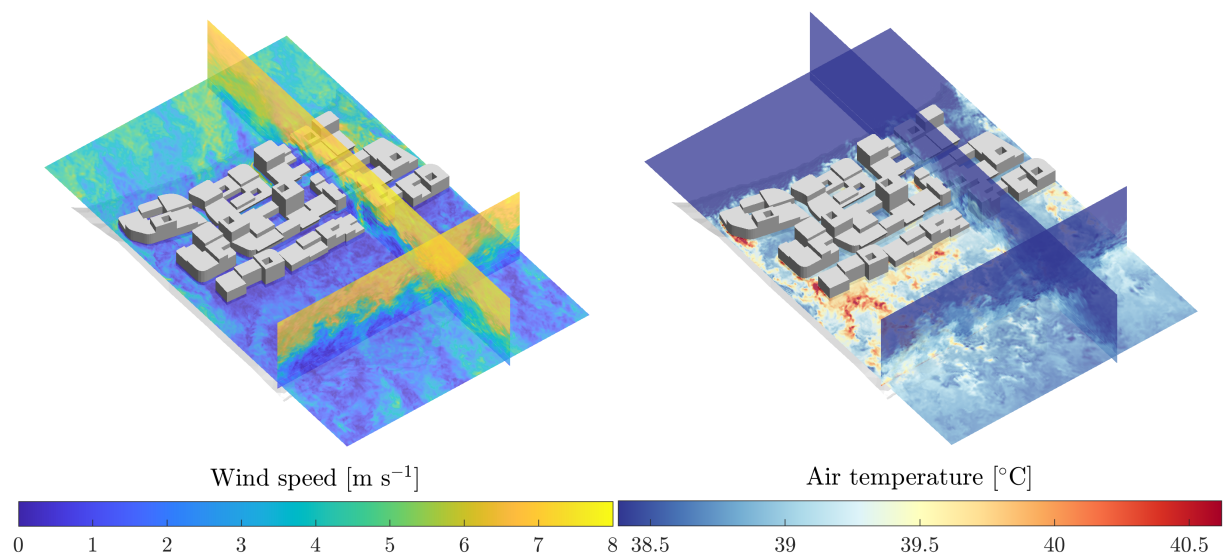


Figure F.1: Instantaneous wind speed and air temperature at horizontal and vertical slices at 1600 LT.

F.2 Chapter 7

F.2.1 Surface energy balance

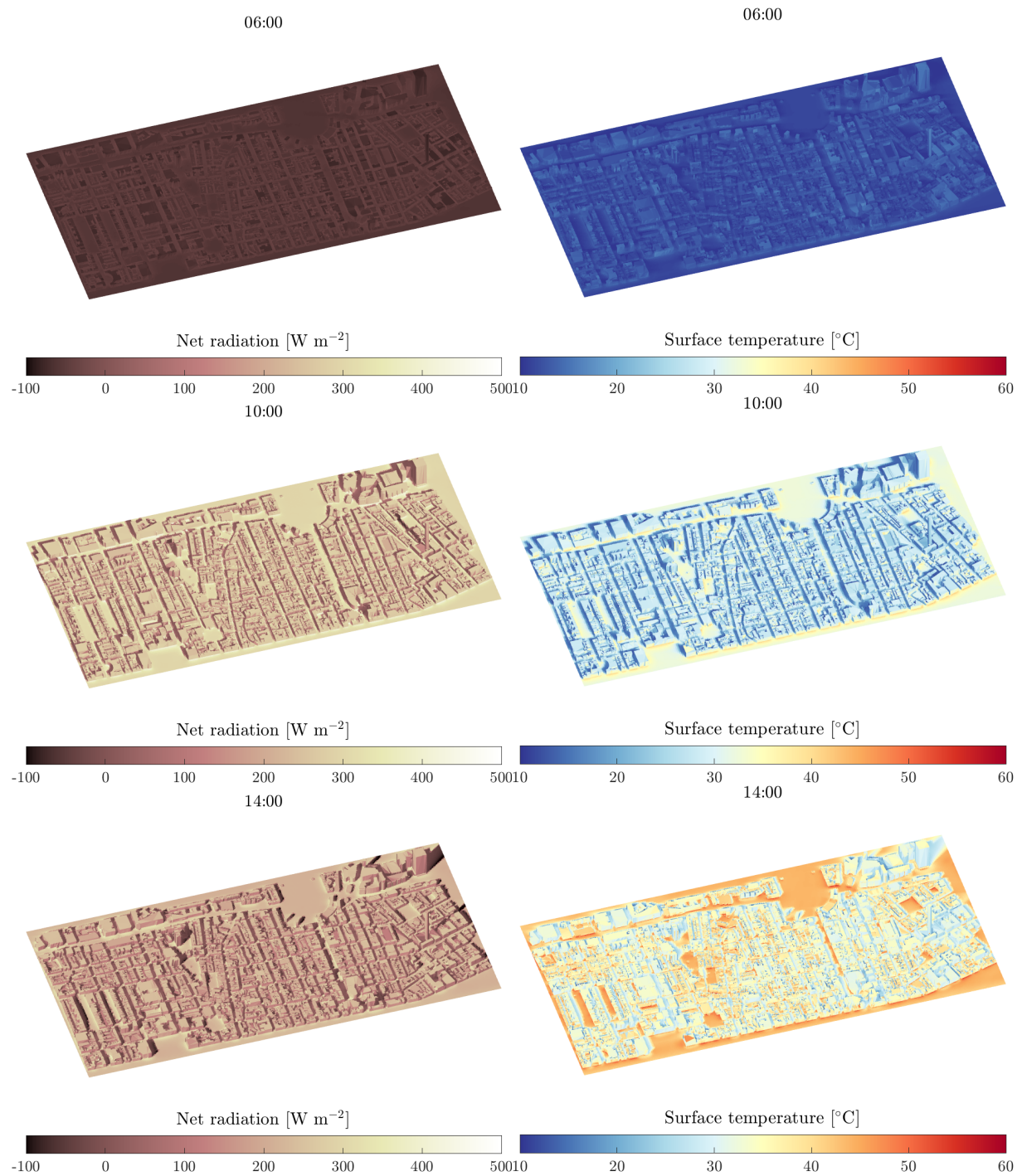


Figure F.2: Evolution of net radiation and surface temperature.

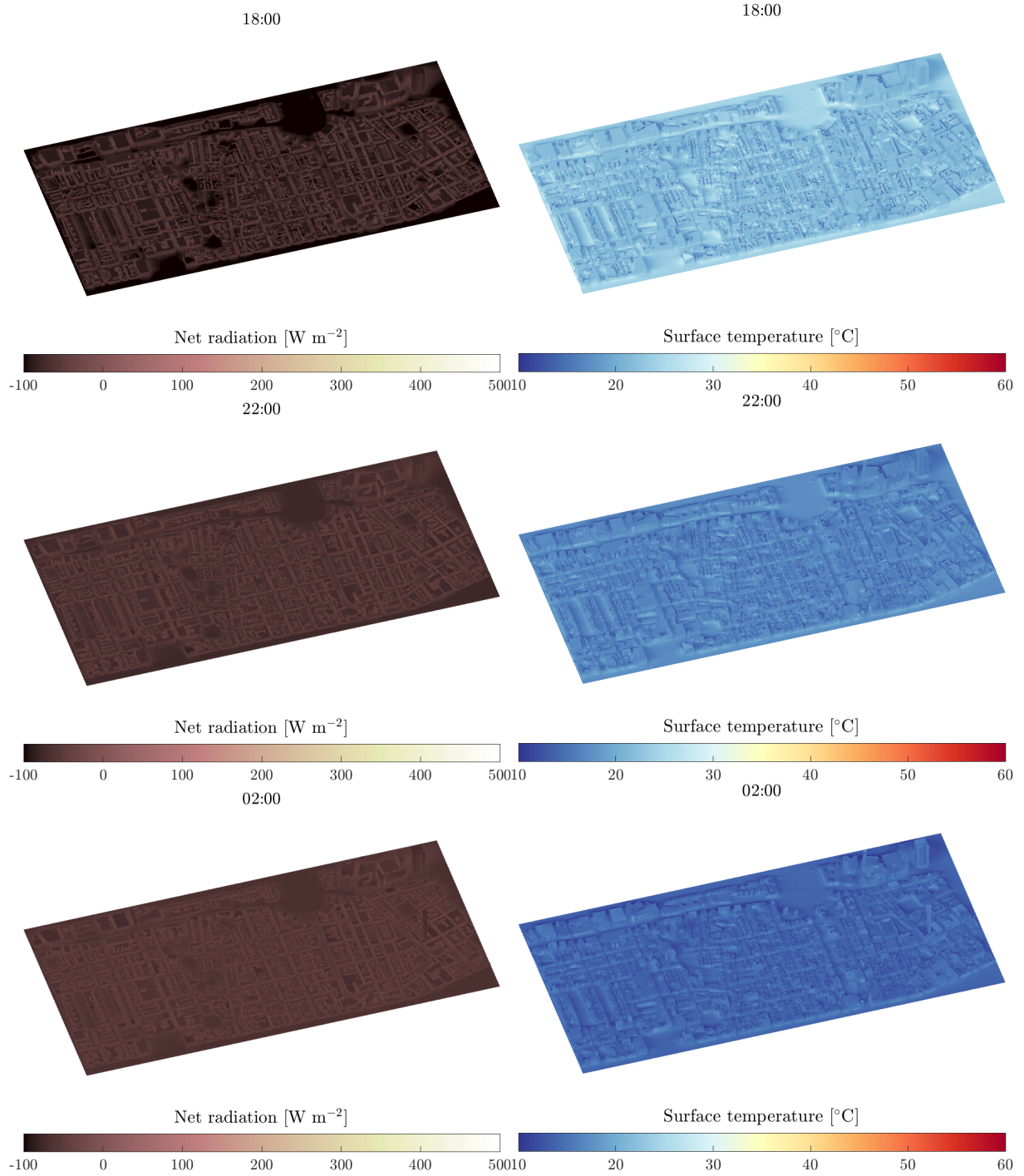


Figure F.3: Evolution of net radiation and surface temperature (continued from Fig. F.2).

F.2.2 Flow

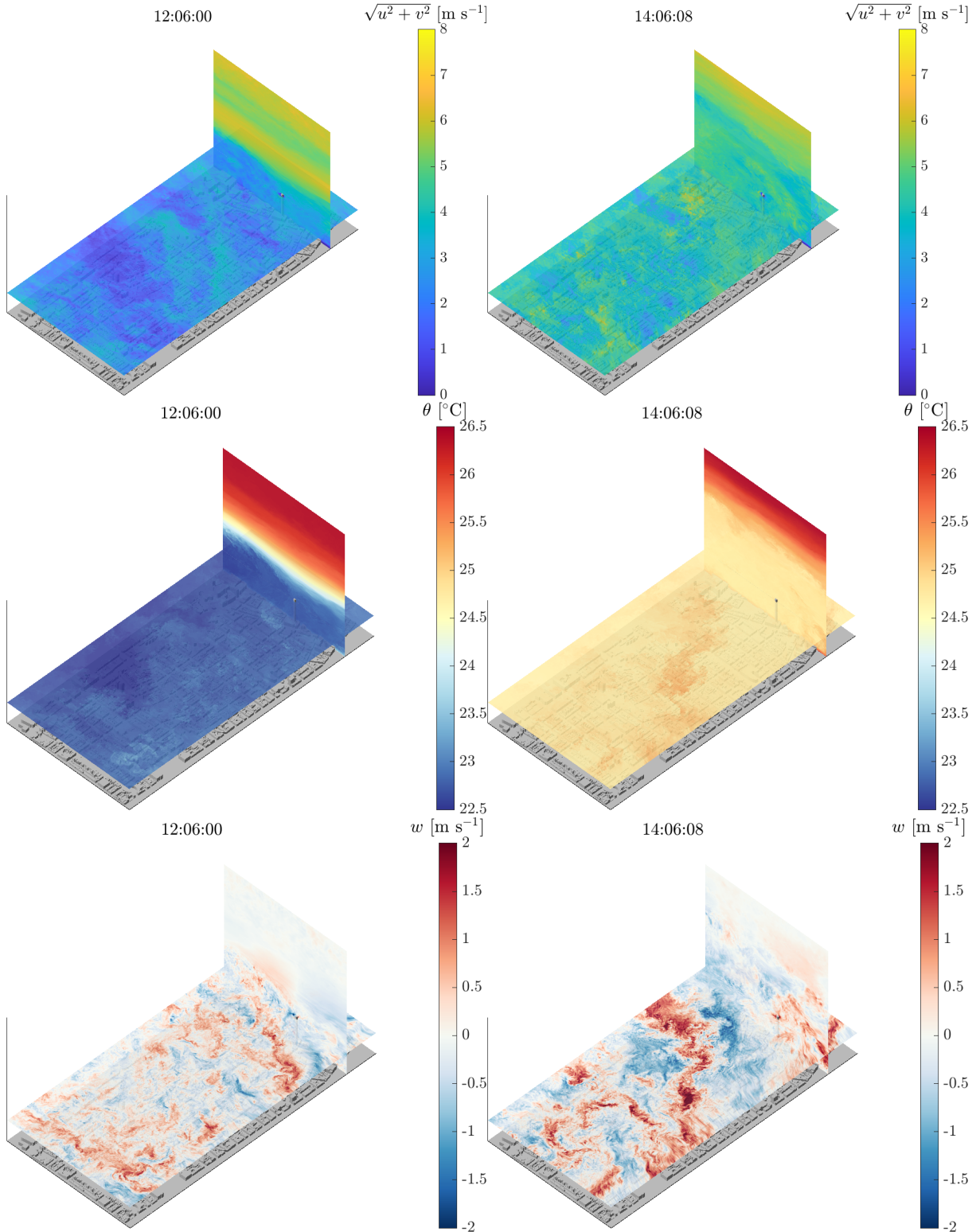


Figure F.4: Evolution of wind speed ($\sqrt{u^2 + v^2}$), air potential temperature (θ), and vertical velocity (w) for case presented in Chapter 7.

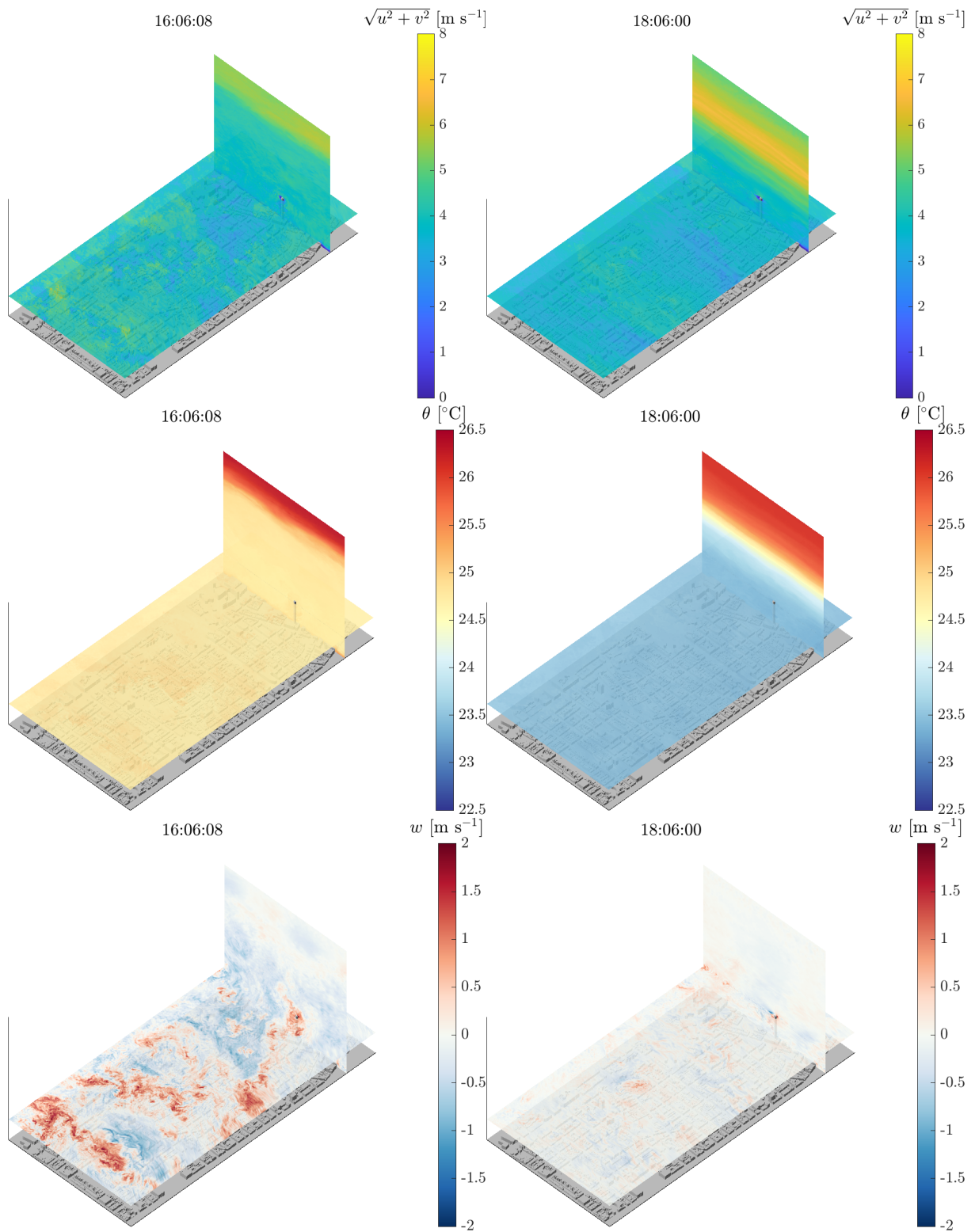


Figure F.5: Evolution of wind speed ($\sqrt{u^2 + v^2}$), air potential temperature (θ), and vertical velocity (w) (continued from Fig. F.4).