Pollutant transport in the Urban Canopy Layer using a Lagrangian Particle Dispersion Model

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Abstract

This thesis studied urban particle dispersion close to source and ground. It used an existing, steady state, three dimensional Lagrangian particle dispersion model, which includes roughness sublayer parameterizations of turbulence and flow. The model is valid for convective and neutral to stable conditions and uses the kernel method for concentration calculation.

Already published corrections to the original model formulation were introduced to the model. An additional model error in the velocity auto-covariance derivative parameterization of the roughness sublayer, detected during the course of this work, was corrected. The impact of these changes were compared to that of a new dissipation rate parameterization in the roughness sublayer, which was based on observations. Furthermore, an earlier work hypothesized that improving the lower boundary condition could improve the model predictions. This modification was realized and its influence compared to the other changes. To reach these goals, the model was initialized and compared with measurements that had been taken during the Basel UrBan Boundary Layer Experiment (BUBBLE), using SF$_6$ as tracer.

One of the corrections to the model formulation, changing the solenoidal probability current, provides better model results, while the rest were only wrong in the publications, not the source code. The newly detected model error has a large influence on the model results. Model performance was neither clearly enhanced nor was it definitely diminished by the new dissipation rate parameterization. Despite this, the present results indicate that the magnitude of the dissipation rate is more important than the shape and derivative of its profile in the roughness sublayer. After correcting the newly detected model error, the results that inspired the modification of the lower boundary condition could no longer be replicated. Consequently, the proposed modification does not improve the model’s agreement with measurements. Additionally, this thesis showed that the model with the drift boundary condition is similarly sensitive to adjustments of the zero plane displacement height and the roughness sublayer boundary height as the original model.
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\( \alpha \) \text{inc} \quad \text{incidence angle between main canyon axis and mean wind speed}

\( \alpha \) \text{street} \quad \text{street canyon direction}

\( \alpha \) \text{wd} \quad \text{mean wind direction}

\( \alpha_a \) \quad \text{angle to choose sign of } y \text{-displacement for canyon drift}

\( \beta_1 \) \quad \text{coefficient in } \Phi_i^*, \text{ introduced by Gibson and Sailor (2012)} \quad \text{s m}^{-1}

\( \beta_2 \) \quad \text{coefficient in } \Phi_i^*, \text{ introduced by Gibson and Sailor (2012)} \quad \text{m s}^{-1}

\( u \) \quad \text{(} \bar{u} + u, v, w \text{)} velocity vector \quad \text{m s}^{-1}

\( x \) \quad \text{(} x, y, z \text{)}, \text{ three dimensional position vector} \quad \text{m}

\( \Delta \Theta \) \quad \text{difference in wall temperature between windward and leeward wall} \quad \text{K}

\( \Delta y_{arc} \) \quad \text{distance between arc receptors along arc} \quad \text{m}

\( \hat{u} \) \quad \text{reference velocity similar to friction velocity} \quad \text{m s}^{-1}

\( d \xi_j \) \quad \text{increment of a Wiener process with mean zero and variance } dt \quad \text{s}

\( dt \) \quad \text{time step} \quad \text{s}

\( du_i \) \quad \text{infinitesimal increment of a velocity component} \quad \text{m}

\( \Theta \) \quad \text{average temperature in street canyon} \quad \text{K}

\( \tau_y \) \quad \text{crosswind integrated concentration} \quad \text{ng m}^{-2}

\( \bar{u}' w_G \) \quad \text{joint moment of } u' \text{ and } w \text{ in the Gaussian distribution} \quad \text{m}^2 \text{s}^{-1}

\( \bar{u}' w \) \quad \text{measured joint moment of } u' \text{ and } w \text{ in the atmosphere} \quad \text{m}^2 \text{s}^{-1}

\( \bar{u} \) \quad \text{mean longitudinal velocity component} \quad \text{m s}^{-1}

\( \bar{u}_{vort} \) \quad \text{circumferential velocity of vortex in canyon} \quad \text{m s}^{-1}

\( u_a \) \quad \text{mean wind speed along main canyon axis} \quad \text{m s}^{-1}

\( u_c \) \quad \text{mean wind speed across main canyon axis} \quad \text{m s}^{-1}

\( \bar{u}_h \) \quad \text{mean horizontal wind speed at roof top level} \quad \text{m s}^{-1}

\( \Phi_i \) \quad \text{probability current following velocity } i \quad \text{m}^{-1}

\( \Phi_i^* \) \quad \text{additional part of probability current } \Phi_i \quad \text{m}^{-1}

\( \Phi_i^C \) \quad \text{convective part of probability current } \Phi_i \quad \text{m}^{-1}

\( \Phi_i^G \) \quad \text{Gaussian part of probability current } \Phi_i \quad \text{m}^{-1}

\( \rho \) \quad \text{Gaussian correlation coefficient between } u' \text{ and } w \quad \text{m}^{-1}

\( \sigma_A \) \quad \text{standard deviation of } P_A \quad \text{m s}^{-1}

\( \sigma_B \) \quad \text{standard deviation of } P_B \quad \text{m s}^{-1}

\( \sigma_{c,y} \) \quad \text{spread of concentration along arc} \quad \text{m}

\( \sigma_{uG} \) \quad \text{standard deviation of Gaussian longitudinal velocity} \quad \text{m s}^{-1}
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\( \sigma_{uwG} \) . . . joint moment of \( u \) and \( w \) in Gaussian probability density function \( \text{m s}^{-1} \)
\( \sigma_{wG} \) . . . standard deviation of Gaussian lateral velocity \( \text{m s}^{-1} \)
\( \tau \) . . . . . . residence time a particle stays trapped in street canyon \( \text{s} \)
\( \tau_{\text{int}} \) . . . . integral scale of turbulent quantity \( \text{s} \)
\( \Theta' \) . . . . temperature fluctuation \( \text{K} \)
\( \varepsilon \) . . . . dissipation rate of turbulent kinetic energy \( \text{m}^2 \text{s}^{-3} \)
\( A \) . . . . . parameter, regulates area of updraft
\( a_{\text{int}} \) . . . . accuracy, between 0 and 1
\( a_i \) . . . . correlated part of acceleration \( \text{m s}^{-2} \)
\( B \) . . . . parameter, regulates area of downdraft
\( B_{D} \) . . . nondimensional bouyancy after Dallman et al. (2014)
\( b_{ij} \) . . . . random part of acceleration \( \text{m s}^{-2} \)
\( C \) . . . . . normalizing factor for kernel function
\( c \) . . . . . local concentration \( \text{ng m}^{-3} \)
\( C_0 \) . . . . Kolmogorov constant of the Lagrangian structure function
\( c_{\text{arcmax}} \) . . . highest concentration along an arc \( \text{ng m}^{-3} \)
\( c_{\text{FN}} \) . . . . area of false negative
\( c_{\text{FP}} \) . . . . area of false positive
\( c_{\text{OB}} \) . . . . area of observation
\( c_{\text{PR}} \) . . . . area of prediction
\( c_o \) . . . . observed concentration at sampler \( \text{ng m}^{-3} \)
\( c_s \) . . . . simulated concentration at sampler \( \text{ng m}^{-3} \)
\( d \) . . . . . displacement height \( \text{m} \)
\( f \) . . . . . transition function
\( g \) . . . . . acceleration due to gravity \( \text{m s}^{-2} \)
\( H \) . . . . . average building height \( \text{m} \)
\( h_i \) . . . . width of the kernel in \( x-, y-, \) and \( z\)-direction \( \text{m} \)
\( i \) . . . . . . \( = 1, 2, 3 \), components in space
\( J \) . . . . . . averaging period of turbulent quantity \( \text{s} \)
\( j \) . . . . . . \( = 1, 2, 3 \), components in space
\( K \) . . . . . . kernel function
\( k = 0.41 \) . . von Kàrmààn constant
\( k_u \) . . . coefficient for roughness sublayer parameterization of \( \overline{u'^2} \)
\( k_v \) . . . . . coefficient for roughness sublayer parameterization of \( \overline{v'^2} \)
\( k_w \) . . . . coefficient for roughness sublayer parameterization of \( \overline{w'^2} \)
\( L \) . . . . Obukhov length \( \text{m} \)
\( m_f \) . . . . weighting function to relate concentration to its density \( \text{ng} \)
\( n \) . . . . . number of particles
\( P_{\text{tot}} \) . . . total probability density function of particle velocities \( \text{s}^2 \text{m}^{-2} \)
\( P_A \) . . . . . . updraft velocity probability density function . . . . . . . . \( s^2 \text{ m}^{-2} \)
\( p_a \) . . . . . . proportionality constant of roof level wind and along canyon wind
\( P_B \) . . . . . . downdraft velocity probability density function . . . . \( s^2 \text{ m}^{-2} \)
\( P_c \) . . . . . . vertical wind speed probability density function . . . . \( s^2 \text{ m}^{-2} \)
\( p_c \) . . . . . . proportionality constant of roof level wind and cross canyon wind
\( P_G \) . . . . . . velocity probability density function in neutral boundary layer \( s^2 \text{ m}^{-2} \)
\( P_u \) . . . . . . longitudinal velocity probability density function . . . \( s^2 \text{ m}^{-2} \)
\( P_v \) . . . . . . lateral velocity probability density function . . . . . . \( s^2 \text{ m}^{-2} \)
\( P_w \) . . . . . . vertical velocity probability density function . . . . . . \( s^2 \text{ m}^{-2} \)
\( P_{uw} \) . . . . . probability density function of correlation between \( u \) and \( w \) . . \( s^2 \text{ m}^{-2} \)
\( Q_i \) . . . . . . model function, derivative of velocity-pdf in regard to velocity . \( s^3 \text{ m}^{-3} \)
\( u \) . . . . . . = \( \bar{u} + u' \) longitudinal velocity component . . . . . . . m s\(^{-1} \)
\( u' \) . . . . . . longitudinal velocity component perturbation . . . . . . m s\(^{-1} \)
\( u_* \) . . . . . . friction velocity . . . . . . . . . . . . . . . . . . . . . m s\(^{-1} \)
\( u_{*L} \) . . . . . local friction velocity . . . . . . . . . . . . . . . . m s\(^{-1} \)
\( v \) . . . . . . lateral velocity component . . . . . . . . . . . . . . . . . . . . . . m s\(^{-1} \)
\( v' \) . . . . . . lateral velocity component perturbation . . . . . . . . . . m s\(^{-1} \)
\( W \) . . . . . . width of canyon . . . . . . . . . . . . . . . . . . . . . . . m
\( w \) . . . . . . vertical velocity component . . . . . . . . . . . . . . . . . m s\(^{-1} \)
\( w' \) . . . . . . vertical velocity component perturbation . . . . . . . . m s\(^{-1} \)
\( w_* \) . . . . . . convective velocity scale . . . . . . . . . . . . . . . . . m s\(^{-1} \)
\( x \) . . . . . . horizontal position along mean horizontal speed . . . . . . m
\( x_p \) . . . . . . \( x \)-position of arc . . . . . . . . . . . . . . . . . m
\( y \) . . . . . . horizontal position perpendicular to mean horizontal speed . . . m
\( z \) . . . . . . = \( z_{\text{AGL}} - d \) vertical position above displacement height . . . m
\( z_* \) . . . . . . upper boundary roughness sublayer, \( d \) subtracted . . . . . . m
\( z_0 \) . . . . . . roughness length . . . . . . . . . . . . . . . . . . . . . . . . . m
\( z_{\text{AGL}} \) . . . . . height above ground . . . . . . . . . . . . . . . . . . m
\( z_{\text{h}} \) . . . . . . average roof level, \( d \) subtracted . . . . . . . . . . . . . . m
\( z_i \) . . . . . . boundary layer height . . . . . . . . . . . . . . . . . . . . . . . m
CORR . . . correlation coefficient
F2 . . . . . . fraction of two
FB . . . . . . fractional bias
MOE . . . . . measure of effectiveness
NMSE . . . normalized mean square error
RD . . . . . relative difference
RMSE . . . root mean square error
1. Introduction

This chapter contains a motivation for the thesis topic (Section 1.1), a short history of the model that will be used throughout the work (Section 1.2) and a short literature overview of the flow characteristics in an urban canopy layer (Section 1.3). Lastly the goals of this thesis are defined in Section 1.4.

1.1. Motivation

Dispersion of air pollutants in urban areas is an important topic, because more than half of the population lives in urban areas (Fernando 2010). Those are particularly affected by pollution, partly due to proximity of possible sources (e.g. traffic, domestic heating, possible disasters) and partly due to the fact that large and complex roughness elements reduce dispersion. The heterogeneous nature of urban areas also increases the complexity of fluid motion, making it therefore harder to measure and simulate than more homogeneous areas like fields or deserts.

Since field experiments in urban areas are not only difficult, but also expensive and therefore rare, computer models of pollution dispersion have a long history. Increasing computing power helps models to evolve to higher complexity, which ideally improves their results. Despite better and better computers, there is still no model that can simulate a situation on a so called “neighborhood scale” (for example one city) with topography that resolves individual houses. One limiting factor is the availability of a good enough topographic map — it would have to resolve all three dimensions — and another factor is the still too high computational effort such a model would require. Therefore a model that can simulate dispersion in the neighborhood scale even without topography is still useful.

Lagrangian models are widespread in use and have advantages over Eulerian models for dispersion modeling (Wilson and Sawford 1996). The foremost advantage of the Lagrangian is the fact that only the flow field has to be known, whereas the Eularian approach also requires knowledge of fluxes. Additionally, the turbulence scheme of Eulerian models can not be as easily changed as in Lagrangian models, which inhibits specialized urban turbulence layers. Attempts in this direction are still being made, for example by Martilli et al. (2002). However, these attempts are usually mesoscale models, which are not suited to describe near-source dispersion because their resolution is too coarse.

The Lagrangian model starting with the work of Rotach et al. (1996), heavily based on
the work of Thomson (1987), and ending with that of Rotach et al. (2004) still has open questions and this thesis investigates some of these.

One result of Rotach et al. (2004) is that modifying the model’s lower boundary condition by making it more “realistic” improves the model performance. Before this modification, a particle that reaches the lower model boundary was simply reflected. After the modification, the particle stays still for a certain so-called residence time, before it is reflected (further explained in Section 2.2.6). This is supposed to simulate trapping inside street canyons, which happens in reality because the model’s lower boundary is not the physical ground (see Section 2.2.6). A large part of this thesis is dedicated to an attempt of improving this residence time approach by an even more realistic formulation. Hence the introduction also features a summary of the flow behavior inside street canyons.

Between the study by Rotach et al. (2004) and this thesis, some additional changes to the model have been made. Gibson and Sailor (2012) point out deficiencies in the original paper (Rotach et al. 1996), investigated in Section 2.4.3. Additionally, while porting the source code from FORTRAN 77 to Fortran 95 in the course of this thesis, an error in the model of Rotach et al. (2004) was discovered (see Section 2.4.2).

1.2. History of the model

Wilson and Sawford (1996) present a review article describing Lagrangian particle dispersion models (LPDM). Roughly speaking, an LPDM follows a particle that is influenced by the average flow field and random turbulence — a so called “random walk”. Then the model repeats this for a large amount of particles and in the end statistically describes the positions of all particles. In this manner information about concentration is obtained.

The mathematical validity of such a model can be proven using criterions. Thomson (1987) compares them and finds that the so called “well mixed criterion” is necessary and sufficient. Simplified, it states that a model that starts with a well mixed particle distribution should keep this distribution. In other words, the well mixed state should be the steady state of the model. Well mixed means uniformly distributed particles in the context of Lagrangian modeling. Thomson (1987) also describes a basic version of modeling equations that fulfill this criterion.

The defining step forward of Rotach et al. (1996) is the combination of convective or neutral to stable atmospheric states, by combining the model equations of Thomson (1987) and Luhar and Britter (1989). Other Lagrangian models can only describe one or the other atmospheric state, not both, which means that an operator has to choose a model depending on the atmospheric condition.

The model of Rotach et al. (1996) uses a box counting method to calculate concentration and is two dimensional. It should be noted that even though the model is called two dimensional and has a vertical and a longitudinal component, fundamentally it is only
1.2 History of the model

Figure 1.1.: The atmospheric layers pertinent to this thesis and how they relate to model geometry. Mixing layer height $z_i$, roughness layer height $z_*$, zero plane displacement $d$, roughness length $z_0$, building height $H$ and street canyon width $W$ are only represented approximately in size. Note that the buildings (grey) are only shown here for reference and do not exist in the model.

a vertical model, since all profiles, model functions and parameterizations only depend on the height. Therefore the longitudinal position does not influence the trajectory of a particle, although its longitudinal velocity does. Consequently, vertical shear is possible, but the model is longitudinally homogeneous. Additionally the model operates only inside the Planetary Boundary Layer (PBL, see Figure 1.1), which is justified for near-source, near-ground simulations (see Section 2.2.6).

The box counting method has certain drawbacks, hence the kernel method (see Section 2.2.7) is introduced in the model. The method is described by de Haan and Rotach (1998) for another model, which is also partly based on the work of Rotach et al. (1996). Furthermore the former two dimensional model is expanded into the third, lateral dimension. However, this new lateral component is independent of the vertical and longitudinal component, so that no lateral shear is possible. Consequently, the model is now horizontally homogeneous.

Several studies at that time (Rotach 1997b, 1999; Rotach and De Haan 1997) show that using a different turbulence scheme in the so called “Roughness Sublayer” (RS, see Figure 1.1) improves the simulation of dispersion over urban areas. The RS lies under the inertial sublayer (IS, see Figure 1.1) and extends to the virtual model bottom, which is at the zero plane displacement $d$ (see Figure 1.1 and Section 2.2.6). It is hypothesized that the RS improves the performance of the LPDM in urban areas because large roughness elements in cities influence the flow field and a specialized parameterization in the RS takes this into account. Rotach (2001) details how to implement the RS in the model.
and compares model output to three field measurements of dispersion experiments. The addition of the RS-parameterization appears to improve the model. However the source height of those experiments was too high to be able to test the hypothesis properly.

A tracer experiment undertaken during the larger Basel UrBan Boundary Layer Experiment (BUBBLE) (Gryning et al. 2005) addresses this limitation with a source height just over roof top level. Rotach et al. (2004) use the model to simulate the experiments and compare with BUBBLE measurements. The parameterized turbulence structure is found to deviate from the measured one. Furthermore, when using the parameterized turbulence profiles as model input, the modeled concentrations are closer to the measured ones than when using turbulence profiles as close as possible to the observations. Rotach et al. (2004) present several hypotheses to explain this and part of this thesis investigates two of them.

Between Rotach (2001) and Rotach et al. (2004) the model code was also used to create a footprint model by running it backwards (Kljun et al. 2002). Despite this, the thereby developed code is not used in Rotach et al. (2004) and also not in this work.

Recently, Gibson and Sailor (2012) have taken a look at the theoretical groundwork of Rotach et al. (1996) and propose some corrections. These will be discussed and, if appropriate, implemented and tested.

### 1.3. Urban canopy layer

The urban canopy layer (UCL) is the lowest atmospheric layer in an urban environment (see Figure 1.1). It forms between buildings, inside street canyons and is characterized by complex flow and turbulence behavior, which depends on many factors.

Ahmad et al. (2005) and Vardoulakis et al. (2003) provide review articles on how street canyons influence flow and dispersion. There are mainly three possibilities to study those effects. First there are wind tunnel or water tank experiments (e.g. Kastner-Klein and Rotach 2004; Uehara et al. 2000), secondly field measurements (e.g. Dallman et al. 2014; DePaul and Sheih 1986; Jackson 1978; Johnson and Hunter 1999; Louka et al. 2000; Nakamura and Oke 1988; Niachou et al. 2008; Zajic et al. 2011) and finally numerical models (e.g. Hunter et al. 1991; Johnson et al. 1973; Kim and Baik 2004; Sini et al. 1996). The following sections describe only the flow inside the UCL for canyons that are formed by linked buildings and have a height $H$ to width $W$ (see Figure 1.1) ratio of about unity. Other width to height ratios or isolated buildings have different flow fields (Oke 1988; Sini et al. 1996).

For wind roughly perpendicular to the canyon axis these circumstances lead to “skimming flow” (Hunter et al. 1991; Oke 1988; Sini et al. 1996). This means that the flow above the buildings is almost decoupled from the UCL and a rotating vortex forms within the street canyon if the wind speed at roof top level is above a threshold of about 1.5 – 2 m s$^{-1}$ for a canyon with height to width ratio of about 1.4 (DePaul and Sheih 1986). Nakamura and
Oke (1988) also find higher scatter for lower velocities in a plot of roof level wind speed versus canyon wind speed. The exact threshold is almost certainly not a fixed value, but depends on at least canyon geometry. However, no study pertaining to this issue could be found. For this work the value of 1.5 m s$^{-1}$ will be used.

The vortex’s orientation is such that the flow is downward on the windward wall of the canyon and upward at the leeward wall (e.g. Niachou et al. 2008). Daberdt et al. (1973) equal “roughly perpendicular” to 30° between wind and canyon direction, using unspecified observations, while Yamartino and Wiegand (1986) found a threshold of about 20°. For unknown reasons the 30° is cited more often (e.g. Eliasson et al. 2006) and therefore will also be used throughout this thesis.

DePaul and Sheih (1986), Daberdt et al. (1973) and Zajic et al. (2014) prove the existence of this vortex for a perpendicular flow in field experiments and others (Johnson et al. 1973; Sini et al. 1996) simulate it using models. In Basel Christen (2005) also observed the vortex for perpendicular cases, as did Eliasson et al. (2006) in Göteborg, although for a deeper canyon. Louka et al. (2000) conclude from their field experiment that the circulation is intermittent, because the 30 minute mean vertical velocity at the top of the canyon is about as large as its scatter of the 1 minute mean. They attribute this to a shear layer at roof level with Kelvin-Helmholtz instabilities, that “flaps”, thus intermittently allowing transport in and out of the canyon.

When the wind flows roughly parallel to the canyon axis, the vortex can form, but only for short periods (Eliasson et al. 2006; Yamartino and Wiegand 1986). On average no vortex forms (Christen 2005; Eliasson et al. 2006) and the flow is channeled into the canyon (Christen 2005; Zajic et al. 2014).

The intermediary case of perpendicular and parallel is the oblique flow case. Therein the vortex forms, but is advected downwind, parallel to the canyon, thus forming a corkscrew motion. This was observed in the field (Johnson and Hunter 1999; Nakamura and Oke 1988; Zajic et al. 2014) and in a wind tunnel study (Wedding et al. 1977).

Recalling that the present model uses the zero plane displacement as its lower boundary (see Figure 1.1) one goal of the present thesis is to add the effects of the UCL to the model of Rotach et al. (1996). To do this without extending the model to the physical ground, a parameterization of pollution transport inside the UCL is necessary. If the model were extended to the ground, which is another possibility of including UCL-effects, a turbulence description would be needed. Due to the horizontally inhomogeneous nature of the turbulence in the UCL, a realistic description is outside the scope of this model, because it is horizontally homogeneous. Therefore turbulent motion is disregarded in the UCL and the proposed modifications will act as a modified boundary condition. Consequently the whole transport inside the street canyons depends on the average flow field. As shown by Christen (2005), the main transport in the UCL is along the canyon axis. The mean horizontal wind speed along and across the canyon can be estimated as follows.
1.3.1. Along canyon flow

Above a threshold velocity (Nakamura and Oke 1988; Santamouris et al. 1999; Yamartino and Wiegand 1986) the along canyon wind speed inside the canyon is directly proportional to the parallel roof top flow. For the street level scale Yamartino and Wiegand (1986) use the relationship

\[ u(z) = \bar{u}_H \frac{\ln \left( \frac{z + z_0}{z_0} \right)}{\ln \left( \frac{z_h + z_0}{z_0} \right)} \]  

(1.1)

to describe the vertical wind speed profile inside a street canyon for an ambient wind direction along the main canyon axis. \( \bar{u}_H \) is the mean horizontal wind speed at roof top level.

Jackson (1978) proposes a power law

\[ u(z) = \bar{u}_H \left( \frac{z - d}{H - d} \right)^\beta \]  

(1.2)

where \( \beta \) is about 0.5, to describe the profile of the horizontal velocity. It has to be mentioned that his experiments were not carried out in a typical street canyon and also largely describe the height above roof level.

A better fitting experiment for this purpose was carried out by Nicholson (1975). For the case of wind parallel to the street she assumed an exponential profile below the mean building height, citing the forest canopy work of Cionco (1965), where

\[ u(z) = u_0 \exp \left( \frac{z \cdot z_0}{0.1H^2} \right) \]  

(1.3)

\( u_0 \) is here the wind speed at the physical ground, which can be calculated from \( \bar{u}_H \) using the same profile:

\[ u_0 = \bar{u}_H \exp \left( \frac{-Hz_0}{0.1H^2} \right). \]

Unlike in the logarithmic profile, which is used above the buildings, here the velocity at the ground \( u_0 \) is not zero. The definition of \( z_0 \) comes from the logarithmic profile.

A downside of using the Nicholson (1975) results is that there are no actual wind measurements to support her wind profile, only a concentration model validated by concentration measurements. Still, Rotach (1995) also found an exponential profile in the UCL for a field experiment in Zürich.

Nakamura and Oke (1988) report a linear relationship between wind speed above the canyon and inside the canyon with slopes from 0.37 to 0.75 and propose 2/3 as an estimate. However, they describe a relationship between the wind speed slightly above roof level (1.2\( z_h \)) and a fixed station inside the canyon (0.06\( z_h \)) instead of the mean wind. Additionally they mention, but do not elaborate, on the influence of the incidence angle except calculating the slope for each of the four quadrants. This influence will be described later.
1.3 Urban canopy layer

1.3.2. Cross canyon flow

The cross canyon wind velocity is, if a vortex has formed, strongly dependent on the position within the canyon. Several studies (e.g. Christen 2005; Eliasson et al. 2006; Yamartino and Wiegand 1986) have attempted to describe this. However, for the purpose of this thesis such detail is not needed and thus will not be discussed further.

What is required is the average circumferential wind speed, which was found to be 1/4 of ambient wind speed for a symmetric canyon and a perpendicular flow by Hoydysh and Dabberdt (1988) in a wind tunnel experiment. Britter and Hanna (2003) list a range from 0.5 to 0.66 for the same value. From Christen (2005) a value of about 0.2 to 0.3 can be derived from the rotational frequency, geometric factors and the average wind profile.

A proportional relationship between the circumferential velocity and the perpendicular roof top velocity is reported by DePaul and Sheih (1986); Santamouris et al. (1999); Yamartino and Wiegand (1986).

1.3.3. Other influential factors

In addition to the factors mentioned above that drive the flow structure in the UCL, some other factors are also influential. Due to various restrictions they will have to be neglected in the model of this work. However, they are mentioned in the following for completeness.

Canyon end effects

Most of the effects described so far pertain to the middle of canyons. In reality street canyons are not so simple, because they can reach intersections or have side canyons. Robins et al. (2002) worked on wind tunnel experiments with intersections where the main street is slightly laterally offset. They found that the magnitude of the offset influences the amount of flow that is channeled into the side street. Additionally they observed that an intersection with no lateral offset lead to a high run to run variability, which indicates an unstable flow. However, when concentration was measured in both side streets, significant levels were not measured far into the side streets. Robins et al. (2002) also write that further inquiry is need to realistically simulate dispersion around intersections and that the phenomenon is highly site specific.

An effect called “intermittent corner vortex” is described by Hoydysh and Dabberdt (1988). Thereby vortices with a vertical rotation axis form at an intersection. The vortices change the concentration distribution inside the street canyon because the concentration converges between two intersections. Due to the model treating the UCL only statistically, both effects have to be neglected.
Different local geometry

Christen (2005) mentions the influence of roof shape on the vortex for the BUBBLE data. This will be ignored from now on, even though a wind tunnel study by Rafailidis (1997) shows “substantial influence of roof shape”, at least in the RS. He finds that slanted roofs improve pollution dispersion compared to flat roofs.

Furthermore, different building heights on the sides of the canyon can also influence the vortex (Hoydysh and Dabberdt 1988; Longley et al. 2004; Xiaomin et al. 2006). Even with a height to width ratio of about unity, Xiaomin et al. (2006) found that sufficiently different building heights (step down) can cause the usual one rotor regime to transition into a multi rotor regime. This effect will also be ignored, because the model does not contain the required topographic information.

Differential heating

The present model does not include radiative heating and all thermal effects are described only by the convective velocity scale $w_*$ and the Obukhov length $L$. Thus it is not possible to describe differential heating of canyon walls due to sun angle, which can influence the vortex. Sini et al. (1996) show with their model how a difference in wall temperature can change the flow regime. Depending on whether the warmer wall is at the leeward or the windward side of the canyon, the vortex can be either reinforced or weakened. Niachou et al. (2008) present a field experiment where in one case the direction of the vortex was even reversed due to thermal effects.

Whether or not it is possible to exclude thermal effects can be decided by a criterion, which is introduced by Dallman et al. (2014). It uses a nondimensional buoyancy

$$B_D = \frac{g \Delta \Theta H}{\Theta \bar{u}_H^2 \left[ 1 + \left( \frac{H}{W} \right)^2 \right]}$$

where $g$ is the acceleration due to gravity, $H$ is the height of the canyon, $W$ its width, $\Delta \Theta$ the absolute difference in wall temperature between windward and leeward wall and $\bar{\Theta}$ the average temperature in street canyon. According to Dallman et al. (2014) a critical threshold of $B_D$ exists when both a thermal circulation and a dynamically driven one exist at the same time. Below the threshold of $B_D$ the dynamic circulation dominates and the thermal circulation can be neglected. The model at hand does this per default and is therefore only viable if $B_D$ is below the threshold. Dallman et al. (2014) find the threshold to be roughly 0.05, while a typical BUBBLE case ($H = 15.1$ m, $W = 15.1$ m, $\bar{u}_H \approx 2$ m s$^{-1}$, $\bar{\Theta} \approx 300$ K) yields $B_D \approx 0.06 \Delta \Theta$. A thermal image taken at 1020 UTC (unknown date) from the Sperrstrasse-tower (position 3 in Figure 2.2) in Rotach et al. (2005) indicates a $\Delta \Theta$ in the order of 10 K. Consequently the Dallman et al. (2014) criterion would be violated by ignoring thermal effects due to differential heating in the model. Since the threshold was determined experimentally using shipping containers on a grass field and so
far not replicated by another study and furthermore the order of $BD$ is not too far off, we feel that it is justifiable to proceed.

Incidence angle

So far only rotational wind speed with flow orthogonal to the canyon axis and along canyon wind speed with flow parallel to the canyon axis has been described. Generally the wind may come from any angle. As already mentioned, a mean vortex forms only for an incidence angle above $30^\circ$ (Dabberdt et al. 1973).

Yamartino and Wiegand (1986) show how an oblique flow can be decomposed into components parallel and perpendicular to the canyon axis using the incidence angle. The resulting components can be used as perpendicular and parallel roof top wind velocities. Niachou et al. (2008) measured decomposition in an experiment, but could no definitively prove it due to insufficient data. For the field experiment of Nakamura and Oke (1988) the wind direction was categorized into four quadrants and a linear relationship between roof top and center canyon horizontal wind speed was found. They did, however, not decompose these wind speeds relative to the canyon direction, but used the horizontal magnitude. Johnson and Hunter (1999) proposed that an along canyon component formed during oblique flow in their field experiment, thereby influencing the vortex.

A numerical study was performed by Kim and Baik (2004) to prove that the incidence angle influences the particle transport in the UCL, although they used square houses instead of canyons. Rodriguez et al. (2013) studied the influence of wind direction error on plume position and found that more complex topography enhances the error.

Stability

Rotach (1995) reports from a field experiment in Zürich that the profile of the mean horizontal velocity not only depends on the incidence angle, but also on the stability in the RS and the UCL. This was tested in a wind tunnel by Uehara et al. (2000) and they found that a stable stratification inhibits the vortex and an unstable stratification increases the strength of the vortex. However, Rotach (1995) found that the atmosphere close to an urban surface is only seldom (“a few events during nighttime in the winter season”) stable and mostly well mixed regarding to temperature. Effects of stability in the UCL will be ignored to simplify the model.

Traffic induced turbulence

Wind tunnel experiments made by Kastner-Klein et al. (2001) show that traffic inside street canyons can influence the transport of particles. Two lane traffic in opposing direction increases turbulence inside the street canyon and disperse the particles faster. Two lane traffic in the same direction influences the mean wind velocity and thereby
also influences average particle transport. A numerical study using a Lagrangian model embedded in a computational fluid dynamic model comes to the same conclusion (Jicha et al. 2000). DePaul and Sheih (1986) measured with hot-wire anemometers that traffic induces turbulence up to a high of approximately 7 meters. This effect will also be neglected due to insufficient data and too high complexity.

1.3.4. Residence time

The residence time $\tau$ is the time a particle stays inside the UCL from the moment it is entrained from above to the moment it reenters the RS above. Louka et al. (2000) calculate it via $\tau = \frac{\text{perimeter of canyon}}{\text{mean wind speed within street}}$ and arrive at 10 s. However, they do not validate this value and use a mean wind speed of 2 m s$^{-1}$, which seems high, given that their measured vertical velocity is usually below 1 m s$^{-1}$.

Eliasson et al. (2006) measure a circulation time of about 1 minute and also mention that it is unclear whether the mean wind speed within the street of Louka et al. (2000) includes an along canyon component. If that were so, the short circulation time of Louka et al. (2000) of 10 seconds would be explained.

Vachon et al. (1999) experimented in a street canyon ($H = 20$ m) with neutral buoyancy balloons, although they were released at street level and therefore had a presumably shorter path to the top of the canyon. About 15% of the total balloons leave the canyon through side streets. The residence times are listed as 15% under 30 s, 57.5% under 60 s, 75% under 90 s, 85% under 120 s, 87.5% under 150 s and 95% under 180 s.

Furthermore, the retention time of particles, defined as the time needed to drop to $1/e$ times the original concentration, was measured to be 0.7–3.8 minutes by DePaul and Sheih (1985) for a canyon with a width to height ratio of 1.5. They observed only cases with roughly perpendicular flow and roof top level wind speeds between 1.7 and 4.5 m s$^{-1}$.

The wind tunnel experiment of Hoydysh and Dabberdt (1988) can be scaled up to a symmetric canyon with 25 m high buildings with 2 m s$^{-1}$ perpendicular roof level wind. Then the residence time of their ground level emissions is listed as 88 s for 33% of the particles, 260 s for 46%, 402 s for 17% and 540 s for 4%.

1.4. Goals and outline

As mentioned before, the aim of this work is to update and extend the model of Rotach et al. (1996) and to study urban canopy effects on near surface dispersion. The model is validated and its performance evaluated by a comparison with measurements of the Basel UrBan Boundary Layer Experiment (BUBBLE). The following objectives will be completed:
1.4 Goals and outline

- Update the model with the changes suggested by Gibson and Sailor (2012) and the correction to an error in the source code and evaluate them.
- Assess the impact of a number of assumptions that are necessary to run the model.
- Study the effects of a dissipation rate profile based on street level measurements — opposed to the general parameterization used before — on the modeled dispersion as proposed by Rotach et al. (2004).
- Investigate canopy effects on urban near surface dispersion by parameterizing drift inside street canyons as a modified lower boundary condition, as suggested by the results of Rotach et al. (2004).

Chapter 2 first gives a brief overview over the BUBBLE. Second, the original model is described. Third, the comparison methods between model output and measurements are specified. Finally, modification to the model are proposed.

Chapter 3 presents and discusses the results of the thesis. It contains some checks whether the modified model violates basic assumptions. Afterwards the model is evaluated in relation to the measurement data. Furthermore, sensitivity studies for some parameters of the modifications are conducted and the modified model is compared to the original model and BUBBLE data.

Finally the results are summarized in Chapter 4 and possible topics of future inquiries are listed.
2. Methodology

Firstly, this chapter outlines the Basel UrBan Boundary Layer Experiment (BUBBLE), which will be used as validation data set. Secondly, the already existing model that was introduced by Rotach et al. (1996) and improved upon by de Haan and Rotach (1998), Rotach (2001) and Rotach et al. (2004), is described. Thirdly, the statistical methods and indices that will be used to describe the model output and its changes are defined. Finally the possible improvements that this thesis suggest are listed.

2.1. Basel UrBan Boundary Layer Experiment (BUBBLE)

The European Cooperation in Science and Technology (COST) action 715 — Urban meteorology applied to air pollution problems — was designed to improve knowledge on the temporal evolution of air pollution. Gryning et al. (2005) call BUBBLE an “offspring” of COST715. Its main goal was the measurement of near-surface vertical turbulence profile and the flow field in and around the urban area of Basel, Switzerland in the years 2001 and 2002 (Gryning et al. 2005).

In the course of this period ground based and remote sensing instruments measured the meteorological conditions in Basel. During an Intensive Observation Period, the BUBBLE tracer experiment, from 15 June 2002 to 12 July 2002, six tracer experiments were conducted in the area “Kleinbasel” (Gryning et al. 2005). Installation of measurement sites required permits, which meant that their position was fixed and had to be planed beforehand (Rotach et al. 2004). Additionally, the analysis and simulation of dispersion during quasi steady-state conditions is easier and so cases that fit both requirements were attempted by using the so called “Clara Wind”. It is a local, thermally driven and north-westerly wind that develops during clear sky afternoons in the summer over Basel (Gryning et al. 2005). On four of the six days the Clara Wind did develop and only those four will be discussed further.

The development of the wind direction during each experiment is visualized in Figure 2.1. During experiment 1, the wind direction was between northwest and north for the first five half hours, before the wind turned to northeast. In the course of experiment 2, the wind came from the west with a small variability. While experiment 3 was undertaken, the wind direction fluctuated between west and north, with a larger variability than during experiment 2. At the time of experiment 4, the wind turned monotonously from roughly
ne northeast during the first half hour, over north, to roughly west-northwest. The importance of these observations are explained in Section 3.3.

Generally the measurement sites were at roof level and therefore inside the RS (Gryning et al. 2005). Supplementary ground level stations were used during one experiment, because the wind direction developed unexpectedly. See tables 2.1 and A.1 for a list and a description of all positions and Figure 2.2 for a visual representation. The rationale for the placement of both source and receptors inside the RS is twofold (Rotach et al. 2004). First, Rotach (2001) demonstrates the importance of correct representation of RS turbulence for urban dispersion modeling. Second, the roof level is directly at the position of at least one pollutant source (domestic exhaust). Due to complex mixing all sources at the street level (traffic) can also be treated as if the source were at roof level, at least if the scale of the described dispersion is larger than the street scale. A tower in a street called “Sperrstrasse” (position 3 in Figure 2.2) was used to measure a concentration profile (3, 10 and 17 m above ground) during the tracer experiments and the data supports the assumption of a uniform concentration inside the street canyons (Rotach et al. 2004).

The Sperrstrasse-tower was also used to measure the meteorological conditions using sonic anemometers, actively ventilated psychrometers and cup anemometers (Christen 2005). It should be mentioned that the coordinate systems of the sonic anemometers used to measure the wind velocity components are rotated such that their x-direction follows the mean wind for each averaging period. Since neither the lateral, nor the vertical mean wind component can be assumed to be zero in any direction due to complex topography and convection, no further rotation was performed.

The tracer experiments used the inert and nontoxic sulfur hexafluoride (SF₆), a method that Gryning (1981) describes in detail, albeit for a different experiment in Copenhagen. The procedure for BUBBLE is described in Gryning et al. (2005) and summarized in Rotach et al. (2004). Essentially SF₆ was released at just over roof level for roughly four
Table 2.1.: Description of measurement sites, based on Gryning et al. (2005). For further details see Table A.1.

<table>
<thead>
<tr>
<th>Site</th>
<th>Name</th>
<th>Description</th>
<th>East</th>
<th>North</th>
<th>Height</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>Parking Novartis Klybeck</td>
<td>flat roof</td>
<td>611692</td>
<td>269037</td>
<td>18.6</td>
</tr>
<tr>
<td>R2</td>
<td>Florastrasse</td>
<td>mobile platform</td>
<td>611400</td>
<td>268214</td>
<td>21.0</td>
</tr>
<tr>
<td>1</td>
<td>Oetlingerstrasse 170</td>
<td>flat roof</td>
<td>611780</td>
<td>268571</td>
<td>18.2</td>
</tr>
<tr>
<td>2</td>
<td>Feldbergstrasse 31</td>
<td>flat roof</td>
<td>611377</td>
<td>268408</td>
<td>19.8</td>
</tr>
<tr>
<td>3a</td>
<td>Tower “Basel-Sperrstrasse”</td>
<td>tower in street canyon</td>
<td>611890</td>
<td>268365</td>
<td>3.0</td>
</tr>
<tr>
<td>3b</td>
<td>Tower “Basel-Sperrstrasse”</td>
<td>tower in street canyon</td>
<td>611890</td>
<td>268365</td>
<td>10.0</td>
</tr>
<tr>
<td>3c</td>
<td>Tower “Basel-Sperrstrasse”</td>
<td>tower in street canyon</td>
<td>611890</td>
<td>268365</td>
<td>17.0</td>
</tr>
<tr>
<td>4</td>
<td>Messe Basel, Halle 1, NE</td>
<td>flat roof</td>
<td>612058</td>
<td>268417</td>
<td>23.9</td>
</tr>
<tr>
<td>5</td>
<td>FMI, Maulbeerstrasse 66</td>
<td>flat roof</td>
<td>612400</td>
<td>268551</td>
<td>29.7</td>
</tr>
<tr>
<td>6</td>
<td>Klingentalschulhaus Kaserne</td>
<td>“castle style” roof</td>
<td>611350</td>
<td>267980</td>
<td>25.9</td>
</tr>
<tr>
<td>7</td>
<td>Manor, Greifengasse 22</td>
<td>flat roof</td>
<td>611603</td>
<td>267838</td>
<td>29.6</td>
</tr>
<tr>
<td>8</td>
<td>Clarastrasse 30</td>
<td>flat roof</td>
<td>611928</td>
<td>267994</td>
<td>24.8</td>
</tr>
<tr>
<td>9</td>
<td>Parking Messe Basel</td>
<td>parking deck</td>
<td>612151</td>
<td>268091</td>
<td>27.9</td>
</tr>
<tr>
<td>10</td>
<td>Schule f. Gestaltung, Bau G</td>
<td>flat roof</td>
<td>612641</td>
<td>268122</td>
<td>28.3</td>
</tr>
<tr>
<td>11</td>
<td>Parking DB</td>
<td>parking deck</td>
<td>612825</td>
<td>268259</td>
<td>11.7</td>
</tr>
<tr>
<td>12</td>
<td>Roche, Bau 74</td>
<td>flat roof</td>
<td>612503</td>
<td>267655</td>
<td>24.9</td>
</tr>
<tr>
<td>13</td>
<td>Schorenweg</td>
<td>ground level</td>
<td>612886</td>
<td>268795</td>
<td>1.5</td>
</tr>
<tr>
<td>14</td>
<td>Bus Station “Lange Erlen”</td>
<td>ground level, sidewalk</td>
<td>612542</td>
<td>269155</td>
<td>1.5</td>
</tr>
<tr>
<td>15</td>
<td>Messe Basel, Halle 1, W</td>
<td>flat roof</td>
<td>612052</td>
<td>268272</td>
<td>23.9</td>
</tr>
<tr>
<td>16</td>
<td>DB-Areal, Erlikönig</td>
<td>ground level, track area</td>
<td>612180</td>
<td>269048</td>
<td>1.5</td>
</tr>
<tr>
<td>17</td>
<td>Bäumlihof</td>
<td>ground level, grassland</td>
<td>613780</td>
<td>268700</td>
<td>1.5</td>
</tr>
<tr>
<td>18</td>
<td>DB-Areal, South</td>
<td>ground level, parking lot</td>
<td>612216</td>
<td>268774</td>
<td>1.5</td>
</tr>
<tr>
<td>19</td>
<td>Schule f. Gestaltung</td>
<td>ground level, park</td>
<td>612660</td>
<td>268143</td>
<td>1.5</td>
</tr>
</tbody>
</table>

hours at a constant rate for each experiment. After one hour, the operators at the receptor sites filled one sample bag over 30 minutes. This duration was felt to balance reduction of variability and preservation of temporal resolution (Rotach et al. 2004). Six bags were filled at each receptor, thereby covering a period of three hours.

The concentration of the samples in the bags was measured using a gas chromatograph with a detection limit of about 5 ng m$^{-3}$ (see Gryning et al. (2005) for details). The calibration procedure described in Gryning (1981) has an accuracy of at least 20% (“conservative estimate”, personal communication Sven-Erik Gryning 2014) and the reproducibility of measurements is about 2% (Gryning 1981, p. 111). The loss due to diffusion of SF$_6$ out of the bags during transport was tested (Gryning 1981) and assumed to be negligible.

Due to fact that the conditions in Basel were not completely stationary (see concentration measurements in Gryning et al. 2005), an additional uncertainty arises from the fact that
the filling of the bags was timed by humans. If the start and end of one averaging period were shifted by, say, one minute, the average concentration during that time could be different than had the bag been filled at the correct time. To estimate how large such an time shift uncertainty would be, each thirty minute averaged concentration time series was linearly interpolated for each station and experiment. Then each averaging period was adjusted by plus or minus one minute and the resulting concentration average calculated. From this, the relative time shift uncertainty of each measurement (for each experiment, station and period) was calculated and its mean was found to be 2.6%. Combined with the relative calibration uncertainty of 20% and the individual measurement error of 2%, the total relative uncertainty for each thirty minute average is 20.3%.

For longer averaging periods (i.e. by averaging over successive samples) the relative time shift uncertainty and the relative individual measurement uncertainty become smaller, since the averaging takes place after the measurements, which are presumably independent. In contrast, the relative calibration uncertainty stays at 20%, even for averaged values.

Another source of uncertainty is the sampling uncertainty that arises from any measurement of any turbulent quantity \( \theta \) and depends on the length of the averaging period. To this end Wyngaard (1973) cites Lumley and Panofsky (1964) for the calculation of the averaging period

\[
J = \frac{2\tau_{\text{int}} \overline{\theta'^2}}{a_{\text{int}}^2 \overline{\theta^2}}. \tag{2.1}
\]

Here \( \tau_{\text{int}} \) is the integral scale of the quantity \( \theta \) and \( a_{\text{int}} \) the desired accuracy or uncertainty of the average.

This formula (2.1) can be used to estimate the sampling uncertainty of the measurements by using the measured concentration as turbulent quantity. As suggested by Wyngaard (1973), the integral time scale \( \tau_{\text{int}} \) is estimated for convective conditions by \( \frac{z}{u} \), where \( z \) is the height of the sampler and the mean horizontal velocity at roof top level \( u_H \) will be used as an approximation for \( u \). The latter is certainly not a perfect solution for all samplers (there are some on the ground), but Wyngaard (1973) called \( \tau_{\text{int}} = \frac{z}{u} \) an “order-of-magnitude estimation” and the formula for \( J \) is only an estimate as well, so the approximation seems justified.

Since the averaging periods for the BUBBLE data are limited to 30 minutes, 1 hour and 3 hours, (2.1) is rearranged to

\[
a_{\text{int}} = \sqrt{\frac{2\tau_{\text{int}} \overline{\theta'^2}}{J \overline{\theta^2}}}. \tag{2.2}
\]

The average of \( a_{\text{int}} \) over all sampler positions for each experiment and the corresponding standard deviation are displayed in Table 2.2. As can be seen from the size of the standard deviations compared to the means, the accuracy is not homogeneous between different stations, even for the same experiments. This is certainly influenced by the estimation of the integral time scale, which is a measure for autocorrelation length. Since
Table 2.2: Sampling uncertainties $a_{int}$ for each experiment and averaging period. Listed are the mean over all sampler positions and the standard deviation in parenthesis as a measure of variability.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>30 min</th>
<th>1 hour</th>
<th>3 hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.07 (0.03)</td>
<td>0.05 (0.03)</td>
<td>0.03 (0.03)</td>
</tr>
<tr>
<td>2</td>
<td>0.08 (0.04)</td>
<td>0.06 (0.04)</td>
<td>0.03 (0.04)</td>
</tr>
<tr>
<td>3</td>
<td>0.15 (0.07)</td>
<td>0.11 (0.07)</td>
<td>0.06 (0.07)</td>
</tr>
<tr>
<td>4</td>
<td>0.09 (0.02)</td>
<td>0.07 (0.02)</td>
<td>0.04 (0.02)</td>
</tr>
</tbody>
</table>

the autocorrelation of concentration in an urban area is presumably dependent on the local topography, a high variability is not surprising. Additionally Table 2.2 shows that increasing the averaging period decreases the sampling uncertainty, which is expected. The downside of longer averaging periods is that the number of data points is reduced. Furthermore, experiment 3 has a larger uncertainty than experiments 1 and 2 by a factor of two. The uncertainty of experiment 4 is higher compared to experiments 1 and 2, although less so than experiment 3. This matter will also be addressed in Section 3.3.

The background concentration of SF$_6$ was measured before each experiment (Gryning et al. 2005; Rotach et al. 2004) and is already subtracted from all subsequent concentration values.

Kleinbasel is a relatively homogeneous urban area with a mean plan area density of 48% (Gryning et al. 2005), which means that about half of the area is covered by buildings. A table of mean roof height and its standard deviation for a 100 m circle around each station can be found in Gryning et al. (2005). The average roof height is about 15.1 m for the whole area. Christen (2005) states a canyon width $W$ to building height $H$ ratio of $H/W = 1$ and a separation distance between two intersections $S$ to $H$ ratio of $S/H = 11$. This constitutes a long canyon and therefore no end effects will be taken into account (see Section 1.3.3).

The convective velocity scale

$$w_* = \left( \frac{g w \Theta'}{\Theta} \right)^{1/2}$$

is calculated for each averaging period and experiment from measurements of the vertical velocity perturbation $w$, the mean temperature $\Theta$ and its fluctuation $\Theta'$. The result is then used as input for the model.

Similar, the friction velocity $u_*$ is also calculated and used as input. However, the standard definition $u_* = \sqrt{\left(\overline{u'w_0^2} + \overline{w_0'^2}\right)}$ is disregarded in favor of a specialized friction velocity $\hat{u}_*$ after Kastner-Klein and Rotach (2004). It has the advantage of being less susceptible to local effects on $\overline{u'w}$. Consequently it is better suited to be used as a representative value for the whole domain, even though it is measured only at one tower.
Kastner-Klein and Rotach (2004) define $\hat{u}_* = \sqrt{-\bar{u}'w_{\max}}$, where $\bar{u}'w_{\max}$ is the maximum value of a function

$$\bar{u}'w(z) = d_1 z^2 \exp(-d_2 z)$$

that is fitted to the measured $\bar{u}'w$-profile. For simplicity and since $\bar{u}'v$ is usually close to zero, all consequent $u_*$ are actually $\hat{u}_*$.

The stability is quantified for each experiment and period by

$$z/L = \begin{cases} 
-k \frac{u_*^3}{w_*^2} \frac{z_i}{z} & \text{for } w_* > 0 \\
\frac{\hat{u}_*}{L} & \text{for } w_* < 0,
\end{cases}$$

(2.4)

where $z$ is height, $L$ is the Obukhov length, $k = 0.41$ the von Kàrmàn constant and $z_0$ the roughness length. Note that a negative $w_*$ does not make sense physically, because $w_*$ describes convective conditions and is always positive under those. If there is no convection, there is no need for $w_*$. However, in (2.4) and some of the following formulas the possibility of a negative $w_*$ is still taken into account to handle edge cases.

Britter and Hanna (2003) cite a roughness length $z_0 = 1$ m for a city of Basel’s topography and this value was already used by Rotach et al. (2004). Christen (2005)
Table 2.3.: Empirical distribution of street directions in degrees, defined like the meteorological wind direction, and their corresponding frequencies for Kleinbasel. The sum of all frequencies has to be unity.

<table>
<thead>
<tr>
<th>street direction $\alpha_{street}$ (°)</th>
<th>5</th>
<th>95</th>
<th>70</th>
<th>160</th>
<th>170</th>
<th>90</th>
</tr>
</thead>
<tbody>
<tr>
<td>relative frequency</td>
<td>0.17</td>
<td>0.17</td>
<td>0.22</td>
<td>0.11</td>
<td>0.16</td>
<td>0.17</td>
</tr>
</tbody>
</table>

proposed $z_0 = 1.5$ m for Basel and the difference in model results for those values will be shown in Section 3.7.3.

The value of the zero plane displacement $d$ is in the range of $0.6–0.85H$ according to Grimmond and Oke (1999). Christen (2005) calculated $d$ for Basel using several methods and got a range of about $0.8–0.9$. Previous to this work the value of $d = 10.1$ m ($= 0.67H$) was used. The influence will be described in a sensitivity study in Section 3.7.3.

Furthermore the height of the roughness sublayer $z_*$ is estimated by Christen (2005) to be about $1.56H$ for Kleinbasel. The model of Rotach et al. (2004) uses $1.477H$ and Section 3.7.3 also contains information about the influence of this value. Raupach et al. (1991) list a range of $(2$ to $5)H$ in their review article for non-urban areas. Rotach (2001) concludes that this range may also be representative for urban areas.

In Section 2.5, a distribution of street directions will be needed. Ideally an objective method would be used to classify and then quantify the distribution, however this lies outside of the scope of this study. Thus the distribution was subjectively extracted from a map (see Figure 2.2) and is listed in Table 2.3. Street directions are defined like the meteorological wind direction (zero degrees at north, clockwise). Moreover, each direction can be equivalently described by the angle $\alpha_{street}$ or the angle $\alpha_{street} + 180^\circ$. This is due to the fact that the wind direction during the simulation decides whether the particles flow up or down the street.

In contrast to Rotach et al. (2004), the measured values of $z_i$ (from Gryning et al. 2005) are used instead of estimated values. The reason is on the one hand that White et al. (2009) show an example where the measured $z_i$ improves the result of a simulation. On the other hand the only reason why Rotach et al. (2004) did not use a measured $z_i$ was due to lack of data availability at that time.

The four successful tracer experiments undertaken within BUBBLE are briefly described in Table 2.4. Exact meteorological conditions and the measurement data set can be found in Gryning et al. (2005).

The experiments will be described from now on using a naming scheme. For three-hour averaged data, where only one data point for each variable and day exists, the first day, 26 June 2002, will be called “experiment 1”. This is repeated in chronological order for experiments 2, 3 and 4. For one hour averaged data, where three data points for each variable and day exist, the day and number of one hour period since start of sampling will be described by a two digit number. The first digit describes the day and the second
**Table 2.4.:** Data about the four successful BUBBLE tracer experiments, adapted after Rotach et al. (2004). Sampler position 3 implies all three samplers (in different heights) of the tower “Sperrstrasse”.

<table>
<thead>
<tr>
<th></th>
<th>Exp. 1</th>
<th>Exp. 2</th>
<th>Exp. 3</th>
<th>Exp. 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Date</td>
<td>26 June 2002</td>
<td>04 July 2002</td>
<td>07 July 2002</td>
<td>08 July 2002</td>
</tr>
<tr>
<td>Release time (CET)</td>
<td>1200–1600</td>
<td>1440–1800</td>
<td>1310–1700</td>
<td>1400–1800</td>
</tr>
<tr>
<td>Sampling time (CET)</td>
<td>1300–1600</td>
<td>1500–1800</td>
<td>1400–1700</td>
<td>1500–1800</td>
</tr>
<tr>
<td>Release rate (g SF₆ s⁻¹)</td>
<td>0.0503</td>
<td>0.0499</td>
<td>0.3008</td>
<td>0.1319</td>
</tr>
<tr>
<td>Source</td>
<td>R1</td>
<td>R2</td>
<td>R1</td>
<td>R1</td>
</tr>
<tr>
<td>Samplers</td>
<td>1–12</td>
<td>1, 3–5, 8–12,</td>
<td>1–4, 6–9, 11,</td>
<td>1–12</td>
</tr>
<tr>
<td></td>
<td>15–17</td>
<td>12, 18, 19</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Release Height (m)</td>
<td>18.6</td>
<td>21.0</td>
<td>18.6</td>
<td>18.6</td>
</tr>
<tr>
<td>Conditions</td>
<td>Strong convection,</td>
<td>Westerly,</td>
<td>Partly cloudy,</td>
<td>Clear sky,</td>
</tr>
<tr>
<td></td>
<td>fairly strong wind, cloudy</td>
<td>strong convection</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Digit the number of the averaging period, so that for example 23 means the second day (04 July 2002) and third (of three, 1700–1800) period. For thirty minute averaged data a three digit number will be used to described the day and the specific one of six averaging periods on each day. The first digit again describes the day, the second is always 0 and the third counts the number of periods since start. For example 402 means the fourth day (08 July 2002) and the second period (1530–1600).

### 2.2. Original Model

This section summarizes the model developed and described by Rotach et al. (1996), which was expanded by de Haan and Rotach (1998), Rotach (2001) and Rotach et al. (2004). Some corrections are listed in Gibson and Sailor (2012).

#### 2.2.1. Basic Model Concept

A Lagrangian Particle Dispersion Model (LPDM) is based on the idea that the dispersion of particles within the boundary layer can be described by an ensemble of independent particles. Each particle is affected by the same velocity field and advected downstream, but additionally by random velocity components that simulate turbulence. After the trajectories of enough particles have been calculated it is possible to obtain the particle concentration (Rotach et al. 1996; Thomson 1987).

The model operates in a natural coordinate system, where $x$ is the horizontal position...
2.2 Original Model

along the mean horizontal fluid velocity, \( y \) the horizontal position perpendicular to the mean horizontal fluid velocity and \( z = z_{AGL} - d \) the vertical position above displacement height \( d \). This is pictured in Figure 1.1.

The longitudinal velocity component \( u \) is decomposed into \( \bar{u} + u' \), with \( \bar{u} \) the mean value and \( u' \) its perturbation. The lateral velocity \( v \) is equal to \( v' \), because the mean lateral wind speed is zero due to the definition of the coordinate system. Similar for the vertical velocity component: \( w = w' \), although its mean is not necessarily zero in the vicinity of an urban canopy; The velocity perturbation components \( u', v' \) and \( w' \) may also be summarized with \( u'_i \), if appropriate, as may the coordinates \( x, y \) and \( z \) with \( x_i \).

To be able to formulate the model certain assumptions have to be made. Molecular diffusion of the particles is neglected, because the typical Reynolds number in the atmosphere is large enough. Particles therefore follow the local velocity field (Thomson 1987). The velocity and position of particles are considered to evolve with a Markov process. This means that the future state of the particle only depends on the present state, not the past. The assumption is only “reasonable”, but enables the use of existing mathematical results (Thomson 1987). Furthermore the random variations of velocities are presumed to be a Wiener process (Thomson 1987), which is similar to Brownian motion. Additionally the particles are assumed to undergo no chemical reactions and the atmosphere is considered to be dry.

With these assumptions it is possible to formulate the Langevin stochastic differential equations (Rotach et al. 1996; Thomson 1987):

\[
\begin{align*}
ds u_i &= a_i(x, u, t)dt + b_{ij}(x, u, t)d\xi_j \\
dx &= udtd
\end{align*}
\]

where \( du_i \) is an infinitesimal increment of a velocity component, \( x = (x, y, z) \) the three dimensional position vector of the particle, \( u = (u' + \bar{u}, v', w') \) its velocity vector, \( dt \) the time step of the model, \( a_i \) the correlated part of acceleration, \( b_{ij} \) the random contribution and \( d\xi_j \) an increment of a Wiener process with mean zero and variance \( dt \). The subscripts, \( i = 1, 2, 3 \) and \( j \) analog, signify the components in space.

An explicit, first order scheme, the forward Euler method

\[
x_i^{\text{new}} = x_i^{\text{old}} + u_i dt
\]

is used to calculate the particle position after each time step. This scheme is unstable for stiff differential equations — like (2.5) — so a small enough \( dt \) has to be chosen to avoid the solution growing too large (see sections 2.2.6 and 3.2.1 for further discussion).

Thomson (1987) shows that the well-mixed criterion is necessary to ensure the correctness of a model formulation. The criterion tests whether particles that are initially well-mixed remain so during the simulation. Well-mixed in this context means that the probability density function (pdf) of the particle’s phase-space distribution is proportional to the pdf
of the fluid elements (i.e. particles behave just like a fluid element would).

The well-mixed criterion also implies that Eulerian pdfs are equal to Lagrangian pdfs (Thomson 1987). Therefore (2.5) is equivalent to the Fokker-Planck equation

$$\frac{\partial P_{\text{tot}}}{\partial t} = -\frac{\partial}{\partial x_i} (u_i P_{\text{tot}}) - \frac{\partial}{\partial u_i} (a_i P_{\text{tot}}) + \frac{\partial^2}{\partial u_i \partial u_j} (B_{ij} P_{\text{tot}}),$$

(2.7)

where $P_{\text{tot}}$ is the pdf of the particle (or Eulerian fluid elements) velocities and $B_{ij} = b_{ik}b_{jk}/2$ with the Einstein summation-convention. For stationary turbulence it can be reduced to

$$a_i P_{\text{tot}} = \frac{\partial}{\partial u_i} (B_{ij} P_{\text{tot}}) + \Phi_i,$$

(2.8)

where $\Phi_i$ satisfies

$$\frac{\partial \Phi_i}{\partial u_i} = -\frac{\partial}{\partial x_i} (u_i P_{\text{tot}})$$

(2.9)

and $\Phi_i \to 0$ when $|u| \to \infty$.

According to Rotach et al. (1996) solutions for $\Phi_i$ cannot be unique, because any function $\Phi^*_i(u_i)$ that is divergence free — in this context deriving by velocity, not space, component — can be added to $\Phi_i$ while still solving (2.9). $\Phi^*$ does, however, change the solution of the flow field (Sawford 1993). Therefore another restriction would be necessary, but none is known to date (Sawford 1993; Thomson and Wilson 2013).

The new idea behind the model started by Rotach et al. (1996) is to create a model that can predict the dispersion of particles in different atmospheric conditions near the ground. Older models of the Lagrangian type had the severe downside that they could either describe convective or non-convective boundary layers (Rotach et al. 1996). This is due to a necessary assumption about the probability density function of turbulence, which is different in convective and non-convective conditions and thus either one or the other case had to be chosen.

### 2.2.2. Probability Density Function

As mentioned, the correlated part of the acceleration $a_i$ in (2.8) can only be calculated if the pdf of the velocity components $P_{\text{tot}}$ is known. The total pdf in the three dimensional model

$$P_{\text{tot}} = f P_u P_c + (1 - f) P_G$$

(2.10)

is constructed by combining the pdfs of two different cases of atmospheric state with a transition function $f$. This is the main difference and improvement introduced by Rotach et al. (1996) compared to other Lagrangian particle models. It enables the model to simulate neutral/stable and convective cases at the same time.

In the convective case neither the longitudinal and lateral wind speed pdfs $P_u$ and $P_v$
are assumed to be correlated, nor the pdf of the vertical velocity

\[ P_c = A P_A + B P_B \, . \] (2.11)

The latter was first introduced by Luhar and Britter (1989) in their one-dimensional, convective model. \( P_c \) is positively skewed for vertical velocities (Rotach et al. 1996) and consists of a combination of

\[ P_A = \frac{1}{\sqrt{2\pi}\sigma_A} \exp \left\{ -\frac{1}{2} \left( \frac{w - \overline{w}_A}{\sigma_A} \right)^2 \right\} \text{ and} \]

\[ P_B = \frac{1}{\sqrt{2\pi}\sigma_B} \exp \left\{ -\frac{1}{2} \left( \frac{w - \overline{w}_B}{\sigma_B} \right)^2 \right\} , \] (2.12a)

the updraft \( (P_A) \) and downdraft \( (P_B) \) components of the vertical wind speed. The parameters \( A \) and \( B \) regulate how strong each component is and can be interpreted as the fraction of up- and downdraft area (Rotach et al. 1996). \( \sigma_A \) and \( \sigma_B \) describe shape of the pdfs and will be determined later (see Section 2.2.3).

The neutral case is a perfectly neutral boundary layer where

\[ P_G = P_u P_v P_w P_{uw} , \] (2.13)

a purely Gaussian distribution, which is taken from Thomson (1987). \( P_u \) is again the longitudinal wind speed pdf, \( P_v \) the lateral wind speed pdf and \( P_w \) the vertical wind speed pdf. \( v \) is assumed to be independent of the other velocity components, whereas the correlation between \( u \) and \( w \) is described by \( P_{uw} \) (de Haan and Rotach 1998). The individual pdfs

\[ P_u = \frac{1}{\sqrt{2\pi}\sigma_uG} \exp \left\{ -\frac{1}{2} \frac{u^2}{(1 - \rho^2)\sigma^2_uG} \right\} \] (2.14a)

\[ P_v = \frac{1}{\sqrt{2\pi}\sigma_v} \exp \left\{ -\frac{1}{2} \frac{v^2}{\sigma^2_vG} \right\} \] (2.14b)

\[ P_w = \frac{1}{\sqrt{2\pi}\sigma_wG} \exp \left\{ -\frac{1}{2} \frac{w^2}{(1 - \rho^2)\sigma^2_wG} \right\} \] (2.14c)

\[ P_{uw} = \frac{1}{\sqrt{(1 - \rho^2)}} \exp \left\{ -\frac{\rho u'w}{(1 - \rho^2)\sigma_uG\sigma_wG} \right\} \] (2.14d)

are described in Rotach et al. (1996) and de Haan and Rotach (1998).

\[ 2B_{ij} = \delta_{ij} C_0 \varepsilon . \] (2.15)
Here $\delta_{ij}$ is the Kronecker delta, $\varepsilon$ the dissipation rate of turbulent kinetic energy and $C_0$ an often discussed constant. Its value is chosen to be 2, see Rotach et al. (1996) and Rotach et al. (2004) for reasoning and details. Therefore,

$$b_{ij} = \sqrt{C_0 \varepsilon}. \quad (2.16)$$

Substituting $B_{ij}$ from (2.15) into (2.8) leads to

$$a_i = \frac{1}{P_{\text{tot}}} \left( -\frac{C_0 \varepsilon}{2} Q_i + \Phi_i \right), \quad (2.17)$$

where

$$Q_i = -\frac{\partial P_{\text{tot}}}{\partial u_i}. \quad (2.18)$$

Since all the pdfs are defined in Section 2.2.2 it is possible (de Haan and Rotach 1998; Rotach et al. 1996) to calculate the different $Q_i$ as

$$Q_u = \frac{u'}{(1 - \rho^2)\sigma_w^2} P_{\text{tot}} + (1 - f) \frac{\rho w}{(1 - \rho^2)\sigma_w^2} P_G, \quad (2.19a)$$
$$Q_v = \frac{v}{\sigma_v^2} P_{\text{tot}}, \quad (2.19b)$$
$$Q_w = f P_v P_u Q_c + (1 - f) \left( \frac{w}{(1 - \rho^2)\sigma_{wG}^2} + \frac{-\sigma_{wG} u'}{(1 - \rho^2)\sigma_{wG}^2} \right) P_G \quad (2.19c)$$

where

$$Q_c = \frac{A(w - \overline{w_A})}{w_A^2} P_A + \frac{B(w + \overline{w_B})}{w_B^2} P_B.$$

The functions $\Phi_i$ are derived in Rotach et al. (1996) and de Haan and Rotach (1998) (for three dimensions) under the assumption of a stationary, horizontally homogeneous boundary layer by splitting $\Phi_i$ into a Gaussian and a non-Gaussian part. The results are based on earlier work (Luhar and Britter 1989; Thomson 1987). Gibson and Sailor (2012) show some corrections to the previously published expressions. The combined results are

$$\Phi_u = P_v \left( \Phi_u^C + (1 - f)\Phi_u^G + \Phi_u^* \right), \quad (2.20a)$$
$$\Phi_v = w v P_{\text{tot}} \frac{1}{\sigma_v} \frac{\partial \sigma_v}{\partial z}, \quad (2.20b)$$
$$\Phi_w = P_v \left( \Phi_w^C + (1 - f)\Phi_w^G + \Phi_w^* \right). \quad (2.20c)$$

$\Phi_u$ and $\Phi_w$ consist of a convective part $\Phi_i^C$, a Gaussian part $\Phi_i^G$ and a third part $\Phi_i^*$, that forms due to the non-uniqueness already mentioned in Section 2.2.1 and some required properties of $\Phi_i$ as shown in Rotach et al. (1996).

The individual parts are,

$$\Phi_u^C = \frac{\partial f}{\partial z} \exp \left( -\gamma w^2 \right) \frac{w}{2\sqrt{2\pi w^2}} \left[ \text{erf} \left( \frac{\overline{w}}{w_A} \right) + 1 \right], \quad (2.21a)$$
$$\Phi_w^C = (I_1 + I_2) \left( \frac{\partial f}{\partial z} P_u + f \frac{\partial P_u}{\partial z} \right) + f P_u \Phi_w^{LD}, \quad (2.21b)$$
using the auxiliary variables
\[
\begin{align*}
\gamma &= \frac{1}{2\sigma_{wG}^2} \\
\hat{u} &= \frac{1}{\sqrt{2(1-\rho^2)}\sigma_{uG}} \left( u' - w \frac{\partial \sigma_{uG}}{\partial \sigma_{wG}} \right) \\
\Phi^I_w &= \frac{1}{2} \left[ \left( -A \frac{\partial \sigma_A}{\partial z} - \frac{\partial A}{\partial z} \right) \text{erf} \left( \frac{w - w_A}{\sqrt{2\sigma_A}} \right) + \left( B \frac{\partial \sigma_B}{\partial z} + \frac{\partial B}{\partial z} \right) \text{erf} \left( \frac{w + w_B}{\sqrt{2\sigma_B}} \right) \right] \\
&\quad + w_A P_A \left[ A \frac{\partial \sigma_A}{\partial z} \left( \frac{w^2}{w_A^2} + 1 \right) + A B \frac{\partial \sigma_B}{\partial z} \left( \frac{w^2}{w_B^2} + 1 \right) + w_B \frac{\partial B}{\partial z} \right] \\
&\quad + \frac{1}{2} \left[ A w_A \text{erf} \left( \frac{w - w_A}{\sqrt{2\sigma_A}} \right) - B w_B \text{erf} \left( \frac{w + w_B}{\sqrt{2\sigma_B}} \right) \right].
\end{align*}
\]
\( \gamma \) has a numerator of 2 in Rotach et al. (1996), however Gibson and Sailor (2012) derived that 1 is correct. Note that in the model code the value 1 is implemented, even if the value of 2 can be found in the original paper. See the appendix of Luhar and Britter (1989) for the derivations of \( \Phi^I_w \) and \( I_1 + I_2 \). The standard deviation of the longitudinal velocity \( \sigma_{uG} \) describes the Gaussian pdf in (2.13), as does the equivalent in the vertical direction \( \sigma_{wG} \) and the correlation coefficient between the Gaussian \( u' \) and \( w \)
\[
\rho = \frac{w G}{\sigma_{uG} \sigma_{wG}}.
\]

Following the approach of Thomson (1987), the appendix of Rotach et al. (1996) lists
\[
\begin{align*}
\Phi^G_u &= \frac{P_G}{2P_v} \left[ \left( \frac{\sigma_{uG}^2}{\sigma_{uG}^2 - \sigma_{uuwG}^2} \frac{\partial \sigma_{uG}^2}{\partial z} + \frac{-\sigma_{uuwG}}{\sigma_{uG}^2 - \sigma_{uuwG}^2} \frac{\partial \sigma_{uuwG}}{\partial z} \right) u' w \\
&\quad + \left( \frac{-\sigma_{uuwG}}{\sigma_{uG}^2 - \sigma_{uuwG}^2} \frac{\partial \sigma_{uuwG}}{\partial z} + \frac{-\sigma_{uuwG}^2}{\sigma_{uG}^2 - \sigma_{uuwG}^2} \frac{\partial \sigma_{uuwG}}{\partial z} \right) w^2 + 2 \frac{\partial w}{\partial z} + \frac{\partial \sigma_{uuwG}}{\partial z} \right]
\end{align*}
\]
\[
\begin{align*}
\Phi^G_w &= \frac{P_G}{2P_v} \left[ \left( \frac{\sigma_{wG}^2}{\sigma_{wG}^2 - \sigma_{wwuG}^2} \frac{\partial \sigma_{wG}^2}{\partial z} + \frac{-\sigma_{wwuG}}{\sigma_{wG}^2 - \sigma_{wwuG}^2} \frac{\partial \sigma_{wwuG}}{\partial z} \right) u' w \\
&\quad + \left( \frac{-\sigma_{wwuG}}{\sigma_{wG}^2 - \sigma_{wwuG}^2} \frac{\partial \sigma_{wwuG}}{\partial z} + \frac{-\sigma_{wwuG}^2}{\sigma_{wG}^2 - \sigma_{wwuG}^2} \frac{\partial \sigma_{wwuG}}{\partial z} \right) w^2 + \frac{\partial \sigma_{wwuG}^2}{\partial z} \right].
\end{align*}
\]
Note that their covariance matrix \( V \) was expanded into the third dimension and the abbreviation \( \sigma_{u_i'u_j} = \sqrt{\bar{u}_i \bar{u}_j} \) for covariances is hereby introduced for any \( i, j = 1, 2, 3 \). Auto-covariances are denoted by \( \sigma^2_{u_i} \). Thereby all covariances that include \( v \) except \( \sigma^2_v \) are zero, because \( v \) is assumed to be independent of \( u \) and \( w \). \( \sigma_{uuwG} \) is the joint moment of \( u \) and \( w \) in the Gaussian pdf.

The last missing pieces are defined in Rotach et al. (1996) as
\[
\begin{align*}
\Phi^*_u &= -\frac{df}{dz} \left[ \frac{\exp \left( -\gamma w^2 \right)}{2\sqrt{2\pi} \sigma_{wG}} \right] w \left[ \text{erf} \left( u' \right) + 1 \right] \\
\Phi^*_w &= -\frac{df}{dz} \left[ \frac{\exp \left( -\gamma w^2 \right)}{2\sqrt{2\pi} \gamma \sigma_{wG}} \right] \exp \left( -u^2 \right),
\end{align*}
\]
although Gibson and Sailor (2012) point out unit inconsistencies. For further elaboration on this matter see Section 2.4.3.
Now $\Phi_u$, $\Phi_v$ and $\Phi_w$ in (2.20) are defined using (2.21), (2.24) and (2.25). Together with $Q_u$, $Q_v$ and $Q_w$ from (2.19), $a_i$ in (2.17) can be calculated if all the covariances, velocities and $\varepsilon$ are known. There are some variables missing, however, that need to be known first. Rotach et al. (1996) define

\begin{align}
\sigma_v &= \sqrt{v^2} \\
\sigma_{wG} &= \sqrt{w^2} \\
\sigma_{uG}^2 &= \overline{u^2} + \frac{\overline{u'w_G}}{\sigma_{uG}^2} f \\
\overline{u'w_G} &= \frac{u'w}{1 - f},
\end{align}

(2.26a)
(2.26b)
(2.26c)

where $\overline{u'w_G}$ is the joint moment of $u'$ and $w$ in the Gaussian distribution and $\overline{u'w}$ the measured joint moment in the atmosphere. Similarly, the notation $\sigma_u = \sqrt{u^2}$ is hereby introduced.

Note that Gibson and Sailor (2012) correct the expression for $\sigma_{uG}$ previously published in Rotach et al. (1996). The expression above is the corrected one. Since the model code already had the correct version since at least 1998, no further inquiry in this matter has been taken.

Rotach et al. (1996) use the assumption that

\begin{align}
\sigma_A &= \overline{w_A} \\
\sigma_B &= \overline{w_B},
\end{align}

(2.27)
as a closure, after Luhar and Britter (1989), to get

\begin{align}
\overline{w_B} &= \sqrt{(\overline{w^3})^2 + 8f^2(\overline{w^2})^3 - \overline{w^3}} \\
\overline{w_A} &= \frac{\overline{w^2}}{2\overline{w_B}} \\
A &= \frac{qw_B}{\overline{w_A} + \overline{w_B}} \\
B &= \frac{qw_A}{\overline{w_A} + \overline{w_B}}
\end{align}

(2.28)
(2.29)
(2.30)
(2.31)

with $q = \frac{1}{\sqrt{1 - \rho^2}}$, and therefore the pdf $P_C$ in (2.11).

### 2.2.4. Transition Function

Another missing piece is the function that lets the model transition between neutral and convective cases. It has to fulfill many requirements (Rotach et al. 1996). Most importantly it has to approach unity in a fully convective boundary layer and should approach zero in a fully neutral one. The latter is not easily possible due to conflicts with other requirements on $f$ (Rotach et al. 1996), but with a trick involving $\delta$ it still does.
The best function to fulfill the requirements and be consistent with the model was found to be (Rotach et al. 1996)

\[ f = C_1(C_2 - \cos g) . \]

The thereby used abbreviations

\[ g = C_3 \pi (1 - \exp(z/L)) , \]
\[ C_1 = \frac{1 - \delta}{2} , \quad C_2 = \frac{1 + \delta}{1 - \delta} , \quad C_3 = 1 - C'_3 \left( \frac{u_*}{w_*} \right)^2 \]
\[ \text{and} \quad \delta = \frac{\alpha_1 w_*}{u_* + \alpha_2} \]

are used to improve readability. Rotach et al. (1996) define \( \alpha_1 = 2.5 \cdot 10^{-2} \text{ m s}^{-1} \) and \( \alpha_2 = 10^{-2} \text{ m s}^{-1} \) because they “proved useful” and \( C'_3 = 1.65 \) by fitting the function to measurement data.

The aforementioned measurements did not include data from experiments inside the UCL. When using the above approach and comparing to actual pdfs of \( w \) measured at the Sperrstrasse tower, Rotach et al. (2004) found that (2.32) does not fit the BUBBLE data well. They attribute this to the fact that (2.32) was not fitted to data where both \( u_* \) and \( w_* \) are large — as they can be for urban areas and are in all BUBBLE cases — and that no measurements inside the UCL were used.

To rectify this, Rotach et al. (2004) fitted a new function

\[ f = \begin{cases} 
C_1(C_2 - \cos g) \tan \left( \frac{\pi z}{16z_*} \right)^2 & \text{when} \quad z \leq 4z_* \\
C_1(C_2 - \cos g) & \text{else},
\end{cases} \]

using the same abbreviations as (2.32). The height of \( 4z_* \) was chosen arbitrarily.

The difference between the two functions \( f \) is depicted in Figure 2.3 on the left panel.
Methodology

Rotach et al. (2004) postulate that the urban effect leads to a more Gaussian pdf of the vertical velocity near the ground, which leads to an \( f \) (2.33) that is closer to zero than the old \( f \) (2.32). Section 3.4 will investigate the influence of this approach.

The right panel of Figure 2.3 shows one problem of the new transition function. Due to the change in curvature between the old and the new function below \( 4z_\ast \), the new \( f \) is no longer continuously differentiable. This is clearly visible in the jump of the solid line at a height of about 50 meter. Since \( \Phi^C_i \) (2.21) and \( \Phi^*_i \) (2.25) depend on \( \frac{\partial f}{\partial z} \), a discontinuity in \( \frac{\partial f}{\partial z} \) leads to a discontinuity in \( \Phi_i \). This potential problem will be investigated in Section 3.2.4.

2.2.5. Parametrization of profiles

Now that all model functions have been defined, it would be possible to calculate the next time step of the model if the velocity field, velocity variances, Reynolds stress, stability, the dissipation rate and other descriptors of the atmospheric conditions were known. Some of those have to be parameterized, because using measurements or numerical weather prediction models as model input is either not possible or prohibitively expensive with the required vertical resolution.

Rotach (2001) shows that it is useful to use different parameterizations in the roughness sublayer and therefore the parameterizations are each split into two parts. The first describes both the inertial sublayer profile and the mixed layer profile at the same time, as proposed by Rotach et al. (1996). The second describes the RS profiles after Rotach (2001). The interface between them is at height \( z_\ast \), as mentioned in Section 2.1. Figure 1.1 shows a visual representation of the mentioned layers and how they relate to model geometry. For an in depth review on the RS, see Roth (2000).

Inertial sublayer and mixed layer

Reynolds stress

\[
\overline{u'w} = -u_\ast^2 \left(1 - \frac{z}{z_i}\right)^\alpha \frac{1}{\Psi} \tag{2.34}
\]

and is parameterized according to de Haan and Rotach (1998) where

\[
\Psi = \frac{\exp \left(10\sqrt{z/z_i} - 5\right)}{1 + \exp \left(10\sqrt{z/z_i} - 5\right)} + \left(1 - \frac{\exp \left(10\sqrt{z/z_i} - 5\right)}{1 + \exp \left(10\sqrt{z/z_i} - 5\right)}\right) \left(1 - \frac{z}{z_i}\right)^\alpha
\]

and either \( \alpha = 1 \) for near neutral conditions or \( \alpha = 1.5 \) for stable conditions (de Haan and Rotach 1998). This formulation incorporates both stable and convective boundary layers at the same time.

Sorbjan (1986) describes the derivative of the mean wind speed in a convective boundary layer \((w_\ast > 0)\) and the formulation of Forrer and Rotach (1997) is used in stable and
neutral conditions. This means that

\[
\frac{\partial \eta}{\partial z} = \begin{cases} \frac{u^*}{kz} \Phi^1_m(\frac{\tilde{z}}{L}) \left(1 - \alpha \frac{\tilde{z}}{z_i}\right)^{2/3} & \text{for } w_* > 0 \\
\frac{u^*}{kz} \Phi^2_m(\frac{\tilde{z}}{L}) & \text{else} \end{cases}
\]

(2.35)

with \( \Phi^1_m = \left(1 - 19.3 \frac{z}{L}\right)^{-1/4} \)

and \( \Phi^2_m = 1 + \frac{z}{L} + \frac{2z}{3L} \exp(-0.35 \frac{z}{L}) \left(1 - 0.35 \frac{z}{L} - \frac{5}{0.35}\right) \),

where \( \alpha = 1 \) (see Rotach et al. (1996) for a discussion) and \( k \) is the von Kármán constant.

The nondimensional stability function \( \Phi^1_m \) comes from Högström (1988) and \( \Phi^2_m \) from Beljaars and Holtslag (1991). This gradient is used to calculate a profile of the mean wind speed by integrating it upwards of a measured wind speed (Rotach 2001).

The vertical velocity variance

\[
\overline{w^2} = 1.5w_*^2 \left(\frac{z}{z_i}\right)^{2/3} \exp\left(-\frac{2z}{z_i}\right) + \left(1.7 - \frac{z}{z_i}\right) u_*^2,
\]

(2.36)

is parameterized according to Gryning et al. (1987) and also describes both neutral and convective cases. As mentioned in Rotach et al. (2004), the model uses a scaled version of this parameterization. Thereby every value is multiplied by the fraction of the observed variance (in 31.7 m) divided by the parameterized variance in that height.

Results of Gryning et al. (1987) and Brost et al. (1982) are used by Rotach et al. (1996) as a foundation for the longitudinal velocity variance in the convective case. When the atmospheric state is neutral (\(|L| > 9900\), an arbitrary, large number) only the second part of Gryning et al. (1987)'s equation applies, because \( w_* = 0 \). When the atmosphere is stable the profile follows the work of Nieuwstadt (1984). Together, this leads to

\[
\overline{v^2} = \begin{cases} 0.35w_*^2 + u_*^2(5 - 4z/z_i) & \text{for } w_* > 0 \\
u_*^2(5 - 4z/z_i) & \text{for } |L| > 9900 \\
4.2u_*^2(1 - z/z_i)^{3/2} & \text{otherwise} \end{cases}
\]

(2.37)

for the longitudinal velocity variance. This variance is scaled identical to \( \overline{w^2} \).

For the lateral velocity variance again the works of Brost et al. (1982) and Gryning et al. (1987) are used for unstable \( (w_* > 0) \) and neutral cases, analogously to the longitudinal velocity variance. Cases with stable conditions are described again by following Nieuwstadt (1984) in deriving the profile. Therefore,

\[
\overline{v^2} = \begin{cases} 0.35w_*^2 + u_*^2(2 - z/z_i) & \text{for } w_* > 0 \\
u_*^2(2 - z/z_i) & \text{for } |L| > 9900 \\
2.9u_*^2(1 - z/z_i)^{3/2} & \text{otherwise}, \end{cases}
\]

(2.38)

also scaled like the other two velocity variances.
Rotach et al. (1996) parameterize the third moment of vertical velocity as

$$\overline{w^3} = 1.3 u_s^3 \left( \frac{z}{z_i} \right) \left( 1 - \frac{z}{z_i} \right)^2. \quad (2.39)$$

They acknowledge that this formulation underestimates the values in the upper part of the atmospheric boundary layer, but the correct formulation (i.e. the one representing the employed data better) does not fulfill the well-mixed criterion (see Rotach et al. (1996) for details).

The dissipation of turbulent kinetic energy is given for a neutral atmosphere ($|L| > 9998$) by Stull (1988, equation 9.5.4a) as

$$\varepsilon = \frac{u_s^3 L}{k z}, \quad (2.40)$$

where $u_{s,L}$ is the local friction velocity. Since $u_*$ is assumed to be constant in the IS, here $u_{s,L} = u_*$. For an unstable, convective boundary layer ($|L| < 9998$ and $w_* > 0$),

$$\varepsilon = \frac{u_s^3}{z_i} \left\{ 1.07 \left( \frac{1 - z/z_i}{k z/z_i} \right)^2 \right\} + \frac{u_s^3}{z_i} \left\{ 1.5 - 1.2 \sqrt[3]{z/z_i} \right\} \quad (2.41)$$

according to Rotach et al. (1996), who combined earlier approaches by Luhar and Britter (1989), Brost et al. (1982) and Grant (1992). If the atmosphere is stable ($|L| < 9998$ and $w_* \approx 0$),

$$\varepsilon = \frac{3.7 u_s^3 (1 - z/z_i)}{k L_L}, \quad \text{where} \quad L_L = \frac{L u_{s,L}^3}{u_s^3 (1 - z/z_i)}, \quad (2.42)$$

according to Stull (1988, equation 9.4.4a).

**Roughness Sublayer**

Rotach (2001) discusses local scaling (not “the theoretical framework of Nieuwstadt (1984)”), which is essentially employing the same functional forms as in the IS in the RS, even though Monin-Obukhov similarity theory is not valid there. However, when using $u_{s,L}$ (2.44) instead of $u_*$, this has proved to be successful (see Rotach (2001) for examples).

In the RS, a different Reynolds stress parametrization after (Rotach 2001) is used:

$$\overline{u'w} = -u_{s,L}^2, \quad (2.43)$$

where

$$u_{s,L} = u_*^{IS} \left[ \sin \left( \frac{\pi}{2} \left( \frac{z}{z_*} \right)^{1.28} \right) \right]^{1/3}, \quad (2.44)$$

where $z_*$ is the height of the RS and $u_*^{IS}$ is the friction velocity in the IS, an input variable as described in Section 2.1. In contrast to equation (1) in Rotach (2001), here the factor of $\pi/2$ inside the sine function is not taken to the power of 1.28. As can easily be seen in his Figure 2., this is correct, because $u_{s,L}$ is fitted to approach $u_*$ when $z$ approaches $z_*$.  

The mean wind profile is calculated as in the IS, namely by using (2.35) and integrating downwards from an input height. Only when the height of the particle is below \( z^* \), the local friction velocity \( u_{*,L} \) is used instead of \( u_\ast \).

(Rotach 2001) also introduced a parameterization for the dissipation of turbulent kinetic energy, analogously to (2.41), only with \( u_{*,L} \) instead of \( u_\ast \).

The three variances of the velocity components are also approximated by linear relationships fitted to BUBBLE data and decrease linearly with height, starting at their corresponding IS-value:

\[
\overline{u'^2} = \overline{u'^2}_{IS} - k_u(z^* - z) \tag{2.45}
\]
\[
\overline{v'^2} = \overline{v'^2}_{IS} - k_v(z^* - z) \tag{2.46}
\]
\[
\overline{w'^2} = \overline{w'^2}_{IS} - k_w(z^* - z), \tag{2.47}
\]

where \( \overline{u'^2}_{IS} \) is the value of \( \overline{u'^2} \) at level \( z^* \), calculated with (2.36), (2.37) or (2.38) (Rotach 2001). \( k_u, k_v \) and \( k_w \) are the fitting parameters for each individual experiment and averaging period.

### 2.2.6. Model Domain

#### Steady state

The model as it was used throughout this work does not create concentration distributions in time, but one stationary concentration field. Since the field measurements (see Section 2.1) are also assumed to be relatively stationary, this poses no problem in comparison. Unlike in the field experiment, the model releases all its particles at the same time, not in a steady stream. This is explained further in Section 2.2.7. During the simulation the particles follow their trajectories as described in Section 2.2.1. Only for the concentration calculation (see Section 2.2.7) the steady state assumption is made.

The simulation ends after a set period of time. Unless stated otherwise, this period is long enough to allow almost all particles to travel further away from the source than all relevant positions, where concentrations are calculated.

#### Frequency of concentration calculation

The concentration calculations are not undertaken every time step to save computing time. Instead, it is done every tenth time step, although this can be adjusted. This is justified, because the kernel method, that will be described in Section 2.2.7, “smears” a particle over a volume. These spheres or “kernels” increase in size as the dispersion increases, which means that they are small at the beginning and larger in the end. At the start they have a radius on the order of 10 meters. Consequently a kernel needs about 10 seconds to travel its own length, assuming a speed of 2 m s\(^{-1}\), which corresponds to ten time steps of one
second. After the first few time steps the radius of the kernels increases above the order of 100 meters.

**Model bounds**

Since the model is Lagrangian and therefore doesn’t need a grid, the position of each particle is calculated and used at floating point resolution. No restriction on $x$- and $y$-direction is imposed.

The model’s vertical top is at the boundary layer height $z_i$ (measured input), and no transport to or from the atmosphere above is possible. This assumption is often used in near surface, close to source concentration models. Furthermore, Section 3.2.3 shows how small its impact is in this case.

When a particle travels to a vertical coordinate $z$ higher than the model top, it is reflected. Thereby the vertical wind speed $w$ has its sign inverted and the new vertical position is calculated by $z_{\text{new}} = 2z_i - z_{\text{old}}$. Hence the absolute travel path of the particle is unchanged (de Haan and Rotach 1998). The sign of the horizontal velocity perturbation $u'$ is also negated to comply with the well mixed criterion, see Rotach et al. (1996) for a discussion on this.

The model’s bottom ($z = 0$) is at the displacement height $d$ above the real ground (see Section 2.1), because the velocity variances are zero below the real height $d + z_0$, at least when they are parameterized as in Section 2.2.5. This is not necessarily so — and certainly not so in reality —, but a choice that was made (Rotach et al. 1996). Alternatively, turbulence parameterizations for the UCL would be needed for the model bottom to be the real ground.

Since no such UCL turbulence parameterization is easily available, the model bottom is at $d$. However, due to the velocity variances becoming zero below $z_0$, the velocity increments do too and a particle advected there would never move again. To avoid this, a particle is reflected when it is transported into this region ($z < z_0$), in a manner analog to the reflection at the model top.

Rotach et al. (2004) describe why an immediate reflection in all cases at the bottom is not optimal, due to the model bottom not being the real ground. In reality particles can enter street canyons (which do not exist in the model) and stay there for the residence time

$$\tau = \frac{2H}{\bar{u}_{\text{vort}}} = \frac{4H}{\bar{u}_H},$$

(2.48)

which depends on the average horizontal wind speed at roof top level $\bar{u}_H$ and the building height $H$ (Rotach et al. 2004). For the mean vortex velocity $\bar{u}_{\text{vort}}$ they use $0.5\bar{u}_H$. It should be mentioned here that the model’s source code of Rotach et al. (2004) mistakenly uses $\bar{u}_H = \bar{u}(H)$ instead of $\bar{u}(z_h)$. Thus the zero plane displacement is not subtracted from the height, taking the wind speed from a higher level and effectively increasing the rooftop
velocity by about 50% on average.

After $\tau$ the particle exits the virtual street canyon again, whereby the sign of its vertical velocity is inverted. All other particle states are retained from before the trapping incident, only the height is increased by one meter to $z = z_0 + 1$. Notably the longitudinal velocity perturbation $u'$ does not have its sign inverted, in contrast to the reflections at either boundary.

The formula for $\tau$ in (2.48) stems from the assumption of a counter rotating vortex (see Section 1.3) with velocity $\bar{u}_{\text{vort}}$ inside the street canyon for a width to height ratio of about unity in all cases. Since the displacement height is about $2/3$ of $H$ (Grimmond and Oke 1999) and the particles travel on average not exactly at the wall or ground, the distance of one vortex rotation is $(2 \cdot 2/3 + 1)H$, approximately $2H$. Not every particle that reaches the model bottom would enter a street canyon in reality, therefore an entering-probability of 33% was chosen by Rotach et al. (2004) to reflect this. The probability describes the probability that the particle hits the street instead of a roof (50% due to geometry) and the probability that the particle is not reflected at the shear layer on top of the street canyon and crosses it instead (66%). These influential assumptions will be relaxed somewhat in the modified model (Section 2.5).

**Time step**

Thomson (1987) suggested a time step criterion to calculate a sufficiently small time step for the model. However, using this minimal time step for all times and all particles would slow down the model considerably. Therefore a default time step of 1 s (see Section 3.2.1 for influence of this value) is chosen and the model functions $a_i$ and $b_{ij}$ are calculated every time step for each particle. If, however, the default time-step is larger than the maximum allowed time-step (Rotach et al. 1996; Schwere et al. 2002; Thomson 1987)

$$dt_{\text{max}} = \min \left( \frac{0.01 \varepsilon}{|w \partial w/\partial z|}, \frac{0.1 \sigma_w}{|a_w|}, \frac{0.1 \sigma_u}{|a_u|}, \frac{0.01 \sigma_w}{|w \partial^2\sigma_w/\partial z^2|}, \frac{0.01 \sigma_u}{|w \partial^2\sigma_u/\partial z^2|}, \frac{10|u'|}{|w \partial v/\partial z|}, \frac{0.02 \sigma^2 u_{wG}}{B} \right)$$

the model creates a sub-time step of size $dt_{\text{max}}$. Then it calculates all model variables and the increments in space and repeats with a time step of $dt_{\text{max}}$ until a full time step $dt$ has been completed. Hence the model can operate with a relatively large time step during normal operation, but still have high temporal resolution when needed.

This need arises when a particle transitions between two zones with a large difference in magnitude of some atmospheric state, i.e. with large gradient. Additionally the time step is bounded because the Langevin equation, on which the model is based, is stiff. The Euler forward scheme that the model uses (see Section 2.2.1) is unstable for this equation, which means that larger time steps increase the chance of numerical instability (Yee and Wilson 2007). This in turn leads to unphysical velocities.

Yee and Wilson (2007) describe the cause for those so called “rogue trajectories” as
twofold. On the one hand rogue trajectories form due to dynamical instabilities in the Langevin equations, additionally exacerbated by the fact that the mean flow field and Reynolds stress tensor are discontinuous in their computational descriptions. On the other hand the already mentioned numerical instability of the simple Euler forward scheme can also not always be controlled with a finite time step. Those two causes can also reinforce each other.

Since no method to suppress the occurrence of rogue trajectories altogether has been found yet (Postma et al. 2012), this model uses a simple "reset" to get rid of them. In each calculation of velocity $P_{\text{tot}}$ appears as denominator (substituting (2.17) in (2.5)). In line of this, an arbitrary lower bound of $10^{-20} \text{ s}^2 \text{ m}^{-2}$ was chosen (Rotach, personal communication) for $P_{\text{tot}}$. When a particle's $P_{\text{tot}}$ becomes smaller than this, its velocities are reset to the average Eulerian velocities in this area.

**Number of particles**

Another model parameter that warrants discussion is the number of particles $n$. Due to the random nature of the model, the result is never exactly the same. This leads to the problem of how to compare different model options when even the same options lead to different results. To solve this problem, it is necessary that the noise created by the random nature is substantially smaller than the signal created by the difference in model options. Only then is it possible to compare the output of different model versions. Obviously the random noise scales inversely with the number of particles, while the signal does not. Therefore more particles are always better, but also take longer to simulate. Section 3.2.2 shows how the noise compares to the signal for identical model runs with the choice of $n = 500,000$ and $n = 50000$ particles. A compromise between computational cost and reproducibility of the results is achieved with $n = 200000$.

**2.2.7. Concentration Calculation**

One common value to describe the distribution of particles at any time step of the model is concentration, the ratio of total particle mass per unit volume. The easiest way to achieve this is the often used box counting method. The model domain is divided into boxes of a certain height, width and length and the number of particles in each box is counted and multiplied by the weight of one particle, then divided by the volume of the box. The problem of this method is that the result is highly dependent on box size (de Haan 1999). Too large boxes smooth the data (e.g. large bias) and too small boxes scatter the data (e.g. large variance).

Therefore this model uses an alternative method called the kernel method, implemented by de Haan (1999). De Haan states that Lorimer (1986) introduced the kernel method for atmospheric dispersion and the latter lists earlier (although non-atmospheric) works.
The kernel method has an advantage over box counting, namely that a smaller number of particles is required to achieve a desired resolution, therefore saving computational costs (de Haan 1999).

The kernel method works as follows. Every particle is “smeared” with a density function

$$K_{\text{de Haan}}(x) = \begin{cases} C(1 - x^T x)^3 & \text{for } x^T x < 1 \\ 0 & \text{else} \end{cases} \quad (2.50)$$

so that it is no longer one mass at one point, but represented by a “kernel” with outwards decreasing density. This density function in (2.50) is triweight and three dimensional. $C = 945/(192\pi)$ is a normalizing factor that ensures that

$$\int_{\mathbb{R}^3} K(x) \, dx = 1,$$

as described by de Haan (1999).

The specific kernel method used here calculates the density function (or rather its width, see (2.51)) for each time step depending on the distribution of the particles. A comparison between different kernel methods by Vitali et al. (2006) shows that this type of kernel method is valid. The concentration

$$c_{\text{de Haan}}(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right),$$

at each desired point $x$, is then simply calculated by adding up the densities of all kernels at that point. $n$ represents the number of particles and $h$ the width of the kernels.

The width of the kernels $h$ is calculated in each time step by

$$h = A(K)n^{-1/7}\sigma,$$

which (de Haan 1999) calls the optimal width. $A(K)$ is, assuming that the distribution of the particles is Gaussian, a factor (see de Haan (1999) for details) and $\sigma$ is the standard deviation of the particle distribution.

The model uses a modified version of the method described above, which was developed, but never published by Peter de Haan (personal communication 2014). The kernel widths

$$h_i = A(K)n^{-1/7}\sigma_i \quad (2.51)$$

are direction-dependent and therefore it is no longer possible to use vector syntax to evaluate the kernel function in the concentration calculation. Hence a new, similar to (2.50), kernel function

$$K(X) = \begin{cases} C(1 - X)^3 & \text{for } X < 1 \\ 0 & \text{else} \end{cases} \quad (2.52)$$

with

$$X_i = \left(\frac{x - x_i}{h_x}\right)^2 + \left(\frac{y - y_i}{h_y}\right)^2 + \left(\frac{z - z_i}{h_z}\right)^2 \quad (2.53)$$
Methodology

is used in the corresponding new local concentration

\[ c(x) = \frac{m_f}{h_x h_y h_z} \sum_{i=1}^{n} K(X_i) . \]  

(2.54)

Additionally, the denominator in front of the sum in (2.54) has a different dimension than the version of de Haan (1999). This solves a unit inconsistency, since his unit of concentration would always be indirectly proportional to length, regardless of the dimension. By dividing by all three \( h_i \) in (2.54) the unit for this three dimensional case is mass over length cubed. \( m_f \) describes the mass of one particle and is calculated by dividing the mass of all particles by the number of particles.

Thus the kernel method could calculate the concentration on each point in the model domain at each time step. In spite of this, the model does not calculate a concentration field at every time step, but only one average field for all time steps. This is justified because the therein calculated field represents a steady state and the measured cases are assumed to be stationary (see Section 2.1).

The mentioned averaging is done by simply adding up the local concentration at each point for all treated time steps. Not all time steps are used to calculate the concentration, see Section 2.2.6. After adding up the local concentrations, the sums are divided by the so called “effective number of particles”, which is the number of particles multiplied by the number of treated time steps.

The reason why the concentration is calculated like this coincides with the fact that the model releases all particles at once, instead of a continuous source like in the experiments. One advantage of this method is that in that way the number of particles always stays the same, which simplifies the flow of the model. Additionally the simulation time is shortened, because the model does not have to reach a steady state first. Since all particles are independent, it does not matter when they follow their trajectories and reach each receptor, or rather when their kernel density is detected by each receptor. Therefore this method does not assume more than a continuous source method would.

To simplify the output data the widely used concept of “arcs” is applied. Figure 2.4 shows that each arc is part of a circle’s circumference that is centered on the mean wind direction and has a constant distance from the source. Multiple equidistant arcs are constructed with increasing distance \( x_p \) from the source and virtual receptors are placed along these arcs at the bottom of the model. The angular distance between adjacent receptors along each arc is constant. Consequently the absolute distance between receptors along each arc is closer the further the arc is to the source (see Figure 2.4).

Along each of those arcs the so called crosswind integrated concentration

\[ c_y(x_p) = \sum_{p=-m}^{m} \frac{\Delta y_{arc,p}}{2} [c(x_p, y_q - 1, 1) + c(x_p, y_q, 1)] \]  

(2.55)

in ng m\(^{-2}\) is calculated. As show in Figure 2.4, \( \Delta y_{arc} \) is the distance with unit meter between two receptors along the arc where the local concentration is calculated. There are
2.2 Original Model

Figure 2.4.: Visual representation of arcs with distance along arc between two receptors $\Delta y_{\text{arc},p}$ exemplary for one case.

A total of $2m + 1$ many receptors along each arc.

Another often used variable is the maximum concentration along each arc called $c_{\text{arc max}}$, which is simply the highest concentration $c$ to occur along one arc.

Additionally the standard deviation of the spacial particle distribution along the arc

$$
\sigma_{c,y}(x_p) = \sqrt{\frac{\sum_{q=-m}^{m} c(x_p, y_q, 1) (|q|\Delta y_{\text{arc},p})^2}{\sum_{q=-m}^{m} c(x_p, y_q, 1)}}
$$

(2.56)
is useful, given the assumption that the center of the plume is along the mean wind direction and therefore the $x$-direction. It is calculated similar to a normal standard deviation (2.58). The obvious first idea to calculate $\sigma_{c,y}$ is to take all particles along one arc, sum up their square distance from the center line, divide by that number of particles and take the square root. Since few particles — those that happen to randomly end up on this position with floating point precision — would actually be on the exact arc, the kernel method is used again. Due to the fact that the local concentration (2.54) is proportional to a “number of particles”, even though those particles are distributed over a kernel, the units of $\sigma_{c,y}$ in (2.56) work out to meter.

In addition to the above quantities the model can optionally output the concentration at each receptor along all arcs and also calculate the concentration at any point that is defined by its absolute position in relation to the source. The latter is useful to calculate the model concentration at the exact sampler positions — including height — of an accompanying experiment.
2.3. Statistical Treatment of Output

2.3.1. Statistical Indices

For an arbitrary value \( \Theta \), Wilks (2011) defines the mean and the standard deviation as

\[
\bar{\Theta} = \frac{1}{n} \sum_{i=1}^{n} \Theta_i \quad (2.57)
\]

\[
\sigma_{\Theta} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\Theta_i - \bar{\Theta})^2} . \quad (2.58)
\]

With these some statistical indices, namely the relative difference (RD), the fractional bias (FB), the normalized mean square error (NMSE), the correlation coefficient (CORR), the root mean square error (RMSE) and the so called fraction of two (F2)

\[
\text{RD} = \frac{1}{n} \sum_{i=1}^{n} \left( \left| \frac{c_{o,i} - c_{s,i}}{c_{s,i}} \right| \right) \quad (2.59)
\]

\[
\text{FB} = \frac{2(c_{o} - c_{s})}{c_{o} + c_{s}} \quad (2.60)
\]

\[
\text{NMSE} = \frac{1}{c_{o}c_{s}n} \sum_{i=1}^{n} (c_{o,i} - c_{s,i})^2 \quad (2.61)
\]

\[
\text{CORR} = \frac{1}{\sigma_{c_{o}}\sigma_{c_{s}}} \sum_{i=1}^{n} (c_{o,i} - \bar{c}_{o})(c_{s,i} - \bar{c}_{s}) \quad (2.62)
\]

\[
\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (c_{o,i} - c_{s,i})^2} \quad (2.63)
\]

\[
\text{F2} = \frac{1}{n} \sum_{i=1}^{n} \begin{cases} 
1 & \text{if } 0.5 \leq \frac{c_{s,i}}{c_{o,i}} \leq 2 \\
0 & \text{else}
\end{cases} \quad (2.64)
\]

can be calculated (Rotach 1997a; Warner et al. 2004a; Wellens 2002). Hereby \( c_{o} \) is the observed concentration, \( c_{s} \) the simulated concentration and \( n \) the number of sampler units.

Warner et al. (2004b) developed the so called “measure of effectiveness” (MOE), another statistical index to compare model output with reality. It is used to describe the accuracy of the model. In contrast to other statistical indices that seek to do so (e.g. NMSE) it can describe under- and over-prediction separately, because it is two-dimensional. To calculate the concentration-based

\[
\text{MOE} = \left( 1 - \frac{c_{\text{FN}}}{c_{\text{OB}}} , 1 - \frac{c_{\text{FP}}}{c_{\text{PR}}} \right) , \quad (2.65)
\]

the “area” of overlap \( c_{\text{OB}} \), “area” of false positive \( c_{\text{FP}} \), “area” of false negative \( c_{\text{FN}} \) and the “area” of prediction \( c_{\text{PR}} \) is used. The “areas” are — for the concentration-based MOE — not areas per se, but concentration sums that are calculated using two vectors \( c_{o} \) and \( c_{s} \).
and the number of samplers $n$ such that

$$c_{FN} = \sum_{i=1}^{n} \max (c_{o,i} - \min (c_{o,i}, c_{s,i}), 0),$$

$$c_{FP} = \sum_{i=1}^{n} \max (c_{i,i} - \min (c_{o,i}, c_{s,i}), 0),$$

$$c_{OB} = \sum_{i=1}^{n} c_{o,i} \quad \text{and} \quad c_{PR} = \sum_{i=1}^{n} c_{s,i}.$$ 

Both dimensions of the MOE (2.65) range between zero and unity, unity characterizing perfect agreement and zero no agreement between measurement and simulation. The first dimension of the MOE describes the decreasing rate of false negatives (less underprediction) and the second dimension the decreasing rate of false positives (less overprediction) (Warner et al. 2004b).

The usefulness of the MOE is laid out in detail by Warner et al. (2004b). When comparing two models A and B, higher values in both dimensions of A mean A is better than B, at least for this specific statistic. If only the first dimension of A is higher (lower) than B while the second is lower (higher), A has a lower rate of under- (over-)prediction, but a higher rate of over- (under-)prediction than B. Lower values in both dimensions of A mean that A is worse than B.

### 2.3.2. Blocked moment bootstrap

Since the scattered nature of the measurements and the heterogeneity of an urban area make sampling errors highly likely and a confidence range for the statistical indices is desired, a resampling approach will be used. Hanna (1989) compares several different resampling methods for air quality modeling evaluation, which were previously described by Tukey (1987). Here the “bootstrap” will be used, since the computing time advantages of the jackknife are no longer relevant with modern computers.

The bootstrap method does not only calculate one value for each statistical index (e.g. NMSE), but a distribution of values. Following Tukey (1987), bootstrapping is realized by drawing a random sample with replacement from the original data set. Thereby the magnitude of the data set is not changed. Consequently it is possible and likely that some data points appear multiple times and others not at all. Afterwards the desired statistical index is calculated from this new data set and stored. Then a new random sample is drawn and the process is repeated for a large number of times.

Hanna (1989) investigated repeats of 10, 100 and 1000 times and found that a larger number of repeats leads to better results. This is generally true, see for example Efron and Tibshirani (1994). As the computing power has increased since, this study will repeat the process 50 000 times.

One problem of bootstrapping as described above — called “seductive bootstrap” —
is that it can sample data sets that have an unrealistic representations of the original data set if that set has distinct groups. For example, imagine a data set consisting of two days of tracer experiments where on one day the source output was ten times as high as on the second day. A fully random approach could draw samples where all data points are from only one day. To alleviate this, Hanna (1989) proposes the so-called “blocked” bootstrap, where the random resampling is forced to draw proportionally from each “block”. Consequently each new data set has the same number of data points from each block as the original data set. In this case each day of experiments is a block, since the days differ in source output, meteorological conditions and choice of measurement positions (see Section 2.1).

The bootstrap method can only work on functional statistics, that means statistics that only depend on the distribution of the sample, not the sample number or order (Efron and Tibshirani 1994). Fortunately, this is true for all the statistical indices listed above.

The output of a bootstrap is a a large number — in this case 50 000 — of the chosen statistic (e.g. NMSE). To analyze this distribution, the mean and the standard deviation are calculated using (2.57) and (2.58) respectively. Following the suggestion of Hanna (1989), the standard deviation is corrected for small sample size $m$ (of the observation-simulation pairs) by multiplying it with $\sqrt{m/(m-1)}$.

From these values a confidence interval of the statistical index is calculated via the Studentized method, which is suggested in Hanna (1989) under the name “moment bootstrap” and earlier by Efron, summarized in Efron and Tibshirani (1994). Thereby a Student-t distribution of the bootstrapped statistic $\theta$ is assumed, which is not always necessarily true. Skewed and multimodal distributions are possible and influence the correctness of this method. The 95% confidence interval is given by:

$$[\bar{\theta} - t_{95}\sigma_\theta; \bar{\theta} + t_{95}\sigma_\theta],$$

(2.66)

where $\bar{\theta}$ is the mean of the statistic $\theta$ and $\sigma_\theta$ is the standard deviation of $\theta$, as described above. The value of $t_{95}$ is the usual Student-t value, depending on degrees of freedom $m - 1$. For $m \rightarrow \infty$, $t_{95}$ approaches 1.96, the Gaussian distribution value.

To reduce the impact of skewed or multimodal distribution of the bootstrapped statistic, the significance of the difference between two distributions (for example the same data from two different model versions) is not estimated by directly comparing the confidence intervals (2.66). Instead, following Hanna (1989) and a similar approach by Irwin (2001), the difference of the statistic is bootstrapped instead. Given model versions A and B, a bootstrap sample is drawn with replacement, the statistics $\theta_A$ and $\theta_B$ (e.g. NMSE) calculated and $\theta_A - \theta_B$ is stored. Then the procedure is repeated 50 000 times, resulting in a distribution of differences. If the two model versions are identical, each difference would be exactly zero. If the 95% confidence interval of the difference between two statistics include zero, the two statistics are not significantly different. If the interval does not
2.3 Statistical Treatment of Output

Figure 2.5.: (a) Comparison between two bootstrap distributions of the first MOE dimension of two different model runs and (b) the bootstrapped difference of the first MOE dimension between the two model runs.

contain zero, they are.

This method is powerful, because it can distinguish between two distributions of bootstrapped statistics that have highly overlapping confidence intervals. Figure 2.5 shows an extreme example. Details of the specific model options will be explained in Section 3.4 but are not important for now, because the following statements are true for any functional statistic and any two different model versions.

Important is that the two distributions of the first MOE dimension in Figure 2.5(a) appear to be highly similar. They are so similar that their means differ only in the second digit after the comma. However, the first run is shifted to the right for all cases, so a purely visual inspection of the distribution invites the conclusion that they are different. Since the bootstrap procedure was repeated for 50 000 times, it is unlikely that this shift is caused by the bootstrap itself.

When looking at the bootstrapped difference between the two first dimension of the MOE of the two runs in Figure 2.5(b), the distribution only contains zero at the very right tail end. Because this tail end is outside the 95% confidence interval, the difference between the two statistics of the runs is significant, even though their means are almost equal.

The success of the method is based on the fact that the difference calculation is undertaken on the same bootstrap sample and thus has the same data set. This means that a difference in the statistic of this bootstrap sample is caused by the change in the model only. Since the procedure is repeated for many different bootstrap samples, the sampling error of the measurement-simulation pair is still being treated the same way as in the bootstrap method without difference.
2.4. Minor Model Modifications

So far the existing model and some auxiliary things have been described. The following section lists the proposed modifications, which were motivated in Section 1.4.

2.4.1. Pseudo-random number generation

The quality of its random numbers is an important part of any stochastic simulation, since a too small degree of randomness will influence the outcome. It is impractical and slow to use true random numbers (e.g. from a hardware source), therefore a series of so called pseudo-random number generators (PRNGs) is being used. Due to the nature of computers, the numbers thus calculated are deterministic, but if a good procedure is used still statistically indistinguishable from true random numbers.

Up to now there was not enough space in publications to treat this topic, even though it is important. Additionally the original model used ran1 and ran2 of Press et al. (1992), but advances in computing power and research into pseudo-random number generation have made them outdated.

Therefore the procedure chosen here is mzran and some variants, which combine a linear congruential generator with a generator that uses subtraction (Marsaglia and Zaman 1994). The resulting integer numbers are transformed into uniformly distributed numbers in (0; 1) as suggested by Marsaglia and Zaman (1994). While not having a long period ($10^{28}$) for modern standards, the procedures are computationally fast and produce good random numbers (Vattulainen 1999).

According to Ripley (1987) the amount of random numbers that can safely be extracted from a good PRNG with period $p$ is proportional to $\sqrt{p}/200$. Since the model needs about ten times the number of particles (per instance of PRNG and time step) and $\sqrt{10^{28}/200}$ is in the order of $10^{12}$, it is possible to run out of good random numbers with these fast PRNGs if a high number of particles or time steps is chosen. To alleviate this problem the PRNGs are reseeded when needed by accessing /dev/urandom on UNIX-like systems or, if that is not possible, by a hashed date and time string with millisecond resolution.

The Wiener increment (Section 2.2.1) requires random numbers with a normal (Gaussian) distribution of mean zero and standard deviation $d_t$. This is achieved by generating Gaussian distributed random numbers of mean zero and unity standard deviation and multiplying with $d_t$ in a later step. The Gaussian distributed random numbers are produced with the Ziggurat algorithm (Marsaglia and Tsang 2000), which is a fast method to transform uniformly distributed random numbers to Gaussian distributed ones. It was slightly modified to use two different PRNGs to choose the rectangle and provide the sample, as suggested in Thomas et al. (2007).

Changing the PRNGs must by definition not affect the characteristics of the model output, because the pseudo-random numbers generated are supposed to be random and
the noise in the model output has to be smaller than the signal. Hence this modification should not change anything. Nevertheless, in Section 3.2 the reproducibility of the results is analyzed. On the one hand to prove that the new PRNGs are implemented correctly and on the other hand to find out how many particles are required to “cancel” out randomness to a sufficient amount, as described in Section 2.2.6.

2.4.2. Corrected derivative of velocity auto-covariance in roughness sublayer

In the model code of Rotach et al. (2004), the formula for the derivative of the three velocity auto-covariances \( \frac{\partial u_i^2}{\partial z} \) in the RS is incorrect. To summarize from the earlier (2.45):

\[
\overline{u_i^2} = \overline{u_{IS,i}^2} - k u_i (z^* - z)
\]

and therefore its derivative has to be \( \frac{\partial \overline{u_i^2}}{\partial z} = k u_i \). However, they use \( \frac{\partial \overline{u_i^2}}{\partial z} = k u_i z \) instead.

As a result, their velocity auto-covariance derivatives are not constant below \( z^* \), as they should be when the function is linear. Additionally there is a small error in the old source code, which results in \( \frac{\partial \overline{v_i^2}}{\partial z} \) being defined twice and \( \frac{\partial \overline{u_i^2}}{\partial z} \) not at all. The latter thereby usually (depending on the compiler and its options) defaults to zero.

One might think that the \( \frac{\partial \overline{u_i^2}}{\partial z} \) do not appear in the model formulas, with the exceptions of the time step criterion in (2.49) and \( \frac{\partial \overline{w^2}}{\partial z} \) in \( \Phi_g^w \) (2.24b). However, for the sake of brevity some derivatives that are required in other equations are neither explicitly listed in this thesis nor the previous works and the \( \frac{\partial \overline{u_i^2}}{\partial z} \) appear there. Those derivatives are straightforward to obtain, so their omission poses no problem.

From now on these corrections will be called ACDC (Auto-Covariance Derivative Correction) and their influence investigated in Section 3.1.

2.4.3. Corrections suggested by Gibson and Sailor (2012)

Gibson and Sailor (2012) introduce some corrections to the model of Rotach et al. (1996), although most of them did not require the code to be changed.

The first correction in their order is the so called “Gaussian Streamwise Turbulence”-correction (Gibson and Sailor 2012), where they derive that the original publication Rotach et al. (1996) was missing the power of two in the enumerator in (2.26c). As mentioned before, this was already correct in the model code since at least 1998 and will not be discussed further.

The “Convective Streamwise Probability Current”-correction is the second one proposed by Gibson and Sailor (2012). They claim that there is a mistake in the formulation of \( \hat{u} \) (their version being (2.22)) in Rotach et al. (1996), namely a \((1 - \rho^2)\)-term missing in the denominator. However, this is not correct, since the original version of Rotach et al.
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(1996) in their notation is

$$\hat{u} = \frac{1}{\sqrt{2}} (V_{11}^{-1})^{1/2} \left( u' - w \frac{\rho \sigma_u}{\sigma_w} \right) , \tag{2.67}$$

where

$$V = \begin{pmatrix} \sigma_{uuG} & \sigma_{vuG} & \sigma_{wuG} \\ \sigma_{wuG} & \sigma_{vuG} & \sigma_{wuG} \\ \sigma_{wuG} & \sigma_{vuG} & \sigma_{wuG} \end{pmatrix} = \begin{pmatrix} \sigma_{uuG}^2 & 0 & \sigma_{wuG}^2 \\ 0 & \sigma_{wwG}^2 & 0 \\ \sigma_{wuG}^2 & 0 & \sigma_{wuG}^2 \end{pmatrix} ,$$

is the covariance matrix of the velocity components. Under the assumption that \( v \) is independent of \( u \) and \( w \), every covariance of \( v \) — excluding the autocovariance — is zero. Thus the inverse covariance matrix is

$$V^{-1} = \frac{1}{\sigma_{uuG}^2 \sigma_{wwG}^2 - \sigma_{uuG}^2 \sigma_{wwG}^2} \begin{pmatrix} \sigma_{uuG}^2 \sigma_{wwG}^2 & 0 & -\sigma_{uwG} \sigma_{wuG}^2 \\ 0 & \sigma_{wwG}^2 - \sigma_{wuG}^2 & 0 \\ -\sigma_{uwG} \sigma_{wuG}^2 & 0 & \sigma_{wuG}^2 \sigma_{wwG}^2 \end{pmatrix} .$$

Therefore the \((1,1)\) matrix element of the inverse covariance matrix

$$V_{11}^{-1} = \frac{\sigma_{wwG}^2}{\sigma_{uuG}^2 \sigma_{wwG}^2 - \sigma_{uuG}^2 \sigma_{wwG}^2} = \frac{1}{\sigma_{uuG}^2 \left( 1 - \frac{\sigma_{uwG}^2}{\sigma_{uuG}^2 \sigma_{wwG}^2} \right)} = \frac{1}{\sigma_{uuG}^2 \left( 1 - \rho^2 \right)} ,$$

and with this \((2.67)\) is evidently equal to

$$\hat{u} = \frac{1}{\sqrt{2(1 - \rho^2)} \sigma_{uuG}} \left( u' - w \frac{\rho \sigma_u}{\sigma_w} \right) ,$$

a reproduction of \((2.22)\) for easier comparison. In conclusion, the expression for \( \hat{u} \) of Gibson and Sailor (2012) is correct, but the earlier expression of Rotach et al. (1996) is correct too and no modification to the model is necessary.

The third correction, named “Solenoidal Probability Current” (Gibson and Sailor 2012), addresses unit inconsistencies by changing \((2.25)\) to

$$\Phi_a^* = -\frac{\partial f}{\partial z} \left[ \frac{\exp \left( -\gamma w^2 \right)}{2\sqrt{2\pi} \sigma_{wwG}} \right] w \left[ \text{erf} \left( \beta_1 u' \right) + 1 \right] \tag{2.68a}$$

$$\Phi_w^* = -\frac{\partial f}{\partial z} \left[ \frac{\exp \left( -\gamma w^2 \right)}{2\sqrt{2\pi} \gamma \sigma_{wwG}} \right] \exp \left( -\beta_2^2 u'^2 \right) , \tag{2.68b}$$

with

$$\beta_1 = \frac{1}{2 \sigma_{wwG}} \tag{2.68c}$$

and

$$\beta_2 = \frac{2}{\beta_1} \tag{2.68d}$$

instead. This correction does solve the unit inconsistency in the older version and will be called Gibson-Sailor-Correction (GSC) from now on. However, it violates the requirement of a divergence free \( \Phi_i^* \) in \((2.9)\), which is explained in Section 2.2.1, and can therefore not be correct.

This violation can be solved by changing the numerator of \( \beta_2 \) to 1 instead, which means
2.4 Minor Model Modifications

\[ \Phi_u^* = -\frac{\partial f}{\partial z} \left[ \frac{\exp (-\gamma w^2)}{2\sqrt{2\pi} \sigma_w} \right] w \left[ \text{erf} \left( \frac{u'}{2\sigma_q} \right) + 1 \right] \] (2.69a)

\[ \Phi_w^* = -\frac{\partial f}{\partial z} \left[ \frac{\exp (-\gamma w^2)}{4\sqrt{2\pi} \gamma \sigma_w \sigma_u G} \right] \exp \left( -\frac{w^2}{4\sigma_u^2} \right), \] (2.69b)

which will be called corrected Gibson-Sailor-Correction (cGSC) from now on.

It is easy to show that (2.69) is divergence free, because using it we get

\[ \frac{\partial \Phi_u^*}{\partial u} = -\frac{\partial f}{\partial z} \left[ \frac{\exp (-\gamma w^2)}{2\sqrt{2\pi} \sigma_w} \right] w \left[ \left( \frac{2}{\sqrt{\pi}} \right) \exp \left( -\frac{u'^2}{4\sigma_q^2} \right) \left( \frac{1}{2\sigma_q} \right) \right] \]

\[ \frac{\partial \Phi_w^*}{\partial w} = -\frac{\partial f}{\partial z} \left[ \frac{\exp (-\gamma w^2)}{4\sqrt{2\pi} \gamma \sigma_w \sigma_u G} \right] (-2\gamma w) \exp \left( -\frac{w^2}{4\sigma_u^2} \right) \]

Since \( \Phi_u^* = \frac{\partial \Phi_u^*}{\partial u} = 0 \) and \( \frac{\partial \Phi_u^*}{\partial w} \) is identical to \( \frac{\partial \Phi_u^*}{\partial w} \) with opposite sign,

\[ \frac{\partial \Phi_u^*}{\partial u} + \frac{\partial \Phi_u^*}{\partial v} + \frac{\partial \Phi_u^*}{\partial w} = 0, \]

as is required in (2.9).

Substituting \( \Phi_i^* \) in (2.20), using either the original version (2.25), cGSC (2.69), or GSC (2.68), leads to \( \Phi_i \) approaching zero as required (see Section 2.2.1) for \( |u| \to \infty \).

Since there is no uniquely true solution for \( \Phi_i^* \) (see Section 2.2.1), both the original version (2.25) and cGSC — not GSC — can be considered correct. Due to the original version (2.25) having unit inconsistencies and GSC (2.68) being truer to the mathematical roots of the expression (Gibson and Sailor 2012), we feel that (2.69) is the best candidate for \( \Phi_i^* \). Section 3.5 shows the influence on the numerical results and Section 3.2.4 proves that GSC is problematic because the divergence violates the well mixed criterion.

### 2.4.4. Dissipation rate parameterization in Roughness Sublayer

In the IS the original \( \varepsilon \)-parameterization (2.41) is still used as described earlier. Conversely, in the RS (upper boundary \( z_* \)) a generalized logit function

\[ \frac{kH \varepsilon}{u_{dIS}^3} = b_1 + \frac{b_2 - b_1}{b_3 + \exp \left( -b_5 \left( \frac{z_{AGL}}{H} - b_4 \right) \right)} \] (2.70)

is fitted to an average profile obtained from observations in Basel (Christen 2005). Note that not the dissipation rate, but a nondimensional dissipation rate is fitted for easier comparison with data from other cities. For the same reason the nondimensional height above ground \( z_{AGL}/H \) is used as well. \( b_1 = 0.7002 \), \( b_2 = 2.3691 \), \( b_3 = 1.7575 \), \( b_4 = 0.8689 \), \( b_5 = 22.4671 \) are the fitting parameters for Basel and the result is displayed in Figure 2.6.

The dissipation rate in Basel was calculated using the so called “inertial dissipation
Figure 2.6.: Nondimensional dissipation rate depending on nondimensional height for one year of BUBBLE (+) and four half-days of Oklahoma (○) measurements with corresponding fits (solid (2.70), dashed (2.71))

As a control and a sensitivity test the data from the Joint Urban 2003 experiment in Oklahoma City (Allwine and Flaherty 2006) is also used to find a new $\varepsilon$-parameterization in the RS. The dissipation rate profiles are taken from Lundquist and Chan (2007), who used the same method as Christen (2005), the inertial dissipation method, to obtain $\varepsilon$-values, described by Piper and Lundquist (2004). Lundquist and Chan (2007) list four different profiles, each for one period of measurements. There are two periods during the day and two during the night. Consequently, the amount of data and thus the representativity of the resulting profile is lower than the profile based on BUBBLE data. Additionally the buildings around the Oklahoma site are higher (about 35 m) and more spread out than the ones in Basel and Lundquist and Chan (2007) describe the dissipation rate as “very high” on all four measurement days. Nevertheless, an exponential profile

$$\frac{kH\varepsilon}{u_{4IS}^3} = a_1 \exp \left( a_2 \frac{z_{AGL}}{H} \right) + a_3$$ (2.71)

is fitted and optionally used by the model in the RS. Note that the average building height $H$ is 35 m (the Oklahoma value) when calculating the fitting parameters, but 15.1 m (the Basel value) when used in the model to calculate $\varepsilon$ and also in Figure 2.6. The fitting parameters are $a_1 = 1.0417$, $a_2 = -2.5473$ and $a_3 = 2.6564$.

Evidently the Oklahoma nondimensional dissipation rate is larger than the one in Basel, although whether the difference is due to the differing average building heights, the little
2.5 Parameterization of drift inside street canyon

An $\varepsilon$-profile has to be continuous in all points. Therefore it is necessary to either force the RS-parameterization to have the same value of $\varepsilon(z_*)$ as the IS-parameterization or the other way around. Since the model is built to simulate pollutant dispersion at the street level, it is presumably more important to have “correct” values closer to the ground. Thus the IS-parameterization (2.41) is scaled via a simple factor to agree with the RS-parameterization in height $z_*$. This procedure is similar to the scaling of the velocity variances in Rotach et al. (2004).

Unfortunately, the piecewise $\varepsilon$-parameterization is not continuously differentiable at height $z_*$ where the IS parameterization and the RS parameterization meet. This might present a problem, because when a particle crosses this region it experiences a sudden change in the value of its $\partial\varepsilon/\partial z$. However, the time step criterion (see Section 2.2.6) is implemented to catch, among others, this very problem. Therefore the problem is circumvented, although at the price of a possible increase in computing time due to a reduced time step.

The influence of the two proposed $\varepsilon$-parameterizations in the RS and the therefore necessary shift in the IS are described in Section 3.6.

2.5. Parameterization of drift inside street canyon

Section 2.2.6 describes how the original model reflects particles at the bottom. Strong assumptions have to be made, for instance the street canyon is always assumed to be perpendicular to the flow and the vortex always forms. Therefore particles are never transported within the street canyon, which is presumably wrong.

However, calculating how far and in which direction a particle is transported by effects within street canyons cannot be done deterministically, because the model does not contain topography and is horizontally homogeneous, in contrast to urban areas in reality. Therefore a statistical approach is necessary, in which only the average flow field influences the particle transport in the UCL. See Section 1.3 for further discussion on this.

Even though the modified model is supposed to improve the parameterization of trajectories in the UCL, some assumptions still have to be made. The first assumption is that a particle that reaches the model bottom does not enter the “correct” virtual street canyon for its touchdown position. This is not possible, because the model does not contain information about the street layout in reality. Instead a street canyon is randomly chosen from a street distribution (see 2.1).

Furthermore, all canyon end effects are ignored. This means that a virtual model canyon

amount of data from Oklahoma or a differing city geometry is unclear. Likely the answer is all of the above. Additionally, the two profiles have a different shape and derivative. This indicates that even a nondimensional $\varepsilon$-profile like the above is not generally representative for every urban area.
is endless and a particle that enters it never meets any side streets or intersections, where more complex flow structures would form (see Section 1.3.3).

Additionally the model does neither include any information about time of day nor about sun angle. Therefore the only information about convection stems from $w_*$ and $L$. This makes it currently impossible to include the thermal effects of differential canyon wall heating, as described in Section 1.3.3.

Another factor that would influence the flow structure in a street canyon is local topography. This includes different wall heights of the lee and windward wall and the shape of the roofs on either side. Section 1.3.3 lists examples of how large these influences can be. Due to the model not containing any non-statistical information about topography, this factor has to be neglected.

Section 1.3.3 also mentions that traffic can influence the flow through a street canyon. Since there is no street map in the model and additionally no traffic data for the BUBBLE, this influence also cannot be described.

Even more assumptions are needed, but those are assumptions about how the flow structure looks like instead of what effects cannot be included. Those will be described in detail in the following.

Fortunately the virtual model bottom coincides well with the top of the vortex under skimming flow (see Section 1.3). Therefore the model bottom is assumed to equal the interface between the RS and the UCL. When a particle reaches the bottom of the modified model a street is randomly chosen from a list of streets. The street data can be estimated from maps (see Section 2.1) and consists of a list of directions for each street type with corresponding frequencies of occurrence.

For instance, an area consisting of a grid of perfectly square blocks in north-south and east-west direction would have two street types ($0^\circ$ and $90^\circ$) with the corresponding frequencies of 0.5 each. In the real world such data is more complex and it will be shown later (see Section 3.7.1) how the choice of street types effects the outcome.

This canyon direction is chosen for each particle and occurrence of trapping individually. Then the incidence angle between the mean wind direction and the canyon is calculated to get the displacement from the effects inside the canyon.

As proposed by Yamartino and Wiegand (1986) the horizontal wind at roof level is mapped to one component along and one component across the main canyon axis. In spite of their use of a transverse wind component ($\sqrt{u^2 + w^2}$) for the cross canyon wind, the vertical component will be neglected for simplicity. Yamartino and Wiegand (1986) also found that the linear coefficient between the along canyon component at roof level and inside the street depends on the azimuth of the approaching flow. This influence will also be ignored. The magnitude of the components depends on the incidence angle and are calculated as follows.
2.5 Parameterization of drift inside street canyon

2.5.1. Along canyon wind parameterization

The average wind speed along the canyon axis $u_a$ can be calculated by integrating (1.1) over the height of the canyon and dividing by the average building height $H$:

$$\bar{u}_a = \frac{1}{H} \int_0^H u(z) \, dz = \frac{\bar{u}_H}{H} \left( H + z_0 - \frac{H}{\ln(\frac{H+z_0}{z_0})} \right).$$

If the values for Basel are used ($H = 15.1$ m and $z_0 = 1$ m) then

$$\bar{u}_a = 0.71 \bar{u}_H.$$

Similar, if the profile of Jackson (1978) (1.2) is averaged and calculated for the BUBBLE circumstances, it leads to

$$\bar{u}_a = 0.85 \bar{u}_H.$$

The third profile (1.3) after Nicholson (1975) can also be averaged to yield

$$\bar{u}_a = 0.73 \bar{u}_H.$$

The obvious flaws in using the three profiles listed above in calculating the mean wind speed (see Section 1.3 for limitations) inside the canyon are somewhat lessened by the consistent outcome of a linear relationship and the similarity of the slopes to the measurements of Nakamura and Oke (1988).

Thus, the mean wind speed $u_a$ inside the canyon, along the main canyon axis, is proportional to the roof level ($z_h$) wind speed and modified by the incidence angle $\alpha_{inc}$ between main canyon axis and mean wind speed such that

$$\bar{u}_a = p_a \bar{u}_H \cos (\alpha_{inc}) \quad (2.72)$$

$\alpha_{inc}$ is defined as always acute and $p_a$ is a proportionality constant that is estimated above to be about 0.8 for Basel.

$p_a$ is unlikely to be less than zero, because that would mean that a flow parallel to the street would reverse direction inside the canyon. Equally unlikely is a near zero positive value, which would mean that the flow is decelerated to near zero inside the canyon. Therefore the smallest physically useful value is assumed to be 0.1.

The largest physically useful value is probably less than unity, although this is not as clear as the smallest value. Due to the gap flow mechanism, it is not inconceivable that the flow would speed up inside the canyon, although no reference to such a case was found. To take note of this, a largest physically useful value of 1.4 was chosen arbitrarily. The influence of this factor will be discussed in Section 3.7.2.
2.5.2. Cross canyon wind parameterization

Similar to the along canyon wind component, the cross canyon wind component $\bar{u}_c$ depends linearly on the roof level wind speed and the incidence angle

$$\bar{u}_c = p_c u(z_h) \sin(\alpha_{inc}).$$  \hspace{1cm} (2.73)

The value of $p_c$ is estimated to be 0.4, see Section 1.3

Since the model at hand does not include thermal effects, the vortex reversal described in Section 1.3 cannot be simulated. Parallel and low wind speed cases, where no vortex forms, will be described without $\bar{u}_c$. Consequently these cases are not taken into account for the calculation of $\bar{u}_c$. Thus $p_c$ is assumed to be positive and nonzero, with a smallest physically useful value of 0.1. No reference to a vortex speeding up faster than the ambient wind speed without thermal involvement was found, thus the largest physically useful value of $p_c$ is assumed to be 0.9.

2.5.3. Residence time

The residence time $\tau$ of a particle trapped in a canyon is estimated as

$$\tau = \frac{2H}{\bar{u}_c} \text{ if } \alpha_{inc} > 30^\circ \text{ and } \bar{u}_c > 1.5 \text{ m s}^{-1}$$  \hspace{1cm} (2.74a)

$$\tau = \frac{2d}{w} \text{ else},$$  \hspace{1cm} (2.74b)

which is simply distance traveled over speed and similar to (2.48). If a vortex forms because the wind speed is high enough (see Section 1.3), the residence time $\tau$ is calculated via (2.74a). Section 2.2.6 justifies the distance of $2H$.

If no vortex forms, (2.74b) is used instead. This happens when either the incidence angle is small ($\alpha_{inc} \leq 30^\circ$) or the roof top velocity is low ($\bar{u}_H \leq 1.5$ m s$^{-1}$). Consequently the residence time depends on the vertical velocity of the individual particle and the zero plane displacement.

As described in Section 1.3.4 it is possible that a particle circulates more than once before it exits the street canyon in perpendicular and oblique cases. To mimic this behavior the residence time of each particle in such a trapping incidence is randomly multiplied by a natural number. The chance that a particle exits the canyon is equal to the chance that it pierces the shear layer on top of the canyon, which is explained in Section 2.2.6 and was chosen to be 0.66 by Rotach et al. (2004).

The hard thresholds of $\bar{u}_c > 1.5$ m s$^{-1}$ and $\alpha_{inc} > 30^\circ$ for the formation of the vortex are certainly not universally true. They should depend on local geometry, but no pertaining literature to this topic could be found.
2.5.4. Drift calculation

The drift of a trapped particle is assumed to be only along the main canyon axis, meaning that no displacement of the particle perpendicular to the canyon takes place. This is justified by the circular motion in orthogonal and oblique cases, the small cross canyon wind component in almost parallel cases and the small canyon width in general.

Since the coordinate system is wind following, there is a displacement in x and y-direction, depending on the angle between the mean wind direction and the canyon direction. The x-displacement is simply added every time step to the x-coordinate of the trapped particle, until it is “released” from the canyon after time $\tau$:

$$x = x + u_a d t \cos (\alpha_{\text{inc}}). \quad (2.75)$$

Because the sign of the displacement in y-direction depends on the absolute angles, a second angle

$$\alpha_a = (\alpha_{\text{wd}} - \alpha_{\text{street}} + 360^\circ) \mod 360^\circ \quad (2.76)$$

is defined, where $\alpha_{\text{wd}}$ is the mean wind direction and $\alpha_{\text{street}}$ the street direction. Then the sign of the y-displacement depends on the quadrant of $\alpha_a$ such that

$$y = \begin{cases} 
  y + u_a d t \sin (\alpha_{\text{inc}}) & \text{if } 0^\circ \leq \alpha_a \leq 90^\circ \text{ or } 180^\circ \leq \alpha_a \leq 270^\circ \\
  y - u_a d t \sin (\alpha_{\text{inc}}) & \text{if } 90^\circ < \alpha_a < 180^\circ \text{ or } 270^\circ < \alpha_a < 360^\circ 
\end{cases} \quad (2.77)$$

After a particle was trapped for the duration $\tau$, it is released back into the model. Thereby all states of the particle are retained from the time step before the trapping incident, except for the vertical velocity $w$, which has its sign inverted and the height $z$, which is set to $z_0 + 1$. Following Rotach et al. (2004), the sign of the longitudinal velocity perturbation $u'$ is not inverted after the trapping, which violates the well mixed criterion. However, it is still inverted for direct reflection at either boundary. The influence of this omission is investigated in Section 3.2.4.
3. Results and discussion

First, this chapter treats the correction of the velocity auto-covariance derivative (see Section 3.1). Second, some model assumptions are verified (Section 3.2). Third a look at the comparison data and the original model results is taken in Section 3.3, before all the proposed changes to the model are investigated. These are in order: the calibration of the transition function in Section 3.4, the Gibson-Sailor-Correction in Section 3.5, the dissipation rate RS-parameterization in Section 3.6 and the drift parameterization at the lower boundary in Section 3.7.

3.1. Corrected derivative of velocity auto-covariance in roughness sublayer

The velocity auto-covariance derivative correction (ACDC) is investigated before anything else, because it corrects an error in the original source code (see Section 2.4.2), not just proposes an alternative.

Figure 3.1 shows how severe the ACDC impacts the dispersion. Both the crosswind integrated concentration in panel (a) and the arc-maximum in panel (b) become about three times larger. The lateral dispersion however is not affected at all. This can be explained because $\frac{\partial u'^2}{\partial z}$ is never actually needed in the model, as opposed to $\frac{\partial u'^2}{\partial z}$ and $\frac{\partial u'^2}{\partial z}$.

The general trend of increased concentration continues in Figure 3.2, where the three-hour averaged experiments 1, 2 and 3 are compared to measurements. At all sampler positions the concentration is higher after ACDC, which is also reflected in the statistics, listed in Table 3.1. This time the data set consists of all thirty minute averages of experiment 1 and 2. The RD, FB and RMSE are significantly worse with ACDC, as is the second dimension of the MOE, which indicates more overprediction. Consequently, the first dimension of the MOE is significantly better, since this describes the underprediction. Also the NMSE and the F2 are better with ACDC, although insignificantly so. The CORR is worse with ACDC, but the difference is insignificantly different from zero.

All in all the correction decreases the agreement of simulated to measured concentration. Since the original version is demonstrably wrong, the correction in the velocity auto-covariance derivative $\frac{\partial u'^2}{\partial z}$ will still be used from now on.
Results and discussion

Figure 3.1.: (a) Crosswind integrated concentration \((2.55)\), (b) maximum concentration along each arc, (c) spread of the concentration along the arc \((2.56)\) for the experiment 1, three-hour average; Comparison between a model with the original version of \(\partial u_i^2 / \partial z\) and the corrected one (ACDC, see 2.4.2).

Table 3.1.: Listed are the bootstrapped means (see Section 2.3.2) of statistical indices (Section 2.3.1) that relate BUBBLE measurements to corresponding model output once using the original \(\partial u_i^2 / \partial z\) and once using the corrected version (see Section 2.4.2), for three-hour averaged values of experiments 1 and 2. Bold values are the best in their column, dark gray background color symbolizes the base version that all other versions are compared to and light gray background means that there is a significant difference (95% confidence) between this value and the base value. The bottom row lists the mean standard deviation (over all versions) of each bootstrapped statistic for reference.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>original</td>
<td>1.18</td>
<td>0.02</td>
<td>2.31</td>
<td>0.50</td>
<td>79.10</td>
<td>0.32</td>
<td>(0.59, 0.60)</td>
</tr>
<tr>
<td>ACDC</td>
<td>1.65</td>
<td>-0.26</td>
<td>2.21</td>
<td>0.50</td>
<td>89.70</td>
<td>0.33</td>
<td>(0.67, 0.51)</td>
</tr>
<tr>
<td>mean (\sigma_{\text{STAT}})</td>
<td>0.27</td>
<td>0.12</td>
<td>0.47</td>
<td>0.06</td>
<td>11.50</td>
<td>0.04</td>
<td>(0.05, 0.04)</td>
</tr>
</tbody>
</table>
3.1 Corrected derivative of velocity auto-covariance in roughness sublayer

Figure 3.2.: Model output, once using the original version of $\partial \overline{u^2} / \partial z$ and once the corrected one (see 2.4.2), compared to corresponding BUBBLE measurements for experiments 1, 2 and 3, three-hour averages. Perfect measurements and a perfect model would align on the first meridian (solid line).
3.2. Model verification

This section checks whether some assumptions are fulfilled by the model, before further inquiries can be taken.

3.2.1. Time step

As described in Section 2.2.6, the choice of time step is generally not arbitrary for a Lagrangian model. It has to be small enough to avoid problems related to the stiffness of the underlying Langevin equation. However, in this particular model, a time step criterion (2.49) is supposed to reduce the time step if the default one is too large for a particular velocity in a particular region.

A test was performed to evaluate the criterion in this regard. If everything works as it should, the choice of time step may not influence the outcome. A too large default time step would simply be reduced in all cases, not just in “problematic” ones.

Figure 3.3 shows the results of this test and as can easily been seen the model performs as expected. Computation time for the run with $dt = 0.1\, \text{s}$ is about four times longer than the run with $dt = 1\, \text{s}$, while the run with $dt = 10\, \text{s}$ is not much shorter. Therefore the

![Figure 3.3](image_url)

**Figure 3.3.** As Figure 3.1, for three identical model runs each with a different default time step $dt = 0.1\, \text{s}, 1\, \text{s}$ and $10\, \text{s}$. 
3.2 Model verification

Figure 3.4.: Experiment 1 through 4, three-hour average, four identical runs, but different random numbers (number of particles is 500 000); The top panel shows the spread (maximum value subtracted by minimum value) of the four runs for each simulated measurement related to the mean simulated concentration (+), representing the random noise of the model. Also in the top panel are the absolute differences between the model mean and the measurements related to the model mean (●), representing the signal. The bottom panel shows the signal to noise ratio (SNR) related to the mean modeled concentration (∗).

default choice of $dt = 1$ s that will be used in all subsequent simulations appears to be justified.

3.2.2. Reproducibility of random results

Due to the random nature of the model (see Section 2.4.1), two simulations with identical input and options do not produce identical output. Therefore it is necessary to use a large enough number of particles so that the intended signal is larger than the random noise (see Section 2.2.6). A strict definition of “large enough” is not trivial and outside of the scope of this work. De Haan (1999) uses 500 000 particles as a “perfect” reference when testing the influence of particle numbers on the kernel method.

Figure 3.4 shows a comparison between four identical runs with 500 000 particles. For each run meteorological input and concentration, measurements used to compare with model output are averaged over three hours. At the top of Figure 3.4 the concentration spread of the four runs is plotted against the concentration mean of the four runs, evaluated at each BUBBLE measurement position. Additionally the absolute difference between the model mean concentration and the corresponding BUBBLE measurement is shown. The latter is thereby generally much larger, indicating that the intended signal — the
difference to measurements — is larger than noise — the spread between the four identical model runs. This observation is quantified in the bottom panel of Figure 3.4 via the signal to noise ratio

\[
\text{SNR} = 10 \log_{10} \left( \frac{\text{signal}}{\text{noise}} \right)
\]

that relates the signal to the noise. It is almost everywhere over 5 dB, except for three measurements, where the model’s predictions are so close to the measurements that the spread of the model runs is in the same order. The spread is about as large as the difference between mean and measurement, thereby resulting in a SNR of close to zero. Since the minimal detection threshold of the measurement is (see Section 2.1) 5 ng m\(^{-3}\), the fact that the SNR is bad for this case will be ignored.

De Haan (1999) used 50 000 as highest non-reference number of particles. Therefore in Figure 3.5 the same procedure as above is repeated with 50 000 particles. Evidently the characteristics of the distribution are similar, only lower. Most of the values are still over 5 dB and the simulations run roughly ten time faster. However, examining the results via the bootstrap method described in Section 2.3.2 shows several significantly different statistics for identical runs with 50 000 particles (not shown). Consequently, 50 000 particles are not enough to yield significant results at the 95% level, because the random noise is too large.

To find a better number of particles, first the model with 500 000 particles is used as a reference. There the bootstrap method does not find significant differences between identical runs. Afterwards lower and lower numbers of particles are tried. It should be
3.2 Model verification

Table 3.2.: As Table 3.1, only for six identical model runs using thirty minute averaged input data from experiments 1 and 2 with 200 000 particles.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>run one</td>
<td>1.39</td>
<td>-0.04</td>
<td>2.65</td>
<td>0.48</td>
<td>87.40</td>
<td>0.29</td>
<td>(0.58, 0.56)</td>
</tr>
<tr>
<td>run two</td>
<td>1.38</td>
<td>-0.04</td>
<td>2.66</td>
<td>0.48</td>
<td>87.73</td>
<td>0.29</td>
<td>(0.58, 0.55)</td>
</tr>
<tr>
<td>run three</td>
<td>1.38</td>
<td>-0.04</td>
<td>2.66</td>
<td>0.48</td>
<td>87.75</td>
<td>0.29</td>
<td>(0.58, 0.55)</td>
</tr>
<tr>
<td>run four</td>
<td>1.38</td>
<td>-0.04</td>
<td>2.63</td>
<td>0.48</td>
<td>87.26</td>
<td>0.30</td>
<td>(0.58, 0.56)</td>
</tr>
<tr>
<td>run five</td>
<td>1.37</td>
<td>-0.04</td>
<td>2.64</td>
<td>0.48</td>
<td>87.37</td>
<td>0.29</td>
<td>(0.58, 0.56)</td>
</tr>
<tr>
<td>run six</td>
<td>1.38</td>
<td>-0.04</td>
<td>2.62</td>
<td>0.48</td>
<td>87.22</td>
<td>0.30</td>
<td>(0.58, 0.56)</td>
</tr>
<tr>
<td>mean σ&lt;sub&gt;STAT&lt;/sub&gt;</td>
<td>0.31</td>
<td>0.13</td>
<td>0.51</td>
<td>0.07</td>
<td>11.78</td>
<td>0.04</td>
<td>(0.05, 0.05)</td>
</tr>
</tbody>
</table>

It is noted that the above method is not robust, because only a limited number of test cases can be simulated. Specific test runs can by random chance appear to have no significantly differences, even though other test runs with this number of particles may.

This subjective testing reveals that about 150 000 particles are the threshold between significant differences and no significant differences at the 95% level. Therefore the number of particles is chosen as 200 000 and this will be used from here on.

Table 3.2 lists the results of the procedure for six identical runs with 200 000 particles. If the random effects of the model would cancel completely, all values in columns would be equal. As it is, the statistical indices do not agree completely, but no significant differences are detected. Those cells would be shaded in light gray.

The number of particles \( n = 200000 \) is larger than previously used for this model, which further mitigates the subjectivity of the above test.

3.2.3. Solid ceiling

Another assumption that the model makes is a solid ceiling (see Section 2.2.6). If the solid ceiling is removed and replaced with a ceiling that permits transport from the PBL to the free atmosphere (but not in the other direction), the concentration at the bottom has to decrease. To test this, the entrainment at the now semipermeable ceiling has a chance of 20% to let a particle go out of the model. Once a particle is in the free atmosphere it is “lost” to the model and is not treated anymore from this point on, neither its trajectory, nor its kernel when calculating the concentration.

As can be seen in Figure 3.6, the difference between the solid and the semipermeable ceiling is negligible. Thus the assumption of a solid ceiling used by this and similar models is valid.
Results and discussion

Figure 3.6: As Figure 3.1, comparison between a run with a solid ceiling (default for this model) and a run where the ceiling allows 20% transport of particles that reach the PBL-free atmosphere interface from below. Those particles are lost and additionally there is no transport from the free atmosphere down.

3.2.4. Well mixed criterion

The well-mixed criterion after Thomson (1987) (see Section 1.2) requires uniformly distributed particles to stay uniformly distributed. This can be easily tested by starting the model with particles equidistantly placed between the model bottom and top with vertical velocity zero. Then the model runs for a certain period (in this case one hour) and afterwards the distribution of the particles is analyzed. Since the model is only vertical (see Section 1.2), the lateral and longitudinal positions do not matter in this context. Unfortunately, this inhibits the use of the kernel method and therefore a simple version of the box counting method is employed instead. Thereby the normalized concentration is calculated by counting the number of particles in a certain height range (five meters wide) and dividing by the ideal distribution, which is number of particles (500 000 in this case) divided by number of height ranges. The result is the normalized concentration for each height interval, which is unity at the start and should stay unity for any amount of time.

Figure 3.7 shows the influence of the calibration of the transition function $f$ to BUBBLE measurements (see Section 2.2.4) on the well-mixed condition. In panel (a) the $f$-calibration is turned off and the model is otherwise in its original state, except for the correction
3.2 Model verification

Figure 3.7.: Test of the well-mixed criterion for runs with the residence time approach (see Section 2.2.6) of Rotach et al. (1996) and different settings: (a) no Gibson-Sailor-Correction (GSC, see Section 2.4.3), no calibration of \( f \) to BUBBLE data (see Section 2.2.4), (b) no GSC, but with \( f \)-calibration and (c) corrected GSC, with \( f \)-calibration; Plotted is the normalized concentration of particles in a given height (bin size 5 m) after one hour of simulation, which would ideally be unity everywhere.

of the velocity auto-covariance derivatives. The test run is undertaken with three-hour averaged meteorological input of experiment 1 for on hour of simulation.

Notable in Figure 3.7(a) is that the normalized concentration is close to unity over the full model height domain, from \( z = z_0 = 1 \) to \( z_i = 1809 \) meters, except below the model bottom at \( z < 0 \). There the trapped particles are not distributed by random and Eulerian motion of the model but fixed at \(-d/2\), the presumed middle of the street canyon. Thus the concentration is not required to be unity and the spikes around \( z = 1 \) meter are expected, because the concentration is zero between 1 and \(-d/2\) meter. Additionally, due to some particles being trapped below the model bottom, the normalized concentration is expected to be slightly less than unity inside the model bounds. This effect is too small to see in the figures however and will be neglected from now on. Consequently, the well-mixed criterion does not appear to be violated in Figure 3.7(a), except for random variations caused by the small height intervals. However, these are to be expected and unavoidable because the high vertical resolution is required later. Note that this is only a rough, visual assessment of how much the well-mixed criterion is fulfilled. Since there is no known reflective boundary condition that complies totally and provably with the well-mixed criterion (Thomson and Montgomery 1994), any such visual inspection can only be superficial. This means that the model will always violate the criterion, but — if
Figure 3.8.: As Figure 3.7, original residence time approach and no \( f \)-calibration for different versions of \( \Phi_i^* \): (a) original formulation, (b) with the Gibson-Sailor-Correction (GSC) and (c) with the corrected GSC (cGSC), see Section 2.4.3;

done correctly — only in a small region or a with small effect.

In Figure 3.7(b) the model options are identical to (a), only the \( f \)-calibration is turned on. There is presumably no difference in the quality of the agreement to the well-mixed criterion compared to (a). This indicates that the original formulation of \( \Phi_i^* \) of Rotach et al. (1996) is indifferent or at least not sensitive to the shape of the transition function \( f \), as it should be.

When using the corrected Gibson-Sailor-Correction (see Section 2.4.3) and the \( f \)-calibration in Figure 3.7(c), there is a small, but still noticeable and not random, reduction of the concentration below roughly 50 m. This is exactly the region where the calibrated \( f \) diverges from the original \( f \) (see Section 2.2.4).

This behavior is investigated further in Figure 3.8, where the \( f \)-calibration is turned off (see Section 3.4 on why it is turned off). As mentioned in Section 2.4.3, the correction of Gibson and Sailor (2012) (GSC) to the \( \Phi_i^* \) of Rotach et al. (1996) has a mistake. The well-mixed test for the original version, the Gibson-Sailor version and the corrected Gibson-Sailor version are displayed in Figure 3.8(a),(b) and (c). This implies a good agreement of the model with the well-mixed criterion, for the original formulation of \( \Phi_i^* \) (a) and the corrected Gibson-Sailor-Correction (c, see Section 2.4.3). The GSC however shows an up to 40% reduction of the normalized concentration in the layer between the ground \((z = 1 \text{ m})\) and a height of about 50 meter. Consequently the GSC violates the well-mixed criterion regardless of the transition function \( f \), which is not surprising given it
3.2 Model verification

Figure 3.9: As Figure 3.7, for runs with cGSC, no \( f \)-calibration and different boundary conditions at the bottom: (a) full reflection at the bottom, (b) residence time approach and (c) drift;

should be divergence free, but is not (Section 2.4.3).

The cGSC on the other hand appears to comply with the well-mixed criterion when the \( f \)-calibration is turned off in Figure 3.8(c), but not when the \( f \)-calibration is turned on in Figure 3.7(c). The reason for this is most likely the influence of \( f \) on \( \sigma_{uG}^2 \) in (2.26c), which is used in \( \Phi^*_i \) with GSC (2.68) and cGSC (2.69), but not in the original version (2.25). Since the calibrated \( f \) is not continuously differentiable, the resulting \( \Phi^*_i \) is not either.

Figure 3.9 pictures the well-mixed test for three different boundary conditions at the model bottom, now using cGSC and no \( f \)-calibration. The first panel (a) shows the height distribution after a simulation with perfect reflection at the bottom, the second panel (b) the residence time approach of Rotach et al. (2004) (see Section 2.2.6) and the third panel (c) the drift approach proposed in this thesis (see Section 2.5).

Notable in Figure 3.9 is that the normalized concentration is close to unity for all three boundary conditions over the full model height domain. While panel (b) and (c) show the aforementioned spike around \( z = 0 \), where the concentration becomes zero below \( z = 1 \) and not equal to zero at \( z = -d/2 \), panel (a) does not. This is easily explained by missing trapping due to immediate reflection.

While earlier it is mentioned that not negating the longitudinal velocity perturbation after a trapping incident (see sections 2.2.6 and 2.5) violates the well-mixed criterion, the effect is too small to be visible in Figure 3.9.
3.3. Model validation and data set

In this section the general model performance shall be investigated and its relation to the BUBBLE data set assessed.

Earlier (Section 2.2.6), the importance of a steady state of the BUBBLE tracer data is already hinted at. In reality a perfect steady state is unlikely, therefore it is important to know by how much reality deviates from it. One way to investigate this assumption lies in the wind direction, which is already described in Section 2.1, accompanied by Figure 2.1. From there we can conclude that the first five half hours of experiment 1 and experiment 2 are likely to comply better with the steady state assumption than the other periods. Especially experiment 4 with its almost steady turning of the wind direction seems likely to pose problems.

Another way to look at the steady state assumption is with the perturbations of the concentration measurements of each sampler and experiment. This data is not displayed in this thesis for brevity, but can be found in Gryning et al. (2005). However, the calculation of the accuracy with a given averaging period in (2.2) already contains all necessary information. Thus it is possible to conclude from Table 2.2 that experiments 4 and especially 3 are less steady than experiments 1 and 2.

To confirm this hypothesis, all thirty minute averaged data sets are simulated and compared to the measurements. The resulting statistics are listed in Table 3.3. Noteworthy is the fact that the source output was different for each day, see Table 2.4. Therefore the RMSE can not be easily compared between different days, while all other statistics are independent of the absolute concentration. Additionally, the statistics in Table 3.3 are not bootstrapped, so one has to be careful when comparing their values. They are only intended to create a rough overview over model simulations of the whole data set.

As expected, the last half hour of experiment 1 seems worse in most statistics than earlier runs of experiment 1, with the exception of the fractional bias. The model seems to be able to simulate the other runs of experiment 1 with good agreement to the measurements, with 101 being the worst. When averaging the data over three hours, the statistics look good, which means that the turning of the wind direction during 106 does not influence the mean steady state too badly. Indicated by the negative FB and the first dimension of MOE being larger than the second, the day is overall overpredicted.

The statistics of all six experiment 2 runs averaged over thirty minutes appear to be similar to each other and generally good, relative to the other values. The first and the last are the worst in most statistical indices. If averaging over thirty minutes, the overall picture is similar to experiment 1, only slightly worse. Generally the concentration values are overpredicted.

Most likely influenced by the unsteady wind direction, all six runs of experiment 3, with the exception of 305, have bad statistics. The RMSE is not as bad as it looks at first glance,
3.3 Model validation and data set

Table 3.3.: Statistics (not bootstrapped) for all thirty minute averaged runs at the top and all three-hour averaged runs at the bottom; simulations with the original model state, except for ACDC (see Section 2.4.2); For the definition of relative difference (RD), fractional bias (FB), normalized mean square error (NMSE), correlation coefficient (CORR), root mean square error (RMSE), fraction of two (F2) and measure of effectiveness (MOE), see Section 2.3.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE (ng m(^{-3}))</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>101</td>
<td>1.96</td>
<td>−1.25</td>
<td>5.77</td>
<td>0.77</td>
<td>86.14</td>
<td>0.50</td>
<td>(0.99, 0.23)</td>
</tr>
<tr>
<td>102</td>
<td>1.88</td>
<td>−0.91</td>
<td>2.07</td>
<td>0.83</td>
<td>76.90</td>
<td>0.36</td>
<td>(0.97, 0.36)</td>
</tr>
<tr>
<td>103</td>
<td>0.61</td>
<td>0.00</td>
<td>0.64</td>
<td>0.81</td>
<td>24.04</td>
<td>0.43</td>
<td>(0.70, 0.69)</td>
</tr>
<tr>
<td>104</td>
<td>0.44</td>
<td>0.33</td>
<td>0.30</td>
<td>0.81</td>
<td>19.92</td>
<td><strong>0.71</strong></td>
<td>(0.65, 0.91)</td>
</tr>
<tr>
<td>105</td>
<td>0.59</td>
<td>0.78</td>
<td>1.06</td>
<td>−0.08</td>
<td>26.50</td>
<td>0.36</td>
<td>(0.41, 0.94)</td>
</tr>
<tr>
<td>106</td>
<td>4.47</td>
<td>−0.37</td>
<td>16.48</td>
<td>−0.43</td>
<td>96.88</td>
<td>0.00</td>
<td>(0.07, 0.05)</td>
</tr>
<tr>
<td>201</td>
<td>3.63</td>
<td>−0.74</td>
<td>1.60</td>
<td>0.55</td>
<td>69.25</td>
<td>0.27</td>
<td>(0.86, 0.39)</td>
</tr>
<tr>
<td>202</td>
<td>0.79</td>
<td>−0.42</td>
<td>0.61</td>
<td>0.78</td>
<td>51.94</td>
<td>0.29</td>
<td>(0.93, 0.61)</td>
</tr>
<tr>
<td>203</td>
<td>1.38</td>
<td>−0.60</td>
<td>2.11</td>
<td>0.42</td>
<td>155.73</td>
<td>0.07</td>
<td>(0.67, 0.36)</td>
</tr>
<tr>
<td>204</td>
<td>1.92</td>
<td>−0.53</td>
<td>1.03</td>
<td>0.91</td>
<td>49.06</td>
<td>0.14</td>
<td>(0.98, 0.57)</td>
</tr>
<tr>
<td>205</td>
<td>0.91</td>
<td>−0.32</td>
<td>0.50</td>
<td>0.79</td>
<td>67.89</td>
<td>0.43</td>
<td>(0.93, 0.67)</td>
</tr>
<tr>
<td>206</td>
<td>1.77</td>
<td>0.72</td>
<td>2.73</td>
<td>0.79</td>
<td>184.40</td>
<td>0.36</td>
<td>(0.36, 0.77)</td>
</tr>
<tr>
<td>301</td>
<td>2.29</td>
<td>−1.45</td>
<td>77.44</td>
<td>0.64</td>
<td>882.67</td>
<td>0.00</td>
<td>(0.40, 0.06)</td>
</tr>
<tr>
<td>302</td>
<td>6.04</td>
<td>−1.20</td>
<td>7.29</td>
<td>0.11</td>
<td>424.13</td>
<td>0.00</td>
<td>(0.53, 0.13)</td>
</tr>
<tr>
<td>303</td>
<td>7.61</td>
<td>−1.34</td>
<td>9.57</td>
<td>0.66</td>
<td>212.46</td>
<td>0.23</td>
<td>(0.97, 0.19)</td>
</tr>
<tr>
<td>304</td>
<td>5.39</td>
<td>−1.10</td>
<td>4.46</td>
<td>0.68</td>
<td>219.61</td>
<td>0.31</td>
<td>(1.00, 0.29)</td>
</tr>
<tr>
<td>305</td>
<td>0.87</td>
<td>−0.54</td>
<td>0.75</td>
<td><strong>0.96</strong></td>
<td>560.49</td>
<td>0.50</td>
<td>(0.95, 0.54)</td>
</tr>
<tr>
<td>306</td>
<td>9.50</td>
<td>−0.49</td>
<td>7.10</td>
<td>−0.18</td>
<td>710.16</td>
<td>0.15</td>
<td>(0.35, 0.21)</td>
</tr>
<tr>
<td>401</td>
<td>0.82</td>
<td>1.41</td>
<td>4.35</td>
<td>0.06</td>
<td>73.76</td>
<td>0.07</td>
<td>(0.17, 1.00)</td>
</tr>
<tr>
<td>402</td>
<td><strong>0.40</strong></td>
<td>0.40</td>
<td><strong>0.28</strong></td>
<td>0.89</td>
<td>66.20</td>
<td>0.64</td>
<td>(0.67, 1.00)</td>
</tr>
<tr>
<td>403</td>
<td>0.91</td>
<td>0.44</td>
<td>2.33</td>
<td>0.56</td>
<td>137.69</td>
<td>0.14</td>
<td>(0.38, 0.59)</td>
</tr>
<tr>
<td>404</td>
<td>1.02</td>
<td>0.08</td>
<td>2.16</td>
<td>0.72</td>
<td>156.02</td>
<td>0.08</td>
<td>(0.47, 0.51)</td>
</tr>
<tr>
<td>405</td>
<td>1.98</td>
<td>−0.12</td>
<td>7.45</td>
<td>−0.01</td>
<td>136.73</td>
<td>0.00</td>
<td>(0.18, 0.16)</td>
</tr>
<tr>
<td>406</td>
<td>0.68</td>
<td>0.79</td>
<td>2.77</td>
<td>0.60</td>
<td><strong>11.06</strong></td>
<td>0.09</td>
<td>(0.27, 0.63)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE (ng m(^{-3}))</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><strong>0.53</strong></td>
<td><strong>−0.33</strong></td>
<td>0.52</td>
<td>0.94</td>
<td><strong>25.93</strong></td>
<td><strong>0.93</strong></td>
<td>(0.90, 0.65)</td>
</tr>
<tr>
<td>2</td>
<td>1.04</td>
<td>−0.44</td>
<td><strong>0.50</strong></td>
<td>0.85</td>
<td>66.40</td>
<td>0.57</td>
<td>(0.95, 0.61)</td>
</tr>
<tr>
<td>3</td>
<td>1.07</td>
<td>−0.61</td>
<td>0.63</td>
<td><strong>0.96</strong></td>
<td>160.26</td>
<td>0.54</td>
<td>(1.00, 0.53)</td>
</tr>
<tr>
<td>4</td>
<td>1.45</td>
<td>−0.68</td>
<td>1.65</td>
<td>0.48</td>
<td>152.40</td>
<td>0.38</td>
<td>(0.85, 0.42)</td>
</tr>
</tbody>
</table>

because the source output is about six times higher compared to experiment 1 and 2. However, when averaged over three hours the fluctuating wind direction seems to average out and the steady state model appears to agree well with the averaged measurements, comparable to experiment 2. The concentration values are overpredicted on average.

With the exception of 401 and 405, the simulations agree well with the measurements for
Results and discussion

Figure 3.10: Ground-concentration field (shaded) at the bottom with simulated concentration at sampler position (x) and measured concentration (thick circle) at the correct z-value. The dashed line and the thin circle show the position of each sampler in the x-y-plane. The thick line represents the difference between measured and simulated concentration: thick circle on top means underprediction, thick circle at the bottom means overprediction; Simulations use the three-hour averaged experiments 1, 2, 3 and 4 at top left, top right, bottom left and bottom right, respectively; experiment 4 for thirty minute averaged data. When looking at the three-hour averaged data however, the statistics are worse than for the other three days. This is most likely induced by the already mentioned shifting wind direction. Overall the day is overpredicted.

Figure 3.10 shows an overview over the four three-hour averaged simulations. At the bottom of each panel the simulated concentration along the arcs (see Section 2.2.7) at a height of one meter is shaded in gray. The plume pattern is visible in all four cases, with low concentrations at lateral outer edges on days 2 and 4, when compared to days 1 and 3. This is caused by a higher overall wind speed during experiments 2 and 4. In the simulation of day 3 the overall concentration appears to be higher, which is consistent with a higher source output (see Table 2.4).
Figure 3.11.: Concentration during experiment 1, three-hour averaged, two arcs in (a) ca. 650 m and (b) ca. 1000 m distance from source; (c) displays a number of samplers that roughly form a center line inside the plume. Plotted are measurements (solid) and the model predictions (dashed). The first arc consists of sampler positions 2, 3, 4 and 5, the second arc is formed by samplers positions 6, 7, 8, 9, 10 and 11, while sampler positions 1, 3, 9 and 12 make up the center line (see Table 2.1).

Furthermore Figure 3.10 shows all 14 sampler positions and concentrations for all cases, although missing data may reduce the number. Thereby the position of each sampler is symbolized by a small, thin circle at the bottom, which is linked by a thin dashed line to the simulated concentration at that specific sampler, symbolized by an x. Linked to this x is a thick line which ends at a thick circle, the concentration measurement at this sampler. The magnitude of the concentrations can be obtained from the logarithmic third axis. Therefore a longer thick line means a higher discrepancy between simulated and observed concentration. If the thick circle is at the bottom of the thick line, the simulation overpredicts and vice-versa.

Figures 3.11, 3.12, 3.13 and 3.14 show similar quantities as Figure 3.10. There the simulated and observed concentration values at the sampler positions are sorted into two arcs and a center line for each day, following the approach of Rotach et al. (2004). To assess the approximation thereby necessary — the positions do not form perfect arcs and lines — see the captions of figures 3.11, 3.12, 3.13 and 3.14 for the individual positions and compare with the map in Figure 2.2. Note that position 3 (“Sperrstrasse”-tower, see Figure 2.2) has measurements in three different height levels (compare Table 2.1), which means that this position shows three measurement and three simulation values, although the latter are too close together to be distinguishable.

Experiment 1 appears to overpredict close to the source and transitions to underprediction the further the samplers are away from the source in Figure 3.10, panel one, and
Results and discussion

Figure 3.12: Concentration during experiment 2, three-hour averaged, two arcs in (a) ca. 500 m and (b) ca. 1200 m distance from source; (c) displays a number of samplers that roughly form a center line inside the plume. Plotted are measurements (solid) and the model predictions (dashed). The first arc consists of sampler positions 1, 3, 7 and 8, the second arc is formed by samplers positions 5, 10 and 12, while sampler positions 3, 10, 11 and 15 make up the center line (see Table 2.1).

Figure 3.11(c), with the threshold being at about 1000 m from the source. According to Figure 3.11(a) and (b), this does not appear to be caused by too high lateral dispersion, since the cross sections of the plume appear to have similar shape along the arcs.

Panel two of Figure 3.10 indicates an overprediction along the plume center line in the three-hour average of experiment 2, because all samplers roughly along the plume center line report lower concentrations than the simulation. This is also clearly visible in Figure 3.12(c) and may be caused by too little vertical or lateral dispersion. Figure 3.12(b) shows that the model predictions at both ends of this arc roughly agree with the measurements, however the center is overpredicted. This points to underestimation of vertical dispersion. The first arc in Figure 3.12(a) partly supports this, since the physical left (positive y-values) side of the arc is near zero in both observation and simulation, while concentrations around the center from −200 m to 200 m are roughly the same, even though the negative side is under- and the positive side over-predicted by about 25%.

During experiment 3, at least when averaging over three hours, the shape of the simulation is similar to that of the observation, only the values are overpredicted. This is visible in the third panel of Figure 3.10 and Figure 3.13. The latter figure also seems to indicate an error in the wind direction, because the peak of the measurements is shifted to the right.

Panel four in Figure 3.10 strongly underpredicts at negative y-positions and strongly overpredicts at the plume center for the three-hour mean of experiment 4. This indicates
that the averaged wind direction is not representative for case 4, most likely caused by the monotonous drift during the experiment. Figure 3.14(a) and (b) support this, because there seems to be a lateral shift of the position of the plume maximum along both arcs. Since the simulated plume center line does not appear to line up with plume center line in reality, the samplers along the center line in Figure 3.14(c) are all overpredicted. This is all consistent with a turning of the wind direction.

As predicted earlier from the time series of the wind direction and the sampling uncertainty of the concentration measurements, the model performance is worse when the situation is not stationary in reality. Therefore, from now on experiments on day 4 will be left out of the analyses, since the day does not appear to be stationary enough. Similarly, data from day 3 will be discarded when treating thirty minute averages, since the high variability of the wind direction also causes a non-steady state. Because averaging over three hours improves this, day 3 data will still be considered for three-hour averages.

Figures with sampler data will show results from model simulations with three-hour averaged data from now on, for the simple reason that higher temporal resolutions lead so many data points that there is hardly anything visible. For calculated statistics — mostly in tables — results from runs with thirty minute averaged values will be shown. Mainly because the number of simulation-observation pairs are six times higher and the statistics therefore more powerful. One has to be careful though, because there is no sixfold increase in sample size, due to the three-hour averaged data being an average.

Figure 3.13.: Concentration during experiment 3, three-hour averaged, two arcs in (a) ca. 650 m and (b) ca. 1000 m distance from source; (c) displays a number of samplers that roughly form a center line inside the plume. Plotted are measurements (solid) and the model predictions (dashed). The first arc consists of sampler positions 2, 3, and 4, the second arc is formed by samplers positions 6, 7, 8, 9, 10 and 11, while sampler positions 1, 3, 9 and 12 make up the center line (see Table 2.1)
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Figure 3.14.: Concentration during experiment 4, three-hour averaged, two arcs in (a) ca. 650 m and (b) ca. 1000 m distance from source; (c) displays a number of samplers that roughly form a center line inside the plume. Plotted are measurements (solid) and the model predictions (dashed). The first arc consists of sampler positions 2, 3, 4 and 5, the second arc is formed by samplers positions 6, 7, 8, 9, 10 and 11, while sampler positions 1,3,9 and 12 make up the center line (see Table 2.1).

Table 3.4.: As Table 3.1, only for model output using the recirculation approach of Rotach et al. (2004) or immediate reflection at the model bottom, for thirty minutes averaged values of experiments 1 and 2.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>recirculation</td>
<td>1.65</td>
<td>-0.27</td>
<td>2.21</td>
<td>0.50</td>
<td>89.67</td>
<td>0.33</td>
<td>(0.67, 0.51)</td>
</tr>
<tr>
<td>reflection</td>
<td>1.57</td>
<td>-0.21</td>
<td>2.21</td>
<td>0.49</td>
<td>86.90</td>
<td>0.32</td>
<td>(0.65, 0.53)</td>
</tr>
<tr>
<td>mean σSTAT</td>
<td>0.32</td>
<td>0.12</td>
<td>0.38</td>
<td>0.06</td>
<td>10.62</td>
<td>0.04</td>
<td>(0.05, 0.04)</td>
</tr>
</tbody>
</table>

An attempt to replicate Figure 15 of Rotach et al. (2004) is pictured in Figure 3.15, with the model in its original state, only with the ACDC (see Section 2.4.2) applied. Some small changes — measured instead of estimated $z_i$, slightly more rigorous discarding of averaged measurements where many are missing — still might affect the outcome however. Therefore deviations are expected and present, notably the general characteristics are different. A general shift to higher concentration predictions is explained by the ACDC (see Section 3.1), but Rotach et al. (2004) found that for each experiment the spread of lower concentration values is higher than that of higher values. This does no longer appear to be the case in Figure 3.15, although the exact reason for this could not be found and the exact same plot as Figure 15 of Rotach et al. (2004) could not be replicated.
Unfortunately, one of the results of Rotach et al. (2004) could not be replicated, due to the ACDC. The result is the fact that the recirculation-boundary condition (see Section 2.2.6) improves the agreement of the model simulated concentration values to the measured ones, which does no longer appear to be true. Table 3.4 shows how immediate reflection at the bottom gives better or almost equal statistics for thirty minute averaged experiments 1 and 2. The RD, FB, RMSE and second MOE dimension are significantly better, while the CORR and the first MOE dimension are significantly worse. The table in Rotach et al. (2004) that is the base for their result mentions “experiment no. 1” as the underlying data, unfortunately without clarifying the averaging period. Regardless, all three possible averaging periods for experiment 1 lead to the same conclusion as Table 3.4 does for a larger number of measurements, namely that the recirculation approach appears to be worse than simple reflection. When the ACDC is turned off, the recirculation approach leads to slightly better model performance than reflection (not shown).
This is unfortunate, because it means that this hypothesis of Rotach et al. (2004) about the model deficiencies, on which part of this thesis is based, were obscured by the model error (see Section 2.4.2) and are therefore erroneous. Nevertheless, the influence of drift on the boundary condition will still be investigated.

### 3.4. Calibration of transition function

Since the recirculation approach does no longer appear to improve the simulation, the $f$-calibration to BUBBLE data (as described in Section 2.2.4) shall too be re-investigated. Section 3.2.4 showed how problematic this can be when combined with the corrected Gibson-Sailor-Correction.

Figure 3.16 shows a comparison of the simulated and observed concentrations at sampler sites during the three-hour averaged experiments 1, 2 and 3. It indicates that at the

**Figure 3.16:** As Figure 3.2, only for models with and once without calibration of the transition function $f$ (see Section 2.2.4) compared to corresponding BUBBLE measurement for experiments 1, 2 and 3, three-hour averages.
## Table 3.5: As Table 3.1, with and without calibration of the transition function \( f \) to BUBBLE measurement (see Section 2.2.4) for all thirty minute averaged experiments of days 1 and 2.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>( f )-calibration</td>
<td>1.65</td>
<td>−0.26</td>
<td>2.22</td>
<td>0.50</td>
<td>89.66</td>
<td>0.33</td>
<td>(0.67, 0.51)</td>
</tr>
<tr>
<td>no ( f )-calibration</td>
<td>1.64</td>
<td>−0.24</td>
<td>2.22</td>
<td>0.50</td>
<td>88.79</td>
<td>0.34</td>
<td>(0.66, 0.52)</td>
</tr>
<tr>
<td>mean ( \sigma_{\text{STAT}} )</td>
<td>0.33</td>
<td>0.12</td>
<td>0.37</td>
<td>0.06</td>
<td>10.53</td>
<td>0.04</td>
<td>(0.05, 0.04)</td>
</tr>
</tbody>
</table>

The majority of the sampler sites the simulated concentrations are lower without the \( f \)-calibration. Consequently, almost all statistics in Table 3.5 are insignificantly improved by turning the \( f \)-calibration off, because the experiments are generally overpredicted (see Section 3.3). In detail the FB and the second MOE dimension are significantly better, while the first MOE dimension is significantly worse. All other statistics are either equal or insignificantly better. The first dimension of the MOE is the extreme case mentioned earlier (Section 2.3.2), where there is a significant difference between the two model version, even though the means differ only in the second digit after the comma and the standard deviation is 0.05. Altogether the difference between the models with and without \( f \)-calibration is not large and mostly insignificant.

### 3.5. Gibson and Sailor (2012)-corrections

Section 3.2.4 shows that the correction of Gibson and Sailor (2012) in \( \Phi^*_i \) (GSC) violates the well-mixed criterion, although this can be corrected (see Section 2.4.3, cGSC). Nevertheless, the influence of GSC and cGSC on the simulated concentration field will be investigated in the following. Since Section 3.2.4 also indicates that the \( f \)-calibration already discussed in Section 3.4 is not compatible with GSC and cGSC, it is turned off in this section.

Figure 3.17 shows a typical example of concentration characteristics, in this case for three-hour averaged experiment 1, although other experiments exhibit the same behavior. In Figure 3.17(a), the crosswind integrated concentration in mg m\(^{-2}\) (2.55) is shown to change its magnitude with the original model the highest and the GSC-model the lowest, but not it’s general shape. The location of the peak is at 50 m for all three model options, although this may be only due to insufficient along-wind resolution. Similarly, the peak of the maximum concentration along each arc in Figure 3.17(b) is highest at a distance of 50 m from the source with the same characteristic as the crosswind integrated concentration: original version highest, similar to the cGSC-model and the GSC-model lower.

Further away from the source, roughly from 100 to 700 m, the crosswind integrated
Figure 3.17.: As Figure 3.1, comparison between the original version of $\Phi_i^*$, the Gibson-Sailor-corrected one (GSC) and the corrected GSC (cGSC) (see 2.4.3) for three-hour averaged experiment 1

concentration is also slightly lower for the cGSC-model and still lower for the model with the GSC, compared to the original version. From about 700 m onwards the three versions can no longer be distinguished from each other in this type of display. The maximum concentration along each arc shows the same behavior, but less clearly. Figure 3.17(c) depicts the lateral spread of the particles, which is highly similar for all three model version over the whole longitudinal range.

The comparison between modeled and observed concentration at the sampler points in Figure 3.18 shows that enabling the GSC in the model generally leads to lower concentrations. Enabling cGSC also leads to lower concentrations, albeit less so than for GSC. It has to be noted that this is not true for all sampler positions, although the outliers are few and no pattern could be found to explain them. Generally the larger concentrations have larger differences between the model versions.

Since the model primarily overpredicts the test cases, this trend of the GSC and the cGSC of leading to lower concentrations improves the statistical agreement to the measured concentrations, which can be seen in Table 3.6. On the one hand the GSC improves the RD, FB, RMSE and second MOE dimension significantly compared to the original version. On the other hand the GSC leads to insignificantly worse NMSE and CORR,
while the first MOE dimension becomes significantly worse. The latter is not surprising, because due to the definition of the MOE its first dimension also becomes smaller when the concentrations do, since it describes the rate of underprediction.

When the model uses the cGSC, the RD, FB, NMSE, CORR, RMSE and the second MOE dimension are improved significantly compared to the original version. The RD, FB, RMSE and second MOE dimension are worse than compared to GSC, but still better than the original model version. This shows that the lower concentrations caused by the cGSC still improve the model performance. As before, this is caused by the general overprediction of the BUBBLE cases.

It was already proven in Section 2.4.3 that the GSC is not correct, so it is clear that it will not be used from now on. The cGSC on the other hand is correct and also meets the well-mixed criterion (Section 3.2.4), but — as mentioned — only when the $f$-calibration (Section 2.2.4) is turned off. Section 3.4 and this section both show that
the specific model change improves the model, although turning off the $f$-calibration only insignificantly. Therefore model performance is better when the $f$-calibration is turned off and the corrected Gibson-Sailor-Correction turned on.

It is interesting that the simulated concentrations are more similar between the models with the cGSC and the original $\Phi^*_i$, compared to the model with the GSC. One could imagine that the inclusion of $\sigma_{uG}$ in both GSC and cGSC, but not the original, could lead to more similarity between the two former, since the difference between them is only a factor of two in one of two dimensions. However, the fact that the concentrations are simulated at the ground likely explains this. Section 3.2.4 proves that the model with GSC underpredicts there, due to a violation of the well-mixed criterion. This further implies that the model might not be as sensitive to changes in $\Phi^*_i$ as Table 3.6 seems to indicate at first glance, at least if the chosen $\Phi^*_i$ is correct.

### 3.6. New parameterization of dissipation rate

To avoid interactions with other model options when looking at the dissipation rate parameterization, the $f$-calibration (Section 2.2.4) and the cGSC (Section 2.4.3) are turned off. The ACDC (Section 2.4.2) is turned on however, since it fixes an error.

Section 2.4.4 describes a new parameterization of the dissipation rate $\varepsilon$ in the roughness sublayer based on BUBBLE measurements. Additionally a parameterization based on data from Joint Urban 2003 in Oklahoma City (see Section 2.4.4) is proposed. Despite the fact that the two parameterizations do neither agree in type of function, nor in magnitude (Figure 2.6), both are used separately for simulations. Using the $\varepsilon$-parameterization based on BUBBLE measurements is intended to test whether a special RS-parameterization of the dissipation rate improves the model. The Oklahoma City one is intended as a basic sensitivity test.

The resulting profiles and their derivatives are shown for one case (experiment 1, three-hour averaged data) in Figure 3.19. Above the height $z_*$, the three $\varepsilon$-profiles on the left

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**Table 3.6.** As Table 3.1, only for different version of $\Phi^*_i$ (see Section 2.4.3); The simulations used are from thirty minute averages of experiment 1 and 2

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>original</td>
<td>1.64</td>
<td>-0.24</td>
<td>2.22</td>
<td>0.50</td>
<td>88.71</td>
<td>0.34</td>
<td>(0.66, 0.52)</td>
</tr>
<tr>
<td>GSC</td>
<td>1.37</td>
<td>-0.08</td>
<td>2.36</td>
<td>0.49</td>
<td>84.51</td>
<td>0.34</td>
<td>(0.62, 0.57)</td>
</tr>
<tr>
<td>cGSC</td>
<td>1.57</td>
<td>-0.20</td>
<td>2.16</td>
<td>0.51</td>
<td>85.89</td>
<td>0.35</td>
<td>(0.66, 0.54)</td>
</tr>
</tbody>
</table>

| mean $\sigma_{STAT}$ | 0.32 | 0.12 | 0.42 | 0.06 | 10.98 | 0.04 | (0.05, 0.04) |
3.6 New parameterization of dissipation rate

Figure 3.19: Three different \( \varepsilon \)-parameterizations described in Section 2.4.4 for experiment 1, three-hour average. On the left side the dimensionless dissipation rates of the model are compared to the BUBBLE-measurements (\( \Diamond \)) and on the right side their vertical gradients are shown.

Panel are identical, only scaled differently by a factor to achieve continuous continuation at \( z_* \). This is obvious, since no other change was made to \( \varepsilon \) above \( z_* \).

Below \( z_* \), they are markedly different in shape, with the Oklahoma City parameterization increasing towards the ground where the other two decrease. Additionally the magnitude of the two newly proposed parameterizations is different, with the BUBBLE parameterization being smaller by a factor of roughly two. For possible reasons for this see Section 2.4.4.

As already mentioned in Section 2.4.4, the vertical gradient of \( \varepsilon \) is not continuous, which can be seen in the right panel of Figure 3.19. This appears to be no problem though, most likely because the time step criterion (see Section 2.2.6) catches the cases where a particle crosses the discontinuity too fast.

Table 3.7 and Figure 3.20 show how the different \( \varepsilon \)-parameterizations affect the simulated concentration at the sampler positions, in comparison to the measured values during BUBBLE. Looking at Figure 3.20, it appears that changing the parameterization of the dissipation rate from the original to the one based on BUBBLE measurements does not influence all sampler positions with the same trend. At some points the BUBBLE-\( \varepsilon \)-parameterization increases and at some points it decreases the sampler concentration. No pattern of which are decreased and which increased can be detected. In contrast, the Oklahoma City-based dissipation rate appears to worsen the agreement to the measurements for most points, often by a larger amount than the difference between the original and the BUBBLE-based one. However, for some points the OC-\( \varepsilon \) improves the agreement, so
Results and discussion

Figure 3.20: As Figure 3.2, model once using the BUBBLE-data based ε-parameterization, once using the Oklahoma City based ε-parameterization and once using the original ε-parameterization; Displayed are three-hour averaged cases 1,2 and 3.

Again no clear trend emerges.

When looking at the statistics of all thirty minutes averaged runs of experiment 1 and 2 in Table 3.7, the model seems to be sensitive to changes in the dissipation rate parameterization. The model with the BUBBLE-based ε has a significantly better FB, but a significantly worse NMSE, RMSE and first MOE dimension compared to the model with the original ε. The other statistics are not significantly different, but are all worse with the BUBBLE-ε. Therefore the new dissipation rate parameterization in the roughness sublayer does not clearly worsen the model agreement, but it seems to.

The model with the Oklahoma City-based dissipation rate on the other hand is certainly worse than the original model in all statistical indices except the first MOE dimension. Significant of those are the RD, FB, RMSE and second MOE dimension.

The effect of the dissipation rate profile shape in the RS seems to be small. This can be illustrated with an arbitrary test case (experiment 1, three-hour averaged data), where
3.6 New parameterization of dissipation rate

Table 3.7: As Table 3.1, only using different dissipation rate parameterizations in the roughness sublayer: the BUBBLE-data based $\varepsilon$, the Oklahoma City based $\varepsilon$ and the original $\varepsilon$ of Rotach et al. (1996), for all thirty minute averaged runs of experiments 1 and 2.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>original $\varepsilon$</td>
<td>1.64</td>
<td>-0.24</td>
<td>2.22</td>
<td>0.50</td>
<td>88.69</td>
<td>0.34</td>
<td>(0.66, 0.52)</td>
</tr>
<tr>
<td>BUBBLE-$\varepsilon$</td>
<td>1.66</td>
<td>-0.20</td>
<td>2.50</td>
<td>0.48</td>
<td>92.36</td>
<td>0.29</td>
<td>(0.63, 0.51)</td>
</tr>
<tr>
<td>OC-$\varepsilon$</td>
<td>2.14</td>
<td>-0.49</td>
<td>3.25</td>
<td>0.47</td>
<td>121.85</td>
<td>0.29</td>
<td>(0.69, 0.42)</td>
</tr>
</tbody>
</table>

mean $\sigma_{STAT}$: 0.38 0.12 0.48 0.06 12.23 0.04 (0.05, 0.04)

Figure 3.21: As Figure 3.1 for experiment 1, three-hour averaged data, comparison between the original model and the model with the two new $\varepsilon$-parameterizations (see 2.4.4)

the effect of the different $\varepsilon$-parameterizations on the plume is shown in Figure 3.21. The crosswind integrated concentration in panel (a) shows no difference at the source and at the peak after 50 m between the three models versions. After the peak, from 100 m source distance onwards, the model with the Oklahoma City-based dissipation rate simulates the highest $c_y$, while model with the BUBBLE-based simulates the lowest concentrations and the original model is in-between. This trend continues, but the differences become smaller.
Table 3.8: As Table 3.1, only using different dissipation rate parameterizations in the roughness sublayer: the BUBBLE-data based $\varepsilon$, the Oklahoma City based $\varepsilon$ (scaled to the BUBBLE based at $z_*$) and the original $\varepsilon$ of Rotach et al. (1996) (scaled to the BUBBLE based at $z_*$), for all thirty minute averaged runs of experiments 1 and 2.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>BUBBLE-$\varepsilon$</td>
<td>1.66</td>
<td>-0.20</td>
<td>2.50</td>
<td>0.48</td>
<td>92.30</td>
<td>0.29</td>
<td>(0.63, 0.51)</td>
</tr>
<tr>
<td>original $\varepsilon$ (BS)</td>
<td>1.65</td>
<td>-0.20</td>
<td><strong>2.47</strong></td>
<td><strong>0.49</strong></td>
<td>91.76</td>
<td><strong>0.30</strong></td>
<td>(0.63, 0.51)</td>
</tr>
<tr>
<td>OC-$\varepsilon$ (BS)</td>
<td><strong>1.64</strong></td>
<td><strong>-0.19</strong></td>
<td>2.49</td>
<td>0.48</td>
<td><strong>91.59</strong></td>
<td><strong>0.30</strong></td>
<td>(0.63, 0.52)</td>
</tr>
<tr>
<td>mean $\sigma_{\text{STAT}}$</td>
<td>0.36</td>
<td>0.12</td>
<td>0.42</td>
<td>0.06</td>
<td>10.99</td>
<td>0.04</td>
<td>(0.05, 0.04)</td>
</tr>
</tbody>
</table>

and become invisible from about 1400 m on.

The same characteristic is also visible in the maximum concentration along the arcs in Figure 3.21(b), although less pronounced. There the differences vanish already at about 500 m.

Lateral spread of the model with the Oklahoma City-based dissipation rate in Figure 3.21(c) grows slower than the original model with increasing source distance, whereas lateral spread of the model with the BUBBLE-based $\varepsilon$ grows faster than that of the original model.

When comparing the two new $\varepsilon$-parameterizations to the original one, the highly similar behavior of the different graphs in all three panels shows that the shape of the profile does not influence the outcome much, as was hypothesized earlier. The shapes of the original and the BUBBLE $\varepsilon$-parameterizations are similar, but different in magnitude. Conversely, the Oklahoma City based dissipation rate profile has a different shape and also a different magnitude. In Figure 3.19, left panel, the magnitudes of the dissipation rate are sorted from Oklahoma City highest, to BUBBLE lowest and the original in the middle. Thereby the differences in the magnitudes are roughly equal. The same ranking can be seen in the graphs in Figure 3.21 with the differences also roughly equal. This indicates that different shape of the Oklahoma City based $\varepsilon$ is less important than the change in magnitude. An alternative interpretation is that the dissipation rate in the roughness sublayer is less important than the one in the Inertial Sublayer and the mixed layer.

To be able to distinguish between those two interpretations, the original and the Oklahoma City-based $\varepsilon$-profiles in Figure 3.19 are scaled (at height $z_*$) to the value of the BUBBLE-based $\varepsilon$ (not shown). In essence, the resulting profiles are identical in the IS and ML and retain their previous shape (see Figure 3.19) in the RS, only scaled to have the same $\varepsilon(z_*)$.

The resulting statistics in Table 3.8 show almost no difference between the actual BUBBLE-based dissipation rate profile (unchanged from before) and the original $\varepsilon$-
parameterization scaled to BUBBLE measurements. Only the first MOE dimension is significantly different, although that is not visible in the first two digits after the period. Similarly, the Oklahoma City-based \( \varepsilon \) only significantly differs in the FB and second MOE dimension. Comparing these results with the results in Table 3.7, it is clear that the main difference between the earlier \( \varepsilon \)-parameterizations lies in their different magnitude in either the IS/ML, the RS or both and that the shape and derivative of the RS-profile plays a smaller role.

### 3.7. Parameterization of drift

For this section the default model options are: ACDC on (Section 2.4.2), \( f \)-calibration off (Section 2.2.4), cGSC on (Section 2.4.3) and the \( \varepsilon \)-parameterization in the RS is based on BUBBLE data (Section 2.4.4). The reasoning for each of options is explained in the corresponding section. In the following, the boundary condition at the bottom of the model is modified to include drift inside street canyons for trapped particles, as described in Section 2.5.

First, a sensitivity study on the street distribution is undertaken in Section 3.7.1. Second, the model’s sensitivity to the two parameters \( p_a \) and \( p_c \) is investigated in Section 3.7.2. Third, a comparison between the model’s sensitivity to several length scales \( (d, z_0 \text{ and } z_*) \) with the drift parameterization on and off is drawn. Lastly, the model’s performance with the drift parameterization is compared to that of other boundary conditions in Section 3.7.4.

#### 3.7.1. Sensitivity to street directions

The estimated street direction distribution for the area of Kleinbasel is described in Section 2.1 and listed in Table 2.3. This distribution is compared to two extremes: only perpendicular and only parallel streets, both relative to the mean wind direction. Thereby the coefficient for the along canyon wind speed \( p_a \) in (2.72) is 0.8 and the coefficient for the cross canyon wind speed \( p_c \) in (2.73) is 0.4, as described in sections 2.5.1 and 2.5.2.

The resulting statistics in Table 3.9 show that there is no clear best version and the significance is generally low. Especially the parallel streets model version, when compared to the model with the estimated street distribution, shows not a single significantly different statistical index. Thereby the RD, the NMSE, the CORR and the RMSE improve, while the other statistics stay the same. Clearly there is no strong sensitivity to this model option.

When comparing the model with perpendicular streets to the model with default streets, the RD, the FB and the second MOE dimension improve significantly. The RMSE and the NMSE improve insignificantly, the first MOE dimension becomes significantly worse
Table 3.9.: As Table 3.1, only using different street layouts (Section 2.5) for all thirty minute averaged runs of experiments 1 and 2.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>street distribution</td>
<td>1.71</td>
<td>−0.23</td>
<td>2.51</td>
<td>0.50</td>
<td>93.95</td>
<td>0.30</td>
<td>(0.64, 0.51)</td>
</tr>
<tr>
<td>parallel streets</td>
<td>1.66</td>
<td>−0.23</td>
<td>2.47</td>
<td>0.52</td>
<td>93.05</td>
<td>0.30</td>
<td>(0.64, 0.51)</td>
</tr>
<tr>
<td>perpendicular streets</td>
<td>1.64</td>
<td>−0.20</td>
<td>2.50</td>
<td>0.50</td>
<td>92.25</td>
<td>0.30</td>
<td>(0.63, 0.52)</td>
</tr>
<tr>
<td>mean σ_{STAT}</td>
<td>0.38</td>
<td>0.12</td>
<td>0.42</td>
<td>0.06</td>
<td>11.09</td>
<td>0.04</td>
<td>(0.05, 0.04)</td>
</tr>
</tbody>
</table>

and the CORR and the F2 stay the same. However, both improvements and decreases are small when compared to those of other model options. Consequently, the sensitivity to this model option is still small.

Somewhat puzzling is the fact that perpendicular streets appear to be, if only slightly, statistically better than the street distribution. This is counter intuitive because perpendicular streets hold particles in place when they become trapped and do not transport them, as the distributed streets and especially the parallel streets do. Since the model still generally overpredicts the concentrations, one would expect that increased dispersion by transport in streets and therefore reduced concentrations would increase the model performance on average.

This behavior might be explained in Figure 3.22, a representative run with three-hour averaged data from experiment 2. Panel (a) shows that the crosswind integrated concentration is highest for the model with perpendicular streets and lowest for the model with parallel streets, from the source to 300 m source distance. In contrast, at a source distance of 300 m the three models show almost equal \( \bar{c}_y \) and from 350 m to 800 m the order is reversed: the perpendicular model is lowest and the parallel model is highest, albeit only slightly so. From there on outward the difference is between the concentrations is practically indistinguishable. The same behavior, only less clear, can be seen in panel (b) for the maximum concentration along each arc, even though the reversal point is shifted to 200 m.

The above described behavior is not restricted to experiment 2, nor to three-hour averaged runs. It happens for all investigated simulations, even though the position of the reversal shifts. Since almost all sampler positions are further away from the source than 300 m, the increased concentration of the model with perpendicular streets close to the source are never compared to measurements and therefore also do not affect the statistics. Further downstream the relationship is reversed and the difference between the models already small, which leads to the perceived insensitivity of the model to street direction distributions. Additionally the lower concentration of the model with perpendicular streets
3.7 Parameterization of drift

in this range leads to a better model performance for test cases, which are generally overpredicted.

The lateral dispersion in Figure 3.22(c) is hardly distinguishable, but highest for the perpendicular model and lowest for the parallel streets. This too seems counter intuitive, because the models with parallel streets and perpendicular streets have no additional transport in y-direction, while the model with the distributed streets does. Consequently the distributed-streets model should have the highest lateral dispersion, but it does not. A fact that might explain this is the increased time particles stay in the model domain for the perpendicular streets model, compared to the model with distributed streets, since they are not transported downstream. During this time the particles can disperse more laterally. The parallel model transports the particles away from the source even faster on average and therefore they spread less laterally. The large difference between the models directly at the source is a numerical artifact from the calculation of $\sigma_{c,y}$ and can be ignored.

3.7.2. Sensitivity to wind speed parameters

The along canyon wind speed parameter $p_a$ and the cross canyon wind speed parameter $p_c$ are used in (2.72) and (2.73) to calculate the along canyon wind speed and the cross...
canyon wind speed inside the virtual streets. A physically realistic range for $p_a$ is defined in Section 2.5.1 as [0.1, 1.4], while $p_c$ is realistically in the interval [0.1, 0.9] (see Section 2.5.2). The default values were derived from literature (see sections 2.5.1 and 2.5.2) and are $p_a = 0.8$ and $p_c = 0.4$ for Basel.

Table 3.10 lists statistical indices that describe the agreement of model simulations to measurements. The runs use thirty minute data of experiments 1 and 2 and all possible combination of $p_a = \{0.1, 0.8, 1.4\}$ and $p_c = \{0.1, 0.4, 0.9\}$. All runs are tested on significant difference to the model with default parameter values.

Altogether, the model with $p_a = 0.1$ and $p_c = 0.9$ has the best statistics. Its RD, FB, RMSE and second MOE dimension are the best of all and significantly better than the default model. Additionally this model has the best NMSE and F2 value, but they are not significantly different from the default. The CORR is unchanged and the first MOE dimension becomes only slightly — although significantly — worse. Since the model with perpendicular streets in Section 3.7.1, which is similar to these settings, also tends to give better results than the model with default drift, this is not surprising. The low $p_a$ effectively turns off along canyon transport and the high $p_c$ shortens the time span that the particles stay trapped. Thus this improvement is in line with the fact that immediate reflection gave better results than the recirculation approach in Section 3.3 with the original model.

In contrast to the best statistical values, the worst appear mostly for the model with $p_a = 1.4$ and $p_c = 0.1$, the polar opposite of the “best” model version above. It has the worst RD, the worst FB and the worst second MOE dimension, the later two being significantly worse than the default. The CORR and the F2 are similar over all models, so

The worst RD, the worst FB and the worst second MOE dimension, the later two being

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_a = 0.1, p_c = 0.1$</td>
<td>1.85</td>
<td>-0.27</td>
<td>2.75</td>
<td>0.49</td>
<td>100.32</td>
<td>0.29</td>
<td>(0.65, 0.49)</td>
</tr>
<tr>
<td>$p_a = 0.1, p_c = 0.4$</td>
<td>1.66</td>
<td>-0.20</td>
<td>2.52</td>
<td>0.49</td>
<td>92.41</td>
<td>0.30</td>
<td>(0.63, 0.52)</td>
</tr>
<tr>
<td>$p_a = 0.1, p_c = 0.9$</td>
<td><strong>1.61</strong></td>
<td><strong>-0.17</strong></td>
<td><strong>2.42</strong></td>
<td><strong>0.50</strong></td>
<td><strong>89.61</strong></td>
<td><strong>0.31</strong></td>
<td>(0.63, <strong>0.53</strong>)</td>
</tr>
<tr>
<td>$p_a = 0.8, p_c = 0.1$</td>
<td>2.05</td>
<td>-0.33</td>
<td>2.58</td>
<td>0.50</td>
<td>99.94</td>
<td>0.30</td>
<td>(0.67, 0.48)</td>
</tr>
<tr>
<td>$p_a = 0.8, p_c = 0.4$</td>
<td>1.71</td>
<td>-0.23</td>
<td>2.51</td>
<td>0.50</td>
<td>94.02</td>
<td>0.30</td>
<td>(0.64, 0.51)</td>
</tr>
<tr>
<td>$p_a = 0.8, p_c = 0.9$</td>
<td>1.64</td>
<td>-0.21</td>
<td>2.44</td>
<td><strong>0.51</strong></td>
<td>91.34</td>
<td>0.30</td>
<td>(0.64, 0.52)</td>
</tr>
<tr>
<td>$p_a = 1.4, p_c = 0.1$</td>
<td>2.14</td>
<td>-0.35</td>
<td>2.46</td>
<td><strong>0.51</strong></td>
<td>98.58</td>
<td>0.30</td>
<td><strong>(0.68, 0.48)</strong></td>
</tr>
<tr>
<td>$p_a = 1.4, p_c = 0.4$</td>
<td>1.78</td>
<td>-0.26</td>
<td>2.52</td>
<td>0.50</td>
<td>95.71</td>
<td>0.30</td>
<td>(0.65, 0.50)</td>
</tr>
<tr>
<td>$p_a = 1.4, p_c = 0.9$</td>
<td>1.69</td>
<td>-0.23</td>
<td>2.48</td>
<td><strong>0.51</strong></td>
<td>93.61</td>
<td>0.29</td>
<td>(0.64, 0.51)</td>
</tr>
<tr>
<td>mean $\sigma_{STAT}$</td>
<td>0.40</td>
<td>0.12</td>
<td>0.42</td>
<td><strong>0.06</strong></td>
<td>11.16</td>
<td>0.04</td>
<td>(0.05, 0.04)</td>
</tr>
</tbody>
</table>
it is probably not important that the “worst” model has the best, but not significantly different, CORR. This shows that transporting particles further for longer deteriorates the model performance, similar to the result with the parallel streets.

### 3.7.3. Sensitivity to length scales

Rotach (2001) already investigates the sensitivity of the model to $z_*$ and $d$, although for an older model version that used a reflective boundary condition at the bottom. This section only briefly investigates whether the newly proposed boundary condition makes the model more or less sensitive to changes in $d$, $z_0$ and $z_*$. Note that this is not supposed to be a complete sensitivity study, because only two values for each length scale are investigated and the different scales are not even permuted with each other. The two values for each length scale are, first, the default value for the model in Basel and, second, a value that is estimated from the results of Christen (2005), as already described in Section 2.1. The simulations use either parameterized drift (see Section 2.5) or the recirculation approach (see Section 2.2.6) as the lower boundary condition.

Table 3.11 shows both model versions with the same changes in the length scales each. The top four rows of values represent the models with recirculation, below that the models with parameterized drift.

The general behavior is similar between the drift-model and the recirculation-model. Increasing the zero plane displacement improves the statistics the most in both cases.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>default</td>
<td>1.58</td>
<td>-0.16</td>
<td>2.40</td>
<td>0.51</td>
<td>88.53</td>
<td>0.31</td>
<td>(0.62, 0.53)</td>
</tr>
<tr>
<td>$d = 13.6$ m</td>
<td><strong>1.32</strong></td>
<td><strong>0.04</strong></td>
<td><strong>2.31</strong></td>
<td><strong>0.53</strong></td>
<td><strong>78.56</strong></td>
<td><strong>0.32</strong></td>
<td>(0.57, 0.60)</td>
</tr>
<tr>
<td>$z_0 = 1.5$ m</td>
<td>1.56</td>
<td>-0.11</td>
<td>2.39</td>
<td>0.50</td>
<td>86.12</td>
<td>0.28</td>
<td>(0.60, 0.54)</td>
</tr>
<tr>
<td>$z_* / H = 1.56$</td>
<td>1.65</td>
<td>-0.21</td>
<td>2.49</td>
<td>0.50</td>
<td>92.56</td>
<td>0.28</td>
<td>(0.63, 0.51)</td>
</tr>
<tr>
<td>default</td>
<td>1.71</td>
<td>-0.23</td>
<td>2.51</td>
<td>0.50</td>
<td>93.99</td>
<td>0.30</td>
<td>(0.64, 0.51)</td>
</tr>
<tr>
<td>$d = 13.6$ m</td>
<td><strong>1.35</strong></td>
<td><strong>0.05</strong></td>
<td><strong>2.36</strong></td>
<td><strong>0.52</strong></td>
<td><strong>78.85</strong></td>
<td><strong>0.33</strong></td>
<td>(0.56, 0.59)</td>
</tr>
<tr>
<td>$z_0 = 1.5$ m</td>
<td>1.67</td>
<td>-0.17</td>
<td>2.42</td>
<td>0.51</td>
<td>89.34</td>
<td>0.26</td>
<td>(0.62, 0.52)</td>
</tr>
<tr>
<td>$z_* / H = 1.56$</td>
<td>1.81</td>
<td>-0.29</td>
<td>2.59</td>
<td>0.50</td>
<td>98.03</td>
<td>0.28</td>
<td>(0.66, 0.49)</td>
</tr>
<tr>
<td>mean $\sigma_{\text{STAT}}$</td>
<td>0.36</td>
<td>0.12</td>
<td>0.44</td>
<td>0.06</td>
<td>11.18</td>
<td>0.04</td>
<td>(0.05, 0.04)</td>
</tr>
</tbody>
</table>
For the modified \(d\)-model, the RD, FB, CORR, RMSE and the second MOE dimension are significantly better than for model with the default \(d\). NMSE and F2 are better as well, although insignificantly so. Only the first MOE dimension decreases, which is not surprising because a larger \(d\) leads to lower simulated concentrations, as is shown in Rotach (2001). Interesting are the facts that the FB is positive and the second MOE dimension is larger than the first. Both suggest a slight underprediction, which is unusual for the model and data set at hand, as described in Section 3.3. This means that the general overprediction of the model can be remedied by choosing a different \(d\).

Increasing the roughness length also leads to different statistics for both drift and recirculation boundary condition. The FB, RMSE and the second MOE dimension are significantly better and the F2 and the first MOE dimension significantly worse. The RD and NMSE are insignificantly better, while the CORR changes insignificantly for both drift-model and recirculation-model, only to worse and better respectively. Altogether this means that the rate of overprediction is increased and the rate of underprediction is decreased, while the difference between simulated and observed value become smaller on average, but also more “bad” values are produced. Therefore it appears that \(z_0 = 1.5\) m is better than \(z_0 = 1.0\) m, but the differences are smaller and less clear than they are for the increased \(d\).

Changing the height of the roughness sublayer \(z_*\) also behaves similarly in both the recirculation-model and the drift-model, although the differences for the recirculation-model are more often significant. Generally the higher roughness sublayer leads to a statistically worse model performance. Specifically the RD, the FB, the RMSE and the second MOE dimension are significantly worse with the new \(z_*\) for both model versions. The recirculation-model also has a significantly worse CORR and F2 with the new roughness layer height, while those values are only insignificantly worse or unchanged for the drift-model. Both model versions have a significantly better first MOE dimension and an insignificantly worse NMSE with the new \(z_*\). In summary, increasing the roughness sublayer height leads to higher concentrations, which decreases the model performance for the test cases, because they are already generally overpredicted.

This seems strange, because usually (Raupach et al. 1991) \(z_* = (2\) to \(5)H\) and here a change from \(z_* = 1.477H\) to \(z_* = 1.56H\) decreases the model performance. However, this is likely linked to the general overprediction of the model. Additionally the model behaves similar to changes in \(z_*\) as it did in Rotach (2001).

It should be emphasized that the above deliberation is not a complete sensitivity study, therefore the magnitude of the model reaction to changes in the length scales cannot be compared. Possibly changes in \(d\) are not as important as changes in \(z_0\) or \(z_*\) when looking at the full range of physically realistic values. Nevertheless, the length scales, except \(z_0\), appear to be able alter the model more than other model options with the exception of the change in the derivative of the velocity auto-covariance profiles.
3.7 Parameterization of drift

3.7.4. Validation of drift parameterization

In this section the different boundary conditions at the bottom will be compared to each other. The recirculation approach (Section 2.2.6) was proposed by Rotach et al. (2004), the parameterized drift in street canyons is explained in Section 2.5 and the immediate reflection is equal to the reflection at the top (Section 2.2.6).

Figure 3.23 shows the plume characteristics for the test case of the three-hour averaged values of experiment 2. In panel (a), the crosswind integrated concentration is lowest for the model with reflection from the source to the peak at about 50 m. This is expected, because reflection moves the particles immediately back into the model domain, where they can continue on their trajectories and on average do so away from the source. From about 1200 m on, the difference to the other models is negligible.

More interesting is the recirculation-model’s $c_y$ compared to the drift-model’s. The recirculation model has the same $c_y$ at the source, but a slightly higher $c_y$ until the peak at 150 m source distance. There the drift-model starts to have the highest $c_y$ and keeps on having it while the difference between the models becomes gradually less and less and vanishes at about 1200 m.
Results and discussion

Figure 3.24.: Fraction of escaped particles plotted against their length of trapping incidence, for three different bottom boundary conditions and experiment 2, three-hour averaged values. Also visible (○) are upscaled values from wind tunnel experiments by Hoydysh and Dabberdt (1988) and balloon measurements (□) of Vachon et al. (1999).

The same behavior can be seen in Figure 3.23(b), only that the differences are smaller and the models cannot be distinguished from about 800 m onwards.

Figure 3.23(c) proves that the lateral dispersion is not responsible for this characteristic, because it is highly similar everywhere. This also indicates that the lateral transport of the drift-model is not relevant to the model result.

Most likely the different behavior of the recirculation and the drift-model can be explained by the fact that the cross canyon wind speed that regulates the recirculation time is smaller for the recirculation approach. The drift model uses a multiplier of $0.4 \cos(\alpha_{inc})$, while the recirculation model uses 0.5. Additionally the residence time of the parameterized drift is randomly multiplied by a natural number to simulate multiple vortex rotations. Thus the drift model traps particles longer and apparently the transport during that time is not enough to offset the difference.

How much longer the trapping in the drift-model lasts can be seen in Figure 3.24. In essence it shows the cumulative frequency distribution of residence times for different model versions for the test case experiment 2, three-hour averaged data, with $u_H = 1.78 \text{ m s}^{-1}$. The almost vertical line at about $\tau = 33 \text{ s}$ represents the residence time of the recirculation-model. All particles stay trapped for the same amount of time and therefore 100% have left after this time. Not visible is the graph of the reflection-model, because there is no trapping in that model.

More interesting is the graph representing the drift-model. There are periods of large “jumps” in the function, which are caused by streets where a vortex forms, because there $\tau$ is always a multiple of the same value (see Section 2.5.3). The periods with smaller slope are the residence times of trapping incidences in canyons without vortex, because
there $\tau$ depends on the individual vertical velocity of each particle (also see Section 2.5.3). Hoydysh and Dabberdt (1988) made wind tunnel experiments, which are scaled up to $H = 25$ m and $\bar{u}_H = 2$ m s$^{-1}$ and also shown in Figure 3.24. Their residence times are generally longer, but it is hard to compare directly, because their buildings are taller and their wind speed higher. However, at least the order of magnitude seems correct.

The balloon residence time of Vachon et al. (1999) is also pictured in Figure 3.24. Generally their balloons leave the street faster than the model releases particles, but they were started at the ground and had therefore less far to travel. Additionally their buildings were taller and they obtained the measurements over several days of changing wind direction and velocity. Still, the shape of the $\tau$ parameterization for the drift model seems to agree well with the measurements.

Figure 3.25 shows a scatter plot, where at almost all sampler positions the simulated concentration of the drift-model is the highest, followed by the model with recirculation.
Table 3.12: As Table 3.1, comparing default drift (Section 2.5), recirculation approach (Section 2.2.6) and direct reflection for 30 minute averaged runs of experiments 1 and 2.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>RD</th>
<th>FB</th>
<th>NMSE</th>
<th>CORR</th>
<th>RMSE</th>
<th>F2</th>
<th>MOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>recirculation</td>
<td>1.58</td>
<td>-0.16</td>
<td>2.40</td>
<td><strong>0.51</strong></td>
<td>88.49</td>
<td><strong>0.31</strong></td>
<td>(0.62, 0.53)</td>
</tr>
<tr>
<td>drift</td>
<td>1.71</td>
<td>-0.23</td>
<td>2.51</td>
<td>0.50</td>
<td>93.93</td>
<td>0.30</td>
<td><strong>0.64, 0.51</strong></td>
</tr>
<tr>
<td>reflection</td>
<td><strong>1.49</strong></td>
<td><strong>-0.09</strong></td>
<td><strong>2.37</strong></td>
<td>0.50</td>
<td><strong>84.94</strong></td>
<td>0.30</td>
<td>(0.60, <strong>0.55</strong>)</td>
</tr>
<tr>
<td>mean σSTAT</td>
<td>0.36</td>
<td>0.12</td>
<td>0.43</td>
<td>0.06</td>
<td>10.99</td>
<td>0.04</td>
<td>(0.05, 0.04)</td>
</tr>
</tbody>
</table>

and then by the reflection-model. This is expected, because only two sampler positions are closer than 300 m to the source and Figure 3.23 indicates that the models behave like this in that range.

Section 3.3 shows that the model currently overpredicts the BUBBLE experiments. Together with the model reaction to the different boundary conditions described above, the statistics in Table 3.12 are not surprising. The model with parameterized drift has a significantly worse RD, FB, RMSE and second MOE dimension than the model with recirculation. The first MOE dimension is significantly better, while the NMSE, CORR and F2 are worse, but insignificantly. This means that the overprediction is increased.

In contrast, the model with immediate reflection at the bottom has a significantly better RD, FB, RMSE and second MOE dimension, while the NMSE is insignificantly better. The CORR and the F2 are insignificantly worse, while the NMSE is insignificantly better. Thus the overprediction is decreased.

In summary, the drift parameterization as described in Section 2.5 decreases the model performance compared to the recirculation approach of Rotach et al. (2004). This could easily be remedied by tuning the wind speed parameters $p_a$ and $p_c$ and also by changing the street distribution, which is already shown earlier. However, this seems disingenuous, because the optimized parameters would not represent realistic conditions and simple reflection fixes the above problems more easily and better.

Another point that could be investigated is the recirculation probability. It is fixed at 66% throughout this thesis, even though this value was chosen quite arbitrarily by Rotach et al. (2004). However, due to reflection improving the model results for BUBBLE compared to parameterized drift, the optimal recirculation probability would be zero.

An additional problem is that the boundary condition with drift introduces a sort of lateral shear, because the particles can now move deterministically oblique to the main wind direction. This technically violates the model assumption that $v$ is independent of $u$. However, the violation is too small to be detected in Section 3.2.4, so the problem is presumably small.
4. Conclusions and outlook

In this chapter important results of this thesis are summarized and a few ideas for future studies are presented. The most important results, first the unexpected and the later those pertaining to the goals defined in Section 1.4 are:

- An error in the original source code for the velocity auto-covariance derivative in the roughness sublayer leads to a drastically different concentration distribution. Unfortunately this means that the results that led to the idea of improving the model by modifying the lower boundary condition can no longer be replicated.

- The model is somewhat sensitive to changes in the solenoidal probability current $\Phi^*$. The one proposed by Gibson and Sailor (2012) improves the model performance for the BUBBLE cases once corrected, because the reduction of the simulated concentration counteracts the general overprediction. The correction is necessary, because the original formulation of $\Phi^*$ by Gibson and Sailor (2012) is not divergence free, which in turn leads to a violation of the well-mixed criterion.

- A different dissipation rate parameterization in the roughness sublayer might improve the model, because it is definitely sensitive to changes in $\varepsilon$. However, the proposed $\varepsilon$ based on BUBBLE data does not appear to clearly improve or worsen the model performance. The alternative dissipation rate based on Oklahoma City data decreases the model result’s agreement with measurements. This means that the more appropriate profile gives better results. Additionally, the present results indicate that the magnitude of $\varepsilon$ is more important than the shape and derivative of its profile in the roughness sublayer.

- An as realistic as achievable drift parameterization at the lower boundary condition changes the model performance, but to the worse for BUBBLE data. However, this is mainly caused by a faulty hypothesis due to the error in the source code mentioned above. The new boundary condition reinforces the now general overprediction of the model. The drift parameterization is sensitive to changes in the wind speed coefficients and less so to the street distribution.

Additional results of this thesis are:

- When the situation in reality is not stationary enough, the model performance is much worse.
Conclusions and outlook

- Problems with the model overpredicting measurements could potentially be solved by increasing the zero plane displacement. The thereby tested value is not an even extreme one, but the result of extensive measurements in Basel, examined by Christen (2005), and was not known at the time of the study by Rotach et al. (2004). Therefore it appears that a better zero plane displacement value leads to a better model performance.

- When looking at sampler position concentrations, a larger amount of particles than previously thought seems to be needed. 200 000 particles appear to work well for a significance level of 95%.

- Changing the boundary condition does not affect the well mixed criterion in any major way, but mistakes in the solenoidal probability current $\Phi_i^*$ does. A not continuously differentiable transition function appears to be problematic if $\Phi_i^*$ depends on $\sigma_{uG}$.

- Calibrating the transition function to measurements changes the model output less than previously assumed. Therefore a correct shape of the transition function $f$ or its continuous differentiability is apparently less important than other factors.

- The assumption of a solid ceiling instead of transport out of the planetary boundary layer is good.

- The impact of the error in the velocity auto-covariance derivative proves that a correct representation of the velocity auto-covariance in the roughness sublayer is essential to the model.

A remaining problem with the model is that the concentrations, especially close to the source, are too high. Since the lateral dispersion appears to work well, this points to the vertical dispersion as culprit. The treatment of the roughness sublayer of Rotach (2001) decreases the velocity variances close to the ground, which results in higher concentrations. Since those concentrations appear to be too high and the modified lower boundary condition increases them even further, it might be possible that the canyon effect in the model should reduce the concentrations at the ground. Of course, in reality canyons trap pollutants, but maybe this effect is already included in the roughness sublayer treatment, so including it additionally in the boundary condition is too much. When looking at the sensitivity of $p_c$, a larger value, which is synonym for a large mean exchange between canyon and model domain above, decreases the concentrations. The results of Christen (2005) show that there are substantial $\mathbf{w}$ at the roof top level, depending on wind and canyon direction, which the model cannot accommodate inside its domain. However, this $\mathbf{w}$ could be incorporated by a modified lower boundary condition. For example, one could increase the vertical velocity after a trapping incident, although this would likely violate the well mixed condition. Another method to include a $\mathbf{w} \neq 0$ could be to modify $\sigma_w$ inside the model domain instead.
In the future, the model should be compared to other tracer experiments in other urban areas to be able to generalize findings. For example, the change in the solenoidal probability current reduces the simulated concentration, which is good for the overpredicted BUBBLE cases. Other cities might be different. The parameterization of the dissipation rate has a similar problem, only the results are inconclusive for Basel, and should therefore also be tested in another city. This is also recommended by Hanna and Chang (2012), who show that model performance is site specific.

When researching the dissipation rate profile, it would be useful to have measurements in the roughness sublayer and the mixed layer simultaneously, because at least the model results indicate that the latter also plays an important role for near ground dispersion.

Instead of improving the lower boundary condition, a better choice of length scales would most likely improve the model performance more. A full sensitivity study over the range of values proposed by Grimmond and Oke (1999) looks promising. Additionally, this should be studied for other areas with different building heights as well.

Another point where large changes in the model can be achieved are the velocity covariance profiles. Much has been done there already by Rotach et al. (2004), but a new city would most likely solidify results.

If one wanted to further improve the drift parameterization at the lower boundary, an objective method to derive a street distribution would likely be necessary. Additionally some method to include thermal effects from differential wall heating should be found, since the literature (e.g. Sini et al. 1996) implies that this changes the flow regime in the UCL. The local topography with different wall heights and roof shapes on sides of the canyon would ideally also be included.

Generally, samplers even closer to the source would be useful when comparing model results to field experiments, because the peak is closer to the source than the BUBBLE-samplers. This was attempted already at BUBBLE, but the peak distance had been underestimated during the planing, because the occurrence of both a large $u_*$ and a large $w_*$ at the same time had not been anticipated.
## A. Appendix

**Table A.1.:** Description of measurement sites, based on Gryning et al. (2005). For site descriptions see table 2.1.

<table>
<thead>
<tr>
<th>Site</th>
<th>East of R1 (m)</th>
<th>North of R1 (m)</th>
<th>East of R2 (m)</th>
<th>North of R2 (m)</th>
<th>Height AGL (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>0</td>
<td>0</td>
<td>292</td>
<td>823</td>
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</tr>
<tr>
<td>R2</td>
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<td>−823</td>
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<td>0</td>
<td>21.0</td>
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<tr>
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References


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Last but not least, I thank my family, friends and fellow students, who have always supported me in my endeavors.
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Datum

Unterschrift