Chapter

METEOROLOGICAL ASPECTS OF AIR QUALITY

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ABSTRACT

This paper provides a survey on the role of the atmospheric boundary layer and its role on air quality. Based on the evaluation of a weather forecast model it is found that the nighttime or stable boundary layer is difficult to forecast. We briefly summarize the relevant processes in this boundary layer prototype, and we discuss their interactions. Next, a climatology of flow meandering and intermittency of the atmospheric turbulence, and its spatial extent under these conditions, is presented based on field observations. Finally, a new formula for the stable boundary layer height is derived.

1. INTRODUCTION

The atmosphere in which we live, consists of a mixture of natural gases (nitrogen, oxygen, water vapor, carbon dioxide and some other spore gases). Human activity leads to several emissions of non-natural pollutants, e.g. by road and air traffic (Charron and Harrison, 2005), industry, agriculture and power plants. Well-known anthropogenic emissions are sulfur dioxide, carbon dioxide, nitrogen oxide, ammonia, methane, volatile organic compounds, and particulate matter. After a primary gas release, several chemical reactions may result in (harmful) reaction products (i.e. secondary pollutants, e.g. Reitebuch et al, 2000), e.g. ozone. Accidents with industrial processes or in traffic might result in a sudden strong emission of pollutants. For example, in the Bhopal (India) disaster a pesticide plant released ~40 tons of methyl isocyanate gas (MIC), killing approximately 3,800 people instantly, and 8,000 others died within two weeks. The incident took place in the early hours of the morning of 3 December 1984 in the heart of the city of Bhopal. Studies showed that the local meteorology (together with the local topography) played an important role in the
dispersion of the MIC over the city of Bhopal (Boybeyi et al., 1995; Sharan et al., 1996). First, the MIC release occurred under calm, clear sky conditions, in a shallow layer close to the ground. Second, a circulation induced by the urban heat island effect between the city and the surroundings, resulted in a flow from the pesticide plant towards the city. As such, it is clear that the local weather can impact on the local air quality.

In addition to anthropogenic sources, a variety of natural sources as forests and wetlands can release several gases and constituents, especially volatile hydrocarbons, ozone and NOx, but pollen and spores as well. Finally, dust emissions due to wild fires, dust storms and volcanic eruptions can have substantial impact on the regional and global air quality and climate (e.g. Mt Pinatubo, 1992).

Some of these primary and secondary emissions can be harmful for human health, natural vegetation and agricultural crops. As an example: long-term exposure of sensitive nature to ammonia and other nutrient rich pollutants has lead to a substantial reduction of the heather vegetation in the Netherlands (Roelofs, 1994; Van Eerden et al., 1998). Also, short term exposure to smog has shown to increase mortality rates in sensitive groups (i.e. the elderly, young children and people with cardiovascular diseases). Stedman (2006) found that for the heat wave in Europe in the summer of 2006, it was due to the poor air quality in the London area that ~21-38 % of the victims were probably not caused by heat stress, but by smog and particulate matter.

Regarding the role of meteorology on air quality, the air mass and the large-scale meteorology determines the background concentrations. In general, air masses from an Arctic or oceanic origin have low concentrations, while air masses with a continental origin are more polluted. Persistent high pressure systems over land collect near surface emissions for a long time period since efficient removal processes (washout and rainout) are absent, and because the air is slowly subsiding. Subsidence causes the air to stabilize and ‘lock’ the polluted near surface air under a so called inversion. On the contrary, in low pressure systems washout and rainout are efficiently active, and the mean upward motions help to remove near surface emissions into the free troposphere aloft.

Given the air mass, the atmospheric flow near the surface consists of irregular and semi-chaotic swirls and vortices of a variety of dimensions (ranging from 1 mm-1 km). These motions are called eddies, and are responsible for the turbulent transport and mixing of the pollutants within a reservoir layer or mixing layer. The turbulent atmospheric mixing also provides lateral dispersion of the released emissions (e.g. from a stack) over a certain width perpendicular to the wind direction. Thus, one may state that to first order the concentration \( C \) is of an air pollutant due to the release of a point source is:

\[
C = Q \left( \frac{U h \sigma_y}{\sigma_z} \right)
\]

with \( U \) the wind speed (ms\(^{-1}\)), \( h \) the mixing height (m), \( \sigma_y \) the dispersion parameter (m), and \( Q \) the source strength (kg s\(^{-1}\)) (Pasquill and Smith, 1983). Thus, high concentrations occur for large \( Q \), and for small wind speed, small mixing height and small dispersion conditions. These conditions occur typically during clear calm nights. Therefore, air pollution concentrations are strongly determined by the basic atmospheric conditions. As such, it is essential to understand the atmospheric processes that govern pollutant concentrations to enable skillful air quality forecasting. A reliable air quality forecast allows for on time and
effective counter measures to reduce the harmful effects on pollutant emissions, and for an effective warning of potential victims. As an illustration, Figure 1.1 shows a thin layer of brownish pollution (probably NO$_2$) on a calm morning in January, with a typical mixing depth of 50 m. The ingredients that govern the air pollutant concentrations are wind speed, mixing height and dispersion parameters. This paper provides a survey on the meteorological issues for air quality. In the next chapter, we introduce the diurnal cycle of the atmospheric boundary layer and its characteristic for wind speed, mixing layer depth and dispersion. Section 3 illustrates the common practice of high resolution weather forecasting for air quality forecasting, and provides an evaluation and identification of typical problematic features in modeling. Section 4 provides an overview of difficulties in understanding the stable boundary layer. Section 5 explains atmospheric dispersion and intermittency of the turbulence in calm nighttime conditions. Section 6 presents some methods for estimation of the nighttime boundary-layer height. A summary of our results will be given in section 7.

Figure 1.1. Illustration of a highly polluted thin stable boundary layer in the early morning of 19 January 2008 in Wageningen, The Netherlands. Photo: G.J. Steeneveld.
2. THE ATMOSPHERIC BOUNDARY LAYER

The Atmospheric Boundary Layer (ABL) is defined as the atmospheric layer adjacent to the Earth’s surface that directly ‘feels’ the effect of the diurnal cycle of wind and temperature at the surface (Stull, 1988). The main characteristic of the ABL is turbulence, which normally mixes air pollutants effectively. Therefore, in air quality literature this layer is often referred to as the mixing height. During daytime, solar radiation heats the surface, which consequently triggers convection by thermals. Figure 2.1 shows a typical diurnal cycle of this layer by observations of wind speed and potential temperature (the temperature of an air parcel when it is adiabatically moved to the surface, $\theta = T + 0.0981z$) from the Cabauw meteorological tower (in the Netherlands, Beljaars and Bosveld, 1997). First, we find that during nighttime strong vertical gradients exist in the potential temperature, and in wind speed. Cold air is built up close to the surface due to radiative heat loss to space, and potentially warmer air remains aloft. This is a stable boundary layer or the inversion layer. Inversion layers inhibit vertical transport and are thus harmful for air quality, so therefore this chapter will largely focus on stable conditions. Stable boundary layers prevail at night, but also during daytime in winter in mid-latitudes as well as in polar regions (Yagüe and Redondo, 1995), and during daytime over irrigated regions with advection. The stable stratification in the morning of the Bhopal accident was one of the causes for the high MIC concentration. On the contrary, during the day all tower levels above 20 m show a nearly uniform wind speed and potential temperature, although it is warmer very close to the surface (unstable stratification).
b)

To understand the ABL diurnal cycle, we need to examine the turbulent nature of the flow in the ABL. Turbulence is the key process for transport and dilution of constituents. Turbulence consists of irregular swirls of motions of different scales superimposed on each other. Turbulence is generated by two mechanisms: *forced convection* (mechanical turbulence) and *buoyancy*. Forced convection occurs when a flow travels over a rough area (with obstacles as grass, trees, cities, hills), and is forced to pass these objects. Wind shear is the source for turbulence in this case. Buoyancy is the effect that warm air parcels have a smaller density ($\rho$) than surrounding colder parcels, and therefore they start to ascend. A characteristic property of turbulence is its effectiveness in transportation of heat, moisture and pollutants. Therefore temperature and wind speed are well-mixed in the ABL, because the turbulence very easily transports heat from the surface upward, and momentum from the free atmosphere downward. Strong boundary layer convection often results in eddies that are sufficiently energetic to mix free tropospheric air (above the ABL) into the ABL. This is called *entrainment*, and is an important contributor to the ABL ventilation, because the imported air is typically cleaner than the ABL air. One can also imagine that the ABL plays a vital role in the exchange of natural (e.g. CO$_2$ and other greenhouse gases) and anthropogenic (e.g. pollutant emission; Neu, 1995) contaminants from the Earth’s surface to the free atmosphere above the ABL (e.g. Pino et al., 2006; Górska et al., 2008).

In the daytime boundary layer, the sun heats the surface and the turbulence is dominantly driven by buoyancy. The boundary layer rapidly grows in the morning, and large convective eddies provide vigorous vertical mixing over typically 1-2 km depth. Then surface emissions are diluted in a deep layer. Godish (2003) shows an evident difference in ABL height climatology between locations in the USA. Northern and coastal station have an average
summertime mixing height of 1000-1200 m, while in desert areas as in Phoenix and Denver the mean mixing height reaches 2600 m. Thus, land use substantially influences the ABL height.

In contrast, at night buoyancy suppresses the turbulence intensity, so only forced convection is a source of turbulence. Therefore, the nighttime boundary layer is much shallower, typically 100-200 m deep, but even 10-50 m is possible for weak winds. Then very high concentrations of (possibly harmful) species may build up in the SBL. During weak winds the suppression of turbulence by buoyancy is larger than the production by wind shear, so as a result the turbulence vanishes. Then, other transport processes than turbulence appear to govern the boundary-layer structure. These are radiation divergence, gravity waves, drainage flows, and heat conduction from the soil, although their role and interactions are not a priori clear for each process until now, and some of them has been only qualitatively understood. Questions such as “What determines the nocturnal cooling timescale at 2 m?” are still not completely answered (Pattantyús-Ábrahám and Jánosi, 2004).

In the next section we will evaluate the mesoscale weather forecast model WRF, which is a state-of-the-art model to provide meteorological information for air quality models.

3. Mesoscale Models for Air Quality Forecasts

Transport and dispersion of pollutants in the atmosphere occurs at first instance at horizontal scales that are much smaller than covered by typical global circulation models/weather forecast models (grid size typically 25 km). Therefore, high resolution weather forecast models, so called meso-scale models or limited area models, are used to forecast the local wind and temperature at much finer resolution (up to 1 km). In that case, the mesoscale model is used to zoom in a specific area of interest. As an example, a sea breeze circulation is a phenomenon on the so called meso-β scale (~100 km), and is usually forecasted with mesoscale model instead of operational global forecast models, because of the restricted resolution of the latter.

Many mesoscale models have been developed during the recent years (e.g. RAMS, MM5, WRF, HIRLAM, AROME, MESO-NH). These models provide the user the possibility to use different calculation methods for the physical processes: the boundary layer scheme, land surface scheme, the radiation scheme, cloud processes, gravity wave drag, and atmospheric radiation. The availability of a myriad parameterizations for each physical process already indicates that no unanimity has been reached for the optimal schemes. We will illustrate some characteristic differences of the forecasted mean and turbulent ABL structure.

3.1. Case Study and Model Set up

In this section, we analyze the ability of the limited area model WRF (version 2.2) to forecast the structure of the ABL for a case study in the Netherlands. We will validate our model forecasts against Cabauw tower observations (e.g. Beljaars and Bosveld, 1997, 51.97°N, 4.93°E, -0.7 m AGL, Figure 3.1), but also with wind profiler data, soundings and
ceilometer observations in De Bilt (20 km north of Cabauw). A ceilometer is an instrument that uses lidar techniques to determine the ABL height.

We selected the period of 30 July 2006, 12.00 UTC to 4 July 2006, 0.00 UTC because this is a clear sky summer period, and many observations are available for model validation. Note that a part of this period is under further study within GABLS3 (Bosveld et al., 2008). Herein column models for the ABL are given the same forecasting task. Their results are evaluated and compared in order to understand model deficiencies and to enable further model development. In this period, The Netherlands are located under a high-pressure system with winds from the southeast. The area consists mainly of grassland and is absolutely flat and relatively homogeneous. Also, the area is characterized by a large water supply and thus a high soil moisture availability. For these simulations the initial and boundary conditions (every 6 hours) were provided by NCEP Final Analysis. The model was run in an area of 1600 x 1600 km with a grid size of 54 km. In this domain, we nested 3 domains with a grid spacing of 18, 9 and 2 km respectively to minimize model errors due to lack of horizontal resolution (Figure 3.1). Moreover, the U.S. Geological Survey provided the land surface properties for the model simulations, such as soil moisture availability, surface roughness, and land use.

The model was run with 3 alternatives for the boundary layer scheme. The first scheme is the so-called MRF scheme (Troen and Mahrt, 1986; Hong and Pan, 1996). This is a first order closure scheme, and the main characteristic of the scheme is that the height dependence of the eddy diffusivity profile is prescribed with a cubic function, and that its magnitude depends on the characteristic velocity scale at the surface layer. Another characteristic is that the scheme allows for non-local counter gradient transport for heat during the day. This extension is needed to represent transport by large eddies on the scale of the boundary layer itself, instead of local transport. A well known disadvantage of this widely used scheme is excessive daytime entrainment at the boundary-layer top, and overestimation of the turbulent transport at night (e.g. Vila et al., 2002; Cuxart et al., 2006, Steeneveld et al., 2008a).

The second scheme has recently been introduced in WRF and is an extension of the MRF scheme. The extensions consist of a) inclusion of prescribed entrainment rate at the top of the boundary layer, b) counter gradient transport of momentum (wind), and c) Prandtl number (i.e. the ratio of diffusivity for momentum and heat) depending on height (see also Noh et al., 2003). As such, we will evaluate whether these modifications circumvent the deficiencies in the MRF scheme. We will refer to this scheme as the YSU scheme.

Finally the third scheme is a 1.5 order closure scheme (MYJ) and uses a prognostic equation for the turbulent kinetic energy (see Stull, 1988; Steeneveld et al., 2008a). Then the eddy diffusivity is determined by multiplication of the turbulent kinetic energy and a length scale. For completeness we mention that we use the Kain-Fritsch cumulus convection scheme, the RRTM scheme for longwave radiation, the Dudhia scheme for shortwave radiation, and the WSM 3-class simple ice microphysics scheme. In the surface layer we use Monin-Obukhov theory as in Janjic (2000), and the 5 layer simple soil scheme is utilized for the soil.
3.2. Results

We will evaluate model forecasts with eddy correlation observations of surface fluxes of sensible heat \( (H) \) and evapotranspiration \( (L_E) \), and next also the profiles of wind speed \( (U) \), potential temperature \( (\theta) \), and specific humidity \( (q) \). Also, we assess the model’s ability to reproduce the 10 m wind speed and ABL height. Since the model probably needs sufficient time to adapt the initial field to its own model physics, we analyze the forecasts after 24 h for the convective ABL and after 36 h for the stable ABL.

Figure 3.2 shows a clear difference in the forecasted profiles during daytime between MYJ on one hand and the other schemes on the other. A characteristic difference is that MYJ forecasts a boundary layer that is typically too shallow and too cold compared to observations. The non-local schemes MRF and YSU simulate an ABL of 1400 m depth, while it is 700 m with MYJ. Furthermore, in the bulk of the ABL MYJ is typically 2 K colder, and 3 g kg\(^{-1}\) more humid than YSU and MRF, and it is evident that MRF and YSU are in closer agreement with the observations. These findings support previous results (e.g. Berg and Zhong, 2005; Steeneveld et al., 2008a). At the same time it is realized that also the wind speed profiles differ substantially. MYJ and MRF forecast similar wind speed profiles close to the surface, while the YSU model provides stronger wind speed close to the surface, and seems to be in closer agreement with the tower observations. This also holds for the individual components, but the wind direction is correctly forecasted by all schemes.

At night the situation is different (Figure 3.3). Although the YSU scheme was intended to improve the daytime representation of the ABL, it also has a clear impact on the full diurnal cycle, and especially on the representation of the nocturnal low-level jet. Normally this phenomenon is a difficult feature to forecast correctly (e.g. Cheinet, 2005, Steeneveld et al., 2008a). The observed LLJ of 12.5 m s\(^{-1}\) at 200 m altitude is best reproduced by YSU, which
forecasts a LLJ of 10 ms\(^{-1}\) at 200 m height. This is substantially better than MYJ and MRF that forecast a weaker LLJ. The improved representation of the LLJ with YSU originates from its daytime modifications, and it can be explained from the Ekman equations. Stull (1988) explains that the sudden decrease of turbulence friction at sunset starts a rotation of the ageostrophic component around the geostrophic wind. As a consequence a LLJ develops. The amplitude of this LLJ is proportional to surface friction at the end of the day. Since this value is larger with YSU, due to the nonlocal momentum mixing, also the friction drop at the end of the afternoon is larger, resulting in a faster LLJ. Consequently the representation of the nocturnal wind maximum improves.

Contrary to the representation of wind speed, the temperature structure and nighttime cooling is better forecasted by MYJ than by the non-local schemes MRF and YSU. This is due to the fact that the MYJ scheme has a smaller turbulent mixing in the boundary layer, which is preferable for SBL modeling (Steeneveld et al., 2008a). At the same time the surface specific humidity is larger with MYJ and in closer agreement with the observations.

We conclude that in the current study the YSU scheme should be preferred for modeling the diurnal cycle. However, especially the representation of the nighttime boundary layer requires improvement.

Figure 3.2. Modeled and observed potential temperature (a) and specific humidity (b) for 1 July 2006, 12 UTC. Black line YSU, dark grey line: MYJ, light grey line: MRF. Asterisk: Cabauw tower observations, open circles: De Bilt radiosonde observations.

Figure 3.3: Modeled and observed potential temperature (a), specific humidity (b), and wind speed (c) for 2 July 2006, 00 UTC. Black line YSU, dark grey line: MYJ, light grey line: MRF. Asterisk: Cabauw tower observations, open circles: De Bilt radiosonde observations.
Figure 3.4 shows the modeled and observed near surface variables. The diurnal cycle of the sensible heat flux is well modeled by WRF, although it is overestimated by ~50 Wm$^{-2}$ by YSU and MRF at noon. The nighttime flux is correctly modeled, although this is usually problematic for models. The relatively high performance may be attributed to the fact that this case has relative high geostrophic wind speed (~7 m s$^{-1}$), and forecast skill breaks down for weak winds.

WRF forecasts the latent heat flux well, although MYJ evapotranspires more than observed, which is a well known model deficiency of MYJ (e.g. Steeneveld et al., 2008a).

The diversity in modeled sensible heat flux is reflected in the forecasted ABL height: MRF and YSU forecast a deeper daytime ABL that is in close agreement with ceilometer observations. At night the model underestimates the ABL height, both compared to the radiosonde and to the ceilometer observations. However, one should realize that no consensus exists on the determination of the stable boundary-layer height from direct model output.
To summarize we find that mesoscale models are well able to reproduce (at least for the current case study) the main characteristics of the boundary layer and its diurnal cycle. However, the model results for stable conditions diverge due to difference in model assumptions. Further research is needed, especially in nighttime conditions (Holtslag, 2006).

4. DIFFICULTIES OF THE STABLE BOUNDARY LAYER

The most relevant processes in the SBL are turbulence, radiative transfer, an elevated nighttime wind maximum (“low-level jet”) near the top of the stable boundary layer (Garratt, 1985), heat conduction in the soil and vegetation, and gravity waves (e.g. Steeneveld et al., 2008b). We will now briefly point out these processes and explain their role.

-Turbulence
Except for the aspect of dispersion and dilution (see section 1), turbulence also plays a role in the determination of the surface sensible heat flux. This is the amount of heat that is transported by the turbulent eddies between the land surface and the atmosphere. The sign of this variable is extremely relevant for air pollution dispersion, since it determines the atmospheric stability. In unstable (daytime) conditions the sensible heat flux is positive (towards the atmosphere), and pollutants are easily vertically mixed and diluted. In stable (nighttime) conditions the sensible heat flux is negative and the sensible heat flux limit the turbulent intensity. Therefore, in stable conditions, pollutants are only hardly mixed or diluted. Thus the sensible heat flux directly governs the mixing regime.

-Longwave Radiative Transfer
Each object that is warmer than the absolute temperature minimum of 0 K emits radiation. This also holds for the air in the atmosphere and in the ABL. Different air layers contain different amounts of absorbing material, such as water vapor, carbon dioxide, ozone etc, and this results in emissivity differences between air layers. The emitted and absorbed long wave radiation differs therefore between the different layers, which consequently results in a net radiative flux divergence, and consequently in net cooling. Especially in the stable boundary layer, the temperature gradients near the surface can become extremely large, and consequently the emitted radiation differs strongly by the different layers (e.g. Hoch et al., 2007; Drie et al., 2007). The potential temperature at a certain level in the atmosphere is amongst others governed by the divergence of the net long wave radiative flux (Rodgers, 1967; Anfossi et al., 1976). Usually a three layer structure is seen in the nocturnal boundary layer: close to the surface a sharp inversion develops due to radiative cooling. In the middle of the SBL, turbulence is dominant and the stratification is limited. Finally, at the SBL top radiative cooling causes a sharp inversion at the SBL top (Garratt and Brost, 1981).

-Soil And Vegetation
At night, conduction enables upward heat transfer from the soil to the surface, and counteracts the surface cooling. On clear nights with weak winds, turbulence cannot be
maintained and therefore both the turbulent sensible and latent heat fluxes vanish. Accordingly, the boundary-layer energy budget is governed by other processes than turbulence. At the surface, the energy budget is in that case solely governed by the net radiation and the soil heat flux. The soil heat flux through the soil depends on the soil material (sand, silt, clay, peat) and the water moisture content of the soil. In the real world, the soil moisture, and thus the soil thermal properties can differ on very small horizontal scales. However, for model applications (see e.g. section 3) the soil is assumed to be homogeneous.

- Elevated Nighttime Wind Maximum

Near the top of the SBL, the wind speed profile is in the idealized case characterized by a small air vertical layer with wind speeds larger than the geostrophic wind speed in the free atmosphere above the ABL. This may occur over large horizontal distances. During daytime, the mean flow is determined by the pressure gradient force, the Coriolis force and the friction that is generated by the ABL turbulence. However, during sunset the turbulent drag suddenly decreases rapidly and the equilibrium is disturbed. As a consequence, the air accelerates in response to the lack of friction in the ABL. The resulting low-level jet (LLJ) or nocturnal wind maximum can act as a second source (beyond the production by near surface wind shear) of turbulence in the stable boundary layer due to the shear above and below the wind speed maximum. On the other hand, the LLJ can also act as a lid on the SBL, because transport across the LLJ is inhibited (Mathieu et al., 2005; Cuxart and Jiménez, 2007), and the LLJ height is thus a relevant height for atmospheric dilution.

- Gravity Waves

A common feature in stably stratified geophysical flows is the ability to support gravity wave propagation (Nappo, 2002). Einaudi and Finnigan (1981) define gravity waves as essentially coherent structures (mainly horizontally propagating) with a speed mostly much less than of the mean wind with horizontal scales less than 500 km and times scales less than a few hours. Gravity waves can be generated by a variety of features: sudden surface roughness changes, convection, and undulating topography, on which we will focus here. Indeed these wave (type) motions are widely observed during special observational campaigns in CASES-99 (Newsom and Banta, 2003). Since gravity waves are able to redistribute energy and momentum, they are important in determining the vertical structure of the atmosphere and the coupling of mesoscale motions to the microscale phenomena.

- Interactions

Figure 4.1 illustrates the above mentioned processes in the SBL, and their interactions (as far as understood at the moment). The main SBL forcings are the pressure gradient force, the Coriolis force, cloud cover, and free flow stability. For example, an increased geostrophic wind speed will enhance the turbulent mixing, and thus give reduced stratification. A reduced stratification will reduce the magnitude of the surface sensible heat flux in the weakly stable regime, and also limits the radiation divergence and thus the clear air radiative cooling. However, in the very stable regime, a reduction of the stratification might result in increased surface sensible heat flux. In both cases the surface energy budget is also altered, resulting in a modified soil heat flux. In the case of ceasing turbulence, the magnitude of the soil heat flux
increases and vice versa. Moreover, this will alter the surface temperature and therefore the outgoing long wave radiation, and so the stratification.

In addition, increased geostrophic wind will under certain conditions increase the impact of wave drag over due to the orography, which at first increase the cyclone filling and thus reduce the geostrophic wind. On the other hand, it will also enhance the low-level jet wind speed. This consequently might result in additional downward turbulent mixing from the jet, which impacts on the stratification again.

One can imagine that the myriad of complex interactions between processes in the SBL have contributed the fact that our current understanding is limited. Therefore, also the representation of the stable boundary layer in atmospheric models in use for weather forecasting, climate and air quality is limited. This regularly results in biased forecasts of weather, air quality and climate (see also section 3).

Figure 4.1. Overview of processes in the stable atmospheric boundary layer and their interactions. Positive interactions are full lines, negative feedbacks are dashed lines (Steeneveld, 2007).
Air quality forecasts are made based on the meteorological variables forecasted by mesoscale models as WRF in Section 3. Apart from the translation of pollutants by the mean wind, pollutants are also mixed away from the plume centerline due to the turbulent nature of the flow. Therefore, the weather dependent dispersion parameters in the $x$, $y$ and $z$ direction $\sigma_x$, $\sigma_y$, and $\sigma_z$ have to be determined to forecast the dispersion of pollutants, such as with Eq. (1.1).

The numerical values of the dispersion parameters depend on the isotropic behavior of the turbulence. In neutral conditions, the dispersion occurs at the same rate in all directions and the turbulence is isotropic. Contrary, for unstable conditions with large thermals in the ABL, the turbulence is evidently anisotropic and $\sigma_x$, $\sigma_y$, $\ll \sigma_z$. However, in stably stratified conditions, vertical motions are suppressed and the turbulence is anisotropic ($\sigma_z$, $\gg \sigma_x$). Since vertical displacement in stratified conditions is limited, one can expect that the dispersion will take place dominantly in the lateral direction. Taylor (1921) derived for the lateral dispersion parameter:

$$\sigma_y^2 = 2\sigma_v^2 \int_0^t (t-\tau)R_1(\tau)d\tau,$$  \hspace{1cm} (5.1)

in which $\sigma_y^2$ is the variance of the lateral wind speed, $t$ is the time after particle release and $\tau$ the time lag over which the Lagrangian auto-correlation function $R_1(\tau)$ has to be determined. For well behaved continuous turbulence, this function is a decaying exponential function. This means that the longer the time difference between particle release is, the lower is their correlation in lateral spread. Note that $T_L = \int_0^\infty R_1(\tau)d\tau$ is defined as the Lagrangian time scale. This is a measure how quickly flow direction of emitted particles become uncorrelated with itself (Stull, 2000). For an exponential decay the integral converges to a finite value, and is therefore $T_L$ is a useful parameter in dispersion models.

At the moment, the behavior of $R_1(\tau)$ and $\sigma_y^2$ under stable condition is under investigation. In this section we determine $R_1(\tau)$ and $\sigma_y^2$ from field observations, as function of classes of atmospheric stability. We utilize long-term observations of a sonic anemometer at 3.44 m above a short grass field in Wageningen, The Netherlands (Jacobs et al., 2003, 2006). The eddy covariance processing software of Van Dijk et al. (2004) is utilized to obtain turbulent fluxes. For this particular study we use the observations for 2006.

The $\sigma_y^2$ at level $z$ can be parameterized from mesoscale model output (since the mesoscale models provide friction velocity $u_*$, sensible heat flux $H$, and thus the Obukhov length $L = -\rho c_p T u_*^3/(g H)$) as follows:

$$\sigma_y^2 / u_* = f \left(\frac{z}{L}\right)$$  \hspace{1cm} (5.2)
The functional form of $f$ is uncertain for stable conditions due to large measurement uncertainties for weak wind conditions (e.g. Mahrt et al., 1998; Mahrt, 1999), and due to self correlation between the dependent and independent variables (Hicks, 1978; Baas et al., 2006). To overcome measurement uncertainties, we selected atmospheric conditions with $U_{10} > 3.0$ ms$^{-1}$ in the following analysis.

Figure 5.1 shows $\sigma_u/u_* \sim 2.2$ for neutral conditions ($z/L=0$), which is consistent with findings of Stull (2000), slightly above the range in a review by Banta et al. (2006) who found that $1.6 < \sigma_u/u_* < 2.1$. More interesting is that for larger stability (i.e. larger $z/L$), $\sigma_u/u_*$ increases, and thus that the variability of the lateral wind speed increases. Finally, we also mention the large uncertainties of these type of observations as shown by the error bars. This uncertainty also increases with stability, due to the fact that turbulent fluctuations are more difficult to measure accurately for stronger stability. It is also therefore that several authors report different empirical formula for Eq. (5.2). The current data analysis suggests 

$$\sigma_u/u_* = 2.2 + 0.86 \frac{z}{L}.$$  However, earlier work by Pahlow et al. (2001) propose

$$\sigma_u/u_* = 2 + 4 \left( \frac{z}{L} \right)^{0.6}.$$ Note that from a theoretical point of view the dimensionless ratio $\sigma_u/u_*$ should become constant for strong stratification (Nieuwstadt, 1984), although none of the parameterizations show this behavior. This is probably caused by the instrumental problems for large $z/L$. Future developments in improving scaling relations for stable conditions will depend on instrument development and refinement of data treatment procedures. For example, Hiscox et al. (2006) measured the plume spread under stable conditions with the innovative lidar technique. This technique has the advantage that dispersion parameter can be obtained with high temporal frequency and directly for a volume.

Figure 5.1. Observed relation between dimensionless lateral velocity variance and atmospheric stability as expressed by $z/L$. Observations for 2006 at the Wageningen field, The Netherlands, are 30 min. averages, and after data screening (see text). Dashed line: Pahlow et al. (2001).
Although the dispersion is controlled by the Lagrangian autocorrelation function, $R_1(\tau)$ is often derived from the Eulerian autocorrelation function by a conversion in time (e.g. Tennekes, 1982). For well behaved turbulent conditions, as for Fig 5.1, the autocorrelation function $R_1(\tau)$ shows a quick decay with delay time. This is illustrated in Fig 5.2a that shows $R_1(\tau)$ for 0-6 UTC at DOY 61 at the Wageningen station. The mean wind amounts about 3-4 ms$^{-1}$ and is from western directions. After approximately 300 sec the $R_1(\tau)$ amounts about 0, as in agreement with the findings of Anfossi et al. (2005).

This picture changes when one considers a more stably stratified night, e.g. 2 Jan 2006 (Fig 5.2b), with mean 10 meter winds of 0.5-1 ms$^{-1}$ from eastern directions. $R_1(\tau)$ now shows a clearly different: $R_1(\tau)$ decreases with $\tau$, but much more slowly than in Fig 5.2a, which means that the wind speed and direction of released particles persistent over a longer time period than for the continuous turbulence. At about 600 sec $R_1(\tau)$ shows a zero crossing. The physical meaning of $R_1(\tau) < 0$ is that particles become anti-correlated, i.e. a particle that has recently been released travels eastwards relative to the coordinate system, while the parcel that was released 800-1000 sec before travels westwards. This is an indication that the flow in the boundary layer is meandering. Finally, only after 1400 sec $R_1(\tau)$ tends to zero. Note that our findings correspond to findings in Anfossi et al. (2005) (their Figure 3).

Meandering flows complicate our ability to model dispersion of pollutants in the atmosphere, because the common methods (i.e. Gaussian Plume Model) are not equipped for this flow type because they assume a linear plume center line. The previous analysis stresses that accurate air quality forecasting needs information on the presence of meandering and if possible also on the time scale of the meandering, i.e. the period.

Figure 5.3 relates the observed minimum value of $R_1(\tau)$ to the wind speed, using half year of observations. It is clear that low wind speeds support substantial negative $R_1(\tau)$, and thus meandering, while for wind larger than 4 ms$^{-1}$ $R_{\text{min}}$ is large. Between wind speeds of 1.5 and 4 ms$^{-1}$ large uncertainty exists on $R_{\text{min}}$, because meandering can apparently not only be described by wind speed, but likely also atmospheric stability is relevant. The current findings for $R_{\text{min}}$ correspond to earlier findings of Anfossi et al. (2005)
Figure 5.2. Observed autocorrelation functions of lateral wind speed component for 1 March 2006 (a) and 2 Jan 2006 (b), 0-6 UTC in Wageningen, The Netherlands. Numbers on top of the graph indicate mean wind speed (first row) and direction (second row) for the corresponding autocorrelation function for the consecutive hours.

Figure 5.3. Observed $R_{min}$ for the year 2006 (0-6 UTC) at the Wageningen station as function of 10 meter wind speed.
5.2. Intermittency in Stable Boundary Layers

Until now we found a clear difference in understanding of stable boundary layers: fully turbulent stable boundary layers are reasonably understood, but our understanding is poor for calm and very stratified conditions. However, for weak wind conditions \((U < 3 \text{ m s}^{-1})\), turbulence is often discontinuous, and of intermittent nature (Holtslag and Nieuwstadt, 1986), and the exchange of heat and momentum may occur in so-called “bursts”, i.e. short episodes of increased turbulence (e.g. Kondo 1978; Weber and Kurzeja, 1991; Van de Wiel, 2002), also known as global intermittency. This coincides with rapid changes in wind speed and temperature. Different physical mechanisms have been suggested to explain the global intermittency. First large shear stress at the low-level jet (LLJ) causes locally increased turbulence that can be transported downwards (Mahrt, 1999). Secondly, passing gravity waves alter the wind speed during passage, and might generate turbulence (Duynkerke, 1991; Nappo, 1991). Thirdly, Businger (1973) explains the global intermittency by decoupling of air in strong stratification so that momentum fluxes are suppressed. Subsequently the pressure force accelerates the flow, and recouples the flow with the surface for several times.

Beyond the exact mechanism, the horizontal extent of this phenomenon is unknown, although this is very relevant for turbulent flux calculations in atmospheric models and dispersion calculations. Intermittently turbulent patches might only occur in a part of a grid cell (Mahrt, 1987). Then, the grid averaged wind speed and temperature gradients are not uniquely related to the mean surface fluxes, and atmospheric models break down (Mahrt, 1998).

Let us illustrate the phenomenon and spatial extent of the intermittent night of 15/16 November 2002 in The Netherlands. The Netherlands were situated in between four weak low-pressure areas and experienced weak winds (typically 2-3 m s\(^{-1}\)) from the southeast.

A) Single Station Observations: The Wageningen Field

At 1830 UTC the screen level temperature drops sharply (from 7 to 2.5°C), and ~1 hour later increases again to 7°C, although the forcing by the long wave incoming radiation (e.g. clouds) does not change (Figure 5.4). Longwave outgoing radiation follows these temperature oscillations. At 2100 UTC another temperature decrease was observed of the same magnitude. Striking is that the temperature decrease occurs while the clouds are coming in, as can be seen in the longwave downwelling flux (LWD). After 2200 UTC the temperatures at 10 cm and screen level are the same. The recorded temperature oscillations coincide with oscillations in wind speed, soil heat flux and wind direction (not shown): high temperatures coincide with a temporary wind speed increase. The surface ground heat flux is less negative during a burst (period of increased turbulence) than during calm conditions. Wind direction shows a small veering when a temperature is increased. Both fluxes of momentum, sensible heat and latent heat are strongly reduced when low temperatures are observed. This overall picture seems to be typical for the Businger (1973) mechanism.

Because little is known whether this phenomenon is locally driven or is present on a larger scale, we use the routine weather observations in The Netherlands (a 300 x 400 km area) to examine the horizontal scale of these events. Observations from coastal station were discarded because they might be influenced by the sea-land transition.
Figure 5.4. Observations of screen level wind speed (U), temperature (T at 1.5 m and 10 cm.), longwave upwelling (LWU) and downwelling (LWD) radiation components at the Wageningen field.

**B) Spatial Development**

To investigate the horizontal extent of the observed oscillations, the 10 min. averaged temperature signal from the 32 automatic weather stations were moving average (MA) filtered with a 2 hour window to suppress the fluctuations of higher frequency. Next, we applied a 30 min MA filter. The resulting signal is used to determine the amplitude, period and number of oscillations at various stations. Figure 5.5 shows the 2m temperature perturbation as observed in Wageningen, Soesterberg and De Bilt (see Figure 5.5d for the locations). Although the different stations are located far apart, and also located over different landscapes and land use, we find a surprising correspondence of the frequency and amplitude of the temperature oscillation.
Figure 5.5: MA filtered temperature signal in Wageningen (a), Soesterberg (b) and De Bilt (c) for the night of 15-16 November 2002. (d) Map of The Netherlands.

Comment [x1]: !!!!!!!!This figure is missing!!!!!!!!!
b) Figure 5.6. Contour plots of maximum temperature perturbation amplitude with 0.8 K as threshold (a), spectral energy (b) and wave period (c).

C) Wavelet Analysis

To analyze the results in section b) with a more objective measure for its intensity, we applied a Morlet wavelet analysis on the temperature observations (Torrence and Compo, 1998). To summarize the information stored in the observed variance, Figure 5.6a shows the maximum temperature perturbation and Fig. 5.6b the integrated variance between 1800 UTC and 2200 UTC over the time scales between 0 and 160 minutes (about 3 hours) for each station. In this manner we neglect the high frequent transition form day to night and the high frequent temperature change due to incoming clouds. The spatial development of the time integrated temperature variance clearly shows that this method confirms the results from section b). Also, Fig. 5.6c shows that the period of the oscillation is approximately similar at
all locations where it has been observed. In this case intermittency is seen in a larger area than
by Kurzeja and Weber (1991) who found intermittency in an at least 30 x 30 km area.

To summarize, global intermittency can occur over large spatial scales (here at least 100
x 100 km). Unfortunately, we are unable identify the physical mechanism of the oscillations.
Local observations at the Wageningen field indicate the Businger mechanism as a possible
mechanism. However, because we can translate the oscillation to De Bilt and Soesterberg,
and because we also found that the phenomenon travels (phase speed about 10 ms^{-1}, not
shown) faster than the typical wind speed (2 ms^{-1}), we also have strong indication that a wave
motion may initiates the oscillations.

**D) A Climatology of Intermittency of Nighttime Turbulence.**

For parameterization purposes in atmospheric models, it is important to know the relative
occurrence of the intermittency in the stable boundary layer, since established methods fail
under these conditions. In very stable conditions, the total turbulent heat transfer can occur in
short bursts: only a few time slots are responsible for the main transport. Then, universal
relations between vertical gradients of wind speed and temperature on one hand and turbulent
fluxes on the other hands are absent, and a more statistical approach could be fruitful (Poulos
and Burns, 2003). Here we will briefly summarize the available tools in the literature, and
provide a climatology of these intermittency indices for a grass field in the Netherlands.

Statistical tools for describing intermittency intensity are:

a) Coulter and Doran (2002) define the *Intermittency fraction* (IF) as the time in which
the individual 1-min fluxes make up the first 50% of the total integrated flux when
accumulated over a certain averaging time. The index ranges from 0 to 0.5, and the
lower the fraction, the stronger the degree of intermittency. In the current analysis we
use 5 min averaged fluxes to examine the degree of intermittency in hourly records.
b) Kurzeja et al. (1988) define a *Gravity wave index* (GWI) for indicating the
intermittency of the turbulence. It is the standard deviation of the vertical velocity
spectrum with a time scale larger than 90 seconds, divided by the total vertical
standard deviation. This index must be derived from power spectra, and if gravity
waves are important the GWI will be much smaller than 1, while GWI will approach
1 for very turbulent cases.
c) Kurzeja et al. (1988) also defines a *Meandering index* (MI) the standard deviation of
the lateral velocity spectrum with a time scale larger than 90 seconds, divided by the
total standard deviation (Nieuwstadt, 1984). This index must also be determined
from power spectra. If meandering occurs, then MI << 1, and the MI will approach 1
for very turbulent cases without meandering.
d) Van de Wiel (2002) defines a Π parameter that is based budget equations for a bulk
model of the stable boundary layer. A bifurcation analysis showed for this system
dynamics approach that Π < 1 indicates intermittent oscillations. Despite the solid
theoretical background of this index, it needs many parameters as input that are
usually not or only known with limited accuracy. These are e.g. pressure gradient,
boundary layer height, surface resistance of the vegetation layer, heat capacity of the
vegetation.
The availability of different indices already indicates that a single index has not proven to be decisive until now.

The observed histograms for the listed indices are depicted in Figure 5.7 and 5.8. We find that the IF has its median around 0.40, and the distribution is heavily skewed. Only 20% of the data has an IF < 0.32. Thus, only a small percentage of the studied nights shows a strong intermittency. The same holds for the Π parameter, which is skewed towards positive values. The criterion for intermittency has been fulfilled for 6.3% of the nights. For MI, only 4.7% of the observations have an MI < 0.7, indicating that meandering is rather scarce according to the criterion. From the analysis of Figure 5.3 we found that 36.6% of the observations shows \( R_{\text{min}} < -0.2 \), and 7.9% showed \( R_{\text{min}} < -0.4 \). As such, MI and \( R_{\text{min}} \) analysis seem to provide consistent results. The GWI is smaller than 0.9 for 6.6% of the time, and the occurrence of intermittency is thus scarce according to the GWI definition.

For all these indices, one must be aware that under very stable conditions, i.e. for which these phenomena are likely to occur, it is more difficult to perform accurate measurements. Therefore one should be careful with the interpretation of the observations.

It is important to remark here that for direct applications in atmospheric models, the degree of intermittency should be expressed in model variables. We attempted to do so by linking the above indices to for example the Richardson number. Although a clear correlation between IF and Ri was found (smaller IF for larger Ri), the substantial data scatter impeded us to find a mathematical expression with sufficient degree of confidence.

The current data analysis was only possible for a single observational field. It is of substantial scientific interest to further study the spatial and temporal development of the intermittency phenomenon. The climatological study Lin et al. (2007) shows that the nighttime stratification in the Oklahoma mesonet observations has substantially decreased during the last decade. Therefore, also climatological trends of intermittency could be expected, and should be analyzed in the near future.
Figure 5.7. Histogram of the intermittency fraction IF (a) and PI (b) as calculated from field observations in Wageningen, The Netherlands over the years 2001-2003.

Comment [x2]: It would be better to have panel a and b on the same page.
6. THE STABLE BOUNDARY-LAYER HEIGHT

The stable boundary-layer (SBL) height ($h$) is an important quantity to describe the relevant processes that govern the SBL development and its vertical structure (Holtslag and Nieuwstadt, 1986). Clearly, the stable boundary-layer height has an impact on the mixing properties of the SBL.

The dispersion of pollutants during stable stratification is strongly affected by $h$ (e.g. Salmond and McKendry, 2005). Release of pollutants below $h$ during periods of weak winds and consequently weak vertical mixing, may result in very high concentrations of primary and secondary pollutants, causing serious consequences for life. Therefore, $h$ is a critical quantity to estimate for meteorological preprocessors in air quality models (Venkatram, 1980; Gryning et al, 1987; Lena and Desiato, 1999; Seibert et al., 2000; Karppinen et al., 2001).

Observing the SBL height ($h_{obs}$) is not straightforward because turbulence is gradually suppressed during stable conditions and it may also show intermittent behavior (e.g. Holtslag and Nieuwstadt, 1986). Vickers and Mahrt (2004, VM04 from now on) found a classical SBL with well-defined surface based turbulence for only 22% of the time for the CASES-99 field campaign. For non-well defined cases, problems occur in measuring $h_{obs}$ because a universal relationship between the profiles of temperature, wind speed and turbulence is lacking. The interpretation of wind speed and temperature profiles is not straightforward in that case, and it is therefore not surprising that several definitions for $h$ are in use nowadays (VM04, Beyrich, 1994).
Despite the uncertainties mentioned above, much work has been done in modeling (scaling) the SBL height ($h_{mod}$) from profile information or from turbulent variables at the surface. However, many of these models have been validated for a limited range of boundary-layer heights or for a single data set. The aim is to present a robust and practical formulation for $h$ based on the governing variables, and based on formal dimensional analysis instead of inverse interpolation. Finally, we discuss and assess the relevance of the Coriolis parameter in practical estimates for $h$.

6.1. Background

The subject of defining and modeling the SBL height has a long history. Well-known definitions for $h$ are (e.g. VM04):

a) a fraction of the layer through which turbulence exists (Lenschow et al., 1988),
b) the top of the downward turbulent sensible heat flux (Caughey et al., 1979),
c) the lowest maximum of the wind speed (often referred to as the Low-Level Jet, LLJ, Melgarejo and Deardorff, 1974), and
d) the top of the temperature inversion or the first discontinuity in the potential temperature profile (Yamada, 1979).

Seibert et al. (2000) state that no final answer is received to the question what is the most suitable height scale to characterize the vertical mixing in the SBL. In principle also subsidence and baroclinicity determine the value of $h$ (Zilitinkevich and Baklanov, 2002; Zilitinkevich and Esau, 2003). However, routine observations of subsidence and baroclinicity are usually unavailable and are therefore not taken into account in this study. Note that the technique of dimensional analysis we use in the second part of the paper is also applicable to other definitions of $h$.

Inspired by the fact that consensus on the SBL height modeling is currently lacking, we use dimensional analysis by using the Buckingham $\Pi$-theorem, without prescribing some particular shape. As governing variables for $h$ we choose (inspired by Zilitinkevich and Mironov, 1996) the surface turbulent buoyancy flux $B_s$, the surface turbulent friction velocity ($u_*$), the Coriolis parameter $f$, the Brunt-Väisälä frequency above the ABL. Note that the $\Pi$-theorem is semi-empirical and only applicable in the range of available observations.

6.2. Observations

Many models for $h$ have been proposed based on a single dataset or on datasets biased towards shallow boundary layers (VM04), and thus universality is not a priori guaranteed for these models. Contrary, the analysis in this paper is based on six observational data sets over different terrain types according to their surface roughness and land use:
a) CASES-99

This measurement campaign was held October 1-31, 1999 near Leon, east of Wichita, Kansas, U.S.A. (37.6486° N, -96.7351° E, and 430 m ASL, Poulos et al, 2002). The area is relatively flat prairie grassland, free of obstacles. We determined $h$ for the 101 profiles using the method in Joffre et al. (2001). They identified $h$ subjectively by inspecting together the wind speed, potential temperature and Richardson number profiles for clear changes below the inversion height that would indicate a change in the structure of the lower atmosphere. This is illustrated in Figure 6.1 for 0700 UTC 23 Oct 1999. The SBL height was based on (1) the LLJ height and ($h_{LLJ}$) and (2) the height of the first discontinuity in the potential temperature profile ($h_0$), from curved to linear in Figure 6.1a. Figure 6.1b illustrates the first peak in the gradient Richardson number at that level. If $h_{LLJ}$ and $h_0$ differ more than 60 m, the data points were rejected. In addition, we selected data for $N > 0.015$ s$^{-1}$, since weaker $N$ could not be determined accurately. The reliability of eddy covariance measurements (10 min. averages) for weak turbulence is questionable, and therefore we disregarded data with friction velocity $u_* < 0.04$ m s$^{-1}$ and sensible heat flux $H > -2$ Wm$^{-2}$.

Figure 6.1. Profiles of potential temperature, wind speed (a) and gradient Richardson number (b) for 23 October 0700 UTC during CASES-99. The arrow indicates the stable boundary-layer height. © American Meteorological Society
b) Sodankylä

This radiosonde dataset is based on the intensive campaign of the international NOPEX/WINTEX program at the observatory of Sodankylä, Finland (67.4° N, 26.7° E, 180 m ASL) between 10-21 March 1997 (Halldin, 1999). The observations were carefully selected by Joffre et al (2001). The terrain around the site is mostly flat, characterized by isolated gently rolling hills (altitude differences 50-150 m), and is covered by sparse forest (mean tree height of ~8 m around the site). The immediate vicinity of the mast was characterized by semi-open pine forest with a mean height $H_r = 8$ m.

c) Cabauw

The first Cabauw dataset has been gathered in the period 1977-1979, The Netherlands (51.971 °N, 4.927 °E; -0.7 m ASL), by Nieuwstadt (1980b), and used in VH96. The data were carefully selected (e.g. filtered for gravity waves) before in VH96.

The Cabauw area is flat and covered with grass with an overall roughness length of 0.20 m (De Rooy and Holtslag, 1999; Van Ulden and Wieringa, 1996). Contrary to the other datasets, the SBL height for this dataset has been observed with a sodar with an uncertainty of about 40% (VH96). However, Arya (1981) and Hicks et al. (1977) found that $h_{LLJ}$ is probably a suitable alternative to represent the observed $h$ with a sodar.

A second Cabauw dataset (‘Cabauw2’) was gathered between August 2003 - April 2004. In this case the observed SBL height was derived from the method described in VH96 instead of the use of a sodar.

d) SHEBA

The SHEBA dataset was obtained over the Arctic ice pack north of Alaska between October 1997 and October 1998. Ice Station SHEBA drifted from approximately 75°N, 144°W to 80°N, 166°W. For this site, $h_{LLJ}$ as observed from radiosondes was taken as $h_{obs}$ provided that this height was also supported by a ‘discontinuity’ in the $\theta$ profile. Similar selection criteria as for CASES-99 have been applied, but with the additional restriction that RH < 0.985 to eliminate the frequently occurring saturated conditions.

e) SABLES98

The final dataset was gathered during the SABLES98 measurement campaign at the CIBA site (41.49°N, 5.47°W, see Cuxart et al., 2000). The observations consist of wind and temperature profiles from regularly launched radiosondes, and from sonic anemometers at 5.8, 13, and 32 m mounted on a tower.

6.3. USING DIMENSIONAL ANALYSIS FOR DERIVATION AN EQUATION FOR THE STABLE BOUNDARY LAYER HEIGHT

A) Three Dimensionless Groups

On the basis of earlier works, we identify that the relevant quantities to describe $h$ are $u_*, f, B_s$ and $N$. Using the Buckingham $\Pi$ theory (e.g. Langhaar, 1951) we find three dimen -
sionless groups:

$$
\Pi_1 = \frac{|B|}{hf u_* N}, \quad \Pi_2 = \frac{kh|B|}{u_*} = \frac{h}{L}, \quad \text{and} \quad \Pi_3 = \frac{N}{f}.
$$

Consequently we may determine the functional form of the surface that describes the relationship between $\Pi_1$, $\Pi_2$ and $\Pi_3$ from observations. This should be a universal relationship if all relevant quantities are included.

Figure 6.2a shows $\Pi_1$ versus $\Pi_2$ on a linear scale for different classes of $\Pi_3$, using Sodankylä observations. Despite the small number of data per class, $\Pi_2$ clearly increases with $\Pi_1$, but levels off at different values for different classes of $N/f$. This relevance of $N/f$ was already mentioned by Kitaigorodskii and Joffre (1988). Note that no data are available for $N/f < 50$ and $N/f > 300$. Furthermore we remark that the plotted dimensionless groups in Figure 6.2 have common terms, and the risk of spurious correlation exists (e.g. Baas et al., 2006). However, it turns out that by randomizing the current datasets the scatter increases. Moreover, below we also use dimensional plots to confirm the performance.

On a log-log scale (Figure 6.2b), we can determine the different slopes for different classes of $N/f$. We propose to fit the data according to $\Pi_1 = d\Pi_2^{\alpha - \beta_1}$. Applying this result and after some re-arrangement we find for $h$:

$$
\lambda = \left( \frac{\frac{1}{\lambda} \frac{\partial}{\partial \theta} \left( \frac{\partial}{\partial \theta} \right) - \frac{C_1}{\lambda} \frac{\partial}{\partial \theta} \right) \right)^{\lambda}
$$

with $\alpha = 3$, $\lambda = \left( C_1 - 0.001 N/f \right)^{-1}$, and $C_1 = 1.8$. The calibration for $\alpha$ and $C_1$ is discussed in detail below, $L$ is the classical Obukhov length (thus including the Von Kármán constant). Note that the innovative aspect of this equation is that the exponent is not constant, but it depends on one of the dimensionless groups. The numerical value 0.001 in $\lambda$ was found by plotting the slopes in Figure 6.5b for different classes of $N/f$ (not shown). In addition, the obtained coefficients (based on Sodankylä observations) were confirmed by using each half of every dataset for calibration and the other halves for validation.

Considering the applicability range of Eq. (6.1), we have to realize that the denominator in the exponent should be positive, hence $N/f < 1800$. With the $N=0.076$ $s^{-1}$ the maximum free flow stability in the dataset, this corresponds to a latitude $|\theta| > 16^\circ$. In addition both $N$ and $L$ need to be larger than zero.
Figure 6.2. Dependence of observed dimensionless groups $B_s/(f N u^* h)$ versus $h/L$ for different classes of $N/f$ on a linear (a) and logarithmic scale (b). © American Meteorological Society
A Monte-Carlo strategy was followed to estimate $\alpha$ and $C_1$ (on Sodankylä (Figure 6.3a) and on the whole dataset (Figure 6.3b)). A clear minimum in the mean is found in the contour plots with $C_1 = 1.8$ and $\alpha = 3$ as optimal estimates and is confirmed using the other statistical quality measures (not shown), and the parameters in Eq. (6.1) can thus be determined with good confidence.

Figure 6.3. Contour plot of the median of absolute error (MEAE in m) for a range of $C_1$ and $\alpha$ for Sodankylä (a) and the total dataset (b). © American Meteorological Society
b) Verification

In this Section we will verify the performance of Eq. (6.1) against the independent data from Cabauw, CASES-99, SHEBA (Figure 6.4b-d, Table 6.1) and a cross validation for Sodankylä (Figure 6.4a). The good performance for Sodankylä is obvious, since these are the same data as used for the calibration. Nevertheless, it seems that the data collapse onto a single curve. This is not trivial and it gives confidence in the method and the variables that we selected. The model agrees well with the CASES-99 (rmse = 53.6 m, but is largely unsystematic) and Cabauw observations (rmse = 80.3 m with rmse-u = 62.6 m), although the scatter is larger for the Cabauw dataset than for the other datasets. This relatively large scatter is probably inherent to the sodar based observations for Cabauw instead of radiosondes profiles for the other datasets (Section 6.3). For SHEBA the model performance is good (rmse = 40.3 m of which 37.6 m is unsystematic), although the model seems to underestimate the observations slightly (Figure 6.4d). Overall, the magnitude of FB < 0.15, which is not achieved for any of the other proposals, and IoA is larger than for Eqs. (6.1) and (6.2). The main improvement by Eq. (6.1) is achieved for shallow boundary layers. In addition to the evaluation of Eq (6.1) in Steeneveld et al (2007) we performed additional testing on a dataset of Cabauw from In addition we tested the Eq. (6.1) on the SABLES98 dataset (Cuxart et al., 2000). The last dataset is gathered in September 1998 over a flat plateau in Spain.

C) On the Relevance of the Coriolis Parameter F: Two Dimensionless Groups Only

The recent literature discusses the variables that govern $h$ (Kosovic and Curry, 2000; Kosovic and Lundquist, 2004). Although $f$ should theoretically play a role in governing $h$ based on it presence in the Ekman equations (at least for neutral boundary layers), we can discuss the relevance of $f$ as compared with $N$ in practical application for the SBL as mentioned in VH96 and Zilitinkevich and Baklanov (2002).

Since free flow stability is always present in the atmosphere and is of order $O(10^{-2})$ while $f$ is typically $O(10^{-4})$, VH96 suggest that the impact of $f$ can be neglected in practice. Mahrt and Heald (1979) and VM04 also argue that the Coriolis parameter is of minor importance since the SBL development is governed by an inertia oscillation. In that case, a pure Ekman boundary layer does not exist and thus the use of $f$ is doubtful.

In addition, if we analyze sodar observations during so-called intermittent nights (e.g. during CASES-99, Van de Wiel, 2002), we find that the boundary-layer turbulence and also the boundary-layer height responds quickly ($< 10$ min) to a change of the near surface turbulence intensity if decoupling from the surface occurs. This suggests that the SBL can react on a timescale much shorter than $f^{-1}$ which is believed to be the governing timescale for the SBL (Nieuwstadt and Duynkerke, 1996). This implies that $f^{-1}$ is not a priori the most dominant timescale for the SBL growth, but that timescales that originate from the interaction with the surface may be more important. Estournel and Guedalia (1990) and VM04 suggest that the roughness length for momentum ($z_0$) is a relevant quantity. Consequently, the relevance of $f$ and $z_0$ will be examined below.
Figure 6.4. Observed and modeled stable boundary-layer height using Eq. (6.1) for Sodankylä (a), CASES-99 (b), Cabauw (c), SHEBA (d), Cabauw2 (e), and SABLES98 (f). Panels a-d: © American Meteorological Society.
Due to the variable nature of $h$, it is useful to adopt statistical techniques to gain insight into the relevant quantities that govern $h$. In this section, we perform a principal component analysis (PCA) on $h_{\text{obs}}$ from all datasets to obtain information about the relative impact of the different variables on $h_{\text{obs}}$. Recall that PCA is a statistical technique in which the total variance of a dataset is decomposed along orthogonal vectors by determining the eigenvalues and eigenvectors of the covariance matrix between the variables. These eigenvectors are sorted in descending order according to the eigenvalues. The eigenvector associated with the largest eigenvalue is called the first principal component (FPC), the second large is called second principal component (SPC), etc. Finally, the data are transformed back into real space, and correlated to the original variables.

Table 6.1. Overview of statistical measure for the new proposals for the SBL height

<table>
<thead>
<tr>
<th>Equation (6.1)</th>
<th>mae</th>
<th>rmse</th>
<th>rmse-s</th>
<th>rmse-u</th>
<th>meae</th>
<th>FB</th>
<th>IoA</th>
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<td>80.3</td>
<td>50.3</td>
<td>62.6</td>
<td>49.9</td>
<td>-0.108</td>
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<td>109.7</td>
<td>77.1</td>
<td>78.1</td>
<td>45.5</td>
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<td>0.831</td>
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<td>53.6</td>
<td>19.0</td>
<td>50.1</td>
<td>33.5</td>
<td>0.114</td>
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<td>39.8</td>
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</tr>
<tr>
<td>SABLES98</td>
<td>43.4</td>
<td>54.3</td>
<td>30.6</td>
<td>44.8</td>
<td>43.0</td>
<td>-0.297</td>
<td>0.562</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Equation (6.2)</th>
<th>mae</th>
<th>rmse</th>
<th>rmse-s</th>
<th>rmse-u</th>
<th>meae</th>
<th>FB</th>
<th>IoA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cabauw</td>
<td>65.1</td>
<td>86.7</td>
<td>57.4</td>
<td>65.0</td>
<td>46.4</td>
<td>0.042</td>
<td>0.795</td>
</tr>
</tbody>
</table>
Table 6.2 shows the absolute values of the correlation coefficients between the observed $u_*$, $N$, $\bar{w}\bar{\theta}$, $f$ and $z_0$ and the FPC. The FPC explained 99.9% of the variance, so the higher principal components can be neglected safely. It appears that the correlation coefficient between $u_*$ and the FPC is large compared to the other coefficients. The quantities $s_w\theta$ and $N$ show a considerably smaller correlation but are still relevant. The Coriolis parameter and $z_0$ have a correlation coefficient of only 0.15 and 0.16 with the FPC respectively. Therefore, the latter quantities are in practice relatively unimportant for $h$ estimation (at least for these datasets). Note that the dominance of $u_*$ gives support to the simple estimate by Koracin and Berkowicz (1988).

Given the discussion above, we may exclude $f$ and $z_0$ from the list of relevant variables, at least for estimation of $h$ in practical applications. Then only two dimensionless groups remain, namely $hN/u_*$ and $hL^*/\bar{L}$ (Figure 6.6a, all data are used). Two regimes can be clearly distinguished. For $hL^*/\bar{L} < 1$ (towards the near neutral limit) $h \propto u_*/N$, in accordance with Kitaigorodskii and Joffre (1988), Van Pul et al. (1994), and VH96.

For $hL^*/\bar{L} > 1$ (towards the very stable limit) the two groups are linearly related on the log-log scale. This means that $h \propto \sqrt{\frac{\bar{L}}{N}}$. Although, it seems that $h$ is independent of $u_*$ in this regime, this is not really the case.

**Table 6.2. Correlation coefficient $r$ between the relevant quantities and the First Principal Component**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$u_*$</th>
<th>$N$</th>
<th>$\bar{w}\bar{\theta}$</th>
<th>$f$</th>
<th>$z_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r$</td>
<td>0.75</td>
<td>0.47</td>
<td>0.37</td>
<td>0.15</td>
<td>0.16</td>
</tr>
</tbody>
</table>
The dependence of $u_*$ comes in via $B_s$, because in the very stable regime the turbulent temperature scale $\theta_*$ is linearly dependent on $u_*$ (Holtslag and De Bruin, 1988; Van de Wiel, 2002). Thus making $B_s$ quadratically dependent on $u_*$ means that $h$ is again proportional to $u_*$, but now with a different factor depending on $N$. Thus our diagnostic equation for $h$ based on the current analysis reads as:

$$h = \begin{cases} 
\frac{10 u_*/N}{32 \sqrt{B_s/N^3}} & \text{for } u_*^2 N/B_s > 10 \\
& \text{for } u_*^2 N/B_s < 10 
\end{cases}$$

Obviously the application of Eqs. (6.1) and (6.2) is limited to cases where $N > 0 \text{ s}^{-1}$.

An alternative formulation is developed with formal dimensional analysis with the same quantities as in the multi-limit equations. The proposed formulation is robust and appears to reduce a significant model bias for shallow boundary-layer heights in comparison with the existing formulations. As such, the proposed formulation appears applicable also for high stability conditions in contrast to existing formulations that primarily are derived for weakly stable cases.

![Figure 6.6a: Relationship between dimensionless groups $hN/u_*$ and $h/L^*$](image)
6.4. An Alternative Theoretically Based Formulation for the Stable Boundary Layer Height

Besides the observational point of view, the SBL height can also be studied more theoretically. The equilibrium SBL height \( h_E \), and its relevance for predicting the SBL structure has been discussed intensively (e.g. Zilitinkevich and Esau, 2003; henceforth ZE03; Steeneveld et al., 2007). Recently, several papers (Zilitinkevich and Mironov, 1996; Zilitinkevich and Calanca, 2002; Zilitinkevich and Baklanov, 2002; ZE03) discuss the relevant processes that govern the SBL height in equilibrium conditions. In these studies, the basic variables governing \( h_E \) are the surface friction velocity \( \*u \), the surface buoyancy flux \( \*w \theta_s \), the Coriolis parameter \( f \) and the free flow stability \( N \). Based on these variables, ZE03 identified three boundary-layer prototypes: the truly neutral \((B_s = 0 \text{ and } N = 0)\), the conventionally neutral \((N\neq 0 \text{ and } B_s = 0)\) and the nocturnal boundary-layer \((N=0 \text{ and } B_s\neq 0)\).

6.4.1. Background

Following the reasoning by ZE03, the SBL depth is defined as the Ekman layer depth \((h_e)\), which is given by the eddy diffusivity \( K_M \) and the Coriolis parameter \( f \) (Stull, 1988):

\[
h_e = \sqrt{\frac{K_M}{f}} \tag{6.3}
\]
For the eddy viscosity $K_M$ ZE03 distinguish between three different boundary layer types, and for each type a characteristic velocity scale $u_T$ and length scale $l_T$:

- Truly neutral: $K_M = u_T l_T = u_T \tilde{h}$
- Conventionally neutral: $K_M = u_T l_T = u_T^2 / N$
- Nocturnal: $K_M = u_T l_T = u_T L$

with $L = -B/\kappa$, the Obukhov length (note the Von Karman constant is not included here).

To obtain an equilibrium height that accounts for all three combined prototypes, the bulk diffusivity $K_M$ can directly be written as:

$$\frac{1}{K_M} = \frac{1}{u_T \tilde{h}} + \frac{1}{u_T^2 / N} + \frac{1}{u_T L}$$  \hspace{0.5cm} (6.7)

Here the proportionality constants are taken 1 for convenience. Consequently,

$$K_M = \frac{u_T^2 \tilde{h} L / N}{u_T \tilde{h} / N + u_T L}$$  \hspace{0.5cm} (6.8)

Combining Eq. (6.8) in Eq. (6.3), solving for $h_\ast = h_E$ and choosing the physical solution in the quadratic equation, we obtain:

$$h_\ast = \alpha \frac{u_T}{N}$$  \hspace{0.5cm} (6.9)

where

$$\alpha = -1 + \sqrt{1 + 4 \left( \frac{u_T}{f L} + \frac{N}{f} \right)}$$  \hspace{0.5cm} (6.10)

The format of Eq. (6.9) was already found earlier in many studies. VH96 found $\alpha$ to be a function of the shear and Richardson number across the SBL, while Steeneveld et al. (2007) derived Eq. (6.10) with $\alpha$ solely depending on the free-flow stability. In any case, Eqs. (6.9) and (6.10) show that $\alpha$ is related to the traditional parameter groups $u_T / (f L)$ (the Monin-Kazanski parameter) and $N/f$ (Kitaigorskii and Joffre, 1988). The numerical value of $\alpha$ is typically 7-13 (e.g., VH96).

Here we compare our result with the proposal from ZE03 that reads as:
\[ h_E = C_R \frac{u'_c}{f} \left( 1 + \frac{C_{uN}^2}{C_{S}^2} \frac{N}{f} + \frac{C_{Ch}^2}{C_{S}^2} \right)^{\frac{1}{2}} \] 

(6.11)

with \( C_R = 0.5 \); \( C_{uN}/C_S^2 = 0.56 \) and \( C_S = 1.0 \). Both proposals will be evaluated against the observations described in the next section.

6.4.3. Results

Results obtained with Eq. (6.11) and Eq. (6.9) with Eq. (6.10) are shown in Figs. 6.7 and 6.8, respectively. Table 6.3 summarizes some statistical quantities for model performance, i.e. mean absolute error (MAE), Systematic RMSE (RMSE-S), median of the mean absolute error (MEAE) and the index of agreement (IoA, Willmott, 1982. The IoA equals 1 for a perfect model performance). Equation (6.9) gives a substantial reduction of the RMSE-S, and an increased IoA compared to Eq. (6.11). Note that for shallow SBLs, mesoscale effects may become important and these may contribute to the bias, since mesoscale effects are not incorporated in the current model. Unfortunately, the proposed interpolation method cannot avoid the negative bias for shallow SBLs.

We realize that the evaluation of the above equations for the equilibrium depth with field data may be troublesome, due complexity of making observations in stable conditions and due to the fact that in reality conditions cannot be controlled. Alternatively, we may consider to explore Large Eddy Simulation results for more controlled testing (as in Esau, 2004). In that case however, we must be aware of the fact that especially in very stable conditions, LES results (profiles of mean and turbulent quantities) are strongly dependent on the model resolution (Beare and MacVean, 2004). Also longwave radiation divergence plays an important role, which is usually not taken into account by LES. Note that the field data used in this study cover a wide range of conditions, including nonturbulent effects such as radiation divergence (e.g. André and Mahrt, 1982).
Figure 6.8. Modeled (Eq. 6.11) vs. observed stable boundary-layer height. © Royal Meteorological Society

### Table 6.3. Statistical Evaluation of SBL height proposals

<table>
<thead>
<tr>
<th>Model</th>
<th>MAE (m)</th>
<th>RMSE-S (m)</th>
<th>MEAE (m)</th>
<th>IoA (–)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eq. (6.10)</td>
<td>78.7</td>
<td>62.9</td>
<td>67.9</td>
<td>0.84</td>
</tr>
<tr>
<td>Eq. (6.11)</td>
<td>100.9</td>
<td>99.3</td>
<td>83.0</td>
<td>0.80</td>
</tr>
</tbody>
</table>

### 6.5. CONCLUSIONS

We propose an alternative method to derive a formula for the stable boundary-layer height when more than one stable boundary-layer prototype contributes to the final boundary-layer height. We directly interpolate the eddy diffusivities of each prototype. The alternative formulation performs well, and reduces the bias of the predicted stable boundary-layer height compared to the original formulation.

### 7. CLOSURE

This chapter discussed the role of the atmosphere, and especially the atmospheric boundary layer on local air quality. We have seen that the background air quality is controlled by the air mass, but that on the local scale the emissions are dispersed under the influence of the boundary layer wind speed, turbulence intensity and the mixing height. These are to a large extent determined by the atmospheric stratification, and these ingredients are required for accurate air quality modeling.

Mesoscale numerical models are used to forecast the local weather conditions that are needed for air quality forecasts. Different model strategies provide different outcome for
turbulence intensity and mixing height. Especially for nighttime conditions (i.e. during stratification) the forecasts diverge between schemes. As such, a research effort into nighttime atmospheric conditions and model improvement is recommended. For example, the intermittent behavior of the nighttime turbulence was shown to be of considerable interest.

Atmospheric dispersion is normally expressed in terms of a weather dependent dispersion parameter. For continuous turbulent conditions, the correlation of lateral movement between released particles soon drops, and becomes approximately zero. However, field observations for calm conditions show meandering flows and intermittent behavior of the turbulence for substantial fraction of nights.

Finally, we discussed the currently available expressions for the nighttime boundary layer height. Recent updates have been validated against field observations, and are ready for use in dispersion models.

Air quality affects the human health and natural and agricultural vegetation, and accurate modeling is requested for correct warnings, and for testing the fulfillment of air quality legislation. Therefore, the current outcome may contribute to further understanding and improved modeling.

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REFERENCES


