Chapter 1

Introduction

1.1 OBJECTIVE OF THE THESIS

The main topic of this thesis is the modeling of the short-range atmospheric dispersion of puffs, a puff being an single instantaneous release of (pollutant, hazardous, or any other) material. The rate of growth of a puff depends on its size; as the puff grows, an increasing part of the spectrum of turbulent eddies will contribute to the puff's enlargement, instead of displacing it as a whole. For short-range applications, when puff sizes are small, this meandering caused by large turbulent eddies dominates the ensemble-averaged dispersion.

Thus the objective of the present thesis is the development of a short-range puff model simulating the instantaneous puff growth apart from the dispersing effect of meandering during the concentration sampling time. Puff growth is adequatly described by relative dispersion parameterizations. The main contribution of this thesis is the development of a scheme to simulate the meandering in three-dimensional space of pollutant puffs. The method adopted is to derive puff center meandering trajectories from stochastic particle paths, supplied by a Lagrangian particle model predicted ensemble-averaged dispersion. That part of the turbulent kinetic energy spectrum which is covered by the puff growth scheme has to be removed from the stochastic particle paths, in order to avoid the double-counting of dispersion. The resulting model approach is called Puff-Particle Model (PPM).

In contrast to relatively dispersing puff models intended for far-field applications like RIMPUFF (Mikkelsen *et al.* 1984) and, which use relative dispersion and aim at resolving the meandering movements by frequently updated flow fields, the artificial meandering of the PPM allows it to be applied in the near field where the small puff sizes would otherwise require flow field updates every few seconds. Several models have been developed based on Gifford's (1959) meandering plume concept to separate the dispersing effect of instantaneous plume (or puff) growth and of meandering (e.g. Hanna 1984, 1986; Savunen and Rantakrans 1997; Sykes 1988). They all have in common that a certain shape of the probability density function of concentration is assumed and that the variance of concentration fluctuations is

derived from the properties of turbulence. SCIPUFF (Sykes 1997) uses a second-order turbulence closure scheme predicting both the mean concentration and its variance. In contrast, the PPM aims at simulating a realistic three-dimensional meandering of the puffs, which allows for the direct determination of the higher moments of concentration, while enabling the individual puffs to account for inhomogeneous conditions.

1.2 ON POLLUTANT TRANSPORT MODELING IN THE PLANETARY BOUNDARY LAYER

1.2.1 Plume, puff and particle atmospheric dispersion models

In this thesis, a number of different studies on air pollution modeling is presented. Atmospheric dispersion is a direct result of atmospheric turbulence. In an Eulerian system, the conservation equation of a scalar quantity (e.g. concentration) contains turbulent fluxes which in general are not known directly. Using K-theory, parameterized eddy diffusivities can be used in order to obtain an analytical solution. When assuming homogeneity, stationarity, and uniform wind speeds regardless of height and eddy diffusivities, an analytical solution can be obtained which is commonly known as Gaussian plume model (e.g. Businger 1982).

Plume models describe the (continuously emitting) release with the use of a plume axis and standard deviations of the pollutant distribution in the lateral and vertical direction as a function of travel time (e.g. Hanna 1982; Sykes *et al.* 1986). The entire plume is always immediately affected by changes of the meteorological conditions at the point of measurement. This lack of causality limits the application of plume models to quasi-stationary conditions beforehand. The major disadvantage of plume models is that their inherent assumptions on homogeneity and stationarity are often not sufficiently fulfilled.

Using a Lagrangian framework, puff dispersion models and stochastic particle models can be distinguished. Puff models cluster the release into consecutively released pollutant puffs. Puffs have a center of mass, which is affected by the flow field, a mass assigned to the puff, and a density distribution (e.g. Mikkelsen *et al.* 1987). Usually, the density distribution is assumed to be Gaussian, so that the concentration can be computed when additionally specifying the lateral, longitudinal, and vertical standard deviations of the density distribution (i.e. puff).

Particle models split the pollutant emission up into discrete particles, which in most cases all have identical masses. The particles act like inertialess infinitely small parcels of air, thus exactly following the local flow field. The particles in these models are assumed to have an additional, stochastic velocity component. When applying 1-particle statistics (Thomson 1987), particle models will predict ensemble-averaged dispersion. This modeling approach allows for non-Gaussian turbulence, especially for the specification of a vertically skewed turbulence probability density function to describe day-time convective conditions (e.g. Luhar and Britter 1989). Using the more complicated 2-particle statistics (Thomson 1990; Borgas and Sawford 1994), relative dispersion is predicted. The major disadvantage of particle models is their need of computing time.

1.2.2 Absolute and relative dispersion

There are two different sampling times, one for the measured meteorological parameters, T_{sM}, and the other for the pollutant concentration prediction, T_{sC}. If the sampling time of an available meteorological information is longer than the desired sampling time of concentration, the dispersion parameterization has to predict the concentration for the concentration sampling time T_{sC}. Then, there is a "gap of dispersion" between T_{sC} and the sampling time of the meteorological input, T_{sM}.

The well-known "absolute" dispersion (so-called 1-particle statistics, or ensemble averaged dispersion), is the ensemble-averaged particle separation with respect to a fixed point in space (Taylor 1921). Richardson (1926) was the first to introduce the concept of relative dispersion, defined as the ensemble averaged separation between pollutant particles released together, i.e. the dispersion around the cluster's center. Gifford (1957a, 1957b) first pointed out that the instantaneous growth of puffs is governed by the concept of relative instead of absolute dispersion. Within the concept of relative dispersion (i.e. 2-particle statistics), turbulent eddies smaller than the actual puff size will contribute to its growth (increasing the ensemble 2-particle separation), while larger eddies move the puff as a whole (without changing the separation of the particles). Mikkelsen *et al.* (1987) derive a set of relative dispersion parameterizations for Gaussian puffs, based on the work of Batchelor (1952).

The missing link between relative and absolute dispersion is the dispersing effect of meandering over time-scales shorter than the averaging time for which the absolute dispersion parameterization applies. Here, "meandering" means movements of the center of the puff or

plume with respect to a fixed point in space. Most formulations of absolute dispersion correspond to an ensemble averaging time of roughly one hour, corresponding to the spectral gap between synoptic and turbulent frequencies. Hence, if $T_{sC} < 1$ hour, or if $T_{sM} > T_{sC}$, or if $T_{sM} < 1$ hour, relative rather than absolute dispersion should be used. For plume or puff models, this means that the meandering has to be treated separately.

1.2.3 Development of the Puff-Particle Model

In order to better understand puff dispersion, in chapter 5 an arbitrary definition of two categories of puff models is introduced. On the one hand, 'plume segment' models, which describe a segment of an ensemble averaged plume by using a puff; their absolute dispersion scheme accounts for the ensemble averaged dispersion (from cluster growth and cluster meandering) during the averaging time T between two consecutive updates of the mean flow field. On the other hand, 'cluster dispersion' models, which interpret a puff as being an instantaneous cluster of pollutants. The spectral gap between turbulent eddies covered by the flow field and those covered by the relative dispersion scheme is simulated with artificial meandering.

The main contribution of the present thesis is the development of the Puff-Particle Model (PPM). The PPM represents the second group of cluster dispersion models. It uses relative dispersion to describe the instantaneous growth of the cluster (puff); the range of turbulent eddies covered by the relative dispersion depends on the size of the cluster. Eddies larger than the cluster will displace the cluster as a whole without dispersing it. This meandering has to be simulated separately.

Within the PPM, the pollutant release is emitted as initially small clusters (puffs), which are advected by the mean wind. Additionally, the puffs exhibit artificial meandering on time scales shorter than the time interval between two consecutive updates of the mean wind field. The dispersing effect of turbulent eddies smaller than the actual size of the puff is described by a relative dispersion parameterization. The turbulent kinetic energy which is not covered by these small eddies is represented by the meandering of the puffs.

There are two ways of looking at the PPM: as a particle model which is speeded up by grouping particles into clusters. The total gain in computing speed is one order of magnitude. (Another factor of 10 can be gained by using an efficient way to estimate the concentration within particle models, see Section 1.2.5). Alternatively, the PPM may be considered as a puff

model with a meandering sub-model, thus allowing the use (and its benefits) of relative dispersion even when frequently updated meteorological information is not available. The basic principle of the PPM, the method to simulate meandering artificially, and a comparison of model results with predictions from other models, are given in Chapter 2

The PPM is a reseach model focussing on the treatment of relative dispersion and puff meandering. Operational puff models like CALPUFF (Scire *et. al.* 1997), U.S. EPA's INPUFF, RIMPUFF (Mikkelsen *et al.* 1984) or SCIPUFF (Sykes 1997), on the other hand, offer a wide range of different parameterizations which are missing in the PPM like, for example, CALPUFF's chemical reaction scheme, RIMPUFF's radiative dose integration capabilities, or SCIPUFF's advanced adaptive grid technique and puff splitting and merging procedures. Besides its main application as a puff meandering model, the PPM can also be driven in a 'plume segment' mode (using absolute dispersion without meandering) and in a 'pure particle' mode.

1.2.4 Avoiding the double-counting of dispersion

The puff-particle approach aims at simulating the dispersing effect of plume meandering by introducing puff center trajectories. These trajectories are determined by the low-frequency part of the turbulence spectrum, since relative dispersion only describes the effects of the high-frequency part. As the puff's size grows, the relative dispersion covers an increasing part of the spectrum (Batchelor 1952; Mikkelsen *et al.* 1987). Therefore, the trajectory of the puff's center of mass has to simulate the effect of a decreasing amount of turbulent eddies, and thus has to become 'smoother' as puff sizes grow.

In the PPM, the stochastic trajectories of the puff centers are derived from (but not identical to) paths of particles as simulated by a fully 3D Lagrangian particle model. The underlying assumption of the particle model employed is that turbulence is a Markov process. This means that the turbulent velocity of any particle at the next time step is fully explained by its current position and velocity. A very effective low-pass filter can be constructed by making use of the fact that the process is Markovian. The corresponding filter eliminates high-frequent stochastic movements and thus produces the required puff center meandering trajectories. These trajectories become smoother (only influenced by large eddies) as the puff grows. The scheme to avoid the double-counting of dispersion is discussed in some detail in Chapter 3.

1.2.5 Density kernels within particle models

In puff models, the computation of a predicted mean concentration at a certain location is done by superimposing the density distributions of all individual puffs at that location. Particle models use a different theory of diffusion than puff models. The Thomson (1987) family of particle models prescribes the (Eulerian) characteristics of turbulence at every point in space, and uses a (numerical) procedure to ensure that the (Lagrangian) motions of the inertialess particles complies with these characteristics. Puff models, on the other hand, aim at separating relative dispersion and dispersion originating from meandering (yielding absolute dispersion). Here, the boundary (a frequency in the spectrum of turbulent kinetic energy) between relative dispersion and dispersion originating from the larger eddies depends on the actual size of the puff in question.

For particle models, it is a common practice to calculate concentration averages over a grid cell in space by counting all particles in a box (a list of examples is given in section 4.2.1). The mass concentration is then obtained by multiplying the number of particles with their mass, and dividing this total mass by the size of the grid box. If the volume average over such a box is what the modeler wants, such box-counting methods are the most efficient.

Often, what is actually needed is the modeled concentration at a given *point* in space. Such point estimations are especially needed when comparing model predictions with measurements from tracer experiments. The “sampling volume” of the concentration measurement units commonly used in such field experiments are by far smaller than the volumes over which the concentration is averaged when employing the box-counting method.

For these reasons, another concentration estimation method is proposed in Chapter 4 of this thesis. It relies on the concept of density distributions of different shape which are ”added” to the particle’s position, i.e. the mass represented by the particle is spread out in space. Such a density distribution around the center of mass is called the density kernel. It has been used first by Lorimer (1986) and Yamada *et al.* (1987) and Yamada and Bunker (1988) within particle models. In the method proposed in Chapter 4, the size (bandwidth) of the kernel distribution is chosen such that the bias and variance of the concentration estimation are jointly minimized.

The kernel method has been widely applied in various fields of science. In atmospheric dispersion modeling, the box-counting method is still used despite its deficiencies. The kernel

method shows most pronounced improvements for concentration predictions in the near-source field, where changes in the particle density are sharp and large proportions of the total number of particles might still be within the volume of few sampling boxes, and for the estimation of surface concentrations, which are of interest for most air pollution simulations, but are likely to show gradients near the surface over distances similar to the vertical extent of box sampling volumes.

Within the PPM, a low-pass filter (which depends on the size of the relatively dispersed puff) removes dispersion from the particle trajectories (cf. previous Section, and Chapter 3). On the contrary, the ”dispersion” added to the model by the numerical kernel bandwidths should not be filtered out of the particle model. It is the smoothing necessary to interpolate between particle positions, and tends to zero as the number of particles approaches infinity, whereas the "overdispersion" (i.e. oversmoothing) caused by the physical sizes remains constant.

1.3 NATURAL VARIABILITY OF POLLUTANT CONCENTRATIONS

1.3.1 Modeling hazardous releases and odor problems

There are different classes of atmospheric pollutants (here, we restrict ourselves to boundary layer pollutants, leaving apart, e.g., gases with greenhouse warming potential). A first group is harmful to the environment (eco-systems, flora or fauna) on a long term basis. Fine particles belong to this first group. The total intake is the important parameter to human health. Whether this intake originates from a high background level or from episodes, is of lesser importance.

The second group can cause impacts on the human health during shorter episodes as well. The main matter of concern is their concentration level during periods of, say, one hour. A member of this group is, for example, ozone. For most species in this group (like NO_x, SO_2, etc.), but not, in general, for ozone, regulatory limits have been imposed both for yearly and (half-)hourly averages (or percentiles thereof). Ensemble-averaged concentration is suited for most applications concerning pollutants from these first two groups.

Atmospheric pollutants of a third group, however, are a health risk on even shorter time scales. Toxic gases can be lethal within minutes or seconds; in general, it is a certain dose (concentration intake integrated over time) which is considered lethal. Such toxic gases can be either emitted during chemical warfare, or as accidental release. Here, the term hazardous

release represents both. Although they do not represent a direct health risk, gases likely to cause odor impacts also belong to this group.

“Assessment of flammability or toxicity on the basis of ensemble-averaged concentrations can be seriously in error. These effects depend on short temporal- and spatial-scale fluctuations and thus the variance is essential for these predictions” (Sykes 1988, p. 354). Short temporal scale effects call for short (concentration) sampling times. This violates a basic assumption of many common air pollution models, since such averaging times are considerably shorter than the spectral gap (approximately one hour). Most models assume that the sampling time is “a time long enough to include most of the turbulent energy spectrum” (Hanna 1982, p. 278).

Often rather than estimating the ensemble-averaged concentration of hazardous material, predictions of a worst-case scenario is needed. This means that the higher moments of concentration have to be predicted as well as the type of distribution, i.e. the probability density function of concentration (which is specific for a given source-receptor configuration, and for a certain concentration sampling time). The need for probability density functions is characteristic for all *a priori* problems (where model outcomes are an input to decision making), in contrast to the more frequent *a posteriori* problems (where a concentration average suffices).

1.3.2 Plume and puff meandering models

„Surprisingly little work has been done in the proper application of statistical analysis techniques to the evaluation of models. Even fewer people recognize that an observed pollutant concentration, averaged over a time, T_a, is a turbulent variable“ (Hanna 1986). Dispersion models, on the other hand, usually predict an ensemble-mean concentration, which cannot be expected to agree with a single observed concentration even if the model were „perfect“.

Many researchers assume a two-scale system where the (turbulent) concentration fluctuations are due to (i) in-plume turbulence; and (ii) intermittency, i.e. meandering of the plume, leading to periods of zero concentration. This two-scale system is based on Gifford’s (1959) fluctuating plume theory, which assumes that a narrow plume with an instantaneous standard deviation σ_{yI} meanders back and forth to give the total standard deviation σ_{yT}. The standard deviation of the meandering motions is σ_{yM}, and the three standard deviations are related by

$\sigma_{yT}^2 = \sigma_{yI}^2 + \sigma_{yM}^2$ (σ_{yI} and σ_{yM} are uncorrelated by definition). If the source aperture is very small, then σ_{yI} is small compared with σ_{yM} at travel times less than the Eulerian time scale, T_E, of the ambient turbulence.

Observations (Fackrell and Robins 1982) show that the most pronounced plume concentration fluctuations are produced very near to the source, and the form of the pdf (probability density function) changes from a near-source exponential to a intermediate-field normal distribution. Despite these forms, the ratio of peak to ensemble-averaged concentrations seems to remain constant. The relative amount of meandering (with respect to ensemble-averages dispersion) depends on atmospheric stability. For stable (night-time) conditions, for example, Hanna (1983) observed very high lateral plume meandering.

Savunen and Rantakrans (1999) present an odor model based on the assumption of a log-normal C-pdf, based on Gifford (1959) and Hanna (1986). Its second moment is estimated as the standard deviation of the meandering motion or, when the plume becomes well-mixed, as the standard deviation of turbulent velocity. Sykes *et al.* (1984) present a second-order turbulence closure scheme which accurately describes the near-field meandering and is able to predict the concentration variance along with the ensemble-mean concentration.

Borgas (1998) and Wilson and Hildermann (1999) focus on the prediction of the highest occurring concentration caused by internal fluctuations. Borgas (1998) uses theoretical relative dispersion considerations to derive the higher moments of the C-pdf, whereas Wilson and Hildermann (1999) use a stochastic Markov process to emulate the time series of internal concentration fluctuations, when the moments of the C-pdf are supplied by any plume meandering model.

1.3.3 Plume meandering during user-specified averaging times

Gifford's (1959) fluctuating plume dispersion model neglects dispersion in the direction of the mean wind, leading to a 'spreading disk' plume dispersion model. The mean concentration distribution as predicted by Gifford's (1959) model is identical with predictions from ensemble-averaged plume models. Additionaly, it predicts statistical properties like the variance of point concentrations. The 'split' between instantaneous plume growth and dispersion due to meandering is a function of down-wind distance, i.e. is different for each 'disk' of the fluctuating plume. These 'disks' do not actually move; it is the statistical property of their movement that is predicted. From this it follows that the statistical properties

of concentration as predicted by the Gifford (1959) approach apply to instantaneous (point) concentrations, i.e. with zero averaging time.

For a non-zero, arbitrary concentration averaging time, however, the correlation of the meandering movements between two neighboring 'disks', or puffs, has to be taken into account. Even though the statistical properties of concentration fluctuations for each point are correct, the statistical properties of concentration *averages* over time differ from non-correlated to correlated meandering. Sykes (1984) and Sykes and Gabruk (1997) present an extension to the Gifford (1959) model, introducing an autocorrelation function for concentration fluctuations. This allows for the computation of the influence of averaging time on the concentration variances.

By using two-particle statistics (Thomson 1990), Thomson (1996) theoretically derives expressions for the second-order moment structure (for different source configurations) of dispersing plumes and puffs in the near, intermediate and far field. This also ensures that the correlation of meandering motions of particles belonging to the same source is taken into account correctly when estimating concentration variances as a function of averaging time.

As has been outlined in Section 1.2, the PPM features stochastic trajectories for the centers of mass of the puffs. This is done to mimic the meandering caused by turbulent eddies larger than the puff itself. The PPM can thus be called a puff-meandering model, coupled with a puff growth parameterization. However, although the corresponding meandering of an individual puff is realistic (i.e. with the correct amount of turbulent kinetic energy), there is no correlation between individual puffs, neither in space nor time. Neighboring puffs will act totally independent of one another. Their trajectories may even cross.

This is a direct consequence of the use of Lagrangian stochastic particle model based on the Markov assumption (thus yielding absolute dispersion, or 1-particle statistics). The Markov assumption implies that the current position, velocity and acceleration of a particle only depend on the corresponding values of the same particle one timestep ago. However, the (spatial and temporal) correlation between parcels of air (represented by puffs) is crucial to the correct estimation of concentration fluctuations. If this correlation (that is, the turbulent eddies themselves) is ignored, the frequency spectrum of simulated concentration is shifted towards higher frequencies. This means that the worst-case episodes are underestimated,

which makes the prediction useless. Thus, by its basic concept, the PPM suffers from the same short-coming as the Gifford (1959) approach.

Therefore, a special plume-puff meandering scheme has been introduced into the PPM (Section 5). It uses “threads of puffs” to represent a plume, or a plume segment. Within such a thread, the puff “knows” the turbulent velocities of its predecessor. Depending on the spatial and temporal separation between the two puffs, the stochastic movements are correlated. This scheme still has some limitations, for example there will be no correlation between two sources which are situated close to each other. However, for a single, continously emitting source, where the average wind speed does not drop below a certain threshold, this scheme is considered to give a realistic (meaning: with the correct spectrum) picture of meandering.

This plume-puff meandering scheme fully models the second of the two time scales of concentration fluctuations (Hanna 1984, 1986): intermittency, i.e. plume meandering. The internal (in-puff, i.e. in-cluster) concentrations fluctuations, however, cannot be modeled with this approach. For this, an additional internal fluctuation model should be used as a postprocessor.

1.4 ADAPTING CONTINOUS PLUME MODELS TO URBAN ENVIRONMENTS

1.4.1 On air pollution modeling within cities

Particle or puff models exhibit advantages over Gaussian plume models as discussed in the previous sections. Their application becomes virtually impossible, however, when it comes to the simulation of an entire year for all sources from e.g. a city. Gaussian plume models are still the method-of-choice for such applications. They have been successfully used for rural single stack configurations. Extensive data sets from corresponding tracer experiments are available and have been used to validate Gaussian plume models (e.g. Hanna and Chang 1993; Olesen 1995; Carruthers *et al.* 1992).

An increasing percentage of the population lives in agglomerations. Cities with their generally high pollutant emission densities affect an increasing population. Technical measures undertaken to reduce air pollution levels addressed heavily polluting industrial activities first. Nowadays, the air pollution level often originates from a countless number of small, not well determined emission sources, especially within cities. Air pollution modeling faces the challenge to shift from the classical single source (with a high stack) dispersion problem, in a

rural surrounding, towards multi-source, multi-receptor situations, in inhomogeneous urban environments.

Although crucial to micro-scale dispersion modeling, very little is known concerning the flow and turbulence structure over built-up areas with irregularly spaced buildings and trees. The latter induce a roughness sublayer (RS), which ranges from ground-level to several times the average obstacle height (Raupach *et al*. 1991). Over urban areas, the vertical extension of the roughness sublayer cannot be neglected. Within this roughness sublayer, the flow and turbulence fields are different from that of the surface layer above (Högström *et al.* 1982; Roth and Oke 1993; Roth 1993; Oikawa and Meng 1995). For example, the Reynolds Stress increases with height (Rotach 1993a). This leads to a smaller gradient of mean wind speed as compared to the 'logarithmic profile' of the surface layer (Rotach 1993a) and the necessity to revise the scaling concept for the turbulence statistics such as velocity variances (Rotach 1993b). Based on these observations, Rotach (1997) proposes a method to introduce the roughness sublayer into existing dispersion models.

1.4.2 Adaptation of a Gaussian plume model

In principle, dispersion modeling over cities could be done with particle models or with puff models like the PPM. Due to limited computational resources, however, Gaussian plume models are still used to handle multi-source / multi-receptor problems. The validity of the Rotach (1997) approach has first been testes with an advanced particle model for a tracer experiment. In this thesis, it then is introduced into a Gaussian plume model which is first validated with two tracer experiments conducted over suburban environments (Section 6). Then, it is applied to the emission inventory of a city for a whole year of meteorological data (Section 7). The method of Rotach (1997) requires changes in the meteorological pre-processor. If the dispersion model uses similarity theory instead of stability classes, the concept of local scaling (the friction velocity being a function of height in the RS) needs to be implemented in the dispersion model itself.

Apart from the RS, the presence of roughness elements also leads to a higher amount of mechanically induced turbulence, as compared to rural environments for the same synoptic conditions. This leads to a tendency of the stability over urban surfaces towards neutral conditions, as compared to the rural areas surrounding the city. One of the more pronounced effects is that there seems to be a minimum value to the Obukhov length, L, such that really

stable as well as free convection conditions hardly ever occur within the center of a city (Hanna and Chang 1992, 1993).

Another characteristic to urban turbulence is the urban energy balance, which differs from the energy balance as it could be observed in the rural environment surrounding the city. The very high fraction of built-up areas leads to a lower albedo, and to a fast run-off of precipitation together with a reduced water storage capacity. Moreover, after the event of snowfall, the over-all albedo changes rapidly away from that of fresh snow, because snow is removed from large parts of the road surfaces, and the remainder of the snow gets dirty.

1.4.3 Limitations to applied modeling

Plume models represent a valid (analytical) solution to the diffusion equation only for idealized circumstances. Stationarity and homogeneity of the turbulence characteristics are requested. In practice, none of these conditions is fully satisfied, but Gaussian plume models have proved to be successful for a variety of applications. As for any other modeling approach, useful results can be obtained as long as the modeler does not interpret the model results in a direction for which no physical parameterizations have been implemented. For example, the homogeneity condition limits the spatial resolution: only concentration predictions averaged over an area of a certain size (for which the city's different areas start looking homogeneous) are reliable.

When adapting continuous plume models to urban environments, in general there is no such thing as an averaged mean wind speed in the lowest few tens of meters, i.e. between the building structures themselves. Plume models can thus not be used in the layer between the buildings. But the majority (in number) of the emission sources, and of the (human) receptors, is situated there. The lowest height which can safely be chosen as the model boundary is the zero plane displacement height (Rotach 1994). Predicted concentrations, too, can only be computed for this minimum height.

An additional source of uncertainty when using plume models within cities is the fact that almost all emissions originate from combustion processes (road traffic, domestic heating, waste incineration, etc.) and thus have a buoyancy induced plume rise. On the aggregated level of gridded emission inventories, the individual characteristics of stacks (like diameter, temperature excess, and vertical exit velocity) are of no importance. An attempt has been made to parameterize the over-all effect of plume rise, and to include this in the model.

1.4.4 Using dispersion models togehter with gridded emission inventories

When applied to an emission inventory, dispersion models will only predict area averaged concentrations, but the measurements will essentially be point concentrations. The latter may be influenced by local emission sources (like major roads), or they may not (giving the urban background concentration). If local influences are present, they may either be resolved by the emission inventory, or they may not.

The representativeness of measurement stations depends on the local influence from roads or near-by buildings. This calls for a detailed investigation of all measurement sites. For any validation of model results, the available point receptor measurements should be classified to at least these three groups (urban background, influenced by major roads with or without local influences). A dispersion model is expected to perform best in predicting the urban background, second-best in predicting concentrations where roads are adequately resolved in the emission inventory, and will show considerable error when local non-resolved effects influence the concentration measurement.

When a concentration measuring unit is positioned such that strong local influences exist (for example in a street canyon), the measured concentration may strongly depend on the mean wind direction. Then, the stationarity condition, and the ensemble-average approach, only allow for concentration sampling times of 24 hours and longer to be compared with the corresponding model predictions. They also do not allow for the comparison of the distribution of hourly concentration, i.e. of quantile-quantile plots of predicted vs. observed concentration, as a model validation tool for such sites with local influences.

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