Dosage-based parameters for characterization of puff dispersion results

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HIGHLIGHTS
- A consistent set of dosage-based parameters for puff dispersion characterization is introduced.
- The scalability and the validity of parameters are confirmed by systematic wind tunnel measurements.
- The effect of the release duration on the parameters is investigated.

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ABSTRACT
A set of parameters is introduced to characterize the dispersion of puff releases based on the measured dosage. These parameters are the dosage, peak concentration, arrival time, peak time, leaving time, ascent time, descent time and duration. Dimensionless numbers for the scaling of the parameters are derived from dimensional analysis. The dimensionless numbers are tested and confirmed based on a statistically representative wind tunnel dataset. The measurements were carried out in a 1:300 scale model of the Central Business District in Oklahoma City. Additionally, the effect of the release duration on the puff parameters is investigated.

1. Introduction
Emergency situations in urban environments often involve instantaneous or short-term releases (puffs) of airborne hazardous materials. The characterization of such scenarios is rather difficult due to the complex flow and dispersion phenomena within the urban canopy layer. Here the building structure has a strong impact on the flow field.

Despite the existence of widely used methods for dispersion estimation, there is no common practice on the characterization of puff dispersion. Books written four decades ago already describe the physics and modelling of puff dispersion (e.g. [1,2]). The Gaussian puff and plume models have been widely applied in the last 50 years for dispersion modelling [2,3]. It is a fast tool, practical in emergency situations. However, the assumptions behind the model might lead to difficulties in predicting the dispersion in an urban environment. Other generally used models are Lagrangian particle models (e.g. [4]) and computational fluid dynamics (e.g. [5,6]). Numerical models and measurements (in wind tunnels and in the field) are often carried out to predict and investigate puff dispersion. For the evaluation of the results mainly case-specific puff parameters are defined.

This paper offers a consistent set of parameters for puff dispersion characterization. The parameters are defined based on the dosage of the puff, providing a uniform, widely applicable criterion. Dimensionless numbers are introduced to convert the parameters from model scale to full scale. The scalability and the validity of the parameters are tested based on systematic wind tunnel measurements providing statistically representative data.

2. Literature review
In the atmosphere a puff is released into a turbulent flow field. Since turbulent flow is random at relevant dispersion scales, it

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will cause the concentration field to be random as well. Consequently, concentration at a particular place and time is assumed to be unpredictable. Due to the turbulence, each realization of puff dispersion will be different from one another. A section of a typical concentration time series of consecutive puff releases is shown in Fig. 1a, demonstrating the variability of the results. Due to the randomness of the processes driving dispersion, Chatwin [7] suggested using Probability Density Functions (PDF) to characterize the variability of puff release dispersion. However, there is still no commonly applied practice on the physical characterization of puff release measurements. During puff dispersion measurements, concentration time series are recorded at defined locations. Based on the time trace, puff characteristics are derived. A typical puff signature taken from a corresponding time series can be seen in Fig. 1b. Typical parameters are the peak (or maximum) concentration, the dosage, the arrival (or travel) time, the peak time and the leaving (or departure) time. From these parameters, further characteristics can be derived, such as the puff advection speed and the duration (or puff retention time). However, the definition of the parameters listed above differs in the literature. Some examples of the different definitions of puff parameters are given by Zheng et al. [8].

The most common practice to define the characteristic times of a puff (such as arrival time, duration and leaving time) is to set an absolute threshold criterion. The puff is considered to be present at the measurement location, when the concentration is exceeding the chosen threshold. The most evident threshold is zero concentration [9]. This might be adequate for characterizing results from a numerical simulation representing an ideal scenario (e.g., [6,10]) or for spectral analysis [11]. For extreme value analysis, when the high concentrations are investigated using the generalized Pareto distribution, problems related to the uncertainty of the low concentrations can be avoided [12]. For toxic or flammable substances, the threshold might be chosen according to acute toxicity limits [13] or lower flammability limits [14]. However, these values are substance specific, with limited transferability to the gases generally used in field trials and wind tunnel measurements. Furthermore, these levels set the threshold rather high compared to the measured concentration. This results in significant wastage of valid data. Therefore, this method is mostly applicable for studies that investigate high concentrations (as in [13,14]).

The threshold used for the evaluation of measured puff data is usually set to a value higher than zero. This is due to the noise inherently present in almost all measured signals and the uncertainty of the measurement devices (including calibration uncertainty).

Techniques involve setting an absolute threshold above zero (e.g. [15]) or applying some kind of baseline removal technique on measured time series (e.g. [16]). In case of a statistically representative dataset with a large number of puff measurements the variability of the results is high. This makes it extremely difficult to define an absolute threshold or a universal baseline, which is sufficient for each puff. (Further discussion on baseline removal techniques and the problems with applying an absolute threshold can be found in [17,18]).

Zhou and Hanna [9] present various approaches to derive the duration of a puff. One of the applied methods is to set the threshold relative to the peak concentration. This method allows defining the threshold independently for each puff. A similar approach was applied for the results of the wind tunnel measurements [19] connected to the DAPPLE field campaign [20]. Here the threshold was related to the 50% of the peak concentration.

The problem yet of using only a threshold criterion is that spikes (caused for example by dust particles entering the measurement volume) might appear in the concentration signal. Such a spike may be large enough to be considered as a valid signal by mistake [21]. Doran et al. [22] define the arrival time as the time after the release, when the concentration first exceeds and remains above an absolute threshold for a specified duration. This method solves the problem related to spikes in the signal. However, setting a minimum duration can also exclude highly intermittent signals, which occur often at measurements taken close to the source location.

The characterization method presented in this paper is based on the dosage of the measured puff. The dosage of the whole measurement signal is taken into account. The background concentration needs to be recorded and subtracted from the measured time series previously. The advantage of taking a defined portion of the dosage as the threshold for characteristic time measures is its cumulative nature. This ensures that spikes have a negligible effect on the puff parameters, while intermittent signals are still taken into account. This consistent definition of puff parameters sets a relative criterion, which can provide different absolute threshold values for each puff. However, the dosage-based criterion is not always the most appropriate to characterize puff dispersion. When the release duration is changing or the exceedence of an absolute threshold is investigated, choosing a threshold-based criterion might be more convenient. As an example, finding the duration, while the concentration is over an absolute threshold (such as exposure limit [13] or flammability limit [14]), the threshold-based criterion is more adequate.
3. Dosage-based puff parameters

The dosage (dos [ppm s], Eq. (1)) of a puff at a certain measurement location is the integral of the concentration (c [ppm], given in parts per million by volume) measured at the location over time (t [s]):

\[
dos = \int_0^T c(t) \, dt, \tag{1}
\]

where \( T \) represents the end of the measurement (detection period) after the cloud of material has left the measurement location (see Fig. 1).

The concentration measure in this paper is given in volume, rather than mass. If the ideal gas law is assumed, under identical boundary conditions the volumes of different type of gases are equal, while their masses are different.

With the exception of the peak time, all characteristic times of the puff depend on the dosage-based criterion. Choosing the 5% and the 95% of the dosage as relative thresholds, the following parameters are introduced:

- dosage (dos [ppm s]): the time–integrated concentration of tracer gas over the detection period,
- peak concentration (pc [ppm]): the highest concentration for the minimum available instrument resolution occurring at the measurement location during the detection period,
- arrival time (at [s]): the time between the beginning of the puff release and when 5% of the total dosage of the puff has reached the measurement location,
- peak time (pt [s]): the time between the beginning of the puff release and when the peak concentration occurs at the measurement location,
- leaving time (lt [s]): the time after the beginning of the puff release when 95% of the total observed dosage of the puff is recorded at the measurement location,
- ascent time (asct [s]): the time interval between the arrival time and the peak time,
- descent time (dscst [s]): the time period between the peak time and the leaving time,
- duration (du [s]): the time interval between the arrival time and the leaving time.

4. Scaling of dosage-based puff parameters

Results of concentration measurements from both wind tunnel and field tests are typically converted to dimensionless values. This ensures that results are comparable and independent from the boundary conditions. Dimensional analysis [23] according to Rayleigh’s method [24] gives the conversion factors for the dosage-based puff parameters to obtain dimensionless values. The selected reference variables for the dimensional analysis are the reference velocity of the approach flow (\( U_{ref} [\text{m/s}] \)), the characteristic (or reference) length scale of the ambient boundary layer (\( L_{ref} [\text{m}] \)) and the volume of the released tracer (\( V [\text{m}^3] \)). Since the aim was to model instantaneous releases, the release duration was not considered as a scaling variable. The release duration was kept constant throughout the measurements. Therefore the transformation of results is restricted to equivalent release periods. Due to the limitations of the wind tunnel measurements, the results are only adequate for neutrally buoyant non-reactive gases released into a neutral atmosphere. Dimensional analysis reveals that the following dimensionless numbers (given by Eqs. (2)–(4)) apply for the puff parameters:

- dosage:
  \[
dos^* = \frac{dos}{V} \frac{L_{ref}^2}{U_{ref}}, \tag{2}
\]
- characteristic times (arrival time, peak time, leaving time, duration, ascent time and descent time):
  \[
t^* = \frac{t}{U_{ref} L_{ref}}, \tag{3}
\]
- peak concentration:
  \[
pc^* = \frac{pc}{U_{ref}^3 V}, \tag{4}
\]

which also converts the time step of the measured concentration time series.

The relationships shown by Eqs. (3) and (4) agree with the Gaussian puff model [2]. Analogue to the definition of the dosage (Eq. (1)) as the time integral of the concentration, the Gaussian plume model is the time integral of the Gaussian puff model [2]. Therefore Eq. (2) can be related to the Gaussian plume model.

For continuous release dispersion measurements, the dimensionless concentration (\( C^* [-] \)) is used to convert the time trace (Eq. (5)). However, Eq. (5) cannot be applied to instantaneous releases, since it depends on the release flow rate (\( Q [\text{m}^3/\text{s}] \)). In case of puff releases, the concentration time trace is nondimensionalised according to the formula of the dimensionless peak concentration (Eq. (4)). Therefore, instead of the flow rate, the total released volume is considered as the scaling parameter.

\[
C^* = C \frac{U_{ref} L_{ref}^2}{Q}. \tag{5}
\]

Results of systematic measurements dedicated to the verification of the scaling are examined to verify the dimensionless numbers listed above (Eqs. (2)–(4)). The effects of the reference velocity and the released amount of tracer gas on the puff parameters were compared to the relationships indicated by the dimensionless numbers. Additionally, the effect of the release duration was investigated, although the aim of the measurements was to examine instantaneous releases.

5. Experimental setup

Results of wind tunnel measurements were analysed to investigate the relationships between the puff parameters and the reference velocity, released amount of tracer gas and release duration. The measurements were carried out in a 1:300 scale model of the Central Business District in Oklahoma City (Fig. 2). The resulting systematic and statistically representative dataset is sufficient for model validation. The basis of these measurements was the Joint Urban 2003 (JU2003) project, one of the most extensive field measurements investigating urban dispersion [25].

The ‘WOTAN’ boundary-layer wind tunnel at the Environmental Wind Tunnel Laboratory in Hamburg with an 18-m-long, 4-m-wide test section was chosen for the measurements. Fast solenoid microvalves mounted in the model for the realization of puff emissions represented ground-level point sources. A laboratory-grade electronic mass flow controller controlled the amount of the released tracer. A bypass release configuration ensured the stability and the repeatability of the release rates. The exhaust velocity and the corresponding momentum of the released material were significantly lower than the wind velocity around the source, hence modelling a
passive emission. Pure ethane was used as a neutral, non-reactive tracer. 2D fibre-optic Laser Doppler Anemometer (LDA) measured the flow field and fast Flame Ionization Detector (FID) measured the concentration. The measurement devices recorded time series with high temporal resolution. The fast FID is able to resolve 1 ppm in model scale, considering the sensitivity, amplification and calibration.

According to Robins et al. [26], dispersion shows puff-like behaviour (corresponding to instantaneous releases), if the arrival time is about three times longer than the release duration. If the release duration exceeds the arrival time, the dispersion has a plume-like behaviour (corresponding to a continuous release). To fulfil the criterion of a puff, the release duration during the wind tunnel measurements was one order of magnitude lower than the arrival time.

To ensure the statistical representativeness of the data, the ensemble size of emitted puffs was chosen to provide a smooth and reproducible frequency distribution of puff parameters for each measurement location. In order to verify experimentally the sufficient ensemble size and analyse the scalability of puff dispersion results, more than 20,000 individual puffs were emitted. For creating a qualified validation dataset, another 35,000 puffs were released with varying wind direction and source location. Harms et al. [27] and Harms [28] provide details on the wind tunnel measurements and the validation exercise. Comparison of the wind tunnel measurement results to the JU2003 field tests show good agreement [27,28].

6. Results

6.1. Scalability tests

During the scalability tests, only one parameter (i.e. the released volume of the tracer gas or the reference velocity) was systematically varied at a time. All other initial and boundary conditions were constant. Fig. 3 and Table 1 illustrate and document the set of test configurations. The measurements were carried out in 2 m height at full scale. The name of the measurement point (e.g. S2_170_AP26) indicates the source number (S2), the wind direction (170°) and whether corresponding data from field measurements is available at the same location from the JU2003 field trials (FP: field measurement point; AP: additional point, measured only in wind tunnel).

Table 1 shows that at each location the puff releases were repeated at least 200 times to ensure proper statistical representativeness. For each recorded puff, the puff parameters were derived from the concentration time trace. The mean value of each puff parameter was calculated for each measurement location. Based on the scatter of the results from repetitive measurements, the uncertainty of the mean puff parameters and the variability of relevant boundary conditions (wind speed, release duration, release flow rate) were defined and shown on the plots as error bars. As example, the results of the scalability tests are shown only for the mean of the distribution of each puff parameter in this paper. Other statistics, such as the median, different percentiles and the RMS values show similar dependence on the reference variables. However, higher-order statistical moments (such as skewness and kurtosis) cannot be scaled with Eqs. (2)–(4) due to their higher-order dependence on the sample, resulting in low robustness.

6.2. Influence of the released amount of tracer gas

To determine the effect of the released amount of tracer on the puff parameters for constant release duration, the flow rate of the release was systematically varied. The released amount of tracer gas has a linear relationship with the peak concentration and the
Table 1
The set of measurements carried out during the scalability tests to investigate the effects of the released amount of tracer gas (a) and the reference wind speed (b) on the dosage-based puff parameters. All values are given in model scale except for the measurement height.

(a)

<table>
<thead>
<tr>
<th>Point name</th>
<th>Number of measurements</th>
<th>Puffs per measurement</th>
<th>$U_{ref}$ (m/s)</th>
<th>Release duration (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S2_170_AP26</td>
<td>5</td>
<td>415</td>
<td>$4.20 \pm 0.01$</td>
<td>$0.30 \pm 0.004$</td>
</tr>
<tr>
<td>S2_170_FP15</td>
<td>3</td>
<td>210</td>
<td>$2.43 \pm 0.01$</td>
<td>$0.49 \pm 0.004$</td>
</tr>
</tbody>
</table>

(b)

<table>
<thead>
<tr>
<th>Measurement points</th>
<th>Measurement height (m)</th>
<th>Number of measurements</th>
<th>Puffs per measurement</th>
<th>Release duration (s)</th>
<th>Flow rate (l/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S2_170_AP26</td>
<td>2</td>
<td>7</td>
<td>220–420</td>
<td>$0.30 \pm 0.004$</td>
<td>$56.4 \pm 0.01$</td>
</tr>
<tr>
<td>S2_170_FP15</td>
<td>2</td>
<td>7</td>
<td>215</td>
<td>$0.29 \pm 0.004$</td>
<td>$158.6 \pm 0.01$</td>
</tr>
<tr>
<td>S2_170_AP30</td>
<td>2</td>
<td>5</td>
<td>220–420</td>
<td>$0.29 \pm 0.004$</td>
<td>$158.2 \pm 0.01$</td>
</tr>
<tr>
<td>S2_170_AP31</td>
<td>2</td>
<td>7</td>
<td>210–245</td>
<td>$0.29 \pm 0.004$</td>
<td>$158.6 \pm 0.01$</td>
</tr>
<tr>
<td>S4_170_FP02</td>
<td>2</td>
<td>7</td>
<td>210–246</td>
<td>$0.29 \pm 0.004$</td>
<td>$158.6 \pm 0.01$</td>
</tr>
<tr>
<td>S4_170_AP32</td>
<td>2</td>
<td>7</td>
<td>210–245</td>
<td>$0.29 \pm 0.004$</td>
<td>$158.6 \pm 0.01$</td>
</tr>
<tr>
<td>S4_170_AP15</td>
<td>2</td>
<td>7</td>
<td>200–280</td>
<td>$0.29 \pm 0.004$</td>
<td>$79.8 \pm 0.01$</td>
</tr>
<tr>
<td>S4_170_AP32</td>
<td>60</td>
<td>7</td>
<td>215–270</td>
<td>$0.29 \pm 0.004$</td>
<td>$158.4 \pm 0.01$</td>
</tr>
</tbody>
</table>

6.3. Influence of the reference velocity

The reference velocity was measured at a height of 267 mm (80 m in full scale) with an LDA and referenced to a Prandtl-tube mounted in the approach flow. The results of the tests investigating the effect of the reference velocity on the puff parameters are shown in Fig. 5. The reference velocity is inversely proportional to the arrival time and the dosage. The peak concentration shows no significant dependency on the reference velocity. Similarly to the influence of the released amount of the tracer gas, the dependencies of the puff parameters on the reference wind speed are also consistent with Eqs. (2)–(4).

6.4. Influence of the release duration

Although the release duration was not considered as a reference variable for the dimensional analysis (since the aim was to model instantaneous releases), the effect of discharge time on the mean values of the puff parameters was also investigated. The layout of the corresponding measurements is shown in Fig. 6 and summarized in Table 2.

During these measurements, the flow rate of the release was constant. Therefore the total released volume of the tracer gas increased with the increase of the release duration. The dosage (Fig. 7a) and the arrival time (Fig. 7b) have a linear relation with the release duration. The reason for the increasing arrival time is its dosage-dependent definition according to the chosen approach. This can be seen in Fig. 7c, where the time series of puffs measured at the same location with different release durations are plotted. The first part of the concentration time series overlap, until the peak concentration of the puff with the shortest release duration is reached (about 0.9 s on Fig. 7c). If the criterion of the arrival time were threshold based, it would not have a dependence on the release duration. However, the other characteristic times (peak time, leaving time, etc.) increase with the increase of the release duration, regardless of the criterion chosen for their definition.

In Fig. 8a the time series of puffs measured at the same location with different release flow rates are plotted. If the release duration is constant and the released volume is controlled by the flow rate (as in Fig. 8a), choosing a threshold-based criterion would mean that the arrival time is dependent on the flow rate (and consequently on the released volume).

The peak concentration also increases with increasing release duration (Fig. 8b). However in case of long release durations, the relation deviates from a linear correlation. The reason behind this lies on the above mentioned findings from Robins et al. [26]. With the increase of the release duration with respect to the arrival time,
Fig. 5. The influence of the reference velocity on the dosage (a), peak concentration (b) and arrival time (c).

Fig. 6. Measurement locations chosen to investigate the influence of the release duration on the puff parameters. The stars are indicating the source locations and the circles are representing the measurement locations.

Table 2
Set of measurements to investigate the effects of the release duration on the dosage-based puff parameters. All values are given in model scale.

<table>
<thead>
<tr>
<th>Point name</th>
<th>Number of measurements</th>
<th>Puffs per measurement</th>
<th>$U_{ref}$ (m/s)</th>
<th>Flow rate (l/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S2,170_AP26</td>
<td>5</td>
<td>250–340</td>
<td>$3.45 \pm 0.01$</td>
<td>$48.5 \pm 0.01$</td>
</tr>
<tr>
<td>S2,170_FP15</td>
<td>6</td>
<td>200–220</td>
<td>$2.42 \pm 0.01$</td>
<td>$158.5 \pm 0.01$</td>
</tr>
<tr>
<td>S4,170_AP33</td>
<td>5</td>
<td>250–320</td>
<td>$3.51 \pm 0.01$</td>
<td>$158.5 \pm 0.01$</td>
</tr>
<tr>
<td>S4,170_FP17</td>
<td>5</td>
<td>200–215</td>
<td>$3.10 \pm 0.01$</td>
<td>$158.5 \pm 0.01$</td>
</tr>
<tr>
<td>S4,150_FP01</td>
<td>5</td>
<td>200–215</td>
<td>$2.48 \pm 0.01$</td>
<td>$158.5 \pm 0.01$</td>
</tr>
<tr>
<td>S2,150_FP09</td>
<td>5</td>
<td>220–280</td>
<td>$2.46 \pm 0.01$</td>
<td>$158.5 \pm 0.01$</td>
</tr>
</tbody>
</table>

Fig. 7. The influence of the release duration on the dosage (a) and arrival time (b). Puff time series measured at the same location with different release durations (c).
the dispersion is changing its behaviour from puff to plume. Consequently, as the release duration increases, its effect on the peak concentration decreases until the puff release is turning into a continuous release and the peak concentration becomes independent from the duration of the release. The dependence on the duration of the release decreases at S2_170_AP26 measurement location first (Fig. 8b). According to Fig. 6, S2_170_AP26 is the closest point to the source location.

7. Conclusions

The dosage-based definition of the puff parameters provides a uniform relative criterion. The dosage-based criterion ensures that possible spikes in the sampled concentration time trace have a negligible effect on the puff parameters, while intermittent signals are still considered. Dimensional analysis provides dimensionless numbers for the scaling of the puff parameters.

The scalability tests consisted of systematic wind tunnel measurements. The provided statistically representative data shows that the dimensionless numbers (Eqs. (2)–(4)) represent proper dependence of the puff parameters on the reference wind speed and the released volume of tracer gas. For constant release duration the dosage and the peak concentration are in linear correlation with the released volume of the tracer gas. The characteristic times are independent from the released volume. The dosage and the characteristic times are in inverse proportion to the reference velocity. The peak concentration is independent from the reference wind speed.

The influence of the discharging time by constant release flow rate was also examined. The released amount of tracer gas increased with the release duration. As the release duration increases, the peak concentration is deviating from its linear dependency on the release duration. This is in agreement with the fact that with increasing discharging time, the puff release is gradually turning into a continuous release. In case of a continuous release, the peak concentration at the measurement location is independent from the release duration.

When the arrival time is defined based on the dosage, it shows a linear relationship with the release duration. Taking a threshold-based criterion instead will ensure that the arrival time does not depend on the release duration. The threshold-based criterion for the arrival time is useful, when the released volume of a puff is controlled by the discharging time. In case of the wind tunnel measurements of the Central Business District in Oklahoma City, the release duration was constant and as short as possible to model instantaneous releases. Therefore in this case the dosage-based criterion was used to derive the arrival times [27].

In a follow-up activity, the effect of the release duration with constant amount of released tracer will be investigated. A dimensional analysis will be carried out where the release duration is also included as a reference variable. This will enable the characterization of short-term releases without the simplification of considering an instantaneous release only. The obtained dosage-based puff parameters will be compared to the results of other approaches found in the literature.

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