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Abstract: When considering accidental or/and deliberate releases of airborne hazardous substances the release duration is often short and in most cases not precisely known. The downstream exposure in those cases is stochastic due to ambient turbulence and strongly dependent on the release duration. Depending on the adopted modelling approach, a relatively large number of dispersion simulations may be required to assess exposure and its statistical behaviour. The present study introduces a novel approach aiming to replace the large number of the abovementioned simulation scenarios by only one simulation of a corresponding continuous release scenario and to derive the exposure-related quantities for each finite-duration release scenario by simple relationships. The present analysis was concentrated on dosages and peak concentrations as the primary parameters of concern for human health. The experimental and theoretical analysis supports the hypothesis that the dosage statistics for short releases can be correlated with the corresponding continuous release concentration statistics. The analysis shows also that the peak concentration statistics for short-duration releases in terms of ensemble average and standard deviation are well correlated with the corresponding dosage statistics. However, for more reliable quantification of the associated correlation coefficients further experimental and theoretical research is needed. The probability/cumulative density function for dosage and peak concentration can be approximated by the beta function proposed in an earlier work by the authors for continuous releases.

Keywords: puff releases; continuous releases; dosages; peak concentrations; exposure statistics

#### 1. Introduction

It is well known that following a short-duration (puff) release, the airborne material that reaches a receptor downwind of the source presents high concentration variability between different realisations of the same short-duration release under the same mean flow conditions, (e.g., [1]). This is mainly due to the local conditions of turbulence which force the material to travel in different pathways in each realisation. An analysis of the experimental data (e.g., [2]) reveals that the variability is reflected on puff-related parameters such as the dosage, peak concentration, arrival time, duration etc. Thus, there is a necessity to quantify the statistical behaviour of these puff-related parameters and especially the ones that concern the human health, i.e., the dosages and the peak concentrations.

There is an important effort in the literature to simulate puff dispersion theoretically/numerically (e.g., [3–6]). Furthermore, in [7] equations are presented for recalculating the continuous-source results to achieve results valid for the short-term source. The outputs obtained were the probability density functions of the puff characteristics: dosage, maximum concentration, and 99th and 95th percentiles of concentrations.



Citation: Bartzis, J.G.; Efthimiou, G.C.; Andronopoulos, S. Modelling Exposure from Airborne Hazardous Short-Duration Releases in Urban Environments. *Atmosphere* 2021, 12, 130. https://doi.org/ 10.3390/atmos12020130

Received: 7 December 2020 Accepted: 17 January 2021 Published: 20 January 2021

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**Copyright:** © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). In addition to the above mentioned variability between different realisations of the same finite-duration release under the same mean flow, for an emergency action plan there is often the need to examine several release scenarios that, among other parameters, concern the release duration itself, which is not known a priori. In computational terms this means that acting in a straightforward manner, this could lead to a relatively high number of simulations to be performed. On the other hand to model an actual exposure scenario in a complex situation such as an urban environment, the use of advanced Computational Fluid Dynamics (CFD) technology is probably the only possibility for producing reliable results.

It is noted that CFD technology is highly demanding with respect to CPU time, especially if the user considers Direct Numerical Simulation (DNS) or Large-Eddy Simulation (LES) approaches. Even for the Reynolds-Averaged Navier–Stokes (RANS) approach, the CPU time is not negligible especially when the number of scenarios to be examined is relatively high.

It is clear from the above that the problem becomes more demanding with respect to the number of simulations if one needs to consider a variety of release durations and in the same time assess the statistical behaviour of the exposure parameters connected to a specific short-duration release.

Therefore, for practical reasons, there is a need to develop simplified but reliable methodologies to cope with this complex problem.

The basic idea here is as follows. When studying release-duration scenarios we can always consider in addition the (single) continuous release scenario. The question is to what degree the exposure parameters, either deterministic or statistical, of a short/finite-duration release are related to the corresponding parameters of a properly defined "equivalent" continuous release. It is noted that the continuous release is a well-studied problem with several existing models able to produce reliable results [8–15].

Closely connected to the behaviour of exposure parameters from both continuous and short-duration atmospheric releases are concentration fluctuations. Indeed, the need to take into account concentration fluctuations in the assessment of hazards from the dispersion of substances has long been recognised (e.g., [16,17]) and concentration fluctuations have been connected to doses in e.g., [18,19]. There is an extended literature in modelling of concentration calculations. The use of analytic forms for calculating the corresponding probability density function (PDF) in open field atmospheric dispersion has been examined in, e.g., [20–25]. The use of a transport equation for the concentration variance was first adopted in [26]. Of particular interest for the present paper is the calculation of concentration fluctuations in dispersion in urban environments or in the vicinity of buildings [27–39]. Several experimental studies of concentration fluctuations of plume (continuous release) dispersion in urban areas or in the vicinity of buildings in real scale or in the wind tunnel have also been reported in the literature [40-44]. Fewer experimental investigations of concentration fluctuations in puffs from quasi-instantaneous releases have been reported (e.g., [45,46]). A recent and most comprehensive review of modelling and experimental research on concentration fluctuations to date has been presented in [47].

The main aim of the present study is to reveal for the first time relationships of exposure parameters of a short/finite-duration release with the corresponding parameters of a properly defined "equivalent" continuous release based on experimental evidence and theoretical considerations. It is noted that if this effort is successful, the benefits could be quite significant, since in most cases a relatively large number of dispersion simulations, reflecting the variety of potential release duration scenarios as well as its stochastic dispersion behaviour, can be replaced by a single continuous release simulation.

The paper presents also experimental evidence that the peak concentration statistics for short-duration releases in terms of ensemble average and standard deviation are well correlated with the corresponding dosage statistics. Finally, the paper presents experimental evidence that the probability/cumulative density function for dosage and peak concentration can be approximated by the beta function proposed in an earlier work by the authors for continuous releases. The structure of the paper is as follows:

- 1. Statement of the hypotheses connecting the short-release ensemble average dosage and its standard deviation with the corresponding continuous-release mean concentration and its standard deviation (Section 2).
- 2. Theoretical establishment of the relationship between short duration release ensemble average dosage and corresponding continuous release mean steady-state concentration (Section 2.1).
- 3. Theoretical establishment of the relationship between short duration release dosage standard deviation and corresponding continuous release concentration standard deviation (Section 2.2).
- 4. Experimental evidence in support of the proposed relationships (Section 3.1).
- 5. Experimental evidence of the relationship between peak concentration and dosage statistics for short-duration releases (Section 3.2).
- 6. Experimental evidence supporting that the probability/cumulative density function for puff ensemble average dosage and peak concentration can be approximated by the beta function (Section 3.3).
- 7. Conclusions (Section 4).

#### 2. Methodology

Let us assume a point source at a given location, releasing a total quantity QT [kg] of a hazardous pollutant within a finite time duration  $\Delta T [s]$ . In this case the corresponding emission rate  $Q [kg \cdot s^{-1}]$  is given by the relation:

$$Q = \frac{QT}{\Delta T} \tag{1}$$

For a finite-duration release, the dosage  $D[kg \cdot s \cdot m^{-3}]$  at a receptor point downstream is defined here as the concentration time integral:

$$D = \int_0^\infty C(t) \, dt \tag{2}$$

where  $C(t) [kg \cdot m^{-3}]$  is the concentration time series at the receptor point. The integration time beyond  $\Delta T$  reflects the increase in cloud passage time due to diffusion processes.

It is noted that if  $\Delta T$  falls well within the ambient turbulence time period's range, the dosage *D*, by integrating different turbulence time periods for each realisation, is expected to have an inherent variability translating to a stochastic behaviour. The problem is to quantify at any receptor point this dosage statistic in terms of the ensemble average  $\overline{D}$ , its standard deviation  $\sigma_D [kg \cdot s \cdot m^{-3}]$  and the appropriate probability/cumulative density function (pdf/cdf). The ensemble here is composed by different dispersion realisations of the release with duration  $\Delta T$ .

Let us in parallel consider the supplementary problem of a continuous release of the same release rate Q which generates at the same receptor point the concentration time series CS(t) [ $kg \cdot m^{-3}$ ]. In principle this time series is infinite in length. If we randomly extract from this time series a piece of time-length  $\Delta T$ , we can calculate a corresponding dosage DS [ $kg \cdot s \cdot m^{-3}$ ] as

$$DS = \int_{\Delta T} CS(t)dt = CS(\Delta T) \Delta T$$
(3)

where  $CS(\Delta T)$  is the time-averaged concentration over  $\Delta T$ . Both *DS* and  $CS(\Delta T)$  are stochastic variables. The *DS* statistical behavior is directly connected to the  $CS(\Delta T)$  statistical behavior. Let  $\overline{CS}(\Delta T)$  and  $\sigma_{CS}(\Delta T) [kg \cdot m^{-3}]$  be the mean and standard deviation

of  $CS(\Delta T)$ , respectively. As  $\overline{CS}(\Delta T)$  is calculated by drawing a relatively large number of "samples" of length  $\Delta T$  from the infinite time series CS(t), it follows that

$$\overline{CS}(\Delta T) \approx \overline{CS} \tag{4}$$

where on the right-hand side  $\overline{CS} = \overline{CS}(\infty)$  is the mean steady-state concentration of the continuous release at the receptor location.

In this study we introduce the hypotheses that the short-release ensemble average dosage  $\overline{D}$  and its standard deviation  $\sigma_D$  are directly related to the corresponding continuous-release mean concentration  $\overline{CS}$  and its standard deviation  $\sigma_{CS}(\Delta T)$ , respectively, as follows:

$$\frac{\overline{D}}{QT} \approx \alpha_m \frac{\overline{CS}}{Q} \tag{5}$$

and

$$\frac{\sigma_D}{QT} \approx \alpha_\sigma \frac{\sigma_{CS}(\Delta T)}{Q} \tag{6}$$

The present emphasis is to test the validity of the above relationships and give a first estimate of the associated coefficients  $\alpha_m$  and  $\alpha_\sigma$ .

It is noted that the above hypotheses are proposed to be valid under any source-tosensor relative location, wind characteristics and local topography. Some inherent uncertainties on the  $a_m$  and  $a_\sigma$  values are expected due to those characteristics' differentiation. Future extensive targeted studies will be needed to quantify such uncertainties.

# 2.1. Finite Duration Release Ensemble Average Dosage $(\overline{D})$ vs. Corresponding Continuous Release Mean Steady-State Concentration $(\overline{CS})$

It is noted that in the remainder, when we refer to a concentration/dosage we mean the excess concentration/dosage that is generated solely from the above-mentioned source, i.e., above background. In other words, the background concentration is considered to be zero.

Following the relatively simple CFD-RANS approach and the eddy viscosity/diffusivity concept (e.g., [48]), the transport equation for the pollutant concentration ensemble average  $\overline{C}(t)$  [kg m<sup>-3</sup>] for a finite duration release, taking into consideration Equation (1), can be expressed as follows:

$$\frac{\partial}{\partial t}(\overline{C}(t)) + \frac{\partial}{\partial x_i}(U_i\overline{C}(t)) = \frac{\partial}{\partial x_i}\left((K_d + K_{ci})\frac{\partial\overline{C}(t)}{\partial x_i}\right) + Q\cdot\delta(\overline{r} - \overline{r_0})$$
(7)

where  $U_i [m \cdot s^{-1}]$  are the mean velocity components,  $K_d [m^2 \cdot s^{-1}]$  is the molecular diffusivity and  $K_{ci} [m^2 \cdot s^{-1}]$  the turbulent eddy diffusivities.

For a finite-duration release, it is reasonable to approximate the ensemble average dosage  $\overline{D}$  at a receptor by the relation

$$\overline{D} = \int_0^\infty \overline{C}(t) dt \tag{8}$$

By analogy, the mean dosage for the corresponding continuous release for a time interval  $\Delta T$ , taking into consideration Equations (3) and (4), would be given by:

$$\overline{DS} = \overline{CS}(\Delta T) \ \Delta T = \overline{CS} \ \Delta T \tag{9}$$

On the other hand, the transport equation for  $\overline{D}$  could be directly derived by integrating Equation (7) over time and taking into consideration Equations (8) and (1):

$$\frac{\partial}{\partial x_i} (U_i \overline{D}) = \frac{\partial}{\partial x_i} \left( (K_d + K_{ci}) \frac{\partial \overline{D}}{\partial x_i} \right) + QT \cdot \delta(\overline{r} - \overline{r_0})$$
(10)

For a continuous source, the governing transport equation for the steady state concentration  $\overline{CS}$  is given by the relationship:

$$\frac{\partial}{\partial x_i} \left( U_i \overline{CS} \right) = \frac{\partial}{\partial x_i} \left( (K_d + K_{ci}) \frac{\partial \overline{CS}}{\partial x_i} \right) + Q \cdot \delta(\overline{r} - \overline{r_0})$$
(11)

We notice that if we replace  $\overline{D} = \overline{CS} \Delta T$  in Equation (10) we end up exactly with Equation (11). In other words, if a spatial function  $\overline{CS}$  is a solution for Equation (11), the function  $\overline{D} = \overline{CS} \cdot \Delta T$  is a solution for Equation (10). This provides the linkage between the ensemble average dosage ( $\overline{D}$ ) from a finite duration release with the steady-state concentration ( $\overline{CS}$ ) from the continuous release. Normalising the relationship  $\overline{D} = \overline{CS} \cdot \Delta T$  by the source release mass QT and taking into consideration Equation (1), we end up with the following relationship between  $\overline{D}$  and  $\overline{CS}$ :

$$\frac{\overline{D}}{QT} = \frac{\overline{CS}}{Q} \tag{12}$$

Comparing Equation (12) with Equation (5) we conclude that the above relevant hypothesis is valid with the associated coefficient  $\alpha_m$  equal to unity. In other words, Equation (12) can be used to estimate the dosage ensemble average at any receptor point caused by a source described by Equation (1) for any release duration provided that the corresponding steady state concentration has been quantified by solving Equation (11).

It is worth underlining here that with only one (steady-state) simulation we are able to estimate the ensemble average dosages for any release duration by using Equation (12).

At this point it should be underlined that the derivation of Equation (12) was possible assuming that the RANS approximation is valid. Thus, in the real problem, the relation (12) could serve as an indicator to what degree RANS approximation is valid.

## 2.2. Short Release Dosage Standard Deviation ( $\sigma_D$ ) vs. Corresponding Continuous Release Concentration Standard Deviation ( $\sigma_{CS}(\Delta t)$ )

Before testing the hypothesis expressed by Equation (6), we need to discuss how we estimate the concentration standard deviation  $\sigma_{CS}(\Delta T)$  in a continuous release which is not a trivial problem.

The fundamental question here is how does the standard deviation  $\sigma_{CS}(\Delta T)$  for the concentration  $CS(\Delta T)$  depend on variable  $\Delta T$ .

Let us assume that the variance  $\sigma_{CS}^2(\Delta T)$  is mainly dependent on the  $\Delta T/T_{CS}$  ratio [49], where  $T_{CS}$  is the turbulent integral time-scale derived from the concentration autocorrelation function  $R_{CS}(\tau)$ :

$$T_{CS} = \int_0^\infty R_{CS}(\tau) d\tau \tag{13}$$

Thus, we are looking for relationships:

$$\sigma_{CS}^2(\Delta T) = \sigma_{CS0}^2 \cdot fs\left(\frac{\Delta T}{T_{CS}}\right) \tag{14}$$

where

$$\sigma_{CS0}^2 = \sigma_{CS}^2 (\Delta T \to 0) \tag{15}$$

and the function  $f_s$  is to be determined. It is noted that  $\sigma_{CS0}^2$  is the variance that is usually directly produced by high time-resolution measurements or/and CFD simulations (e.g., [27]) in which the time resolution is usually of the order of seconds.

We try to address the problem theoretically first and assume well-mixed conditions and the von Karman power spectra [50] for concentration frequency spectra  $S_{cs}(n)$  [51]:

$$\frac{nS_{cs}(n)}{\sigma_{cs0}^2} = \frac{0.58nT_{cs}}{\left[1 + 1.49(nT_{cs})^2\right]^{5/6}}$$
(16)

The parameter *n* denotes the frequency. Signal integration over  $\Delta T$  means that all frequencies below  $1/\Delta T$  will disappear. A simple approximation of the power spectra of those filtered signals could be the original power spectra with a frequency cutoff  $1/\Delta T$ . This approximation includes the assumption that the expected distortion of the new power spectra near the cutoff frequency region is insignificant, especially if one takes into consideration that the overall power contribution comes mainly from the low frequency region as this can be seen also in Equation (16).

Based on the above assumptions the standard deviation of the filtered concentration signal can be expressed by the simplified approximation:

$$\frac{\sigma_{cs}^2(\Delta T)}{\sigma_{cs0}^2} = f_S\left(\frac{\Delta T}{T_{CS}}\right) \approx \int_0^{1/\Delta T} S_{cs}(n) dn \tag{17}$$

Equation (17) has been integrated numerically and then simple fitting relationships have been attempted to fit the obtained numerical results. It was possible to fit those numerical data with the following relationship:

$$f_S\left(\frac{\Delta T}{T_{CS}}\right) \approx \frac{1}{1 + 0.232\Delta T/T_{cs}} \tag{18}$$

To investigate to what degree Equation (18) is realistic, we considered the 1:225-scale wind-tunnel experiment in a semi-idealised urban area (Michelstadt) which is part of the online validation data base CEDVAL-LES (https://mi-pub.cen.uni-hamburg.de/index. php?id=6339). More details for the data and data treatment are given in [52]. Concentration time series from 196 sensors have been generated in that experiment. Each sensor contains 55,000 concentration high time-resolution ( $\Delta \tau_0 = 1.125s$ ) measurements.

Here, in each sensor time-averaged concentration time series were obtained for time intervals  $\Delta T$  in the range from  $\Delta \tau_0$  to  $1500\Delta \tau_0$ . In total,  $196 \times 1500 = 294,000$  time-averaged concentration time series were produced, and the concentration variance ratios  $\sigma_{CS}^2 / \sigma_{CS0}^2$  for each time series were calculated. The results are given in Figure 1 as function of  $\Delta T / T_{CS}$ .



**Figure 1.** The concentration variance ratio  $\sigma_{CS}^2 / \sigma_{CS0}^2$  as a function of  $\Delta T / T_{CS}$  compared with analytic functions  $f_S(\Delta T / T_{CS})$ .

In Figure 1 the concentration variance ratio is compared with two curves: one corresponding to the theoretical relationship (18) and one corresponding to the following empirical relationship that seems to fit better the experimental results.

$$f_S\left(\frac{\Delta T}{T_{CS}}\right) \approx \frac{1}{1 + 0.42\Delta T/T_{CS}} \tag{19}$$

It is interesting to see that the theoretical curve (18) is not only well correlated with the experimental data, but it is also serving as their upper bound. One explanation could be that in the theory the pollutant is assumed to be well mixed along all turbulent scales, an assumption which is not always true in reality.

It is worth underlying here that the formulation (18) sets the concentration fluctuation statistics as a function of the integration time interval in a completely new basis with solid roots in the theory. The replacement of the fitting parameter 0.232 by the value 0.42 as suggested in Equation (19) was obtained from only the above wind tunnel experiment but with a relatively dense sensor network reflecting a considerable variety of downwind distances, orientations with respect to the wind direction and local geometric characteristics. This gives some validity in the direction of obtaining a value applicable for dispersion in urban environments. Obviously more experimental work including the real atmospheric environment will be needed.

In the remainder we adopt the more realistic Equation (19) to estimate standard deviations in the various time intervals  $\Delta T$ .

## 3. The Experimental Evidence: The S2 Michelstadt Experiment for Puff and Continuous Releases

As stated above, an important effort here is to seek experimental evidence on the dosage statistics relationships between puff and continuous releases.

The present study is considered as a first attempt to examine to what extent such a hypothesis is realistic and therefore is limited to the S2 Michelstadt Experiment for puff and continuous releases. The selection of this particular experiment is justified by the fact that it is a well-studied experiment and it has been numerically simulated in the past [53–55]. The S2 source is located on the ground in an open space as shown in Figure 2.



**Figure 2.** Top view of the buildings configuration in the Michelstadt wind-tunnel experiment (**left**); source and receptors locations for the S2 Michelstadt puff experiment (**right**).

The sensors are located at 7.5 m above ground (in real scale). In this study the three sensors shown in Figure 2 were considered which are common for both the puff and continuous releases.

In case of the continuous release the flow rate of the tracer gas was  $0.5 \text{ kg s}^{-1}$  while in case of the "instantaneous" (short-duration) release the released quantity per puff was 10 kg and the release duration per puff was 29 s. In total, 286 puffs were released with a time distance between two successive releases of the order of 10 min.

For each puff the experiment produced measurements for several parameters such as dosage, peak concentration and peak concentration based on 15-s average, together with concentration signal time characteristics such as arrival, peak and departure times.

#### 3.1. The Puff Releases vs. the Continuous Release Comparisons

The present puff release experimental data study strengthens the hypotheses that the dosage is the key defining parameter and the peak concentrations can be derived from the dosages not only in terms of ensemble averages and standard deviations but also in terms of pdf/cdf. What is needed on this problem is further scientific evidence to quantify more precisely their respective correlation factors although the  $\sigma/m$  (standard deviation over mean) ratio shows a bit more clearly a relationship close to unity.

As mentioned above, the problem in this section is finite-duration release dosage quantification both in terms of ensemble average and standard deviation. We tried to seek experimental evidence for the proposed interrelationship by performing puff releases vs. continuous release comparisons in the abovementioned S2 Michelstadt experiment.

To ensure intercomparison data coherence all 286 experimental puffs were considered including the non-detected puffs at the sensors shown in Figure 2 as well. The undetected puffs were included assigning a zero value for the dosage. The dosage data for the puff releases and the steady-state concentration data for the continuous release at the three sensors are summarised in Table 1. It is noted that following the formulation of Equations (5) and (6) the dosage ensemble averages and corresponding standard deviations are normalised by the total puff mass release ( $m = \overline{D}/QT$  and  $\sigma = \sigma_D/QT$ ), while the steady state concentrations and corresponding standard deviations are normalised by the total puff mass release ( $m = \overline{CS}/Q$ ,  $\sigma = \sigma_{CS0}/Q$  and  $\sigma(29s) = \sigma_{CS}(29s)/Q$ ). In this table, the concentration turbulence time scales as estimated from the continuous concentration signal are included as well.

<b>Table 1.</b> The S2 Michelstadt experiment: data for the 286 puff releases and the continuous release (for the puff releases
$m = \overline{D}/QT$ and $\sigma = \sigma_D/QT$ ; for the continuous release $m = \overline{CS}/Q$ , $\sigma = \sigma_{CS0}/Q$ and $\sigma(29s) = \sigma_{CS}(29s)/Q$ ).

Sensors	Puff Releases			Continuous Release			
	Non Detected	Normalise (ppm	Normalised Dosage (ppm s/kg)		Normalised Concentrations (ppm s/kg)		
	Puffs	m	σ	m	σ	σ (29 s)(*)	Scales (s)
S2P7	31/286	124.73	116.60	125.85	145.06	114.36	19.20
S2P19	44/286	86.42	88.99	32.27	43.44	39.58	59.54
S2P22	4/286	85.49	62.56	78.79	56.20	49.31	40.69

(\*) Estimated from Equations (14) and (19).

It can be seen from Table 1 that not all puffs were detected in each sensor. The sensor S2P19 shows the lowest detection ratio indicating a relatively higher degree of unstable flow behaviour.

In Figure 3 the puff release normalised ensemble average dosage is compared with the equivalent continuous release steady state normalised concentration to test the validity of Equation (12). The comparison is fairly good with the largest discrepancy in the sensor S2P19. This sensor is associated with the highest number of undetected puffs. Such behaviour is expected to be associated with significant flow unsteadiness [56]. It should be noted that in the present approach the key assumption is that the RANS approximation is valid. Apparently, this assumption in the neighbourhood of the sensor S2P19 is ques-



tionable. In fact, there are many studies in the literature revealing the RANS weakness in replicating unsteady flows (e.g., [57–61]).

**Figure 3.** Puff release normalised ensemble average dosage vs. continuous release normalised mean steady state concentration: ensemble averages and means as expressed in Equation (12).

Figure 4 shows the intercomparisons of the  $\sigma/m$  ratios for the puff release normalised dosage and the continuous release normalised steady-state concentration. It is noted that for the continuous release the standard deviation  $\sigma(29s)$  of the normalised steady-state concentration is derived by the relationships (14) and (19) using the concentration signal standard deviation ( $\sigma_{CS0}$ ) and autocorrelation time ( $T_{CS}$ ) and the puff release duration ( $\Delta T = 29s$ ).



**Figure 4.** Puff release vs. continuous release intercomparisons:  $\sigma/m$  ratios

It is shown that the correlation between the steady state and the puff releases  $\sigma/m$  ratios is quite good and close to unity.

Thus, the present results support the hypotheses as expressed by Equations (5) and (6). The first estimate of the associated coefficients is:

$$\alpha_m \approx \alpha_\sigma \approx 1 \tag{20}$$

This is an important finding that strengthens the hypothesis that prediction of puff release dosage statistics can be derived directly from the equivalent continuous release concentration statistics.

#### 3.2. The Puff Release Experiment Peak Concentrations

In case of a finite-duration release, sometimes in exposure studies we are interested not only in the dosage but in the peak concentrations as well. Here it is examined to what degree the peak concentrations are correlated with the corresponding dosages. We focus on the peak concentrations given by the experiment, i.e., the directly measured peak concentrations and the 15-s time-averaged peak concentrations. The data in terms of ensemble averages (m) and standard deviations ( $\sigma$ ) normalised by the single puff mass release rate at the three sensors are summarised in Table 2.

**Table 2.** The puff releases dosage and peak concentration (m: ensemble average,  $\sigma$ : standard deviation) normalised by the released puff mass and the puff release rate, respectively.

Sensor	Normalised Pea (ppm	k Concentration ·s/kg)	15-s Time-Averaged Normalised Peak Concentration (ppm·s/kg)		
	m	σ	m	σ	
S2P7 S2P19 S2P22	160.00 53.66 63.80	121.92 49.21 48.67	88.05 29.51 36.91	69.26 29.08 27.15	

In Figures 5 and 6a a comparison is shown between dosages and peak concentrations in terms of ensemble averages and  $\sigma/m$  (standard deviation over ensemble average) ratios at the three sensor locations.



Figure 5. Puff releases: ensemble average (m) values of peak concentrations vs. dosages.



**Figure 6.** Puff releases:  $\sigma/m$  ratios of peak concentrations vs. dosages.

It seems that there is a correlation for both parameters (i.e., m and  $\sigma/m$ ) connecting peak concentration and dosages. The present results indicate a correlation factor in the order of unity. However, further investigations are needed to draw more precise estimations.

An important question that also needs to be answered is how the concentrations averaged over larger time intervals behave. In Figure 7 we compare the ensemble average peak concentrations with the ensemble average peak concentrations derived from moving concentration averages over 15 s. There is almost a perfect correlation with an estimated factor of 0.554. A lower value than unity was expected due to concentration signal 15-s time filtering. However further experimental evidence is needed before any factor value assessment is attempted.



**Figure 7.** Puff releases: ensemble average (*m*) values of time-averaged ( $\Delta \tau = 15 s$ ) peak concentrations vs. measured peak concentrations ( $\Delta \tau_0 = 0.666s$ ).

In Figure 8, it is interesting to see that the  $\sigma/m$  ratios are also correlated by a factor of unity.



**Figure 8.** Puff releases:  $\sigma/m$  ratio of time-averaged ( $\Delta \tau = 15 s$ ) peak concentration vs.  $\sigma/m$  ratio of measured peak concentrations ( $\Delta \tau_0 = 0.666s$ ).

#### 3.3. Dosage/Peak Concentrations Pdf/Cdf for Puff Releases

The continuous release dosage and concentration statistical behaviour in terms of probability density function (pdf)/cumulative density function (cdf) has been extensively discussed in [52]. The beta function seems to be the appropriate generic approximation for the concentration/dosage pdf. Here we will examine to what degree the beta function as applied in [52] is also the proper pdf/cdf approximation for the puff release dosage and peak concentration.

In Figure 9a–c the theoretical (beta function) vs. experimental cdf's are given for puff dosages and peak concentrations.



Figure 9. Cont.



**Figure 9.** Puff releases: Beta function vs. experimental cumulative density function (cdf) for (**a**) dosage, (**b**) peak concentrations and (**c**) 15-s time-averaged peak concentrations.

It is noted that a perfect fir would follow the 1:1 line. Figure 9 shows that the beta function as introduced in [52] seems to be a good pdf/cdf approximation not only for dosages but for peak concentrations as well. This means that if the ensemble average and standard deviation for those parameters are known or can be predicted, the detailed pdf/cdf can be also adequately approximated.

### 4. Conclusions

The exposure due to airborne hazardous releases of short time duration is stochastic in nature and strongly dependent on the release duration. Its assessment often requires a relatively large number of dispersion simulations especially if one needs to consider a range of release durations and at the same time reveal the statistical behaviour of the associated exposure parameters due to atmospheric turbulence. The present analysis introduces the novel approach to replace all the above-mentioned simulation scenarios by only one simulation corresponding to a continuous release scenario and derive the exposure parameterisation for each individual scenario by simple relationships. The present analysis was concentrated on dosages and peak concentrations, the primary parameters in assessing downstream exposures.

Having established the steady-state concentration  $\overline{CS}$  of the corresponding continuous release and its standard deviation  $\sigma_{CS0}^2$  (either from high-time-resolution experimental measurements or from CFD modelling), the dosage ensemble average for short-duration releases is given by Equation (5), its standard deviation is given by Equations (6), (14) and (19), while its pdf/cdf is given by the beta function introduced by [52]. The associated coefficients are given by the Equation (20). All those relationships are as valid as the RANS approximation expressed by Equation (7).

Furthermore, the present experimental data analysis supports the hypothesis that the peak concentration statistics for short-duration releases in terms of ensemble average and standard deviation are well correlated with the corresponding dosage statistics. However, for more reliable quantification of the associated correlation coefficients, further experimental and theoretical research is needed. The pdf/cdf of peak concentration from short-duration releases can also be approximated by the beta function proposed by [52] for continuous releases.

It should be underlined that the whole methodology does not depend on source strength or sensor distances from the source. Although the presented theoretical evidence is rather solid, increasing the degree of confidence and reliability, the presented methodology evaluation is based on rather limited experimental data mainly due to a relatively small number of existing measuring sensors in the wind-tunnel experiments. There is a need for further research especially in expanding the relevant experimental data base.

**Author Contributions:** Conceptualisation, methodology, writing—original draft preparation, J.G.B.; software, validation, formal analysis, G.C.E.; writing—review and editing, S.A. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

**Data Availability Statement:** The experimental data used in this study were made available in the framework of the COST Action ES1006 http://www.elizas.eu/.

Acknowledgments: The authors kindly acknowledge the support of COST Action ES1006 (http://www.elizas.eu/).

Conflicts of Interest: The authors declare no conflict of interest.

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