



UDINEE: Evaluation of Multiple Models with Data from the JU2003 Puff Releases in Oklahoma City. Part II: Simulation of Puff Parameters

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Abstract

The capabilities of nine atmospheric dispersion models in predicting near-field dispersion from puff releases in an urban environment are addressed under the Urban Dispersion INternational Evaluation Exercise (UDINEE) project. The model results are evaluated using tracer observations from the Joint Urban 2003 (JU2003) experiment where neutrally-buoyant puffs were released in the downtown area of Oklahoma City, USA. Sulphur hexafluoride concentration time series measured at ten sampling locations during four daytime and four night-time puff releases are used to evaluate how the models simulate the puff passage at the measurement locations. The neutrally-buoyant puff releases in the JU2003 experiment are the closest scenario to radiological dispersal device (RDD) releases in urban areas, and therefore, UDINEE is a first step towards improving the emergency response to an RDD explosion in the urban environment. We investigate for each puff and sampler the model capability of simulating the peak concentration; the peak and puff arrival times; and time duration, defined as the period over which concentrations exceed 10% of the peak concentration. This analysis points out differences on the performance of models: the fraction within a factor-of-two values ranges from 0.10 to 0.6 for peak concentration, from 0 to 1 for the peak and arrival times, and from 0 to 0.8 for the time duration. The results reveal that the characteristics of the release site largely influence the model simulation as it affects initial puff size and the initial downwind spread of the puff.

Keywords Atmospheric dispersion models · JU2003 field experiment · Performance analysis · UDINEE project · Urban dispersion

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1 Introduction

Atmospheric dispersion models (ADMs) are used for assisting emergency management planning and response associated with the release of hazardous materials in the atmosphere (e.g. Bradley 2007; Benamrane et al. 2013; Benamrane and Boustras 2015). The dispersion of radioactive material from a radiological dispersal device (RDD) (e.g. Andersson et al. 2009; Di Lemma et al. 2014), for example, due to its likely use in urban environments, poses a challenge for ADMs. It is in populated areas where a proper estimation of the radioactive dispersion is indispensable to minimize possible health risks associated with RDD explosions (e.g. Jonsson et al. 2013).

Understanding the transport and dispersion of pollutants in urban environments is difficult (e.g. Hosker 1984), as it largely depends on the city-scale flows above and within the urban canopy layer, and the urban atmospheric boundary-layer characteristics. Britter and Hanna (2003) review mean flow, turbulence and dispersion in urban areas. Advancements in computing resources during the last few years have improved the simulation by atmospheric models of urban flow and its short time-scale variability (e.g. Blocken 2015). Because of this progress, a wide range of ADMs can now simulate air pollution dispersion in cities (e.g. Baklanov et al. 2009; Lateb et al. 2016; Wingstedt et al. 2017).

To support decision making dealing with the atmospheric dispersion of airborne harmful materials, predictions of ADMs must be able to provide adequate description of the atmospheric processes (Ribeiro et al. 2014). To increase the confidence in decision making based on ADM predictions requires establishing the ADM capabilities and limitations. The variability between model predictions should also be characterized and quantified (COST ES1006 2015). Both purposes are achieved through comparison of model predictions to tracer and meteorological observations provided by field campaigns (e.g. Rao 2005).

Model evaluation criteria depend on the context in which models are used (Steyn and Galmarini 2008). Moreover, observations from field campaigns must fulfil certain requirements to be used for evaluating urban ADMs (Schatzmann and Leitl 2002), so as to resolve the short time-scale variability in meteorological conditions and pollutant concentrations inside the urban canopy layer (Britter and Hanna 2003). The meteorological and tracer observations measured during the Joint Urban 2003 (JU2003) field campaign (Allwine and Flaherty 2006) perfectly fulfil these requirements. In addition, during the JU2003 experiment, 40 instantaneous puff releases (25 daytime and 15 nocturnal) were performed.

Under the Urban Dispersion INternational Evaluation Exercise (UDINEE) project, nine ADMs have been evaluated using the subset of the observations from the JU2003 database measured during the set of puff releases performed over ten intensive operational periods. The puff releases in the JU2003 experiment (Clawson et al. 2005) were chosen because one of the UDINEE objectives is to better understand modelling capabilities for RDD scenarios. A radiological dispersal device is typically associated with the explosive dispersal of radiological materials in urban areas, and due to the heat associated with the explosion, these explosive releases are characterized by buoyancy (e.g. Sharon et al. 2012). The instantaneous non-buoyant puff releases at ground level in the JU2003 experiment are the closest scenario to RDD releases in urban areas, and therefore, the JU2003 database based on puff releases is an excellent resource for evaluating the application of ADMs in RDD-like releases in urban environments.

From the basis of this exceptional field experiment, UDINEE with its multi-model approach provides an important contribution towards the study of RDD explosions and the associated emergency response in urban environments. Under the UDINEE project,

observations and model predictions were made available to all participants through the ENSEMBLE web-based platform (<http://ensemble.jrc.ec.europa.eu/>), hosted at the European Commission Joint Research Centre (Bianconi et al. 2004; Galmarini et al. 2004, 2012).

In our study, we examine how the models simulate the puff passage at the measurement locations (a companion study is devoted to the comparison of observed and predicted concentration levels, see Hernández-Ceballos et al. 2019). We evaluate for each puff and sampler the model capability to match the peak concentration, the peak and puff arrival times, and the time duration (the period over which concentrations exceed 10% of the peak concentration). Predictions of the dispersion coefficients (σ_y , σ_z) and their spatial and temporal variability are also evaluated. To achieve this purpose, simulations from the nine ADMs participating in the UDINEE project are compared with sulphur hexafluoride (SF₆) time series measured from eight puff releases. The impact of modelling thermal effects (day–night stability differences or neutral atmospheric conditions) on the performance of models is also discussed.

2 Methodology

2.1 Observed Time Series

A comprehensive description and technical details of the JU2003 experiment are given in Clawson et al. (2005). In this field campaign, SF₆ concentration time series with a temporal resolution of 0.5 s were measured for each puff by fast-response tracer gas analyzers. In this analysis, and in agreement with Hernández-Ceballos et al. (2019), we take as reference the SF₆ concentrations from the four puffs released during the third and eighth intensive operating periods (IOP3 and IOP8), which were carried out during daytime and night-time respectively. The selection of both intensive operating periods is based on the large availability of predictions (eight out of the nine models simulated the dispersion of the four puffs each released in IOP3 and IOP8), and tracer measurements in each one, thus guaranteeing the largest statistical sample.

Clawson et al. (2005) show a summary of the meteorological conditions during the July 2003 study period, calculated over all fixed anemometers at street level and on building tops, mean wind direction was 196° during IOP3 and 157° during IOP8, whilst a relative narrow range of wind speeds was also encountered in both intensive operating periods (3.7 m s⁻¹ in IOP3 and 3.8 m s⁻¹ in IOP8) (Zhou and Hanna 2007). During the JU2003 experiment, there were no large diurnal differences in urban boundary-layer stability. Hanna et al. (2007) reported that slightly unstable conditions prevailed during both day and night intensive operating periods, while Hertwig (2007) indicated that differences in stability existed between the daytime and night-time releases during the JU2003 experiment. A detailed characterization of the mean and turbulent atmospheric parameters governing the observed tracer distributions in each intensive operating period is addressed in Brown (2004) and Hanna et al. (2007).

Each puff was released at a height of about 2 m above street level by popping a balloon containing a known mass of SF₆ (Fig. 1), which is a highly inert tracer gas and has relatively low background levels (about 5 pptv, see Martin et al. 2011). The release times range from 0900 to 1000 CDT (Central Daylight Time) for IOP3 and from 0500 to 0600 CDT for IOP8 (CDT = UTC – 5 h). To ensure that SF₆ concentrations in each sampling

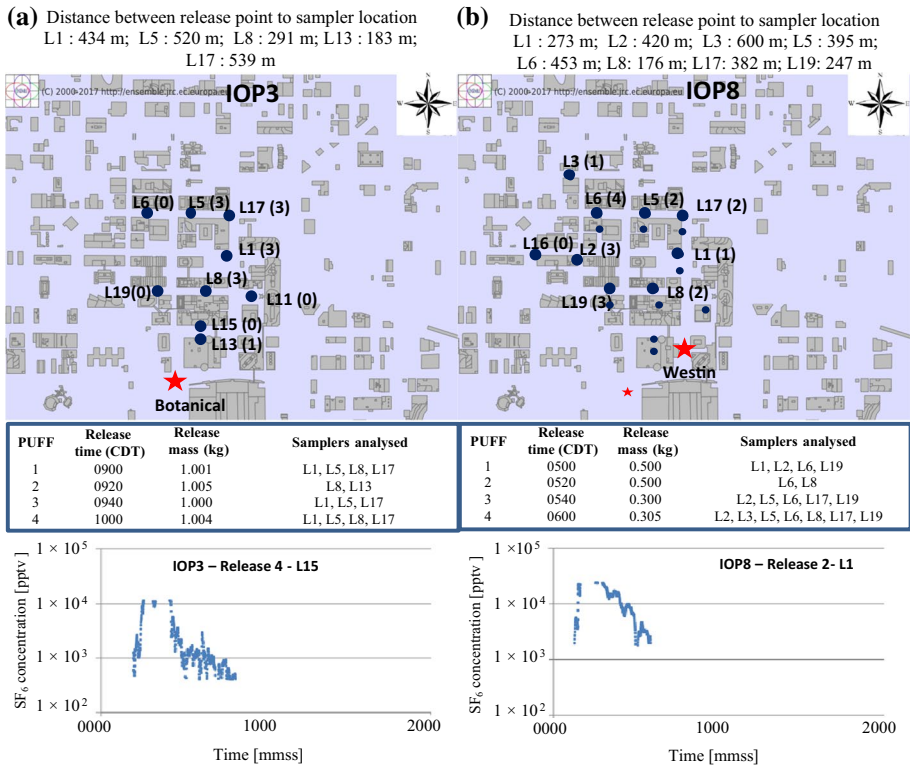


Fig. 1 View of SF₆ source and the fast-response tracer gas analyzers on the UDINEE modelling domain during IOP3 and IOP8. In brackets and in each table are indicated the number of puffs analyzed in each measurement location in each intensive operating period (maximum observed >400 pptv). Below, concentration time series from fast-response sampler L15 during IOP3 release 4 and L1 during IOP8 release 2 are shown

location were from the latest puff released, the puffs were released every 20 min in each IOP. Figure 1 shows the locations of the release points and the nine fast-response tracer gas analyzers that remained stationary in IOP3 and IOP8 (the number 5 was mobile and it is not considered in our study). As can be seen van-mounted fast-response tracer gas analyzers were deployed at about 2 m above ground level (a.g.l.), in different configurations depending on the release location and wind direction. The fast-response tracer gas analyzers were positioned to the north–north–east of the release point in IOP3 and to the north–west in IOP8. The distance from the release points ranges from 183 (L13) to 539 m (L17) in IOP3 and from 176 (L8) to 600 m (L3) in IOP8 (Fig. 1).

Clawson et al. (2005) provide information on the calibration of fast-response tracer gas analyzers, with eight calibration standards used ranging in concentration from pure air to over 10,000 pptv SF₆. The calibration standards had a manufacturer-listed concentration uncertainty of ±5%. Considering this value, it is reasonable to expect accuracy variations up to ±10%. All of the average recovery values are within this range. The standard deviations for all of the groups reported were less than 9%, which should be a reasonable estimate of instrument precision.

Following the criterion applied in Hernández-Ceballos et al. (2019), a SF₆ concentration of 400 pptv is assumed to account for the minimum threshold in the observations. For an equal comparison, we wished to use only those puff and sampler data in each intensive operating period when a clear concentration signal is available, and observed maximum concentration is above 400 pptv. This value agrees with the typical limit of quantitation (*LOQ*) for each intensive operating period and fast-response tracer gas analyzer reported in Clawson et al. (2005), and at the same time, it limits the presence of residual tracer from an earlier puff, which is of vital importance in order to correctly identify the main puff passage at each sampler.

2.2 Participating Models and Modelling Input Variables

In the context of UDINEE, six modelling groups from Europe and two modelling groups from North America simulated the dispersion of the puff releases that occurred during the JU2003 experiment. The nine ADMs, listed below, have been evaluated; for more information see Hernández-Ceballos et al. (2019).

- Emergency Source Term Evaluation—Chemical, Biological, Radiological and Nuclear (ESTE CBRN) (ABmerit (Slovakia); Čarný et al. 2015).
- Canadian Urban Flow and Dispersion System (CUDMS) (Meteorological Service of Canada (Canada); Benbouda 2007; Hogue et al. 2009).
- Parallel-Micro-SWIFT-SPRAY (PMSS) (France Atomic and Alternative Energies Commission (France); Oldrini et al. 2017).
- Micro SWIFT-SPRAY (MSS) (L’Istituto di Scienze dell’Atmosfera e del Clima (Italy), Anfossi et al. 2010; Tinarelli et al. 2012).
- Numerical atmospheric-dispersion modelling environment (NAME) (UK National Weather Service (United Kingdom); Jones et al. 2007).
- NAME-Urban (UK National Weather Service (United Kingdom); Jones et al. 2007).
- Quick Urban and Industrial Complex (QUIC) (National centre for Nuclear Research (Poland); Pardyjak and Brown 2001, 2002).
- ADREA-HF (National Centre for Scientific Research “Demokritos” (Greece); Bartzis 1991; Venetsanos et al. 2010).
- Urban dispersion model (UDM)/second-order closure Integrated Puff (SCIPUFF) (Defense Threat Reduction Agency (United States); Hall et al. 2003; DTRA 2008; Sykes et al. 2016).

We need to consider that a single model realization cannot reproduce a single realization of one puff dispersion in a turbulent flow, as measured in the JU2003 experiment. Considering this, part of the bias is unavoidable and arises from the very stochastic nature of the turbulent flow. An observed ensemble average should be obtained from a group of puffs released under identical (or similar) conditions. However, a large number of such puffs is required for a statistically stable ensemble, but is impossible to achieve in a field program (Chang and Hanna 2004).

UDINEE does not aim at an identification of the best or worst model, as different urban geometries, meteorological conditions, set of models, boundary conditions, and diffusion schemes, should be taken into account. UDINEE aims at evaluating the overall performance of the models analyzed and the state-of-the-art in urban dispersion modelling, as well as explaining the differences between the model results and the dependence

on input assumptions made by the project participants. With this aim, each model is identified hereafter by an anonymous code (M1–M10). For more information on the characteristics and performance of each model, see other articles in this special issue.

The information provided to all modellers participating in the UDINEE project to simulate the SF₆ dispersion resulting from each puff releases was:

- Source location and height (2 m a.g.l.), release times and mass released (Fig. 1);
- Meteorological information: 10-s average time series of wind direction and speed, temperature and relative humidity measurements by the Portable Weather Information Display System (PWIDS) sensor No. 15. This sensor was located 10 m above the roof of the Post Office (40 m a.g.l.) and 1 km upwind of central business district. Also available are 10-min average time series of wind direction and speed for the 20 DPG sonic anemometers, all located in the downtown street canyons at heights of 8 m a.g.l. on small towers and sited above 5 m or more from the nearest building. All participating models were run using the meteorological time series from the PWIDS sensor (Hernández-Ceballos et al. 2019).
- Geographical information System (GIS) shapefiles of the Oklahoma City centre, which contains building heights and coordinates. The urban canopy of Oklahoma City was highly inhomogeneous. The tallest building in the urban core during the JU2003 experiment was approximately 152 m (Burian et al. 2003).

The simulations were conducted for an urban domain covering the downtown Oklahoma City area (1.6 km × 1.4 km² in size and from zero to 402 m a.g.l.). The horizontal grid size selected is 5 × 5 m² and 57 vertical levels are defined according to exponential grid spacing. There were modelling groups performing the simulations in different grid spacing (see Table 1 in Hernández-Ceballos et al. 2019), and model data were interpolated onto the common grid. The simulation domain and the complex of buildings in the area are shown in Fig. 1.

2.3 Definition of Puff Parameters

Modelled time series of SF₆ concentrations with temporal resolution of 0.5 s were requested at the measurement locations (blue dots in Fig. 1) from each UDINEE participant. We note that the ADMs used in this context provide ensemble-averaged concentrations at the time resolution of the meteorological input variables. Thus, the ADM predictions cannot be representative of the intrinsic atmospheric variability at a frequency of 0.5 s from the single realization given by measurements. Several of the Lagrangian models do not directly calculate time series with a temporal resolution of 0.5 s. To fulfil the UDINEE requirements, these models produced averaged time series at the sampling sites with a lower temporal resolution (20 s or 1 min), and the corresponding 0.5-s time series are obtained by interpolation. The Eulerian models, in contrast, provide instantaneous ensemble-averaged values at the time instances every 0.5 s.

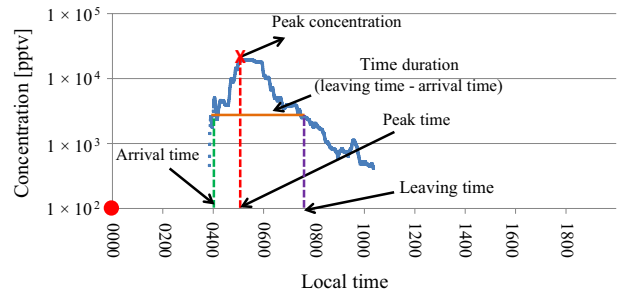
Figure 2 is an observed concentration time series (in logarithmic scale) illustrating the parameters that are used in the current study to characterize the puff passage at each measurement location. We note that peak concentrations are calculated using normalized concentrations to the release mass (Q) of each puff (Fig. 1). The rest of parameters are invariant to normalization. As defined by Zhou and Hanna (2007):

Table 1 Numbers of concentration samplers for IOP3 and IOP8 with stated performance for individual model

		IOP3 (36 samplers)						IOP8 (36 samplers)						
<i>N</i>	Acceptable > 400 pptv	Zero-zero =0 pptv	False negative $C_{O,max} > 400$ ppv, $C_{P,max} < 400$ pptv	False positive $C_{O,max} < 400$ pptv, $C_{P,max} > 400$ pptv	<i>N</i>	Acceptable > 400 pptv	Zero-Zero =0 pptv	False negative $C_{O,max} > 400$ ppv, $C_{P,max} < 400$ pptv	False positive $C_{O,max} < 400$ pptv, $C_{P,max} > 400$ pptv	<i>N</i>	Acceptable > 400 pptv	Zero-Zero =0 pptv	False negative $C_{O,max} > 400$ ppv, $C_{P,max} < 400$ pptv	False positive $C_{O,max} < 400$ pptv, $C_{P,max} > 400$ pptv
M1	28	23	3	0	2	—	—	—	—	—	—	—	—	—
M2	—	—	—	—	—	36	33	0	0	36	33	0	0	3
M3	30	27	0	0	3	36	31	0	2	36	31	0	2	3
M4	26	22	0	2	2	15	10	0	5	15	10	0	5	0
M5	30	27	0	0	3	36	33	0	0	36	33	0	0	3
M6	28	15	5	8	0	29	14	0	12	29	14	0	12	3
M8	31	27	1	0	3	26	14	0	10	26	14	0	10	2
M9	25	16	5	4	0	23	18	0	5	23	18	0	5	0
M10	30	27	0	0	3	35	11	0	21	35	11	0	21	3

N is the number of samplers where the listed model made predictions

Fig. 2 Concentration time series from fast-response sampler L01 during IOP3 release 3 and puff parameters for statistical study. Red dot on the x axis indicates the release time of the puff



- Peak concentration (C_{max}) is the 0.5-s maximum concentration in each time series (red cross in Fig. 2);
- Peak time is the difference between the time when the peak concentration is reached and the release time of each puff (red dot in Fig. 2);
- Arrival time is the time difference between the release time and the time when the concentration is greater than or equal to $0.1 C_{max}$ for the first time;
- Time duration (D_t) is the time period over which concentrations exceeds 10% of the peak concentration (C_{max}).

Based on the previous parameters, the following dispersion coefficients have also been estimated,

- Standard deviation of the concentration time series (σ_t), based on the approach used by Hanna and Franzese (2000) for non-Gaussian distributions (e.g. time series with outliers and/or two or more peaks). Thus, σ_t is calculated as

$$\sigma_t = D_t / 4.3 \quad (1)$$

where 4.3 is the width of a normal distribution at 0.1 of its maximum value (Doran et al. 2007; Zhou and Hanna 2007).

- Along-wind dispersion coefficient (σ_x) is the standard deviation of spatial concentration distribution (Hanna and Franzese 2000), and is calculated as

$$\sigma_x = u \sigma_t \quad (2)$$

where u indicates the effective puff speed at which the puff is moving; u is not the instantaneous puff speed, but the average puff speed over its trajectory from the source position to the sampler position. The speed is calculated as the straight-line distance from the source to the sampler, x (Fig. 1) divided by the peak time (Zhou and Hanna 2007).

2.4 Metrics for Evaluating Model Performance

Quantitative comparisons assess whether the simulation of the aforementioned parameters at receptors points can match the observed ones, and the degree of scatter. The primary quantitative performance measures used to assess the prediction skill of the models are the geometric mean (MG), geometric variance (VG), fraction of predictions within a factor-of-two and a factor-of-five of observations ($FAC2$ and $FAC5$), and its use was suggested

by Hanna and Chang (2012) for ADM evaluation. These measures are generic and apply to any kind of data pairings, including paired in space (sampler) and time (puff), and any kinds of variables, including peak concentration, the peak and puff arrival times and time duration. According to Chang and Hanna (2004), MG and VG values may be more suitable for dispersion modelling because of concentrations spanning many orders of magnitude. These measures have been used in the statistical evaluation of other dispersion models (e.g. Hendricks et al. 2007; Schatzmann et al. 2010). A perfect model has values of MG , VG , $FAC2$ and $FAC5 = 1$. To evaluate and compare how models simulate the variability of the derived parameters with distance and time, the coefficient of determination (R^2) is used. This coefficient is a statistical measure of how close the data are to the fitted regression line, which ranges from zero (none of the variability explained) to 1 (all variability explained).

3 Results

Tables 1 and 2 present quantitative performance measures for the nine models used in UDINEE, with concentrations paired in space and time. Table 1 has been generated using the complete set of sampling data for each model and for the four release periods during IOP3 and IOP8 respectively. The total number of samplers for each intensive operating period is 36 (nine fast-response tracer gas analyzers and four puffs during each intensive operating period) (Clawson et al. 2005). The Table includes samplers where either maximum observed ($C_{O,max}$) or predicted ($C_{P,max}$) concentration is less than the minimum threshold (400 pptv) used in this analysis (Sect. 2.1). Hence, Table 1 includes a listing of the number of samplers for each model that indicate acceptable ($C_{O,max} > 400$ pptv; $C_{P,max} > 400$ pptv), false negative ($C_{O,max} > 400$ pptv; $C_{P,max} < 400$ pptv), false positive ($C_{O,max} < 400$ pptv; $C_{P,max} > 400$ pptv) and zero-zero ($C_{O,max} = 0$; $C_{P,max} = 0$) pairs of values.

The number of modelled SF_6 time series with acceptable samplers varies between models and intensive operating periods (Table 1). These differences arise because several models simulated zero concentration values during the sampling period (20 min) at some samplers in which puffs were actually measured. There are only “zero-zero” cases for IOP3, mostly due to the fact that the observed and predicted plumes (models M1, M5 and M6) were shifted to the east after the release, and hence were off of some samplers located to the north of the release point (Hernández-Ceballos et al. 2019). The zero-zero category has no cases for IOP8, due to the observed plumes stayed over the sampler network, and the predicted plumes were either relatively broad (models M3 and M5) or spread laterally much more to the west than the observed plume (models M4 and M9) (Hernández-Ceballos et al. 2019). IOP8 has many more false negative than false positive pairs. In contrast, the number of false negative and false positive is similar in IOP3, because both observed and predicted plumes were broad in the east-north-east direction.

Clawson et al. (2005) explains that the samplers were occasionally saturated (i.e., concentrations exceeded the maximum concentration measurement capability). Figure 1 shows two examples of this behaviour from sampler L15 during IOP3 and sampler L1 during IOP8. We have removed these time series in the results shown in Table 2, which only considered those samplers (N value) where the observed and predicted SF_6 maximum concentrations exceed the minimum threshold of 400 pptv and the maximum is properly measured. In total, 13 and 18 SF_6 time series in IOP3 and IOP8 (see the samplers analyzed in

Table 2 Number of concentration samplers for IOP3 and IOP8 with stated performance for individual models and puff parameter

N	Peak concentration			Peak time			Arrival time			Time duration		
	FAC2	FAC5	>FAC5	FAC2	FAC5	>FAC5	FAC2	FAC5	>FAC5	FAC2	FAC5	>FAC5
IOP3 (time series = 13)												
M1	13	7	2	4	13	0	11	2	0	11	2	0
M2	-	-	-	-	-	-	-	-	-	-	-	-
M3	13	8	3	2	4	8	0	3	10	11	2	0
M4	13	4	7	2	13	0	13	0	0	7	6	0
M5	13	5	5	3	10	3	13	0	0	2	11	0
M6	6	2	3	1	3	3	5	1	0	2	2	2
M8	13	2	6	5	13	0	12	1	0	3	7	3
M9	7	4	1	2	7	0	7	0	0	6	1	0
M10	13	4	7	2	0	12	0	7	6	4	8	1
IOP8 (time series = 18)												
M1	-	-	-	-	-	-	-	-	-	-	-	-
M2	18	4	8	6	14	4	10	3	5	2	10	6
M3	16	5	3	8	13	3	10	6	0	7	8	1
M4	6	2	2	2	4	2	4	2	0	2	3	0
M5	18	7	3	8	11	7	15	3	0	0	12	6
M6	11	1	1	9	3	5	5	2	4	3	4	4
M8	9	4	2	3	5	4	7	2	0	2	3	4
M9	7	3	3	1	7	0	7	0	0	4	2	1
M10	6	2	3	1	6	0	3	2	1	1	2	3

N is the number of samplers where the observed and predicted maximum concentrations are above 400 pptv. FAC5 values are calculated excluding pairs within FAC2 values

Fig. 1) are used to evaluate how the models simulate the puff passage at the measurement locations.

The results of this multi-model quantitative comparison are organized in two subsections. In Sect. 3.1, we show the performance of models in simulating the peak concentrations, the peak and puff arrival times and the time duration, while Sect. 3.2 is dedicated to displaying how the models simulate the temporal and spatial variability of the dispersion coefficients (σ_r , σ_y).

3.1 Simulation of Observed Puff Parameters

Two panels are shown for each parameter, with each being the corresponding scatter plot with the observed (horizontal axis) and predicted (vertical axis) values for each intensive operating period (Fig. 3a–d for IOP3 and Fig. 3e–h for IOP8). Each point represents the observed-modelled pair for a given puff and sampler. In the scatter plots, straight lines corresponding to *FAC2* and *FAC5* (without *FAC2*) agreement are also plotted. The model performance metrics for each puff parameter are shown in Table 2 (*FAC2* and *FAC5*) and in Fig. 4 (*VG* vs *MG*).

3.1.1 Peak Concentration Normalized by the Emission Mass

Figure 3 shows the two panels of the maximum 0.5-s concentrations for each intensive operating period. The scatter plots reveal differences between models based on the large and different spread of the points around the main diagonal. Visual inspection shows more spread during night-time (IOP8) than during daytime (IOP3).

In general, several potential factors, such as transport distance, wind speed and direction, and turbulence patterns can potentially account for the range of observed maximum concentrations. Flaherty et al. (2007) reported the critical influence of the wind direction on the variability in the concentrations measured for different release periods, and how the highest concentrations measured at the crane site occurred when the wind direction was within 20° of the ideal transport direction. For deviations greater than 20°, concentrations drop off rapidly as only the far edges of the plume are observed, or the plume misses the receptor completely.

On average, there are also differences between the daytime and night-time normalized maximum concentrations. Observed peaks average about 8 pptv kg⁻¹ during daytime and about 16 pptv kg⁻¹ at night. Not all of the models match these day–night differences in the normalized maximum concentrations. Models M4, M6, M3 and M5 present higher mean peaks during night-time and models M8, M9 and M10 during daytime. These differences between models can be attributed to the consideration of day–night thermal differences in the simulations (e.g., the tracer vented upwards, with upward motions more intense during daytime, and therefore favour lower concentration levels during daytime puffs). Flaherty et al. (2007) and Finn et al. (2010) reported, from enhanced dispersion during convective conditions, that the daytime vertical profiles of the SF₆ tracer generally show a lower magnitude and exhibit a more uniform vertical distribution than the night-time profiles. In contrast, if day–night stability differences are not considered, the differences between modelling predictions can be associated with the changes in the release location and flow dynamics in the urban area.

Low *FAC2* values are obtained in both intensive operating periods, with a range from 0.15 (M8) to 0.61 (M3) during daytime, and from 0.10 (M6) to 0.38 (M5) at night

Fig. 3 Scatter plots for, **a** peak concentrations (in pptv kg^{-1}), **b** peak time (in seconds), **c** arrival time (in seconds), and **d** time duration (in sec) predicted and observed paired in space (same sampling location) for IOP3. Scatter plots for, **(e)** peak concentrations (in pptv kg^{-1}), **(f)** peak time (in seconds), **(g)** arrival time (in seconds) and **(h)** time duration (in seconds) predicted and observed paired in space (same sampling location) for IOP8. The axes of the plots are logarithmic for concentrations and linear for the times. Points are plotted for individual models under the condition that observed and predicted peak concentrations must both exceed the threshold of 400 pptv

(Table 2). There are more points largely underpredicting ($> FAC5$) the observed peak values in IOP8 than in IOP3. In addition, the largest overprediction in IOP3 is seen on both the lowest and the highest observed peak concentrations, while the largest overprediction is concentrated at low peak concentrations in IOP8.

On average, peak concentrations are overestimated in both intensive operating periods (MG values average about 1.3 in IOP3 and 1.9 in IOP8, Fig. 4). Three models (M4, M8 and M9) underestimate and two models (M6 and M3) overestimate the observed peak concentrations in both intensive operating periods. A change in the behaviour of models M5 and M10 between daytime and night-time is observed. With the exception of model M6 in IOP8, VG values < 100 in both intensive operating periods (Fig. 4). The large bias obtained for M6 is mainly caused by the large overprediction registered in three measurement locations in IOP8 respectively (Fig. 3e–h).

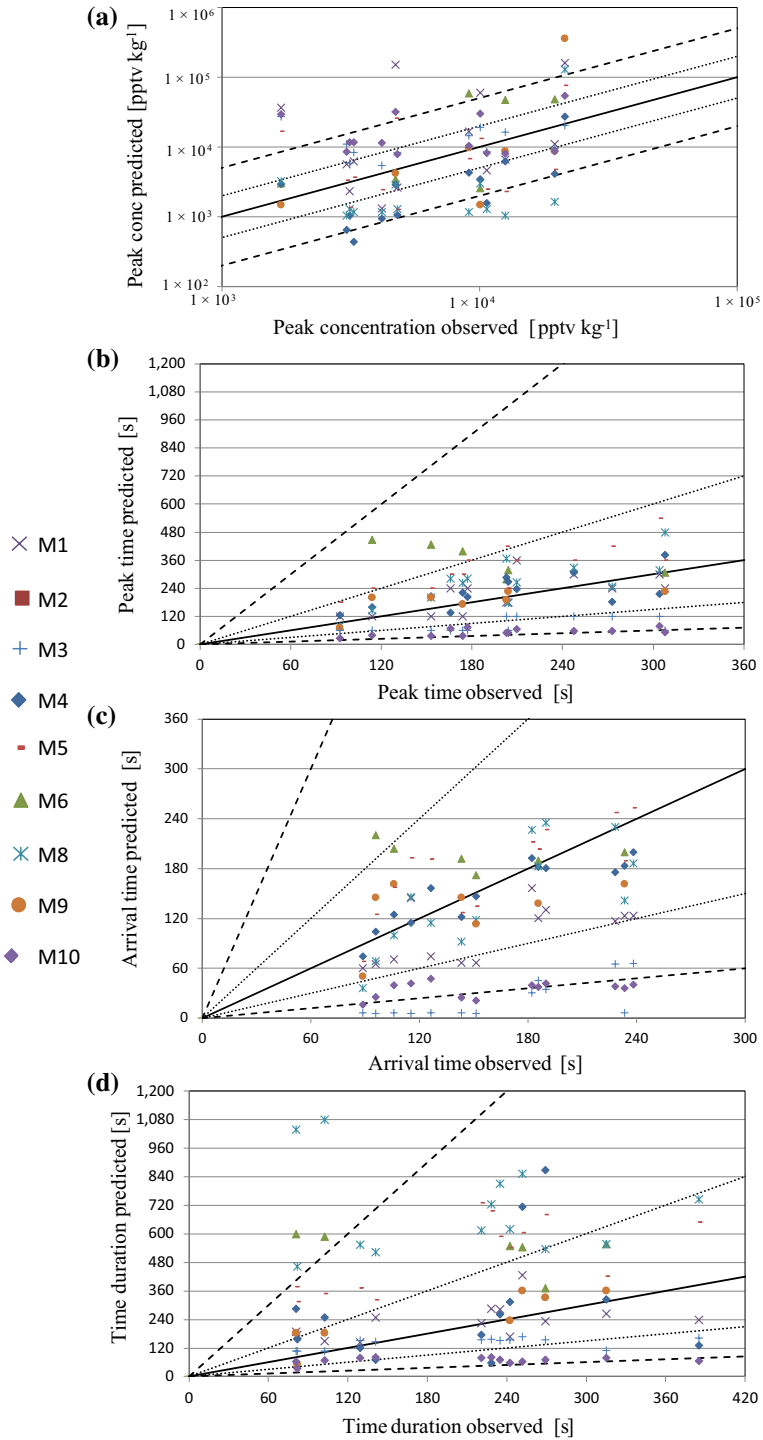
3.1.2 Peak Time

The scatter plots for the peak times are shown in Fig. 3a–d (IOP3) and Fig. 3e–h (IOP8). Based on the scatter diagrams, there are large differences between them. On average, all models present larger peak times during night-time, which is in agreement with the average values from observations (about 201 s in IOP3 and 224 s in IOP8).

Despite the different scatter, most of the predictions fall within a factor-of-two of observations in both intensive operating periods, pointing out the $FAC2$ values (100% of the predicted samplers) of models M4, M1, M8 and M9 during daytime, and of models M9 and M10 during night-time (Table 2). In contrast, models M10 and M3 in IOP3 and model M6 in IOP8 have the highest percentage of points falling within a factor-of-five. Looking at Table 2, and with the exception of model M10 in IOP3 and model M6 in IOP8, predicted peak times are mainly below $FAC5$ of the observations (above 95% of the points).

The MG values (Fig. 4) indicate that the models overestimate or underestimate the peak times independently of the intensive operating period. The MG values show that six out of eight models clearly overpredict the observed peak times ($MG > 1$) in IOP3, with a maximum MG value of 1.9 (M6). The maximum VG value in IOP3 is 6.1 (M10), while the rest of the models keep VG values below 2.4 (Fig. 4). In IOP8, seven out of eight models overpredict the observed peak times ($MG > 1$), with a maximum value of 3.2 (M6). IOP8 presents low VG values, with an average of about 2, which indicates that the spread is limited to a small number of pairs.

Comparing the scatter, model M6 is highlighted, since many predictions are flat and high in both intensive operating periods (Fig. 3). In the case of IOP8, this model largely overestimates the peak times at eight samplers (peak concentration is predicted just at the end of the sampling period). Analyzing the observed time series at these samplers (puffs 1, 2, 3, 4 from L06, puffs 1, 3, 4 from L02, and puff 3 from L08), the common characteristic is the presence of more than one peak and a relatively long time duration of the time series. Zhou and Hanna (2007) identify some of these outliers in the peak time, which were



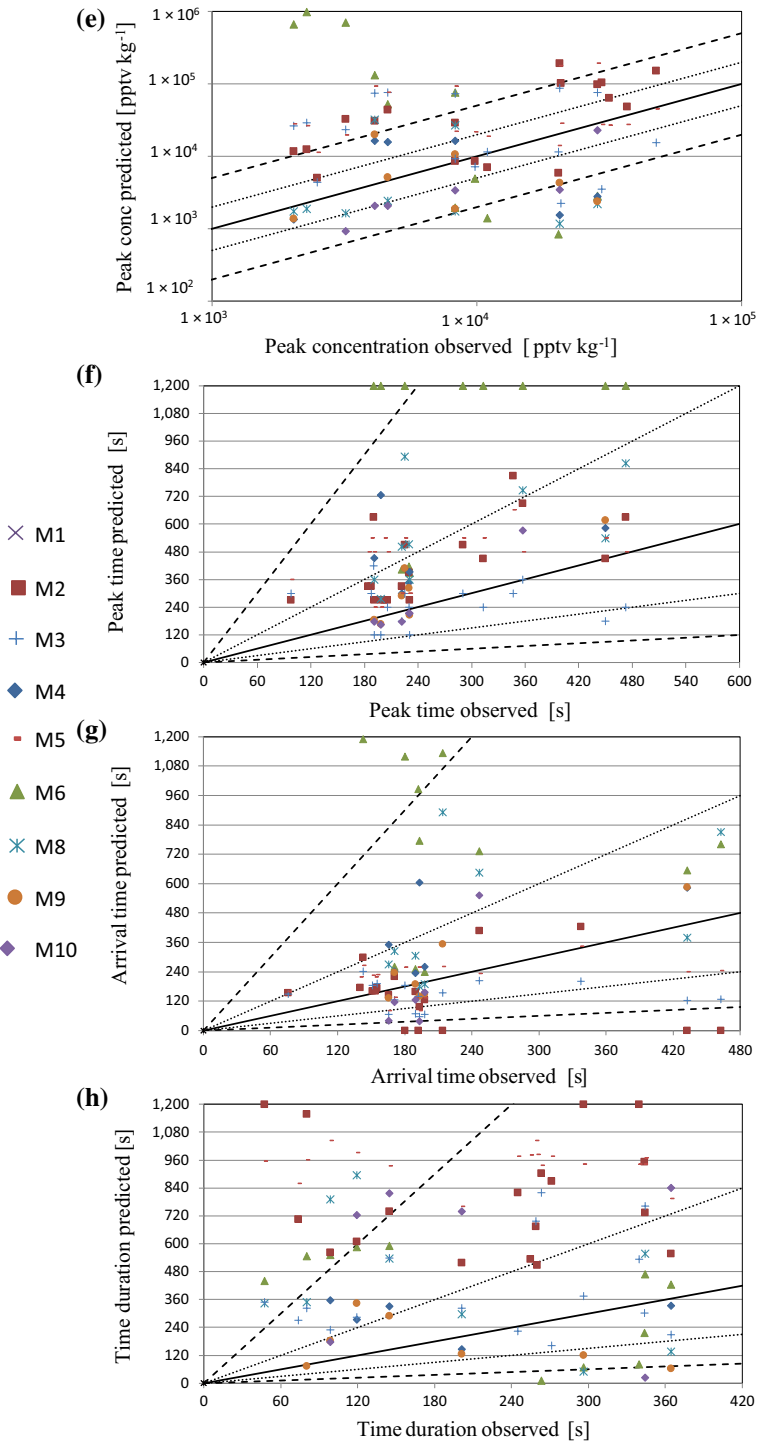


Fig. 3 (continued)

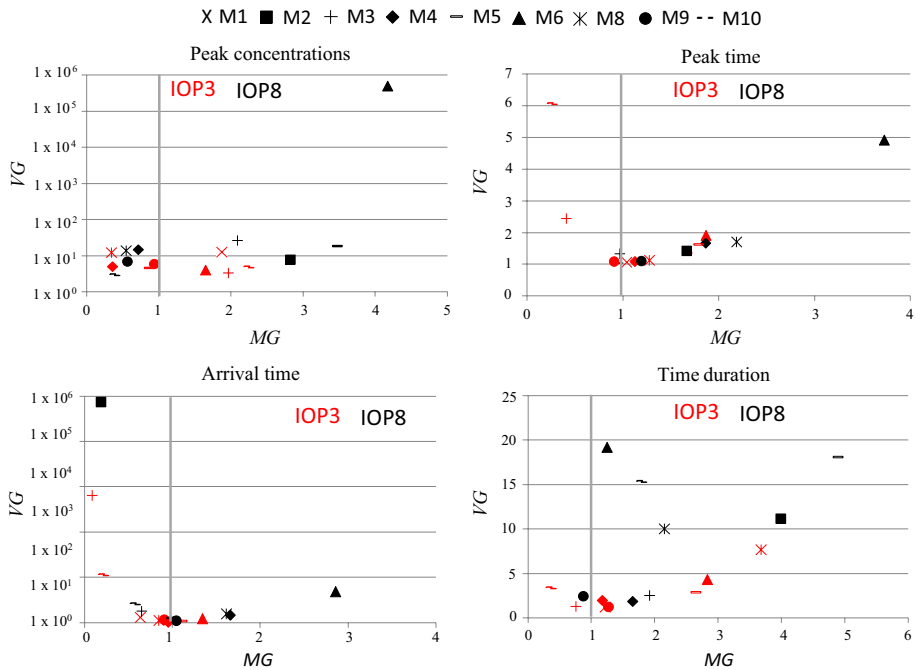


Fig. 4 Diagrams (VG vs MG) for the performance of models in simulating each puff parameter. Each model is identified by its anonymous code. Red colour is for IOP3 and black colour is for IOP8. Note the differences in scales

associated with the location of the samplers near to and/or behind large buildings. Considering this information, model M6 could therefore have difficulties in simulating the physical processes determining the puff dispersion in these specific samplers.

3.1.3 Arrival Time

Figure 3 shows the scatter plots for predicted and observed arrival times for each intensive operating period. Visually, the distribution of the points is completely different in each one. The scatter also points out how the agreement looks better below 180 s in both, which suggests a better representation of the small puff arrival times, i.e. fast puffs and/or nearby samplers to the release point. This result is in agreement with the increase in the complexity of matching the observed puff concentrations with increasing the distance of the sampling site from the release point. Hernández-Ceballos et al. (2019) report that the models tend to increasingly underestimate concentration as the puff moves away from the source. This behaviour is strongly influenced by the complex circulations and turbulence patterns generated by the buildings in the built-up urban area.

In IOP3, and with the exception of M3 and M10, the models present high agreement with observations [$FAC2$ values range from 0.8 (M6) to 1.0 (M4, M5, M9)] (Table 2). In the case of M3 and M10, there are many points underestimating the observed values above a factor-of-five (77% of the points for M3 and 46% for M10), which consequently causes the minimum $FAC2$ value ($FAC2$ is zero for models M3 and M10). In IOP8,

although the spread of the points is larger, most of them fall within a factor-of-two of observations, in a range from 0.45 (M6) to 1.0 (M9) (Table 2). Only M6 shows a larger percentage of points ($\geq 50\%$) within or above a factor of five of observed arrival times.

On average, the *MG* values show different trends in IOP3 ($MG=0.8$) and in IOP8 ($MG=1.2$). In IOP3, with the exception of M6 and M5 ($MG>1.0$), the models underestimate the arrival time ($MG<1$) in a range from 0.1 (M3) to 0.9 (M4) (Fig. 4). In the case of IOP8, while three models (M2, M3 and M10) underestimate the arrival of the plume (MG values average about 0.5), there are five models overestimating its arrival (MG values average about 1.8). Model M6 reaches the maximum *MG* value (2.9).

The *VG* value is below 10 in most of the models and in both intensive operating periods (Fig. 4). The highest *VG* values ($VG>100$) correspond to M3 in IOP3 and M2 in IOP8. These large values relates to the large underestimation of the arrival time at most of the receptors in the case of model M3 in IOP3, and in five receptors in the case of model M2 in IOP8.

3.1.4 Time Duration

Scatter plots for the time duration are depicted in Fig. 3. We note the large spread in both plots and how models tend to largely overpredict the observed time duration during IOP8 (night-time), whilst there appears to be more balance between the points around the line of best fit during IOP3 (daytime hours). According to the meaning of this parameter, i.e. time period over which concentrations exceed the 10% of the peak concentration, these results suggest day–night stability differences, if thermal effects are taken into account. Differences can be, for instance, in the simulation of building wake effects, which contribute to the puff elongation by retaining and then releasing tracer over the city. This mechanism contributes to the asymmetry of the puff about their maximum values (Doran et al. 2007).

On average, the *FAC2* value is higher in IOP3 (0.5) than in IOP8 (0.3), and it is important to point out that all models present improved *FAC2* values during IOP3 (daytime) (Table 2). The majority of points in most of the models are within a factor-of-five in both intensive operating periods and an increase in the number of predicted values above the *FAC5* value is registered overnight. This result reveals how the characteristics of the sampler location inside the urban canopy can affect the agreement between observed and predictions at a particular receptor (given that they are placed in different locations for the different intensive operating periods). In this sense, the location of the sampler can cause it to be affected either by the edges or by the middle of the spreading cloud of tracer material.

In terms of *MG* values, seven out of eight models overpredict the time duration in IOP8, with values in a range from 1.2 (M6) to 4.0 (M2) (Fig. 4). In contrast, model M9 underpredicts the observed time duration, with an *MG* value of 0.9. In the case of IOP3, three models predict a shorted puff duration at the receptors (*MG* values are 0.4 for M10 and 0.8 for M3) while the rest of them predict a longer duration with an average value of 2.1 and a maximum value of 3.7 (M8). On average, the *VG* value is larger during IOP8 (it averages about 10) than during IOP3 (it averages about 3), in agreement with the large scatter shown. The highest *VG* value is obtained for M6 in IOP8 (at around 20) and the lowest for M1 and M9 ($VG=1.2$) (Fig. 4), for which most of the points fall along the perfect agreement line.

3.2 Dispersion Coefficients

The purpose here is to evaluate how models capture the relationships between, (i) σ_t and peak time, and (ii) σ_x and downwind distance from the release point in IOP3 and IOP8. We apply a linear relationship to quantify the association between these variables. However, we need to keep in mind that due to the effect of buildings and street canyons on urban dispersion, these relationships may not actually be linear in an urban environment, as they are in open fields (e.g. Hanna and Franzese 2000). Many studies have been carried out to investigate the influence of buildings on the airflow and concentration fields (e.g. Zhang et al. 2015, Ricci et al. 2017). The wind field within the street canyons can look very different from the average wind field with along-street flow and large-scale turbulent eddies. In this sense, Flaherty et al. (2007) show how the presence of buildings channels the plume, shifts its transport direction, and makes it wider than a non-channelled plume.

By analyzing these relationships, and according to Zhou and Hanna (2007), we also investigate the model predictions about the initial size and spread of the puff. The intercept value of the linear relation between σ_t and peak time (at peak time = 0) represents the measure of the initial puff size (in seconds), while in the relationship between σ_x and downwind distance, the intercept value (at distance from the release = 0) represents the initial downwind plume spread (in metres).

The value of both intercept values relates to the influence of buildings around the source location. In this sense, the four puffs were released in the midst of tall buildings (on the east side of Broadway across from the Westin Hotel) during IOP8, while they were released in a park upwind of the area of tall buildings (near the Myriad Botanical Gardens) during IOP3 (see Fig. 1, and Clawson et al. 2005). Figures 5 and 6 show the graphical relationship between variables, and Table 3 summarizes the values obtained for the elements of each linear relation (slope, y-intercept and R^2 values). The observed values have been generated using the complete set of samplers (Fig. 1), while for each model, we have considered the number of samplers where each model made predictions above 400 pptv (N value in Table 2).

3.2.1 Variation of the Standard Deviation of the Concentration Time Series with Peak Times

The observed relationship between these two variables is different in each intensive operating period (Fig. 5). From observations, while σ_t values seem to increase with peak times during IOP3 (daytime—positive linear correlation with $R^2=0.43$), σ_t values are more spread out and seem to decrease drastically as peak time increases in IOP8 (overnight—negative linear correlation with $R^2=0.18$). Some of the models (Table 3) also catch these differences between intensive operating periods. In IOP3, the models present a positive linear correlation between these two variables and four of them (models M6, M9, M5, M10) improve the coefficient of determination between the observed values. In the case of IOP8, there are four models (M6, M8, M3, M10) following the negative linear correlation obtained from observations, and the R^2 values range from 0.05 (M8) to 0.59 (M10).

The observed and predicted intercept values (Table 3) reflect the impact of the release site characteristics on the initial puff size. In all of the models, the linear relationship presents a larger intercept value in IOP8 than in IOP3, in line with the different characteristics of the release sites. In IOP3, six out of eight models have a larger intercept value than with

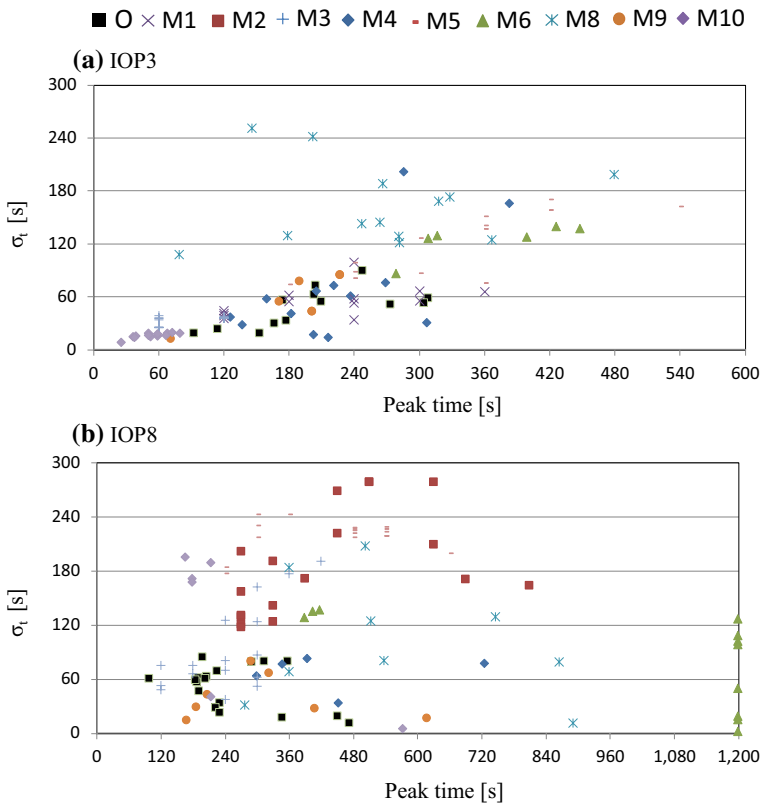


Fig. 5 Observed and predicted σ_t versus peak time for IOP3 and IOP8. Note the differences in peak time scales

the observations (5.08 s), with the maximum value reached by M8 (about 160 s). It should be pointed out that two models (M4 and M9) present a negative intercept value, i.e., initial puff size. A possible cause of this result could be in the simulation of the puff hold-up in the wakes of large buildings upwind of the sampler locations, which influence the effective intercept term (Zhou and Hanna 2007). In IOP8, only one model (M3 with -2.70 s) presents a negative intercept value while the rest of the models give an average initial puff size of about 113 s, with a maximum value of 231 s (model M10) and a minimum one of 48 s (model M9), while the observations yield 78.3 s.

3.2.2 Variation of the Along-Wind Dispersion Coefficient with Downwind Distance

The set of observed σ_x values present rather small differences with distance in both intensive operating periods (Fig. 6). There is a positive and low-slope linear relation with increasing downwind distance from the release point in both (0.23 in IOP3 and 0.09 in IOP8), with R^2 values of 0.42 during IOP3 (daytime) and 0.04 during IOP8 (overnight). Differences between models and between intensive operating periods (day–night) results are pointed out. In IOP3, most of the points from models are close to the observed values with the exception of M8, which clearly provides bigger σ_x values than those found from

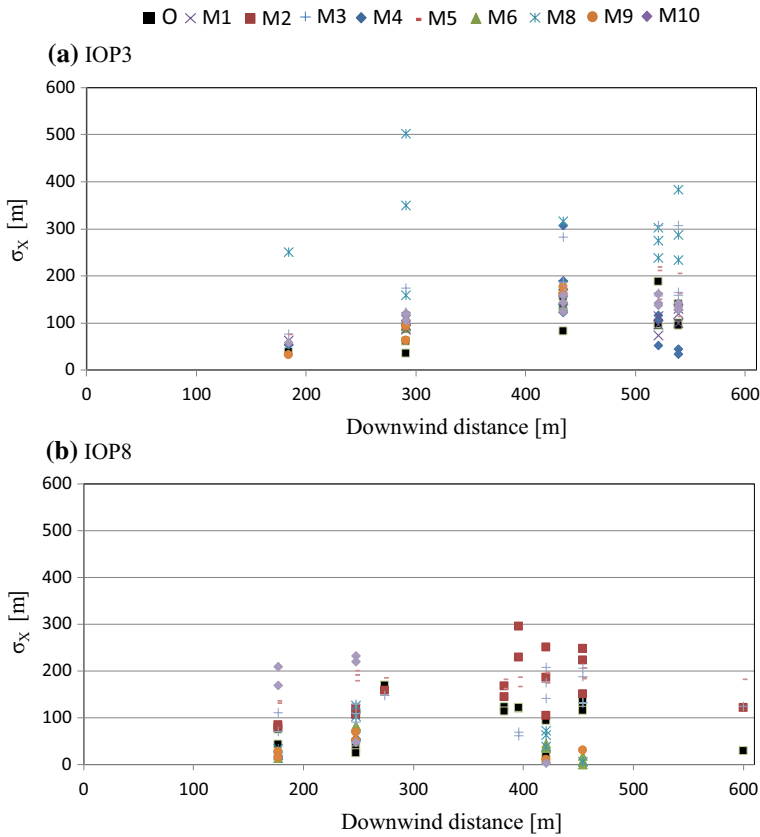


Fig. 6 Observed and predicted σ_x versus downwind distance in IOP3 and IOP8

observations at the same distances. In the case of IOP8, there is a large amount of scatter around observations. In general, the variance between these two parameters is captured and better explained by most of the models in each intensive operating period, with the exception of models M4, M1, M8 and M3 in IOP3 and of model M8 in IOP8 (Table 3). These differences between models can be partly justified by the relationship between duration time and σ_x (Sect. 2.3) and so, the large scatter obtained in the simulation of the time duration in each IOP.

The intercept term of this linear relation represents the initial downwind plume spread (in metres). The intercept value calculated from observations is 1.4 m in IOP3 and 50 m in IOP8. It is necessary to point out that the derived initial σ_x obtained for IOP3 is similar to the initial puff size (1 m) in the JU2003 experiment. In contrast, for IOP8, the intercept value (51.1 m) is in the line with the one obtained in Zhou and Hanna (2007) of about 40 m and therefore, much larger than the physical puff size of the JU2003 experiment. Most of the models present a non-zero and positive intercept value, which suggest the simulation of the “hold-up” effect caused by the retention and subsequent release of airborne material by the buildings (Doran et al. 2007). Five out of eight models present larger intercept values in IOP3, in a range from 30 (M5) to 309 m (M8), and 6 out of 8 in IOP8, with values from 55 m (M2) to 342 m (M10). There are models predicting negative intercept values in

Table 3 Observed and modelled slope, intercept and coefficient of determination (R^2) values of the variation of puff parameters with time and distance

	σ_t versus peak time			σ_x versus downwind distance		
	Slope/600	y-intercept (s)	R^2	Slope	y-intercept (m)	R^2
IOP3						
O	0.21	5.08	0.43	0.23	1.40	0.42
M1	0.11	30.19	0.27	0.09	72.95	0.12
M2	–	–	–	–	–	–
M3	0.10	24.95	0.30	0.34	37.83	0.32
M4	0.50	–45.34	0.41	0.02	106.00	0.00
M5	0.30	19.49	0.64	0.28	30.53	0.57
M6	0.20	51.38	0.54	0.50	–52.24	0.86
M8	0.01	160.10	0.00	–0.07	309.05	0.01
M9	0.41	–18.19	0.67	0.58	–88.28	0.94
M10	0.15	7.91	0.65	0.17	55.54	0.62
IOP8						
O	–0.10	78.30	0.18	0.09	51.10	0.04
M1	–	–	–	–	–	–
M2	0.16	116.54	0.23	0.31	55.63	0.28
M3	0.39	–2.70	0.49	0.16	72.84	0.17
M4	0.01	60.66	0.01	0.52	–76.13	0.99
M5	0.03	205.97	0.05	0.08	147.90	0.23
M6	–0.09	168.21	0.37	–0.18	104.02	0.39
M8	–0.07	140.89	0.06	–0.06	76.93	0.03
M9	–0.03	48.08	0.03	–0.04	49.12	0.06
M10	–0.41	231.40	0.59	–0.77	342.52	0.50

600 means the downwind distance until the linear relation is valid

each intensive operating period, M6 and M9 in IOP3 and M4 in IOP8. This negative value indicates the simulation of more upwind dispersion of the puff in the early phase of the dispersion.

4 Influence of Atmospheric Stability

As in Hernández-Ceballos et al. (2019), the statistical measures presented in the previous sections show variability among different models in the simulation of the puff dispersion. As expected in complex built environments and in agreement with COST ES1006 (2015), the performance of models is influenced significantly by the location of sources (e.g. open space such in IOP3, and inside a complex building structure in IOP8) and receptor points.

The impact of using fixed or time-varying inflow conditions on the performance of models was addressed in Hernández-Ceballos et al. (2019). Another key factor contributing to differences between models is if and how they treat the effect of atmospheric stability on puff dispersion. Many studies have reported the significant effect of atmospheric stability on pollutant dispersion in the urban environment (e.g. Kumar et al. 2006; Yassin 2013). In

urban areas, during the day, surfaces are more reflective and become hotter and thus, producing more convective eddies. As a result, urban areas are rarely as stable, and hence, the performance of models could change in case stable or unstable atmospheric stratification is considered in their computations. Significant day–night differences in puff dispersion and concentration variability have also been reported (e.g. Finn et al. 2010; Franzese and Huq 2011). Marked differences of about a factor of three or four between concentrations data during day and night releases have been observed, as well as, night-time plumes are more likely to have reduced concentration fluctuation intensities relative to daytime plumes. In contrast, Hanna et al. (2007) concludes that the effects of atmospheric stability are minimal in the downtown area.

Table 4 shows whether models simulating IOP3 and IOP8 assumed day–night stability differences or neutral atmospheric conditions. Whilst there are four models (M9, M3, M5, M10) assuming different stability between day and night intensive operating periods, there were five models (M1, M2, M4, M8, M6) in which neutral atmospheric conditions without any thermal effect were established for simulating both IOPs. We need to point out that M2 and M1 simulated only one intensive operating period respectively (see Sect. 2.1).

Looking at the results shown in Table 3, the model simulations using day–night stability differences are acceptable (>400 pptv) for 84% and 82% of the total simulated samplers in IOP3 and IOP8 respectively, while the percentage is lower for those using neutral stability (67% and 66% of the simulated samplers in IOP3 and IOP8). In addition, considering the percentage of false negative samplers predicted by each group of models, those applying day–night stability differences present a lower percentage than those using neutral stability in each intensive operating period. It is for 3% and 8% of the total simulated samplers in IOP3, and for 21% and 25% in IOP8 respectively.

Considering the performance measures of *MG* and *VG* obtained simulating the maximum concentrations (Sect. 3.1), differences are also observed between both groups of models. In IOP3 (daytime) and applying neutral stability conditions, *MG* values average about 0.7, which suggests a mean underprediction bias of about a factor of 2, and it has range from 0.30 to 1.87. In contrast, the average of *MG* values is 1.35, which suggests mean overprediction bias of about a factor of 2, and the range is 0.32–2.25 considering day–night stability differences. The range of *VG* values is higher for neutral, between 5.0 and 97.2, than for day–night stability conditions, between 3.4 and 39.2. In IOP8 (night-time), *MG* values average about 0.9 for neutral and 1.2 for day–night stability differences,

Table 4 Modelling of thermal effects (day–night or neutral)

	Neutral or day–night stability
M1	Neutral atmospheric conditions without any thermal effects
M2	Neutral atmospheric conditions without any thermal effects [Background turbulence scheme (Hanna)]
M3	Parametrization scheme to diagnose heat flux; cloud fraction
M4	Neutral atmospheric conditions without any thermal effects
M5	Parametrization scheme to diagnose heat flux; cloud fraction
M6	Neutral atmospheric conditions without any thermal effects
M8	Neutral atmospheric conditions without any thermal effects
M9	Boundary conditions dependent on the evaluated atmospheric stability category
M10	Boundary-layer model as part of SCIPUFF

while the average of VG values decreases about three orders of magnitude using day–night atmospheric conditions. These results suggest that there is a change between underestimation and overestimation by using neutral conditions or day–night stability differences, and that the largest modelled bias in the simulation of maximum concentrations tend to appear simulating the puff dispersion using neutral atmospheric conditions.

Taking as reference the coefficient of determination calculated between σ_t and peak time, and σ_x and downwind distance from the release point in IOP3 and IOP8, we have also found that models using day–night stability differences improve the percentage of explained variance. For σ_t vs peak time, the mean R^2 is 0.30 for neutral and 0.56 for day–night differences in IOP3, while it is 0.16 and 0.29 respectively in IOP8. In the case of σ_x versus downwind distance, models using day–night stability differences improve largely the mean R^2 value in IOP3, from 0.24 to 0.61, while IOP8 is the only case in which the neutral models present a mean R^2 (0.42) higher than those applying day–night differences (0.24). The latter obtain the highest R^2 value in each intensive operating period, with the exception of IOP8 and of σ_x versus downwind distance. These results, hence, suggest that those models applying day–night stability differences tend to yield a better fit than neutral ones.

It is often assumed when simulating transport and dispersion in the urban environment that stability conditions are neutral. Lundquist and Chan (2007) indicated that for long-duration releases under moderate wind conditions and within a built-up area the assumption of neutral stability is accepted. The results shown in this analysis looks contradictory with this suggestion, and point out the need to consider even slight unstable conditions in the simulation of daytime and night-time releases. To achieve this, there is a need to have sufficient meteorological input variables and data to address atmospheric stability to model urban dispersion.

5 Conclusions

Under the UDINEE project, nine ADMs of different levels of complexity were evaluated and compared with tracer measurements from the subset of instantaneous puff releases performed during the Oklahoma City Joint Urban 2003 field experiment. This study has investigated the model capability in simulating the characteristics (concentrations and timing) of the fast-response time series, as well as how models simulate the initial dispersion phase of the puff dispersion. To this purpose, we have compared observed and modelled SF_6 concentrations, with time resolution of 0.5 s and concentrations above 400 pptv, corresponding to four puff releases each in IOP3 (daytime) and IOP8 (night-time).

Overall, the point-by-point quantitative comparison of the simulated and observed parameters has shown that models better capture the arrival and peak times. There are specific samplers in which puff parameters were poorly simulated, showing how the characteristics of the sampler location inside the urban canopy can affect the agreement between observations and predictions. Within this mean behaviour, it should be pointed out that there were noticeable differences between models, both in simulating the parameters and between day and night predictions. These differences are also observed in the results obtained for the dispersion coefficients. It is important to emphasize that the evaluation results here are based on two out of 10 intensive operating periods of the JU2003 experiment.

UDINEE has highlighted differences in ADMs and in the parametrization schemes, in simulating the propagation of the plume from an instantaneous source of release in an urban environment. Our analysis demonstrates that knowledge of concentration variability is potentially very significant for urban emergency-response planning. In this sense, and in the present framework, the impact of atmospheric stability on the performance of models has also been investigated. An improvement in the performance of models (e.g. increase the percentage of acceptable samplers, a decrease in the percentage of false negative samplers, an improvement in the simulation of maximum concentrations, and in the relationships between dispersion coefficients with time and distance) has been observed by using day–night stability differences. This result indicates the need to have sufficient meteorological input variables and data to quantify atmospheric stability in simulating urban dispersion.

It appears that there is still need for more work to further improve the present modelling tools, and the UDINEE project has been proven to be a good platform to foster collaborations among modelling groups. The large amount of data produced under the UDINEE project and already stored in the ENSEMBLE system should support detailed studies of urban dispersion models. By building on the current experience and promoting community work, it is expected that additional analysis can be efficiently conducted to improve the currently available modelling systems. This dispersion dataset is a valuable asset, not only for developing advanced tools for emergency-response situations in the event of a toxic release, but also for refining air-quality models. More work is needed to investigate the sensitivity of the model results to different modelling options, different urban geometries and different meteorological conditions.

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