

1 EXPERIMENTAL DATA AND CFD PERFORMANCE FOR CLOUD 2 DISPERSION ANALYSIS: THE USP-UPC PROJECT

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17 **Abstract**

18 Forecasting the behaviour of a flammable or toxic cloud is a critical challenge in quantitative risk
19 analysis. Recent literature shows that empirical and integral models are unable to model complex
20 dispersion scenarios, like those occurring in semi-confined spaces or with the presence of physical
21 barriers. Although CFD simulators are promising tools in this regard, they still need to be fully
22 validated with comprehensive datasets coming from experimental campaigns designed ad-hoc. In this
23 paper, we present an experimental campaign carried out by a joint venture between University of São
24 Paulo and Universitat Politècnica de Catalunya to investigate CFD tools performance when used to
25 analyse clouds dispersion. The experiments consisted on propane cloud dispersion field tests
26 (unobstructed and with the presence of a fence obstructing the flow) of releases up to 0.5 kg/s of 40 s
27 of duration in a discharge area of 700 m². We provide a full 1-s averaged propane concentration
28 evolution dataset of two experiments, extracted from 29 points located at different positions within the
29 cloud, with which we have tested FLACS® CFD-software performance. FLACS reproduces
30 successfully the presence of complex geometry, showing realistic concentration decreases due to cloud
31 dispersion obstruction by the existence of a fence. However, simulated clouds have not represented the
32 whole complex accumulation dynamics due to wind variation.

1 **Keywords:** consequence analysis, propane, field tests, computational fluid dynamics, FLACS
2 software.

3 **1 INTRODUCTION**

4 Dispersion of hazardous gas releases occurring in transportation or storage installations represent a
5 major threat to health and environment. Therefore, forecasting the behaviour of a flammable or toxic
6 cloud is a critical challenge in quantitative risk analysis. Cloud dispersion is often analysed using
7 Gaussian and integral models that usually provide reliable and fast results for dispersions in simple
8 scenarios, i.e. unobstructed, over flat terrain; however, these models show limitations when applied to
9 study dispersions over terrains with any degree of complexity, like in offshore production units,
10 refineries or industrial plants. Obstacles present in the cloud scattering path interact with the gas flow
11 and generate turbulence causing an important effect in the cloud dispersion. The impact of the
12 geometry on dispersion has to be necessarily evaluated to perform an accurate dispersion analysis and
13 simple models are not able to tackle it. The latter treat terrain complexities by means of a surface
14 roughness parameter, which becomes a very imprecise and unrealistic approximation when modelling
15 dispersion with complex local geometries.

16 The interest of Computational Fluid Dynamics (CFD) codes to solve complex flow related problems
17 has been extended within the scientific community, together with the increase on computational
18 capacity. One of the areas where CFD has already shown its potential is in risk analysis, and more
19 particularly in dispersion. Although CFD tools spend significantly more time to perform dispersion
20 analysis, they allow taking into account the geometry of elements present in real scenarios, such as
21 barriers or semi-confined spaces. A comparative study between the use of an integral model and a
22 CFD tool to evaluate dispersion analysis is reported by Schleder & Martins (2013a); in this study, a
23 LNG (liquefied natural gas) leakage in a semi-confined space was simulated using the UDM (unified
24 dispersion model (Haper, 2009) model and the FLACS CFD-simulation tool (GexCon AS, 2013),
25 showing the latter the ability to realistically peak the concentration variations due to the presence of an
26 obstacle placed at the dispersion path, which led to an increase of the LFL (lower flammability limit)
27 distance reached by the vapour cloud. Sklavounos & Rigas (2006) compared the performance of the

1 CFD code CFX(Ansys Inc., 2011) with two traditional models –SLAB (Ermak, 1990) and DEGADIS
2 (Reynolds, 1992) – when challenged to simulate also an experimental LNG release. Their results
3 showed that the CFD code presented better accuracy than the integral models when reproducing
4 concentration distributions in the dispersion field.

5 In recent years the use of CFD tools to perform dispersion analyses has been increased and although
6 they have been proven promising, they still present some challenges to overcome. As shown by
7 Plasmans et al. (2012), large differences may arise among simulation results when using different CFD
8 tools and/or different CFD analysts to assess the same dispersion scenario. In CFD simulations, a wide
9 range of computational parameters must be set by the user, which may affect the results significantly.
10 For instance, in a typical simulation the user must select the variables of interest, has to be able to
11 choose a turbulence model from a set of available options, must define the computational domain and
12 mesh, must specify the boundary conditions, the methods of discretization and the convergence
13 criteria, among others. Sensitivity tests and validation studies have been conducted during the last
14 years in order to provide insights on how to appropriately set CFD simulations (e.g. Sklavounos and
15 Rigas, 2006; Cormier et al., 2009; Tauseef et al., 2011), but to do that, reliable experimental data is
16 needed. There are few reported field experiments in the literature dealing with dispersion and even less
17 dealing with dispersion in environments with some degree of complexity. The majority of these tests
18 were performed decades ago, and the data generated is not comprehensive enough for an exhaustive
19 evaluation of CFD tools performance.

20 **1.1 Literature review on dispersion experiments**

21 Most of the field tests performed in the past involved LNG dispersions, since during the decades of 70
22 and 80 a huge effort was conducted in order to fully understand the behaviour of LNG when released
23 accidentally (e.g. Blackmore, Eyre and Summers 1982; Koopman et al., 1982; Goldwire et al., 1983).
24 More recently, experiments involving LNG releases on water have been performed (Hanlin, 2006).
25 Field tests involving other substances such hydrogen or tracer gases are found in smaller proportion
26 (Middha & Hansen, 2009; Bilotft, 2001; Allwine and Flaherty, 2007), although the tests involving the
27 former substance have been increased in last years.

1 Among the more classical dispersion field tests used for validation purposes, the Falcon and the Burro
2 series (reported by Koopman et al. 1982 and Brown et al. 1990, respectively) have to be highlighted.
3 Both tests consisted of LNG spills; the Burro tests were undertaken at an open area without obstacles
4 whereas the Falcon tests were performed in a terrain with obstacles. These tests have been extensively
5 used for models validation (e.g. Ermak, Chan, Morgan, & Morris, 1982; Gavelli, Bullister, & Kytoma,
6 2008; Hansen, Gavelli, Ichard, & Davis, 2010). However, it is important to note that the tests were
7 made decades ago, when the range of measurement and data logging equipment was not as
8 comprehensive as nowadays and therefore data available from these tests is scarce for an overall CFD
9 validation exercise.

10 Later on, Gaz de France and Associates (Butler and Royle, 2001) conducted experiments involving the
11 dispersion of a dense gas in an environment with obstacles. However, the project was focused on flash
12 fires and not on cloud dispersion. In most trials, the cloud was ignited few seconds after the gas release
13 started and therefore, it hardly dispersed. Still in the 2000 first decade, the tests MUST (Biltoft, 2001),
14 MID05 (Allwine and Flaherty, 2007) and MKOPSC (Cormier et al., 2009) were carried using tracer
15 gas (the first two) and LNG as substances. They were undertaken by a consortia involving private
16 companies; therefore, only a small portion of the collected data is publicly available through published
17 reports, which hampers its use to perform validation studies. More recently, in 2010, the Jack Rabbit
18 test was conducted in order to assess the behaviour of a cloud generated by a large amount of
19 ammonia released instantaneously in a terrain depression, and although it is rated as a test with
20 obstructions, its scenario is very restricted since the obstruction is just the result of the changing slope
21 in the terrain (Hanna et al., 2012). It is worth to note that most published data only contain values of
22 peak concentrations or concentrations in a specific moment after the release. Concentration evolution
23 with time and space can be hardly found in the literature which reduces the possibility to explore CFD
24 validity for dispersion studies.

25 **1.2 The USP-UPC Project**

26

1 As the literature review shows, there is a lack of complete experimental data to assess the use of CFD
2 tools for consequences analysis involving dispersion of flammable and toxic substances. To overcome
3 this drawback, a joint venture between University of São Paulo (USP) and Universitat Politècnica de
4 Catalunya (UPC) has recently been established to investigate the performance of CFD tools when
5 analysing cloud dispersion of flammable/toxic substances by means of ad-hoc experimentation.
6 The first stage of the experiments planned in this project was undertaken at Can Padró Security and
7 Safety training site during 22nd-25th July of 2014 and consisted of LPG clouds formation and
8 dispersion tracking. Eleven trials were performed, comprising a total amount of around 70 kg of LPG
9 emitted. The vapour clouds were intensively monitored to determine concentration evolution with time
10 and space.
11 The paper at hand provides a description of this first USP-UPC campaign and gives details of the
12 experimental data of two of the trials and their simulation using FLACS simulation software, which is
13 a CFD tool specifically developed for consequence analysis. The objectives of this paper are to offer
14 new sets of experimental cloud dispersion data to the international community and to show
15 preliminary results of CFD performance to simulate two of the experiments, as an example of the
16 potential uses of the data gathered during the tests.

17 **2 EXPERIMENTAL SET-UP**

18 The field tests consisted of continuous releases of LPG in the atmosphere with the subsequent
19 resulting cloud formation. LPG composition consists of 97% propane (volume), 1.5% butane and
20 1.5% of other gases such as hydrogen and nitrogen. Experiments were intensively monitored and
21 concentration was characterized as a function of time and space. The LPG was stored in a 4 m³
22 pressurized vessel (saturation pressure at ambient temperature) located roughly 45 m apart from the
23 cloud dispersion path on an upper site, at a relative elevation from the ground of 15 m. The fuel
24 flowed through a 40 mm diameter pipe with a total length of 50 m down to the release point, which
25 was located at 1.5 m high (Figure 1).
26 Pressure and temperature were monitored at the release point by an electronic pressure transmitter
27 (Barksdale, type UPA5) and two K-type thermocouples located 0.05 m upstream of the outlet orifice,

1 both recording at a frequency of 4 Hz. This data was used to calculate the mass flow rate and the jet
2 velocity at the outlet orifice assuming isentropic expansion between the stagnation point and the
3 orifice jet exit, by applying the appropriate thermodynamic relationships.
4 Additionally, sensors were deployed over a 700 m² area (35 m in release direction and 20 m in cross
5 direction). 47 self-powered electrochemical oxygen sensors (2FO flue gas sensor of CiTicel) were
6 placed at 19 different locations within the discharge area at three different heights: 0.1, 0.6 and 1.3 m
7 (Figure 2). We choose this type of sensors as an indirect measure of LPG concentration, since we
8 assumed that any decrease in the concentration of oxygen was caused by displacement of oxygen by the
9 LPG vapour. Oxygen sensors were made of a galvanic cell, being the current flow between the cell
10 electrodes proportional to the oxygen concentration to be measured. The sensors contained a bridge
11 resistor to provide a voltage power (mV) output. A small amount of oxygen was consumed in the cell
12 reaction in order to produce the current flow and the subsequent voltage power output. Assuming an
13 atmospheric oxygen concentration of 20.9% (volume) and an atmospheric nitrogen concentration of
14 79.1% , the LPG vapour concentration $[LPG_v]$ could then be expressed as:

15

$$16 \quad [LPG_v] = 1 - [O_2] - \frac{79,1[O_2]}{20,9}$$

17

18 Being $[O_2]$ the oxygen concentration detected by the sensors.

19 Some of the experiments were designed to investigate the influence of an obstruction placed in the
20 dispersion path; thus, in some trials a 1.3 m-height 1 m-width fence was placed perpendicular to the jet
21 direction at the centreline of the sensors array 10 m apart from the release point.

22 Furthermore, 1 meteorological station (Vantage Vue Wireless of Davis Instruments) and 5 ultrasonic
23 wind sensors (WindSonic OP1 of Gill Instruments) were used to monitor the weather conditions.

24 Wind direction and speed measurements were made at a frequency of 1 Hz; the wind sensors were
25 placed at 1 m height at position W1A and at 1 m and 2 m height at positions W2AB and W3AB (see
26 Figure 2). Ambient temperature and relative humidity was obtained by means of the meteorological
27 station located at the site.

1 In order to register and store the sensors data, one datalogger model DT85 of DataTaker Loggers, with
2 2 expansion modules CEM20 and one data acquisition system model Field Point of the National
3 instruments were used. The data were recorded at a rate of 4 hertz.
4 Eleven trials were taken with different releases rates and spill durations. In the present paper only two
5 of these trials are presented and intensively discussed: P25_2 and P25_3. These trials were chosen due
6 to the similarity of initial conditions: the former consisted of a release of 8 kg with no obstacles and the
7 second consisted of a release of 6 kg in the presence of the fence, both releases with 40 s duration. Figure
8 3 shows an instant of trial P25_2. It can be observed the release point, several masts used to sustain the
9 temperature and oxygen sensors (positions 1, 2, 3, 4, 5, 8 and 10 as detailed in Figure 2) the 3 higher
10 masts (positions W1, W2 and W3) used to support the anemometers and the vapour cloud formed.

11

12 **3 CFD MODELLING**

13 The CFD simulations were performed using FLACS[®] software (GexCon). FLACS is a CFD tool that
14 was specifically developed for consequence modelling. It uses conservation equations for mass,
15 energy, and momentum; it solves Reynolds Averaged Navier-Stokes (RANS) equations based on the
16 standard k- ϵ turbulence model of Launder & Spalding (1974). According to HSE (2013), RANS
17 approach is widely accepted in engineering CFD studies; it is based on the concept of separating the
18 fluid velocity components and scalar quantities (pressure, temperature, concentration) into mean and
19 fluctuating components, then transport equations are used to evaluate the model. The model of
20 Launder & Spalding (1974) is based on the turbulent kinetic energy and its dissipation rate; the
21 magnitudes of these two variables are calculated from transport equations and solved simultaneously
22 with those governing the mean flow behaviour.

23 **3.1 Physical settings of the scenarios**

24 CFD simulations of trials P25_2 and P25_3 were performed to challenge FLACS against the
25 experimental data. The scenario conditions used to perform the simulations are presented in Table 1.
26 Values of ambient temperature, ambient pressure, relative humidity and wind direction and speed were

1 considered as the median of the recorded values during the duration of each test. In a previous
 2 sensitivity analysis reported elsewhere (Schleder, 2015) we found that environmental variables did not
 3 show high sensitivity scores, so that we relied on the experimental measurements to set our
 4 simulations. The ground roughness was assumed equal to 0.03, which is the typical value for concrete
 5 surfaces (GexCon AS, 2013). The Pasquill class used was E – slightly stable. At the moment of the
 6 trials, there was a cloud cover of around 80% and it had been raining during 2 hours prior to the
 7 beginning of the tests. This condition reduced considerably the heat emitted from the ground leading
 8 to stable atmospheric condition.

9 The pressure and temperature ranges at the outlet orifice are detailed on Table 1 by the minimum and
 10 the maximum values registered during the duration of the trials. 1s averages of the measured
 11 temperature and pressure values were used to calculate the release rate. As previously mentioned, the
 12 jet velocity at the outlet orifice and the mass flow rate were calculated assuming isentropic expansion
 13 between the stagnation point and the orifice jet exit; the total amount of fuel released was obtained by
 14 the integral of the mass flow rate during the release. The simulations were performed by considering a
 15 1 second-averaged variable mass flow rate.

16 Table 1 - Scenario conditions

Variable	Unit	P25_2	P25_3
Ambient Temperature	°C	21.2	22.5
Ambient pressure	hPa	993	993
Relativity humidity	%	86.8	86.9
Wind direction	°	185	235
Wind speed at 1 m high	m·s ⁻¹	0.49	0.70
Pasquill Class	-	E	E
Ground roughness	m	0.03	0.03
Discharge direction	-	horizontal	horizontal
Discharge height	m	1.5	1.5
Release duration	s	40	40
Temperature release range (min/max)	°C	-28.1/4.7	-28.41/10.26
Pressure release range (min/max)	bar	0.1/1.2	0.1/1.3
Amount of fuel released	kg	8.0	6.5
Discharge rate (min/max)	kg·s ⁻¹	0.04/0.38	0.08/0.39

17

1 **3.2 Domain and grid definition**

2 The simulation domain was discretized using a single block Cartesian grid, defined following FLACS
3 user manual guidelines (GexCon AS, 2013). An orthogonal base X, Y and Z was used, being X
4 horizontal and parallel to the jet direction, Y horizontal and perpendicular to the jet direction and Z
5 vertical. The domain extended 50 m in the X direction (from 5 m before the release point to 45 m after
6 the release point), 48 m in the Y direction (centred on the release point) and 10 m in the Z direction
7 (from the ground level). As such, the release point coordinate was (0, 0, 1.5) in our domain. The
8 domain was defined using two types of meshes (Figure 4a): the former being a coarse (macro) grid,
9 representing the zone where the dispersion is expected to occur; and the latter being a fine (micro)
10 grid, representing two different swaths intersecting around the release point: one vertical, formed by a
11 mesh of cells at the centreline of the dispersion path, and the other horizontal, formed by a mesh of
12 cells centred at 1.5 m height (i.e. release height).

13 The cells were represented by 1 m edge cubes at the macro grid. In order to set the micro grid we
14 followed the FLACS guidelines (GexCon AS, 2013); which specifies that the area of the expanded jet
15 (A_{jet}) must be solved in only one cell and that the area of this cell across the jet (A_{cv}) should be larger
16 than the area of the expanded jet but not larger than twice A_{jet} (Figure 4b). The jet area expected after
17 the expansion at ambient pressure was estimated using the FLACS jet utility –which is based on a
18 one-dimensional model for the release of an ideal gas from a pressurized reservoir through a nozzle
19 into an open atmosphere (GexCon AS, 2013)– and the dimensions of the cell across the jet were
20 defined so that the area fell between the specified limits. Thus, the width and height of the micro grid
21 cells were fixed at 0.04 m (as a function of the jet area expected after the expansion at ambient
22 pressure).

23 The FLACS guidelines also recommend that the aspect ratio (the ratio between the smallest and
24 largest side of the cell) of the micro grid has to be not larger than five (due to stability of the numerical
25 solution); thus, the length of the cells was fixed at 0.20 m. Next, the cells nearby the leak were
26 smoothly increased to the macro grid resolution (see Figure 4a), maintaining the maximum change in

1 grid resolution from one grid cell to the next one less than 40% (as recommended by the FLACS
2 guidelines).
3 Finally, monitoring points were inserted in the simulation specifications at the same locations where
4 the sensors were placed in the field, which allowed the measured values of concentration and
5 temperature to be compared with the simulated values.

6 **4 RESULTS AND DISCUSSION**

7 As previously mentioned, one of the aims of this study is to offer new sets of cloud dispersion data to
8 the international community to: i) be used for models validation studies and to ii) provide new insights
9 of gas dispersion phenomena in realistic environments. The most relevant data acquired during P25_2
10 and P25_3 tests are presented in this section and more detailed information is included in annex A (i.e.
11 LPG release rates and concentration evolutions with time and space). It has to be said that it had been
12 raining during 2 hours prior to the beginning of the tests and some sensors did not work well due to
13 accumulated water over the sensor output.

14 Another aim of this study was to investigate at an initial stage the CFD performance when challenged
15 to reproduce cloud dispersion in complex scenarios. To address this objective concentration was
16 defined as the main variable of interest.

17 **4.1 Trial P25_2**

18 Figure 5 a) shows experimental versus simulated values of peak LPG concentrations calculated from
19 12 active oxygen concentration sensors at the centreline during trial P25_2. The experimental data fits
20 within a range of 0.01% - 7.43% of LPG. As expected, the highest concentrations were measured in
21 the first 5 m from the release point in the area where the jet was expected.

22 The CFD performance when challenged to simulate P25_2 experimental scenario was evaluated using
23 the factor of two (FAC2) range, which analyses whether the simulated values fall within a \pm factor of
24 two of the measured data. This factor is widely used for CFD validation purposes. It was one of the
25 parameters recommended by Weil et al. (1992) and Hanna et al. (2004) to evaluate air quality models,
26 later on, it was recommended by HSE in the Model Evaluation Protocol (Ivings et al. 2007) and more

1 recently it was used by Coldrick et al. (2009) and Ivings et al. (2013). It has to be also noted that the
2 authors have already applied this criterion in previous studies (Schleder & Martins, 2013, Schleder et
3 al. 2014). FAC2 confidence limits are included in the previous figure as dashed lines. 75% of the
4 plotted points fit within this range.

5 In Figure 5 a), it can be observed how only three points did not adjust to the FAC2 range. Two of them
6 were representing the concentrations measured by two sensors placed 2 m apart from the release point
7 at 0.1 and 0.6 m high, respectively. In those locations, the simulated values (both <0.1%) were
8 significantly lower than the measured concentration real sensors (0.3 % and 2.2% respectively). These
9 two points are the ones with their respective symbols fully stepping on the abscissa axis. The third
10 sensor was placed 5 m from the release point at 0.6 high. The simulator also failed when trying to
11 predict the maximum LPG concentration at a point (5, 0, 0.6), since the simulated value (0.3%) was
12 significantly lower than the measured concentration (1.28%).

13 The same FAC2 analysis was performed considering all the sensors that worked well during the tests
14 (Figure 5 b)), not just those located at the centreline. Compared to Figure 5 a), the agreement was
15 poorer, with 60% of the plotted points within the FAC2 range. The simulator had bigger errors when
16 simulating concentrations out of the dispersion path axis, where turbulence may have bigger effects; 5
17 out of 10 concentration values located at the left hand side of the dispersion path following the jet
18 direction (2 m of displacement in y direction), and 4 out of 7 values located at the right hand side (also
19 2 m displaced) fell out of the FAC2 limits, showing a clear underestimation tendency

20 *4.1.1 Concentration dynamics with time of trial P25_2*

21 Concerning the evolution of the concentration with time, FLACS was able to peak the general trend
22 for most of the sensors, excepting those placed near the source term (in the first 5 m of the discharge
23 path) in which the simulator underestimated significantly the measured values, as previously noted.

24 Figure 6 and Figure 7 show two examples of the LPG comparison of the real/simulated concentration
25 evolution with time plotted for two oxygen concentration sensors, the first located at the centreline 9
26 m apart from the release point (sensor 6A at a height of 0.1 m) and the other located 15 m apart from

1 the release point, at the centreline too (sensor 16B, at a height of 0.6 m). Measured release rate (which
2 acts also as input in the FLACS scenario) is also plotted for comparison purposes.

3 Regarding the sensor 6A, it can be observed how simulated concentration is more sensitive to release
4 rate changes than the real concentration. As such, an initial peak (simulated, 1.3%) can be found
5 around 5 s, which is the response of a maximum release rate occurring roughly one second before. The
6 real concentration evolution is smoother, nevertheless showing also a peak (of around 1%) one second
7 later than the simulated one. This tendency can still be observed when paying attention to the release
8 rate drop occurring 14 s after the start of the test: simulated concentration reacts accordingly showing
9 a drop 5 seconds after, whereas the real concentration takes longer to descend, showing a minimum 8
10 seconds after the release rate drop. Certainly, there is an increasing delay between the dynamics of the
11 simulated cloud and the real one, and as such the simulated cloud dilutes faster than the real one. This
12 is due to the fact that the simulated cloud is not able to pick the accumulation that the real one
13 experienced. This becomes more evident 25 seconds after the start of the release, when real
14 concentration in sensor 6A increases, while the simulated one decreases according to the pattern
15 shown by the release rate evolution. Furthermore, it is also possible to note greater oscillations on the
16 measured concentration values compared to the predicted values.

17 Sensor 16 B behaves in a similar way: although the first concentration maximum is accurately picked
18 by the simulated cloud (both in terms of absolute value and instant of time), the simulated cloud
19 disperses faster, not showing the accumulation registered by the real sensor. Also, simulated
20 concentration curve is smoother compared to the real evolution.

21 One of the reasons that could explain these particular lacks of accuracy could be found in the
22 simulated wind. A constant wind is considered in the simulations, which gives reasonably good results
23 when simulating concentration in the centreline (note that variations of $\pm 20\%$ of mean wind speed did
24 not increase the simulator performance -data not shown). However, FLACS loses accuracy when
25 simulating concentrations at location out of the dispersion path axis. During the execution of the test,
26 there were oscillations on wind speed and direction, the wind speed ranged between $0.03 \text{ m}\cdot\text{s}^{-1}$ and
27 $1.02 \text{ m}\cdot\text{s}^{-1}$ and the direction between 63° and 287° . With a simulated wind dynamics simpler than the
28 real one, FLACS may represent less turbulent eddies than the real ones occurring in the experimental

1 site. Therefore, the simulated cloud disperses smoothly than the experimental cloud. However, in
2 order to verify this hypothesis more experimental data covering a wider range of wind conditions
3 would be needed as well as better representation of wind profile in the simulations.

4 **4.2 Trial P25_3**

5 Figure 8 a) presents measured versus simulated values of peak LPG concentrations at the centreline
6 calculated from 12 active oxygen concentration sensors during the trail P25_3. The trial P25_3 was
7 undertaken some minutes after trial P25_2; thus, the values in Figure 8 correspond to the same sensors
8 of the centreline that did work well during trial P25_2.

9 In this case, 83% of the predicted/measured points also fit well within the range of factor2. As in the
10 previous trial, for the two sensors placed 2 m apart from the release point, at 0.1 and 0.6 m high, no
11 significant concentrations were predicted.

12 In addition, performing the same FAC 2 analysis considering all the sensors (not just those located at
13 the centreline), 70% of the points were found to fit well within the FAC 2 range. Similarly to trial
14 P25_2, the agreement decreased when adding concentration values measured out of the dispersion
15 path axis. In this case, however, the simulator bias did not show a clear tendency, presenting
16 over/underestimated values in similar proportion.

17 *4.2.1 Concentration dynamics with time of trial P25_3*

18 Figure 9 and Figure 10 show two examples of the LPG concentration evolution with time calculated
19 from two oxygen concentration sensors, one located at the centreline, 1 m after the fence (0.6 m high,
20 sensor 11B) and the other, located at the same place, but at a height of 1.3 m (sensor 11C). Concerning
21 sensor 11B, it can be seen how both concentration curves, measured and simulated, present a very
22 good agreement. It is worth noting that there is a time delay (of around 4 s) when comparing predicted
23 vs. measured peak concentrations, but in this case the first maximum is the one corresponding to the
24 measured concentration. Despite this initial delay, however, the simulated cloud again seems to dilute
25 faster than the real one. The effect of the fence can be clearly observed in both real and simulated
26 curves; although the release rate keeps around $0.15\text{-}0.2 \text{ kg}\cdot\text{s}^{-1}$ during the last period of the experiment

1 (between 28 s – 38 s), concentration values show a general decreasing trend. Again, it can be clearly
2 seen how the simulated curve is smoother than the real one, for the above mentioned reasons.
3 Concentration evolution of sensor 11C is rather well simulated too. In this case, the simulated cloud
4 shows a maximum peak in the 11C sensor location faster than the real one. However, the simulated
5 cloud dilutes faster. Interestingly, the simulated cloud fails to represent the complex accumulation
6 dynamics detected by the real sensor occurring from 30 seconds after the release. Rather, simulated
7 concentration becomes negligible during this particular period.

8 **4.3 Cloud concentration profiles**

9 Figure 11 and Figure 12 show the cloud concentration profile at the centre plane of the cloud path
10 ($Y=0$) 10 s after the release start, for trials P25_2 and P25_3 respectively. Some monitor points with
11 their related concentrations (experimental and simulated) are gathered in the box. In monitoring points
12 of Figure 11, the mean error between measured and simulated values was 13%. It is worth noting that,
13 at this instant, concentrations were low and although maximum errors of around 39% were found (e.g.
14 error in 11C), they do not represent large discrepancies, e.g. the maximum difference between the
15 simulated and the measured volumetric concentration is only of 0.41% (sensor 11C).
16 Concerning to trial P25_3 (Figure 12) the mean error between simulated and experimental
17 concentration was 18%, with a maximum error of 36% when simulating the concentration of the
18 sensor 16B (errors roughly of the same order of magnitude than ones computed for the trial P25_2).
19 Moreover, it is possible to verify the influence of the fence placed 10 m apart from the release point on
20 the cloud dispersion, since part of the cloud is trapped before the barrier. In P25_3, the simulated
21 propane concentration at locations 11B, 11C, 16A and 16B were significantly lower than the
22 concentrations simulated at the same positions for trial P25_2, with decreases between 13% and 44%.
23

24 **5 CONCLUSIONS AND FUTURE WORK**

25 This paper presented the first stage of the experimental campaign undertaken by the joint venture
26 between University of São Paulo and Universitat Politècnica de Catalunya envisaged to provide

1 experimental data about gas dispersion with the aim of investigating the performance of CFD tools for
2 cloud dispersion of flammable/toxic substances modelling.

3 The literature review show evidence that data on concentration of toxic or flammable clouds as a
4 function of time and space are very scarce. Usually the experimental data is presented in graphs of
5 concentrations at specific instants and positions, and in most cases, only peak values are provided. The
6 data provided here is much comprehensive than any other published experimental dataset concerning
7 cloud dispersion, which will be particularly suitable for the scientific community to perform complete
8 models validation and comparison studies, and conduct time dependent analysis of cloud dispersion
9 behaviour.

10 The tests performed by USP-UPC consisted of continuous LPG releases at the atmosphere and the
11 subsequent monitoring and characterization of the cloud concentration and temperature. Some of the
12 trials undertaken were designed to investigate the influence of an obstruction placed in the path of the
13 vapour flow. We provide comprehensive LPG concentration data of two particular tests: trials P25_2
14 and P25_3. These trials are similar in release conditions; however, the former is a release without
15 obstacles and the second has an obstruction 10 m apart from the release point.

16 Some preliminary analysis comparing LPG concentration data of these two tests with CFD simulations
17 were presented. In general terms, the CFD-based simulator has shown good performance when
18 simulating cloud concentration. It has to be highlighted that FLACS passes with good accuracy the
19 FAC2 test, which is a well-established and standardized indicator for model validation purposes.

20 FLACS shows mean errors of 13% for unobstructed scenarios, and of 18% for obstructed ones, which
21 are acceptable given the general dynamics of the experimental tests (i.e. unsteady release rate and
22 wind fluctuations in speed and direction). Moreover, FLACS seems to successfully reproduce the
23 presence of complex geometry and its effects on cloud dispersion, showing realistic concentration
24 decreases due to cloud dispersion obstruction by the existence of a fence.

25 FLACS performance may be improved by setting the scenario considering more complex wind
26 dynamics as the ones encountered during the field tests, at the expense, however, of the simulation
27 runtime. To the best of our knowledge, a variable wind profile in CFD simulations has never been

1 considered for dispersion analysis, however real scenarios are far from having stable wind. This is
2 surely a relevant point which shall be explored in our future work.

3

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FIGURE CAPTIONS

Figure 1. Layout of the propane installation

Figure 2. Oxygen sensor array (blue points); the numbers are identifiers of the masts where the sensors were attached and the letters A, B and C represent the sensors height, at 0.1 m, 0.6 m and 1.3 m respectively. (e.g. the mast “3ABC”, located at the centreline of the dispersion path 5 m apart from the release point, sustained sensors at three heights: 0.1 m, 0.6 m and 1.3 m). The yellow points named W1-W3, represent the location of the anemometers at 1 m height (A) and 2 m height (B).

Figure 3. Photo of trial P25_2, showing the release point and masts; at 40 s from the beginning of the release and release rate of 0.17 kg/s.

Figure 4. a) Grid representation; b) micro grid cell containing the release point. A_{jet} is the jet area expected after the expansion at ambient pressure and A_{cv} is the area of the cell across the jet. For both areas, the following relation must be fulfilled: $A_{jet} < A_{cv} < 2 \cdot A_{jet}$

Figure 5. Comparison between simulated peak concentration and experimental data of a) centreline monitored points b) all monitored points of trial P 25_2

Figure 6. Measured and simulated concentrations at sensor 6A position, in the centreline, 9 m from the release point 0.1 m high.

Figure 7. Measured and simulated concentrations at sensor 16B position, in the centreline, 15 m from the release point 0.6 m high.

Figure 8. Comparison between simulated values and experimental data of a) centreline monitored points b) all monitored points of trial P 25_3.

Figure 9. Measured and simulated concentrations at sensor 11B position in trial P25_3 (1 m after the fence at 0.6 m high).

Figure 10. Measured and simulated concentrations at sensor 11C position in trial P25_3 (1 m after the fence at 1.3 m high).

Figure 11. Cloud profile concentration of Trial P25_2 at centreline, 10 s after the release start.

Figure 12. Cloud profile concentration of Trial P25_3 at centreline, 10 s after the release start.

FIGURES

Figure 1

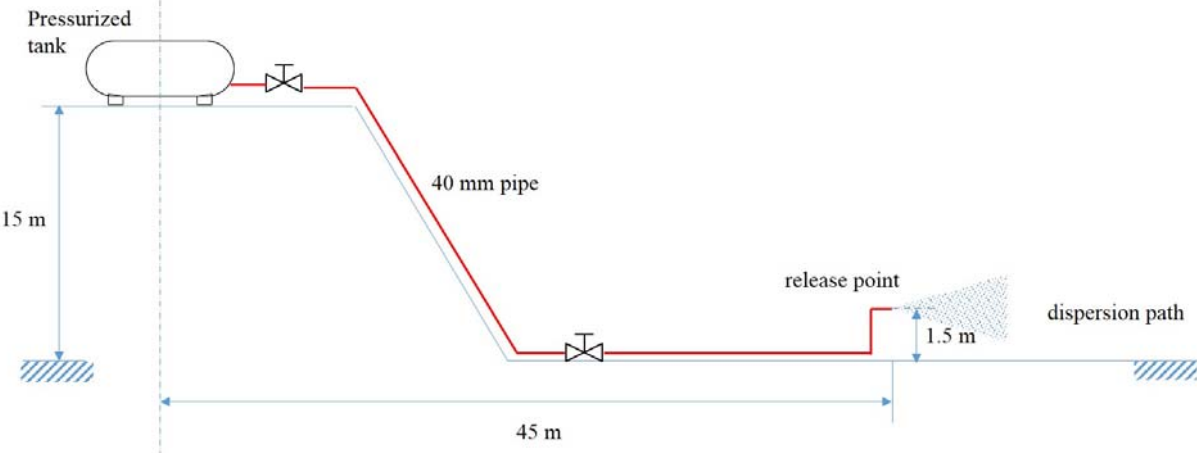


Figure 2

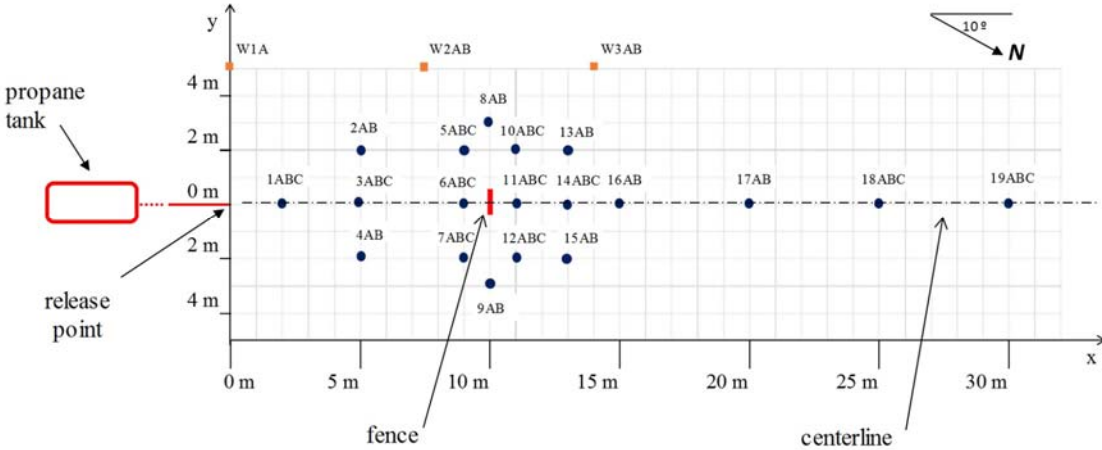


Figure 3



Figure 4

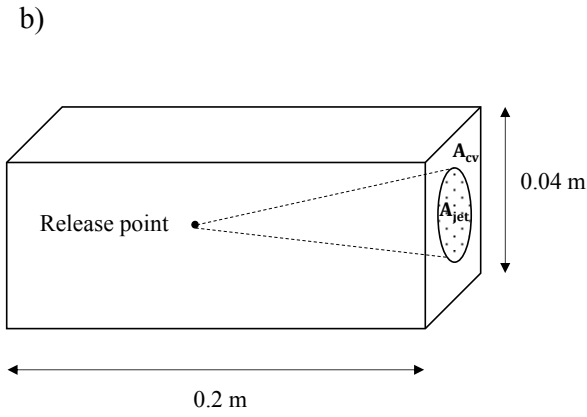
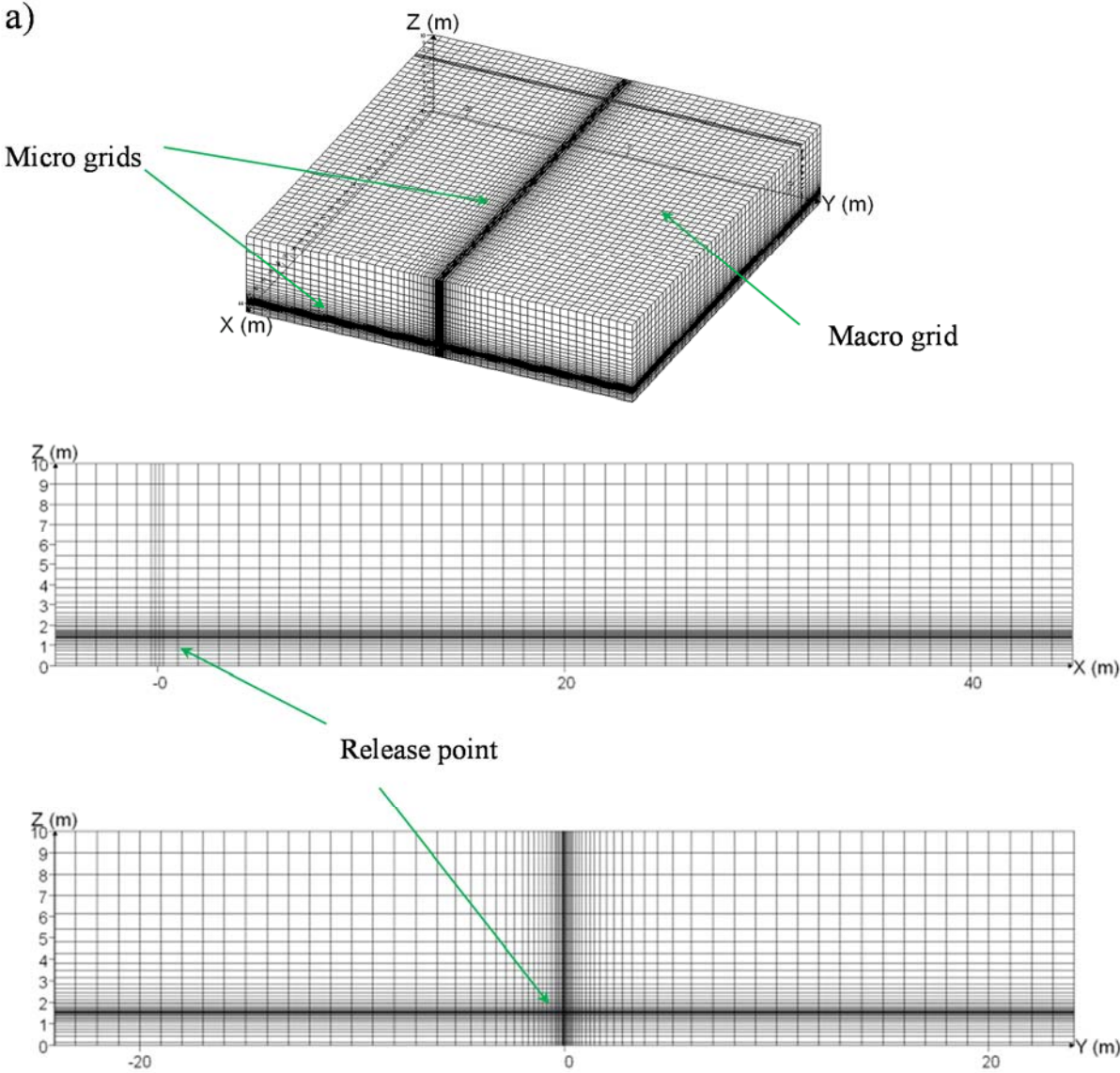


Figure 5

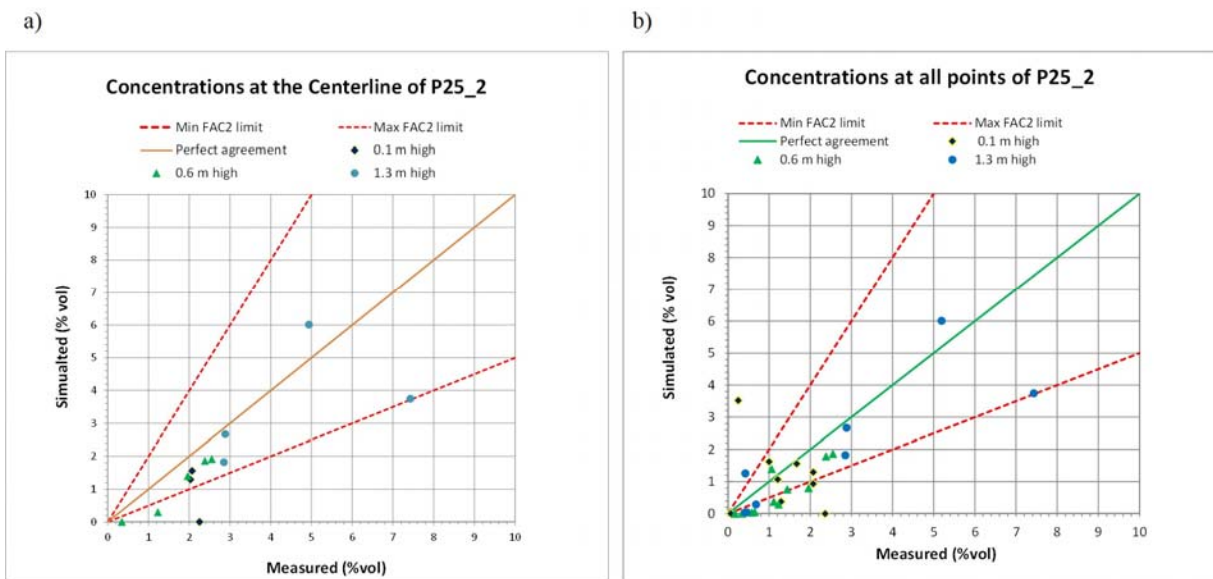


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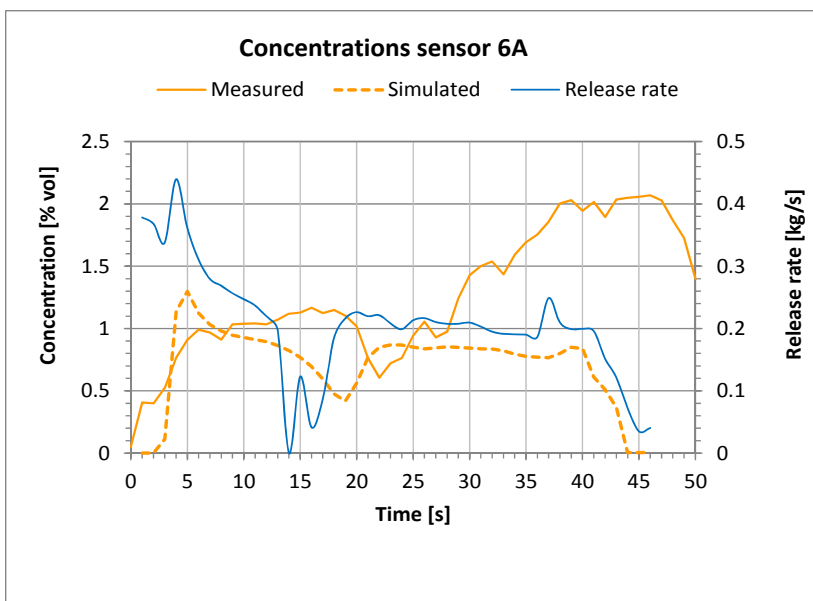


Figure 7

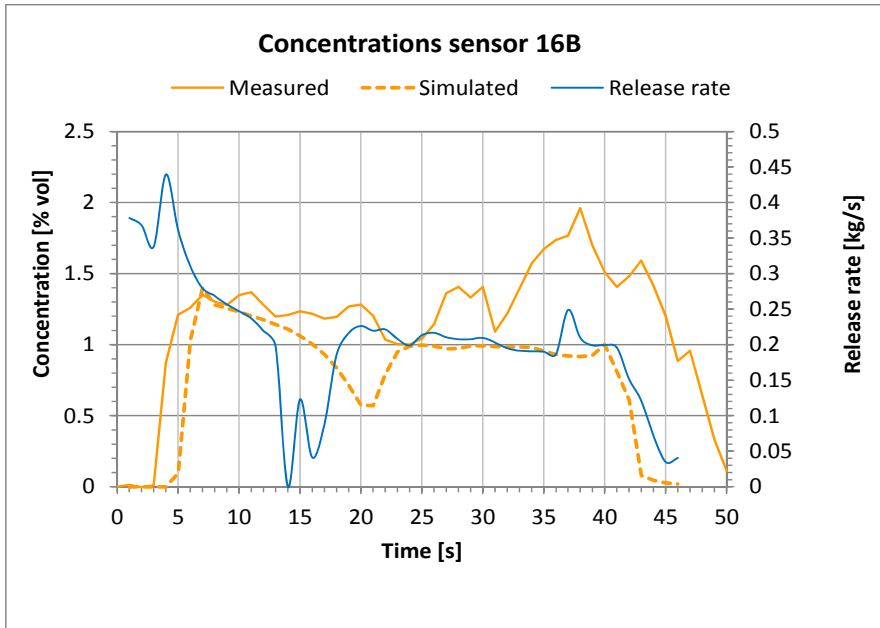


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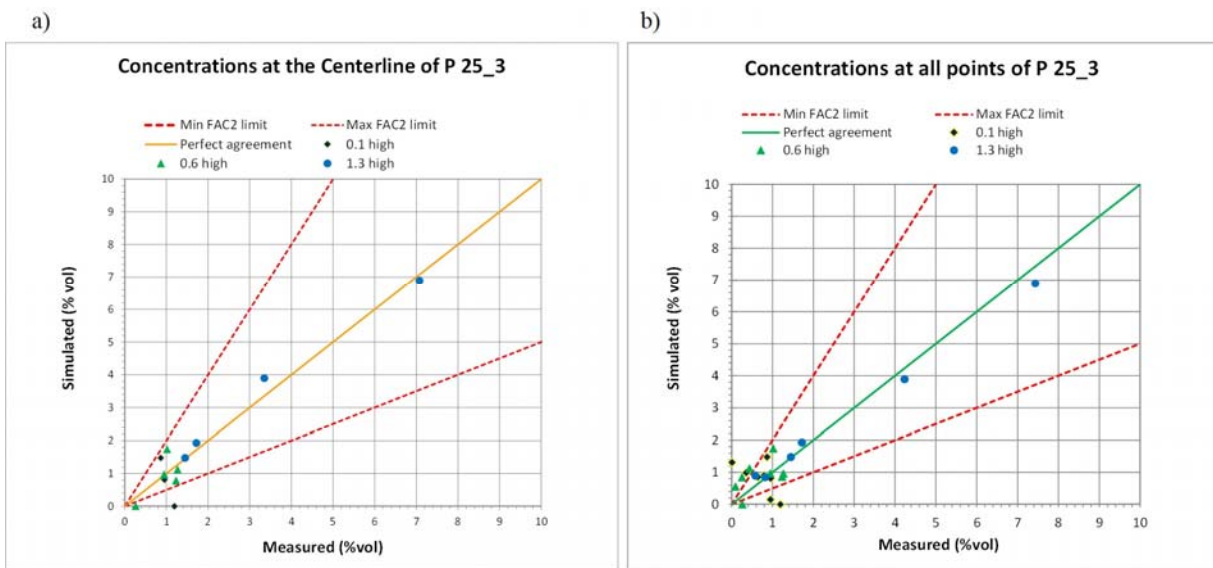


Figure 9

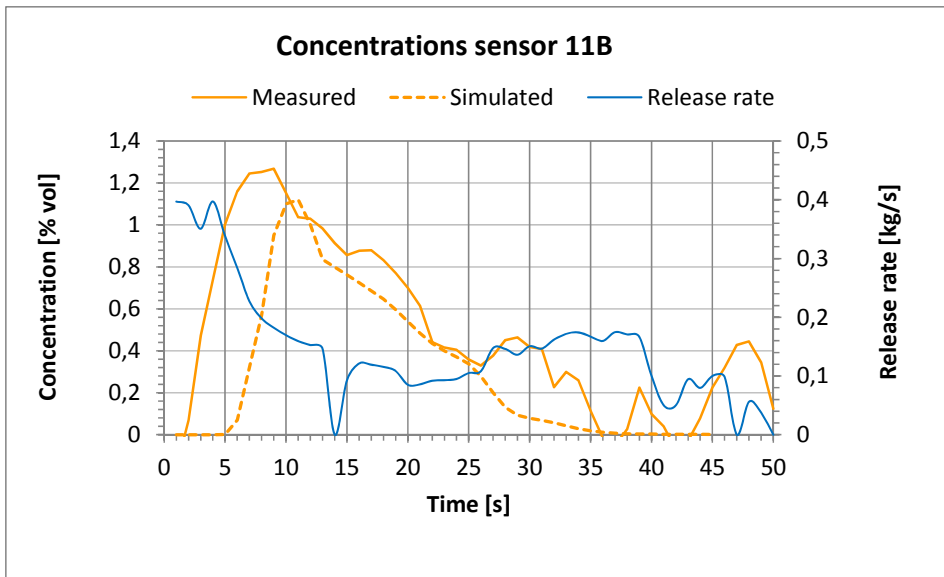


Figure 10

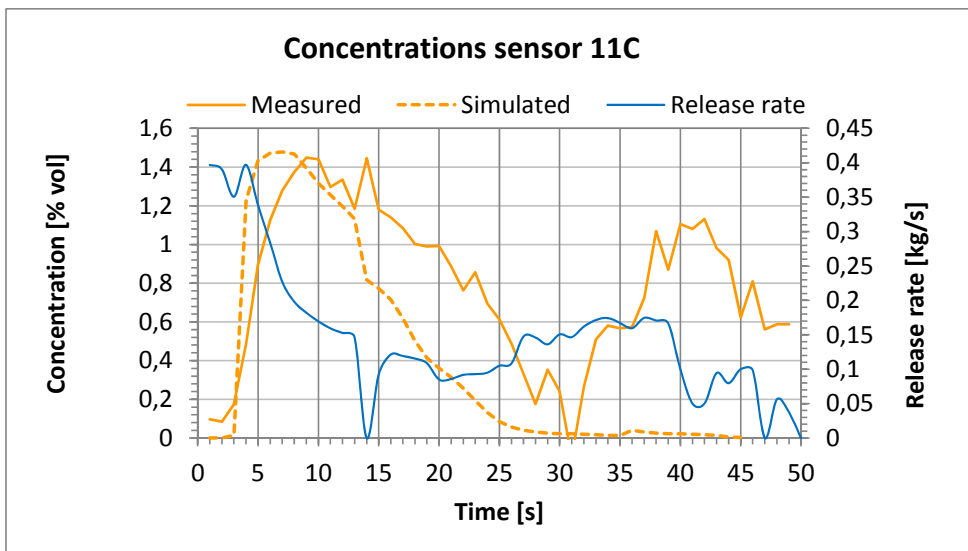


Figure 11

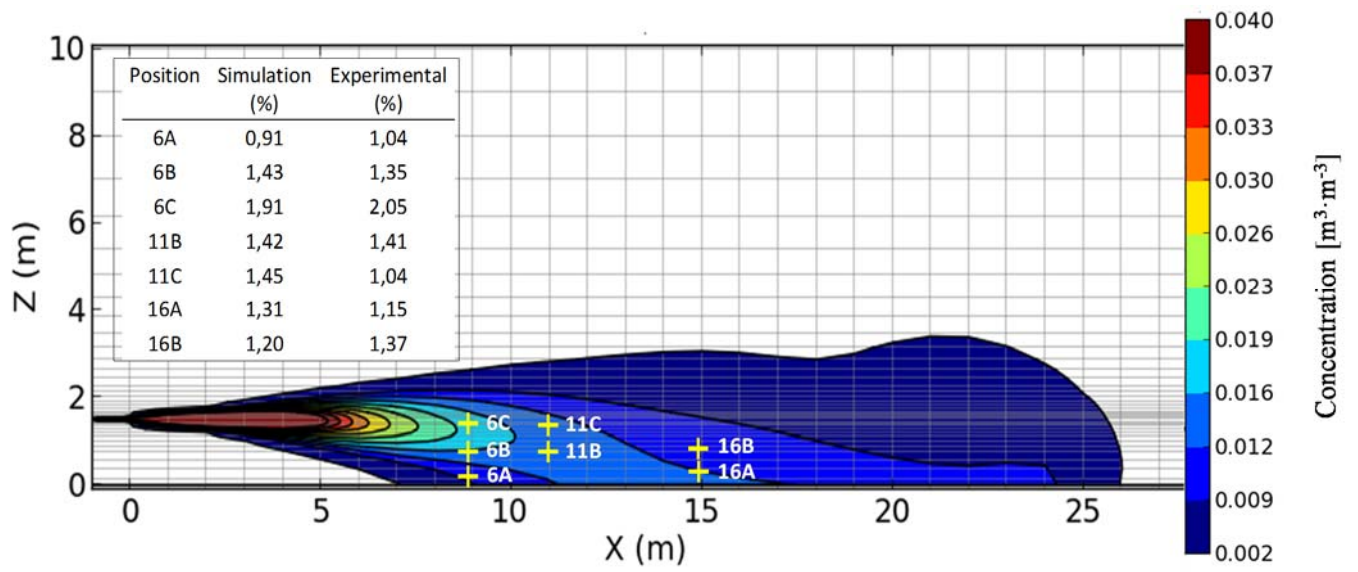
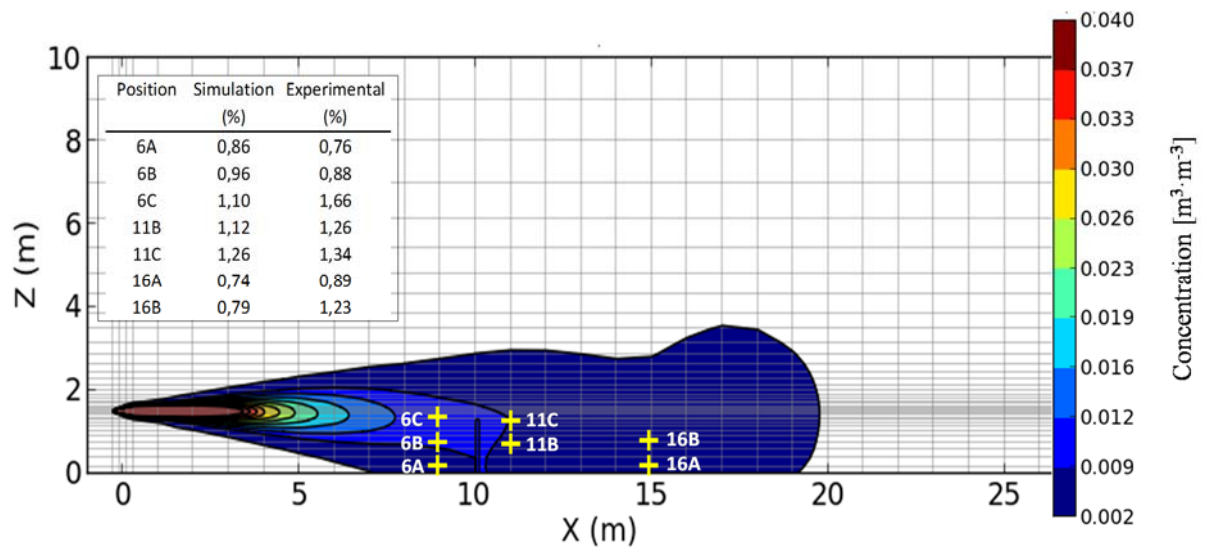


Figure 12



ANNEX A

In this Annex concentration values and release rates of trials P25_2 and P25_3 are presented. The concentration measures are presented as function of time for each sensor placed in the field tests; the trials presented here were carried out in a very cloudy day with scattered showers; the rain before the trials created a more stable atmosphere; however, several sensors did not work well due to accumulated water over the sensor output. In the following tables only the measured values corresponding to the sensor that worked well during the trials are presented. The concentrations and release rates provided are both 1 s-averaged.

Table A 1 shows the discharge rate of trial P25_2; Table A 2 and Table A 3 show the concentrations for each active sensor of trial P25_2; Table A 4 shows the discharge rate of trial P25_3; Table A 5 and Table A 6 present the concentrations for each active sensor of trial P25_3.

Table A 1- Release rate of trial P25_2.

Time [s]	Temperature at outlet orifice [°C]	Pressure at outlet orifice [hPa]	Release rate [kg.s⁻¹]
1	4.68	590	0.38
2	-10.94	1070	0.37
3	-11.97	740	0.34
4	-7.85	480	0.44
5	-1.77	320	0.36
6	2.17	230	0.31
7	4.02	190	0.28
8	4.40	170	0.27
9	3.99	160	0.26
10	3.06	140	0.25
11	2.08	130	0.24
12	0.77	110	0.22
13	-1.92	90	0.20
14	-4.98	0	0.00
15	-10.52	40	0.12
16	-15.03	10	0.04
17	-25.14	30	0.09
18	-26.98	70	0.19
19	-27.56	100	0.22
20	-27.90	110	0.23
21	-27.93	100	0.22
22	-27.91	100	0.22
23	-27.92	90	0.21
24	-27.95	80	0.20
25	-27.76	90	0.21
26	-28.01	100	0.22
27	-27.96	90	0.21
28	-27.99	90	0.21
29	-28.02	90	0.21
30	-28.07	90	0.21
31	-28.09	80	0.20
32	-28.05	80	0.19
33	-28.07	80	0.19
34	-28.10	70	0.19
35	-28.13	70	0.19
36	-28.09	70	0.19
37	-28.05	130	0.25
38	-28.07	90	0.21
39	-28.12	80	0.20
40	-28.15	80	0.20

Table A 2 -Concentrations of trial P25_2 (sensors 1A to 7B).

Sensor	1A	1B	1C	3B	3C	4A	4B	5A	5B	5C	6A	6B	6C	7A	7B
y [m]	0.0	0.0	0.0	0.0	0.0	-2.0	-2.0	2.0	2.0	2.0	0.0	0.0	0.0	-2.0	-2.0
x [m]	2.0	2.0	2.0	5.0	5.0	5.0	5.0	9.0	9.0	9.0	9.0	9.0	9.0	9.0	9.0
z [m]	0.1	0.6	1.3	0.6	1.3	0.1	0.6	0.1	0.6	1.3	0.1	0.6	1.3	0.1	0.6
Time [s]															
1	0.05	0.09	0.44	0.07	0.38	0.01	0.10	0.00	0.06	0.14	0.41	0.29	0.30	0.45	0.44
2	0.34	0.18	2.16	0.14	1.05	0.06	0.17	0.00	0.08	0.18	0.40	0.56	0.62	0.35	0.34
3	0.51	0.24	3.41	0.30	2.07	0.07	0.05	0.00	0.08	0.18	0.52	0.86	1.10	0.32	0.32
4	0.46	0.34	3.81	0.43	2.58	0.09	0.07	0.00	0.06	0.13	0.76	1.12	1.71	0.27	0.30
5	0.34	0.25	4.06	0.44	2.96	0.12	0.07	0.00	0.11	0.12	0.91	1.33	1.95	0.16	0.25
6	0.49	0.16	4.23	0.53	3.13	0.13	0.07	0.07	0.22	0.16	0.99	1.44	1.93	0.13	0.18
7	0.49	0.02	4.47	0.58	3.31	0.20	0.06	0.14	0.24	0.19	0.97	1.41	2.01	0.28	0.11
8	0.52	0.00	4.58	0.48	3.39	0.22	0.06	0.13	0.13	0.23	0.91	1.34	2.04	0.36	0.00
9	0.48	0.00	4.53	0.50	3.43	0.21	0.05	0.08	0.17	0.33	1.03	1.40	2.10	0.54	0.06
10	0.39	0.02	4.62	0.51	3.47	0.20	0.05	0.16	0.25	0.31	1.04	1.40	2.10	0.27	0.22
11	0.31	0.08	4.44	0.51	3.46	0.15	0.04	0.11	0.19	0.24	1.04	1.35	2.05	0.19	0.32
12	0.27	0.12	4.51	0.54	3.41	0.10	0.05	0.00	0.07	0.13	1.03	1.41	2.01	0.13	0.22
13	0.05	0.19	4.53	0.57	3.31	0.20	0.06	0.00	0.00	0.08	1.07	1.51	2.01	0.04	0.04
14	0.00	0.08	4.62	0.50	3.28	0.25	0.06	0.00	0.00	0.17	1.12	1.48	2.04	0.06	0.05
15	0.00	0.00	4.55	0.36	3.18	0.21	0.06	0.00	0.06	0.27	1.13	1.51	1.94	0.19	0.17
16	0.00	0.00	4.50	0.54	3.24	0.11	0.06	0.00	0.15	0.25	1.17	1.55	1.96	0.21	0.11
17	0.00	0.00	4.47	0.50	3.16	0.00	0.06	0.00	0.12	0.27	1.12	1.56	1.98	0.29	0.17
18	0.00	0.01	4.24	0.30	3.20	0.00	0.05	0.09	0.10	0.16	1.15	1.57	1.98	0.12	0.36
19	0.00	0.05	4.28	0.34	3.29	0.00	0.04	0.15	0.06	0.14	1.10	1.51	1.97	0.20	0.54
20	0.00	0.05	4.54	0.36	3.34	0.00	0.03	0.12	0.03	0.11	1.02	1.36	1.97	0.33	0.49
21	0.03	0.15	5.21	0.33	3.35	0.00	0.03	0.00	0.01	0.10	0.76	1.31	1.98	0.35	0.35
22	0.37	0.26	5.24	0.34	3.47	0.00	0.03	0.00	0.04	0.15	0.61	1.45	2.00	0.29	0.15
23	0.44	0.27	5.28	0.49	3.54	0.00	0.03	0.00	0.06	0.20	0.72	1.53	2.04	0.41	0.10

Sensor	1A	1B	1C	3B	3C	4A	4B	5A	5B	5C	6A	6B	6C	7A	7B
y [m]	0.0	0.0	0.0	0.0	0.0	-2.0	-2.0	2.0	2.0	2.0	0.0	0.0	0.0	-2.0	-2.0
x [m]	2.0	2.0	2.0	5.0	5.0	5.0	5.0	9.0	9.0	9.0	9.0	9.0	9.0	9.0	9.0
z [m]	0.1	0.6	1.3	0.6	1.3	0.1	0.6	0.1	0.6	1.3	0.1	0.6	1.3	0.1	0.6
24	0.32	0.25	5.41	0.68	3.66	0.01	0.03	0.00	0.06	0.18	0.76	1.62	2.12	0.51	0.22
25	0.26	0.17	5.56	0.41	3.79	0.02	0.02	0.00	0.06	0.17	0.94	1.63	2.22	0.65	0.52
26	0.26	0.09	5.66	0.28	3.93	0.08	0.02	0.00	0.09	0.34	1.05	1.68	2.29	0.57	0.59
27	0.25	0.05	5.77	0.20	4.08	0.13	0.01	0.00	0.20	0.33	0.93	1.68	2.35	0.59	0.55
28	0.17	0.06	6.10	0.48	4.21	0.07	0.01	0.00	0.14	0.21	0.97	1.76	2.42	0.65	0.54
29	0.20	0.14	6.18	0.78	4.24	0.00	0.00	0.00	0.08	0.14	1.24	1.90	2.51	0.61	0.56
30	0.37	0.14	6.30	0.77	4.34	0.00	0.00	0.00	0.05	0.11	1.43	2.01	2.59	0.64	0.54
31	2.25	0.07	6.51	0.73	4.40	0.00	0.00	0.00	0.02	0.10	1.50	2.02	2.63	0.78	0.54
32	1.10	0.08	6.52	0.72	4.49	0.00	0.00	0.00	0.02	0.08	1.54	2.07	2.70	1.00	0.65
33	0.44	0.09	6.39	0.68	4.51	0.00	0.00	0.01	0.02	0.05	1.43	2.20	2.73	0.95	0.64
34	0.36	0.11	6.31	0.74	4.60	0.00	0.00	0.10	0.03	0.08	1.59	2.29	2.77	0.81	0.54
35	0.32	0.14	6.41	0.89	4.70	0.00	0.00	0.24	0.07	0.05	1.69	2.39	2.84	0.87	0.51
36	0.29	0.13	6.59	1.12	4.72	0.00	0.00	0.30	0.10	0.06	1.75	2.44	2.88	0.77	0.51
37	0.36	0.08	6.73	1.19	4.75	0.00	0.00	0.03	0.08	0.11	1.86	2.48	2.85	0.86	0.46
38	0.36	0.15	6.91	1.05	4.80	0.00	0.00	0.02	0.05	0.11	2.00	2.51	2.77	0.70	0.39
39	0.29	0.15	6.91	1.00	4.74	0.03	0.00	0.00	0.05	0.09	2.03	2.55	2.68	0.38	0.30
40	0.25	0.09	7.06	1.23	4.84	0.05	0.00	0.00	0.06	0.07	1.95	2.43	2.59	0.33	0.24
41	0.25	0.15	7.43	1.20	4.94	0.06	0.00	0.02	0.01	0.01	2.01	2.43	2.55	0.42	0.27
42	0.27	0.21	7.42	1.15	4.90	0.10	0.00	0.00	0.00	0.00	1.90	2.47	2.47	0.68	0.35
43	1.56	0.18	7.7.43	0.86	5.19	0.13	0.00	0.00	0.00	0.05	2.03	2.44	2.33	0.67	0.23
44	2.36	0.19	7.40	0.78	5.13	0.10	0.00	0.18	0.00	0.04	2.05	2.41	2.19	0.57	0.21
45	0.77	0.20	7.35	0.85	4.57	0.06	0.00	0.18	0.00	0.03	2.06	2.28	2.09	0.49	0.31
46	0.33	0.18	4.32	0.82	3.81	0.06	0.00	0.14	0.23	0.07	2.07	2.15	1.79	0.36	0.39
47	0.24	0.12	2.08	0.67	2.50	0.15	0.00	0.16	0.36	0.13	2.03	2.05	1.59	0.24	0.36

Sensor	1A	1B	1C	3B	3C	4A	4B	5A	5B	5C	6A	6B	6C	7A	7B
y [m]	0.0	0.0	0.0	0.0	0.0	-2.0	-2.0	2.0	2.0	2.0	0.0	0.0	0.0	-2.0	-2.0
x [m]	2.0	2.0	2.0	5.0	5.0	5.0	5.0	9.0	9.0	9.0	9.0	9.0	9.0	9.0	9.0
z [m]	0.1	0.6	1.3	0.6	1.3	0.1	0.6	0.1	0.6	1.3	0.1	0.6	1.3	0.1	0.6
48	0.10	0.12	0.56	0.51	1.79	0.09	0.00	0.28	0.42	0.20	1.87	1.91	1.22	0.11	0.35
49	0.27	0.13	0.00	0.13	1.08	0.10	0.00	0.39	0.48	0.42	1.73	1.57	0.79	0.05	0.29
50	0.40	0.11	0.00	0.00	0.67	0.08	0.00	0.40	0.58	0.37	1.40	1.23	0.54	0.07	0.25
Minimum	0.00	0.00	0.44	0.00	0.38	0.00	0.00	0.00	0.00	0.01	0.40	0.29	0.30	0.04	0.00
Maximum	2.36	0.34	7.43	1.23	5.19	0.25	0.17	0.40	0.58	0.42	2.07	2.55	2.88	1.00	0.65
Values averaged by 1 s															

Table A 3 -Concentrations of trial P25_2 (sensors 7C to16B)

Sensor	7C	9A	10A	10B	10C	11B	11C	12A	12C	13A	15A	15B	16A	16B
y [m]	-2.0	-3.0	2.0	2.0	2.0	0.0	0.0	-2.0	-2.0	2.0	0.0	0.0	-2.0	-2.0
x [m]	9.0	10.0	11.0	11.0	11.0	11.0	11.0	11.0	11.0	13.0	15.0	15.0	13.0	13.0
z [m]	1.3	0.1	0.1	0.6	1.3	0.6	1.3	0.1	1.3	0.6	0.1	0.6	0.1	0.6
Time [s]														
1	0.08	0.00	0.13	0.18	0.15	0.13	0.00	0.02	0.00	0.00	0.00	0.00	0.08	0.01
2	0.07	0.00	0.00	0.11	0.20	0.27	0.16	0.05	0.00	0.00	0.00	0.04	0.11	0.00
3	0.05	0.01	0.00	0.19	0.25	0.76	0.62	0.05	0.00	0.00	0.04	0.05	0.21	0.01
4	0.02	0.07	0.36	0.32	0.31	1.18	2.85	0.50	0.18	0.00	0.63	0.17	0.55	0.87
5	0.00	0.00	0.29	0.36	0.43	1.36	0.00	0.36	0.39	0.07	0.66	0.17	0.91	1.21
6	0.03	0.00	0.44	0.41	0.39	1.53	0.17	0.23	0.42	0.06	0.51	0.26	1.16	1.26
7	0.00	0.00	0.76	0.39	0.49	1.50	0.98	0.26	0.30	0.23	0.69	0.37	1.24	1.35
8	0.00	0.00	0.82	0.44	0.57	1.49	1.18	0.18	0.24	0.39	0.81	0.40	1.09	1.30
9	0.00	0.00	0.68	0.34	0.44	1.48	1.40	0.06	0.19	0.47	0.67	0.42	1.09	1.28

10	0.02	0.00	0.37	0.32	0.42	1.45	1.40	0.10	0.03	0.49	0.59	0.28	1.15	1.35
11	0.00	0.00	0.01	0.30	0.43	1.41	1.04	0.10	0.00	0.37	0.52	0.27	1.15	1.37
12	0.00	0.00	0.03	0.30	0.36	1.36	1.25	0.00	0.00	0.22	0.63	0.20	1.15	1.28
13	0.00	0.00	0.00	0.27	0.25	1.45	1.75	0.00	0.00	0.16	0.57	0.02	1.05	1.20
14	0.00	0.00	0.00	0.17	0.26	1.46	1.44	0.00	0.00	0.03	0.25	0.00	0.99	1.21
15	0.00	0.00	0.00	0.15	0.39	1.45	1.33	0.00	0.00	0.00	0.25	0.00	1.08	1.24
16	0.00	0.00	0.00	0.36	0.34	1.42	1.71	0.00	0.00	0.00	0.23	0.00	1.08	1.22
17	0.04	0.00	0.00	0.42	0.51	1.44	1.80	0.00	0.00	0.01	0.18	0.05	1.06	1.18
18	0.21	0.00	0.05	0.26	0.47	1.50	1.49	0.05	0.00	0.02	0.47	0.20	1.11	1.20
19	0.25	0.00	0.00	0.14	0.32	1.41	1.54	0.03	0.00	0.01	0.67	0.44	1.17	1.27
20	0.20	0.00	0.00	0.06	0.19	1.06	1.77	0.00	0.10	0.03	0.65	0.54	1.11	1.28
21	0.14	0.00	0.00	0.04	0.26	1.03	1.47	0.01	0.17	0.00	0.98	0.48	1.07	1.20
22	0.07	0.00	0.00	0.08	0.53	1.11	1.46	0.20	0.18	0.00	0.89	0.49	0.89	1.04
23	0.04	0.00	0.00	0.12	0.43	1.18	1.56	0.40	0.14	0.00	0.93	0.47	0.68	1.00
24	0.01	0.00	0.10	0.27	0.49	1.30	1.59	0.41	0.00	0.00	1.00	0.49	0.86	1.00
25	0.02	0.00	0.06	0.43	0.36	1.42	1.68	0.38	0.00	0.00	0.93	0.66	0.97	1.04
26	0.05	0.00	0.22	0.52	0.42	1.53	1.78	0.61	0.04	0.00	0.78	0.71	1.10	1.14
27	0.09	0.00	0.08	0.44	0.50	1.56	1.79	0.52	0.18	0.00	0.93	0.79	1.19	1.36
28	0.11	0.00	0.24	0.41	0.52	1.60	1.81	0.80	0.34	0.00	0.82	0.56	1.21	1.41
29	0.12	0.00	0.14	0.40	0.48	1.69	1.78	0.69	0.33	0.00	0.89	0.44	1.25	1.33
30	0.24	0.00	0.01	0.33	0.35	1.83	2.15	0.71	0.20	0.00	0.62	0.26	1.28	1.41
31	0.45	0.00	0.00	0.20	0.21	1.88	2.09	0.68	0.03	0.00	0.72	0.25	1.42	1.09
32	0.42	0.00	0.00	0.21	0.17	1.97	1.94	0.61	0.00	0.00	0.94	0.37	1.57	1.22
33	0.33	0.00	0.00	0.14	0.13	2.04	1.93	0.56	0.00	0.06	1.12	0.51	1.74	1.39
34	0.28	0.00	0.00	0.27	0.16	2.08	2.01	0.59	0.00	0.13	1.18	0.70	1.88	1.57
35	0.25	0.00	0.43	0.63	0.15	2.15	2.02	0.65	0.00	0.00	1.28	0.72	1.94	1.67
36	0.04	0.00	0.75	0.59	0.05	2.36	1.91	0.74	0.00	0.00	1.26	0.49	1.92	1.74
37	0.00	0.00	0.87	0.37	0.00	2.38	2.28	0.66	0.00	0.06	1.45	0.70	1.97	1.77

38	0.00	0.00	0.86	0.29	0.00	2.33	2.12	0.81	0.00	0.35	1.33	0.85	2.06	1.96
39	0.00	0.00	0.80	0.31	0.05	2.31	1.90	1.00	0.00	0.38	1.43	0.93	2.07	1.70
40	0.00	0.00	0.81	0.46	0.00	2.25	2.00	1.13	0.00	0.54	1.53	0.99	1.99	1.51
41	0.00	0.00	0.89	0.71	0.03	2.29	1.92	1.21	0.00	0.87	1.44	0.96	1.92	1.41
42	0.00	0.00	0.98	0.50	0.07	2.22	1.60	1.17	0.00	0.90	1.29	0.87	1.81	1.48
43	0.01	0.00	1.00	0.55	0.22	2.03	1.38	1.03	0.00	1.13	1.25	0.87	1.77	1.59
44	0.08	0.00	1.29	0.77	0.34	1.90	1.24	0.95	0.00	1.30	1.36	1.06	1.76	1.42
45	0.11	0.00	1.04	0.75	0.46	1.87	1.25	1.03	0.00	1.34	1.46	0.95	1.54	1.20
46	0.08	0.00	0.85	0.68	0.53	1.86	1.16	0.96	0.00	1.29	1.67	1.02	1.51	0.89
47	0.06	0.00	0.87	0.77	0.68	1.67	0.92	0.83	0.00	1.31	1.55	0.87	1.62	0.96
48	0.08	0.00	1.05	0.78	0.53	1.42	0.55	0.74	0.00	1.32	1.46	0.78	1.34	0.64
49	0.00	0.00	1.12	1.11	0.64	1.09	0.35	0.61	0.00	1.44	1.27	0.71	1.04	0.33
50	0.00	0.00	0.93	0.72	0.57	0.87	0.19	0.45	0.08	1.40	1.01	0.18	0.90	0.11
Minimum	0.00	0.00	0.00	0.04	0.00	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.00
Maximum	0.45	0.07	1.29	1.11	0.68	2.38	2.85	1.21	0.42	1.44	1.67	1.06	2.07	1.96
Values averaged by 1 s														

Table A 4 - Release rate of trial P25_3

Time [s]	Temperature at outlet orifice [°C]	Pressure at outlet orifice [hPa]	Release rate [kg.s ⁻¹]
1	10.26	740	0.40
2	-12.66	1330	0.39
3	-11.85	880	0.35
4	-7.46	380	0.40
5	-2.45	240	0.34
6	1.84	170	0.28
7	3.23	110	0.23
8	4.44	90	0.20
9	5.07	80	0.18
10	5.46	70	0.17
11	5.58	60	0.16
12	5.52	50	0.15
13	5.17	50	0.15
14	4.75	0	0.00
15	4.19	40	0.09
16	3.23	30	0.12
17	2.49	30	0.12
18	0.93	30	0.12
19	-0.89	30	0.11
20	-4.10	20	0.09
21	-10.30	20	0.09
22	-14.08	20	0.09
23	-22.00	20	0.09
24	-26.70	20	0.09
25	-27.21	20	0.11
26	-27.86	20	0.11
27	-28.13	50	0.15
28	-28.35	40	0.15
29	-28.41	40	0.14
30	-28.34	50	0.15
31	-28.30	40	0.15
32	-28.23	50	0.16
33	-28.18	60	0.17
34	-28.24	60	0.17
35	-28.30	60	0.17
36	-28.32	50	0.16
37	-28.16	60	0.17
38	-28.16	60	0.17
39	-28.26	60	0.17
40	-28.30	80	0.17

Table A 5 - Concentrations of trial P25_3(sensors 1A to 6C).

Sensor	1A	1B	1C	3B	3C	4A	4B	5A	5B	5C	6A	6B	6C
y [m]	0.0	0.0	0.0	0.0	0.0	-2.0	-2.0	2.0	2.0	2.0	0.0	0.0	0.0
x [m]	2.0	2.0	2.0	5.0	5.0	5.0	5.0	9.0	9.0	9.0	9.0	9.0	9.0
z [m]	0.1	0.6	1.3	0.6	1.3	0.1	0.6	0.1	0.6	1.3	0.1	0.6	1.3
Time [s]													
1	0.19	0.00	0.21	0.05	0.00	0.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	0.06	0.00	1.64	0.03	0.86	0.47	0.00	0.00	0.00	0.00	0.00	0.00	0.25
3	0.05	0.00	2.76	0.15	1.51	0.62	0.00	0.00	0.00	0.00	0.16	0.22	0.76
4	0.00	0.00	3.36	0.44	2.21	0.69	0.00	0.00	0.00	0.00	0.35	0.63	1.20
5	0.00	0.00	3.72	0.41	2.63	0.65	0.00	0.00	0.00	0.00	0.80	0.91	1.56
6	0.08	0.05	3.86	0.59	2.91	0.69	0.00	0.00	0.00	0.00	0.86	0.92	1.69
7	0.07	0.19	3.80	0.83	3.04	0.67	0.00	0.00	0.00	0.00	0.79	0.90	1.72
8	0.16	0.26	4.19	0.93	3.12	0.80	0.00	0.04	0.00	0.00	0.76	0.89	1.69
9	0.25	0.15	4.21	0.94	3.12	0.89	0.00	0.23	0.00	0.00	0.73	0.88	1.65
10	0.19	0.00	4.31	0.75	3.04	0.94	0.00	0.33	0.00	0.00	0.65	0.92	1.54
11	0.00	0.00	4.39	0.59	2.96	0.95	0.00	0.21	0.00	0.00	0.82	1.02	1.58
12	0.00	0.00	4.33	0.52	2.92	0.77	0.00	0.16	0.00	0.00	0.86	0.89	1.48
13	0.00	0.00	4.20	0.61	2.86	0.52	0.00	0.30	0.00	0.00	0.76	0.69	1.34
14	0.00	0.06	3.76	0.61	2.75	0.28	0.00	0.45	0.02	0.00	0.68	0.58	1.19
15	0.33	0.06	3.65	0.56	2.64	0.28	0.00	0.40	0.09	0.00	0.63	0.56	1.08
16	0.36	0.15	3.88	0.44	2.52	0.31	0.00	0.79	0.00	0.00	0.50	0.47	0.94
17	0.00	0.26	3.75	0.29	2.45	0.17	0.00	0.53	0.00	0.00	0.40	0.36	0.74
18	0.00	0.12	3.65	0.24	2.44	0.00	0.00	0.03	0.00	0.00	0.44	0.40	0.70
19	0.00	0.01	3.58	0.33	2.38	0.00	0.00	0.00	0.00	0.00	0.27	0.36	0.63

Sensor	1A	1B	1C	3B	3C	4A	4B	5A	5B	5C	6A	6B	6C
y [m]	0.0	0.0	0.0	0.0	0.0	-2.0	-2.0	2.0	2.0	2.0	0.0	0.0	0.0
x [m]	2.0	2.0	2.0	5.0	5.0	5.0	5.0	9.0	9.0	9.0	9.0	9.0	9.0
z [m]	0.1	0.6	1.3	0.6	1.3	0.1	0.6	0.1	0.6	1.3	0.1	0.6	1.3
20	0.00	0.00	3.50	0.40	2.32	0.15	0.00	0.00	0.00	0.00	0.16	0.27	0.64
21	0.00	0.00	3.27	0.31	1.99	0.35	0.00	0.00	0.00	0.00	0.05	0.16	0.51
22	0.00	0.00	3.49	0.25	1.91	0.23	0.00	0.63	0.00	0.00	0.03	0.00	0.37
23	0.00	0.00	3.79	0.29	2.01	0.05	0.00	0.73	0.00	0.00	0.12	0.00	0.34
24	0.00	0.00	3.64	0.31	2.04	0.26	0.00	0.47	0.00	0.00	0.11	0.06	0.36
25	0.00	0.00	3.57	0.47	2.04	0.33	0.00	0.49	0.00	0.00	0.09	0.04	0.43
26	0.00	0.00	3.61	0.63	2.09	0.47	0.00	0.41	0.00	0.00	0.09	0.02	0.50
27	0.01	0.00	3.73	0.43	2.26	0.51	0.00	0.25	0.00	0.00	0.00	0.02	0.46
28	0.07	0.00	3.99	0.41	2.26	0.65	0.00	0.00	0.00	0.00	0.00	0.10	0.45
29	0.23	0.00	4.46	0.45	2.23	0.75	0.00	0.00	0.00	0.00	0.00	0.16	0.49
30	0.45	0.02	4.48	0.55	2.26	0.72	0.00	0.00	0.00	0.00	0.11	0.24	0.63
31	0.44	0.06	4.56	0.61	2.26	0.65	0.00	0.00	0.00	0.00	0.11	0.31	0.71
32	0.52	0.02	4.82	0.76	2.23	0.65	0.00	0.00	0.00	0.00	0.19	0.31	0.67
33	0.51	0.21	5.00	0.92	2.30	0.73	0.00	0.00	0.00	0.00	0.41	0.28	0.62
34	0.61	0.25	4.93	0.79	2.45	0.46	0.00	0.00	0.00	0.00	0.48	0.26	0.29
35	0.40	0.26	5.07	0.65	2.57	0.00	0.00	0.00	0.00	0.00	0.41	0.28	0.10
36	0.20	0.17	5.12	0.80	2.70	0.00	0.00	0.00	0.00	0.00	0.51	0.31	0.26
37	0.22	0.10	5.33	0.71	2.74	0.00	0.00	0.00	0.00	0.00	0.36	0.34	0.28
38	0.36	0.03	5.89	0.61	2.85	0.00	0.00	0.00	0.00	0.00	0.41	0.26	0.24
39	0.68	0.03	6.57	0.58	3.03	0.00	0.00	0.00	0.00	0.00	0.46	0.13	0.14
40	0.66	0.14	6.80	0.35	3.16	0.07	0.00	0.00	0.00	0.00	0.44	0.00	0.00
41	1.19	0.10	7.08	0.25	3.35	0.60	0.00	0.00	0.00	0.00	0.41	0.00	0.00
42	0.68	0.03	6.57	0.64	3.55	0.83	0.00	0.00	0.00	0.00	0.47	0.00	0.00
43	0.68	0.06	6.63	0.68	3.66	0.92	0.03	0.00	0.00	0.00	0.45	0.24	0.23

Sensor	1A	1B	1C	3B	3C	4A	4B	5A	5B	5C	6A	6B	6C
y [m]	0.0	0.0	0.0	0.0	0.0	-2.0	-2.0	2.0	2.0	2.0	0.0	0.0	0.0
x [m]	2.0	2.0	2.0	5.0	5.0	5.0	5.0	9.0	9.0	9.0	9.0	9.0	9.0
z [m]	0.1	0.6	1.3	0.6	1.3	0.1	0.6	0.1	0.6	1.3	0.1	0.6	1.3
44	0.67	0.09	6.69	0.37	3.79	1.00	0.08	0.00	0.00	0.00	0.56	0.50	0.55
45	0.66	0.11	6.75	0.28	0.14	0.91	0.05	0.00	0.00	0.00	0.77	0.75	0.81
46	0.66	0.14	6.80	0.93	4.03	0.77	0.05	0.15	0.00	0.00	1.06	1.04	0.70
47	0.79	0.13	6.80	1.32	4.23	0.54	0.07	0.04	0.00	0.00	1.35	0.83	0.45
48	0.93	0.12	6.89	1.11	4.23	0.42	0.37	0.51	0.00	0.00	1.31	0.66	0.21
49	1.06	0.11	6.99	0.65	3.44	0.07	0.18	0.18	0.00	0.00	1.07	0.59	0.05
50	1.19	0.10	7.08	0.14	2.89	0.02	0.17	0.00	0.00	0.00	1.00	0.25	0.00
Minimum	0.00	0.00	0.21	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Maximum	1.19	0.26	7.08	1.32	4.23	1.00	0.37	0.79	0.09	0.00	1.35	1.04	1.72
Values averaged by 1 s													

Table A 6 -Concentrations of trial P25_3 (sensors 7A to 15A)

Sensor	7A	7B	7C	9A	10B	11B	11C	12A	12C	13A	15A	16A	16B
y [m]	-2.0	-2.0	-2.0	-3.0	2.0	0.0	0.0	-2.0	-2.0	2.0	-2.0	0.0	0.0
x [m]	9.0	9.0	9.0	10.0	11.0	11.0	11.0	11.0	11.0	13.0	13.0	15.0	15.0
z [m]	0.1	0.6	1.3	0.1	0.6	0.6	1.3	0.1	1.3	0.6	0.1	0.1	0.6
Time [s]													
1	0.01	0.00	0.00	0.10	0.00	0.00	0.70	0.01	0.38	0.00	0.05	0.00	0.00
2	0.00	0.00	0.00	0.01	0.00	0.07	0.10	0.01	0.06	0.00	0.05	0.00	0.00
3	0.06	0.00	0.11	0.00	0.00	0.47	0.08	0.01	0.00	0.00	0.07	0.00	0.00
4	0.48	0.00	0.18	0.00	0.00	0.73	0.17	0.01	0.00	0.00	0.65	0.33	0.43
5	0.43	0.00	0.18	0.06	0.00	1.00	0.48	0.01	0.00	0.00	0.81	0.65	0.70

Sensor	7A	7B	7C	9A	10B	11B	11C	12A	12C	13A	15A	16A	16B
y [m]	-2.0	-2.0	-2.0	-3.0	2.0	0.0	0.0	-2.0	-2.0	2.0	-2.0	0.0	0.0
x [m]	9.0	9.0	9.0	10.0	11.0	11.0	11.0	11.0	11.0	13.0	13.0	15.0	15.0
z [m]	0.1	0.6	1.3	0.1	0.6	0.6	1.3	0.1	1.3	0.6	0.1	0.1	0.6
6	0.40	0.00	0.39	0.19	0.00	1.16	0.90	0.01	0.01	0.00	1.04	0.80	1.00
7	0.47	0.00	0.51	0.14	0.00	1.25	1.13	0.01	0.05	0.11	1.18	0.95	1.08
8	0.58	0.00	0.56	0.14	0.00	1.25	1.28	0.01	0.11	0.26	1.26	0.84	1.23
9	0.63	0.00	0.71	0.11	0.00	1.27	1.37	0.01	0.30	0.30	1.23	0.92	1.23
10	0.64	0.25	0.72	0.04	0.00	1.15	1.45	0.01	0.14	0.18	1.23	0.87	1.19
11	0.50	0.10	0.71	0.04	0.00	1.04	1.44	0.01	0.12	0.20	1.22	0.74	1.14
12	0.34	0.16	0.60	0.00	0.00	1.03	1.30	0.01	0.20	0.33	1.10	0.63	1.05
13	0.42	0.05	0.55	0.00	0.00	0.98	1.33	0.01	0.23	0.43	0.97	0.57	1.00
14	0.39	0.11	0.55	0.00	0.03	0.91	1.18	0.01	0.19	0.37	0.98	0.53	0.96
15	0.50	0.09	0.63	0.13	0.18	0.86	1.45	0.01	0.21	0.26	0.89	0.35	0.73
16	0.51	0.05	0.65	0.36	0.29	0.88	1.18	0.01	0.21	0.00	0.79	0.38	0.84
17	0.51	0.06	0.60	0.00	0.44	0.88	1.14	0.01	0.17	0.00	0.69	0.38	0.79
18	0.56	0.12	0.48	0.01	0.51	0.83	1.08	0.01	0.28	0.00	0.66	0.28	0.69
19	0.64	0.17	0.51	0.07	0.60	0.77	1.00	0.01	0.25	0.00	0.63	0.26	0.59
20	0.56	0.25	0.42	0.16	0.20	0.70	0.99	0.01	0.58	0.00	0.49	0.20	0.57
21	0.56	0.06	0.35	0.14	0.00	0.61	0.99	0.01	0.32	0.00	0.47	0.00	0.45
22	0.38	0.00	0.26	0.00	0.00	0.44	0.89	0.01	0.09	0.00	0.29	0.00	0.18
23	0.37	0.00	0.15	0.00	0.00	0.42	0.76	0.01	0.00	0.00	0.20	0.00	0.11
24	0.37	0.00	0.08	0.00	0.00	0.41	0.86	0.01	0.00	0.00	0.21	0.00	0.00
25	0.15	0.00	0.14	0.00	0.00	0.36	0.70	0.01	0.00	0.00	0.10	0.00	0.00
26	0.00	0.00	0.26	0.00	0.00	0.33	0.61	0.01	0.00	0.00	0.00	0.00	0.00
27	0.10	0.03	0.21	0.00	0.00	0.38	0.49	0.01	0.00	0.00	0.00	0.00	0.00
28	0.00	0.12	0.21	0.00	0.00	0.45	0.33	0.01	0.00	0.00	0.00	0.00	0.00
29	0.02	0.00	0.07	0.00	0.00	0.46	0.18	0.01	0.14	0.00	0.00	0.00	0.00

Sensor	7A	7B	7C	9A	10B	11B	11C	12A	12C	13A	15A	16A	16B
y [m]	-2.0	-2.0	-2.0	-3.0	2.0	0.0	0.0	-2.0	-2.0	2.0	-2.0	0.0	0.0
x [m]	9.0	9.0	9.0	10.0	11.0	11.0	11.0	11.0	11.0	13.0	13.0	15.0	15.0
z [m]	0.1	0.6	1.3	0.1	0.6	0.6	1.3	0.1	1.3	0.6	0.1	0.1	0.6
30	0.22	0.00	0.00	0.00	0.00	0.42	0.35	0.01	0.24	0.00	0.00	0.00	0.00
31	0.12	0.00	0.06	0.00	0.00	0.41	0.24	0.01	0.16	0.00	0.00	0.00	0.00
32	0.09	0.00	0.21	0.00	0.00	0.23	0.00	0.01	0.00	0.00	0.00	0.00	0.00
33	0.10	0.00	0.25	0.00	0.00	0.30	0.26	0.01	0.00	0.00	0.02	0.00	0.00
34	0.40	0.00	0.14	0.29	0.00	0.26	0.51	0.01	0.00	0.00	0.09	0.00	0.01
35	0.59	0.00	0.19	0.33	0.00	0.11	0.58	0.01	0.13	0.00	0.17	0.00	0.15
36	0.23	0.00	0.05	0.25	0.00	0.00	0.57	0.01	0.03	0.00	0.20	0.00	0.16
37	0.13	0.00	0.35	0.20	0.00	0.00	0.57	0.00	0.00	0.00	0.13	0.00	0.07
38	0.28	0.12	0.54	0.15	0.00	0.03	0.72	0.01	0.00	0.00	0.20	0.00	0.02
39	0.39	0.23	0.57	0.06	0.00	0.22	1.07	0.00	0.00	0.00	0.55	0.00	0.00
40	0.41	0.22	0.55	0.02	0.00	0.10	0.87	0.00	0.00	0.00	0.75	0.00	0.13
41	0.41	0.20	0.53	0.00	0.00	0.04	1.10	0.00	0.00	0.00	0.90	0.00	0.31
42	0.38	0.20	0.53	0.00	0.00	0.00	1.08	0.00	0.00	0.00	0.99	0.00	0.59
43	0.35	0.19	0.57	0.00	0.00	0.00	1.13	0.00	0.00	0.00	1.09	0.00	0.61
44	0.32	0.19	0.62	0.00	0.00	0.08	0.98	0.00	0.00	0.00	1.24	0.00	0.97
45	0.29	0.18	0.67	0.00	0.00	0.22	0.92	0.00	0.00	0.00	1.40	0.00	1.13
46	0.36	0.18	0.71	0.00	0.00	0.32	0.62	0.00	0.00	0.00	1.44	0.00	1.15
47	0.43	0.25	0.82	0.00	0.00	0.43	0.81	0.00	0.00	0.00	1.30	0.00	1.11
48	0.49	0.32	0.93	0.00	0.00	0.44	0.56	0.00	0.00	0.00	1.39	0.00	1.24
49	0.56	0.40	1.04	0.00	0.00	0.35	0.59	0.00	0.00	0.00	1.57	0.00	1.47
50	0.56	0.47	1.15	0.00	0.08	0.12	0.59	0.00	0.00	0.00	1.43	0.00	1.46
Minimum	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Maximum	0.64	0.47	1.15	0.36	0.60	1.27	1.45	0.01	0.58	0.43	1.57	0.95	1.47
Values averaged by 1 s													

