Comparisons of experimental measurements and large eddy simulations for a helium release in a two vents enclosure

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Abstract

This work takes place in the context of potential hazards in the use of hydrogen in fuel cells. The present article describes comparisons between PIV measurements performed on a two vented cavity with an helium injection and Large Eddy Simulation of the same configuration. A two vented cavity is chosen because a quasi state is reached rapidly and it facilitates both CFD calculations by reducing the CPU costs and also enables statistical treatment of the data, the temporal averaging being possible at steady state. At the same time, this configuration is close to fuel cell designs, except for the set-up reduced size. We also describe the experimental set-up and the care which has to be taken to produce Particle Image Velocimetry velocity fields. The final goal of the paper is to validate a L.E.S approach as a good replacement to experiments, since access to both velocity and concentration fields is required to improve existing simplified models. Indeed, most of the 2 vents models rely on simplified assumptions such as a constant entrainment coefficient, a bi-layer formation which is not always the case in real situations.

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benchmarks have been published on closed, one vented and two vented cavities [11–18]. They showed satisfactory agreement between CFD and experimental concentration measurements for jet releases of helium. On the other hand, for plume releases, R.A.N S models for turbulence proved to be significantly more diffusive than measurements [13,15]. Only “coarse” Large Eddy Simulation with Smagorinsky models for turbulence capture correctly the maximum concentration [18] but with still a strong diffusion for the minimum concentrations (being higher than expected).

On the experimental side, PIV measurements can mostly been achieved on small set-ups, the maximum reasonable size of a velocity field being around 40 cm with a 8Mpx PIV camera. Very few measurement exist on a free jet at a meter scale, and to our knowledge none on a set-up as large as a fuel cell. As a result, we decided to develop two types of research jointly: to characterize the flow in vented cavities through highly resolved L.E.S numerical simulations [19,20] and to perform PIV measurements of the flow in a small enough experimental set-up. This volume limitation is actually of the same order for the CFD approach due to the need to represent spatial scales close to the Kolmogorov length.

In this paper, we present an experimental set-up designed to perform injection and dispersion of helium in a 2 vented box with Particle image velocimetry measurements. Comparisons between experimental measurements and numerical results obtained for the same configuration [21] are presented. This article largely validate the L.E.S numerical approach although some difficulties are shown to remain.

The first section of this paper presents briefly the context of this work. In the second section the experimental setup is described. In the third part, statistical operators and statistical independence of the data is discussed. At last, in the fourth part, the numerical approach is briefly presented and comparisons between experimental and numerical results are discussed.

### Experimental setup

#### Choice of the experimental set-up

The experiment is carried out on a parallelepiped cavity. In order to reach rapidly a quasi steady state, two vents are considered inside the cavity and located respectively at the bottom and at the top of the same solid wall boundary, Fig. 1.

The height of the set up has been set to 15 cm in order to have a high spatial accuracy of the PIV measurements. Indeed with a 8Mpx camera and a window size of 16px, the physical size of the window is around 0.6 mm which is about 3 times the Kolmogorov scale. With a window shift of 8px, we have access to information very close to the Kolmogorov scale. The width of the set-up is chosen around 5 cm, which is slightly more than the expected turbulent spreading of the plume in order to limit jet/wall interaction. After machining of the box panels in Plexiglas, the internal dimensions of the cavity are $W \times L \times H = 4.9 \times 5 \times 14.9 \times 10^{-2} m^3$.

The injection diameter of 10 mm and the flow rate of 5NL/min were chosen to ensure a laminar to turbulent transition in the mid height of the enclosure predicted to occur at $H/d > 5$ [22], as well as a jet to plume transition. The injection pipe length is over 30 diameters long and a laminar Poiseuille flow is insured upwind at the inlet centered at the base of the box.

At last, vents of equal size were chosen and to be smaller than the expected so called Linden’s top homogeneous layer [10], with a surface area $5 \times 2.9 \times 10^{-4} m^2$. We will see in the results section that this Linden bi-layer structure doesn’t occur in this configuration (personnal communication shows that a higher injection flow rate is required).

Flexi-glass of thickness $5 \times 10^{-3} m$ is used for the solid wall boundaries.

#### 3/8 m$^3$ experimental configuration

**Environment:** This experimental set-up is located inside a 30 m$^3$ garage, Fig. 2, fully isolated with styrilidur panels. Temperature variations monitored with a Pt100 sensors are below 0.1°C over an hour. Daily temperature variation is below 0.5°C and temperature is monitored during experiments. The garage itself is part of a warehouse with small daily temperature fluctuations (1°C on average). The garage is also fully sealed, except with the presence of two circular vents of 30 cm diameter in order to evacuate potential accumulation of helium. Residual velocities in the garage are not measurable in comparison with the velocities at the experimental set-up vents (which are the entry/exit interfaces between the box and the room), that is lower than a few cm/s. We notice that the laser power supplies have been placed outside of the garage to reduce the potential natural convection that could have been induced if located inside the garage.

**Experimental build-up:** The cavity and the whole instrumentation, that is camera and laser are tighten together with Bosch aluminium profiles, Fig. 3. This ensures the required perpendicularity of the cavity main axis, the camera and the laser light sheet. Adjusting feet below the bosc profiles allow as well to set up the horizontality of the base Bosch profiles and therefore the verticality of the side walls of the experimental cavity.

**Injection:** We inject pure helium through a cylindrical pipe with a unique constant mass flow-rate $Q = 5$ NL/min into a two vented parallelepiped enclosure filed initially with air at rest. Normo-Liters per minute is a mass flow rate in that it is the volumetric flow rate that would occur at 0°C injection’s temperature. At the 25°C injection temperature of our experiments, the volumetric flow rate of helium is therefore $Q = 5 \times (273+25)/273 = 5.45$ l/min. That mass flow rate is controlled with a Brooks (1–20 NL/min range) gas flow controller. That mass controller had been calibrated within the last 6 months and ensures an accuracy better than 1% error at the chosen flow rate.

**Physical properties:** All the physical properties of the light helium gas are referred to with the $u_{in}$ subscript (meaning “injected”), while the subscript $u_{am}$ is used to denote the ambient air. Both injection temperature and garage temperature have been checked to be at 25°C within the error limit of the sensor (around 1°C for portable TC used at beginning of experiments, fixed Pt100 were used for monitoring during experiments and set-up qualification) (See Table 1).

**Optical devices:** The laser beam is produced either by a double cavity 200 mJ Yag laser (Quantum), or a continuous 5
Fig. 1 – Experimental set-up.

Fig. 2 – Garage containing the experimental set-up.

Fig. 3 – Experimental set-up with Bosch aluminium profiles for assembly. Quantum pulsed Yag laser is presented.
Watts laser. The laser beam is then changed into a plan with a semi-cylindrical lens and thickness of the plan is adjusted with a divergent and a convergent lenses. Those lenses are fixed on the quantum laser exit, or on a specific bench screwed to the Bosch profiles. Positioning of the different systems is done with micro-metric screws. With the 2 cavities pulsed yag laser, a PIV 8Mpx camera is used (CMOS) and with the continuous laser, a 1Mpx 2 kHz camera is used ( cinevision). Lenses used on the camera are full frame designed Carl Zeiss 35 mm, 50 mm and 85 mm with wide opening (better than 2). Those expensive lenses have very reduced distortion (less than 0.7% geometrical deformation at the edges). In practise, the geometrical distortion is even lower due to the reduced size of the sensor (half the full frame size). PIV measurements won’t therefore be affected by the geometrical distortion. At last the semi-cylindrical lens can rotate in order to adjust the verticality of the laser plan.

Seeding: Particles are needed in order to visualise the flow and carry on with PIV measurements. The seeding is realized with a theater smoke generator. The smoke is made of around 1 µm droplets, which last around 15 min before evaporation. Their size is small enough to ensure no drift in our experimental condition and their motion will represent accurately the gas flow in the room and in the cavity. Indeed, rapidly the fog is sucked into the box through the bottom vent and rejected through the top vent. Droplets volume concentration is such that roughly 10 drops can be seen on a PIV sub-window of 600 µm, that requires a spacing of approximately 200 µm between droplets, that is 200 diameters. The required volume fraction is therefore roughly 1/200^3 which is close to 10^{-5}%. We can assert that during experiments, image control shows than we never exceed a concentration of 10^{-3}%. We underline this to assert that fog has no significant influence on the gas volumic mass, it would modify it by less than 0.1%. Fog influence is therefore negligible compared to helium influence on the mixture density.

PIV specifications

A laser sheet of less than 1 mm thickness is enlightening a vertical plan, Fig. 4. The fog droplets are enlightened by the laser. For the Yag pulsed laser, the pulse lasts 6 ns and freezes the droplets at their positions. For the continuous laser, the fast camera shutter can be adjusted from 2 to 10 kHz at the cost of a loss of light on the images. In practise we limit ourselves to a 3 kHz shutter speed. Particle movements are not frozen, and droplets are seen as short spheres or even lines instead of dots. This doesn't affect too much in practise the quality of the results although it may theoretically reduce the measurements accuracy.

As said, the pulsed laser (10 Hz) is in used in association with a 8 Mpx PIV camera, whereas the continuous laser is used with a 1 Mpx fast camera (2 KHz). With the fast camera we perform measurement at the injection and also near the bottom vent. With the PIV camera, we cover the full enclosure but with slow frequency acquisitions of 1 Hz (to perform time averaged statistics). But every acquisition is made of two pictures separated by a small time interval (250 up to 750 µs). The PIV process consists in splitting each camera pictures in sub-windows. We use 16 x 16 pixels windows. Those windows might overlap and we choose a 8 pixels overlapping. A pair of images separated by a time interval is selected. Cross correlations of the light signal are done on each pairs of sub-windows, Fig. 5. The cross correlation signal contains a principal peak (maximum value) and secondary peaks. The location of the principal peak is the most probable displacement of the particles in the sub-window. The velocity is obtained by dividing with the time interval.

It is important to note that accuracy of the measurement depends on the displacement of the particles on the image. Theories indicate that the position of the peak might be determined with sub-pixel accuracy (around 0.1 to 0.2 pixel). Therefore a 10 pixels displacement of the correlation peak will lead to a 1–2% error. A smaller displacement will evidently lead to higher errors: the smaller displacement, the higher relative error. Nevertheless the absolute error remain the same. That is why we want to select time intervals between pictures that maximise the displacement of particles on the sub-windows. On the other hand, a too large displacement leads to the risk of particles leaving the window before the second picture is taken. The correlation peak will correlate first image particles with particles on second image which have entered the window (other particles in fact). The correlation peak position will be a wrong indication of the particles displacement. Therefore two opposite notions coexist: accuracy of the displacement calculation and probability to measure the right displacement.

At last, the picture’s quality is of importance as well. If too many particles exist on the picture, they might hide each other and correlation between two successive pictures might be incorrect. If too few exist, errors connected to leaving or entering of particles between pairs of image might also lead to errors. On average we try to seed the ambient gas in order to have around 10 particles on the sub-windows. Practically, we calculate velocity fields using the free software GPIV delivered on Ubuntu Linux distributions. We use 16 x 16 px sub-frames with a 8 px shift and a predictor/corrector algorithm with distorted images capability. Basically, an estimate of the velocity is made with the procedure described above, then sub-framed are moved and distorted according to that first prediction. A new velocity field is calculated and an iterative process is engaged until converged to a certain accuracy.

Fig. 4 – Illustration of the laser plan creation and camera measurements.
Measurement accuracy

Image quality: In order to improve the final image quality, we operate different treatments. The first treatment is to calculate an image where at each pixel, we calculate the minimum pixel value of all the images. We then subtract this image to all the original images. This helps to remove all the background light and light reflections on the picture. We also replace all the walls (where there is obviously no flow) by the a fixed random image of particles. This helps to post-treat the images with no artifacts in the wall regions, where velocities will be calculated as zero thanks to the fixed particles artificially located in the walls. No other treatment (luminosity, contrast etc...) is done since it proved to be useless.

Time steps adjustment: The second important choice to make is the time step between images forming a pair. For the fast camera, the frequency of acquisition is 2 kHz. We can pair successive images or 1 every 3 or more pictures. In practise, we pair every successive images when we are interested at the velocities in the jet, the time step is therefore of 500 μs? For the flow fields around the bottom vent, we select a time step of 1 ms by dropping 1 every 2 pictures. We have analysed more thoroughly the selection of time steps with the yag cavity laser since time interval between cavities can be chosen as wished. We calculated that a 250 μs time step is ideal for the jet region with largest velocities (around 1 up to 2 m/s), whereas a time step of 750 μs is best suited for the outer jet region where velocities range between 0.1 up to 0.5 m/s. We therefore have to calculate twice the full picture fields and collect the velocity fields in the regions depending on the time step used.

Signal noise ratio: That parameter indicates the ratio between the maximum value of the first correlation peak and the second peak maximum value. GPIV software opts the inverse ratio, the smaller the value, the most probability to measure the correct velocity. We plot an example of the signal to noise ratio on a 2D plan, Fig. 6. The GPIV signal to noise ratio is close or higher to one in the regions where velocity is maximum. Is expected since particles might exit the sub-windows. Furthermore it has to be noticed that a small region near the injection hardly contains particles. Indeed injected helium contains no seeding and no mixing with the seeded air is occurring there. This might also lead to bad SNR in the vicinity of injection. In practise we consider the region located up to 2 cm above region as unusable for measurements. We won’t compare PIV results with CFD results in that region, although plots will contain that region.

We assessed that almost 95% of the data are associated with a GPIV SNR below 1 (that is a standard SNR above 1). We also plot, Fig. 7, the time averaged velocities calculated versus the GPIV SNR. For a given GPIV SNR, we include all the data with a lower GPIV SNR to calculate the average. We observe that for a GPIV SNR below 1, the average is not modified. For GPIV SNR above 1, the average is modified but only by less than 1%. For data associated with a GPIV SNR higher than 1, velocities may be wrong (by a 100%) but they only merely contribute to an error on the time averages. This is due to the fact that less than 5% of the data are concerned. Nevertheless, only data with a GPIV SNRS lower than 1 will be used to calculate the statistical quantities. This is a common procedure in PIV techniques.

Steadiness: We are interested in quasi steady states. Although it has no connection with PIV accuracy, it is also an important aspect of experiments qualification to ensure that our data are indeed produced during a quasi steady state. We will discuss more in depth this aspect in the next section.

Measurement errors: All the preceding qualifications lead to expect an absolute accuracy better than 0.2px for the displacement calculations with a 95% confidence. Our time steps strategy, based on separating varying regions of the flow based on the velocity intensity, lead to an expected absolute error of 8 cm/s in high velocity regions (the maximum velocity being around 2 m/s) and an absolute error lower than 3 cm/s in the lowest velocity regions (velocities range between 0 up to 0.6 m/s).

Time aliasing: We checked that no slow periodicity/aliasing phenomenon interfere when doing acquisition at 1 Hz with the pulsed laser. We performed up to 7 Hz acquisitions with the pulsed laser and 2 khz acquisitions on a fast camera which excluded that results at 1 Hz could be affected by such a problem.

Representativeness: A last important point is the representativeness of the velocity measurement. Indeed smoke droplets velocities are measured. First the PIV method requires that velocities of the different droplets present in a PIV windows are similar (the differences between velocities
Second, in our specific case of air/helium mixing if regions of pure helium - therefore with no droplets - coexist with regions of air in a same PIV window (this happens only in thin eddy structures with adjacent layers of helium and air), the droplets are representative of the mixture velocity only if helium and air have close velocities in the PIV window. Both issues are addressed at the end when we ensure that windows are small enough to reduce velocity variations influence. The 16px wide windows represent areas of the mixture of around 0.6 mm width. Although helium or air volume concentration show strong gradients in the laminar region of the jet (from 1 to 0 across the jet boundary), velocities don’t exhibit such stiff gradient. Based on CFD results, we observe that the maximum velocity gradients are of 1 m/s on 1 cm (for example in Fig. 18), which makes it less than 6 cm/s on a PIV window. This is compatible with an expected 8 cm/s error in the high velocity regions. Same observations are made in low velocity regions indicating a correct choice of the window size. Furthermore, for the case of a presence of air/helium adjacent layers in a window, the observed width of each layer is around 0.2 mm or less (about the size of the CFD calculated Kolmogorov scale) associated with velocity differences less than 2 cm/s and therefore negligible.

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Fig. 6 – Example of a signal to noise ratios distributions in $y=0$ and $x=-0.5$ plans.

Fig. 7 – Test of the influence of GPIV SNRS Threshold on time averaged velocities. (a) Measurements performed in $yz'$ and (b) measurements performed in $xz$.
Reproducibility: A strong attention has been put on reproducibility of the results. The presented experiment has been redone at least 20 times in the xOz plan with different types of material (fast cameras, PIV cameras, PIV lasers, continuous laser, fog generators or oil droplet generator), at different places (the garage has been moved from one warehouse to another) and different seasons (slight temperature differences of a few degrees). Results are always reproduced within the expected experimental error. For the other plans of measurement, the experiments are systematically redone 3 times only to check for human errors in the process since reproducibility has already been demonstrated. Indeed only the visualisation map is changed, the experiment itself is always the same (same flow rate etc ...).

We illustrate, Fig. 8, velocity profiles in the vertical plan perpendicular to the vent centered on the jet axis (xOz), for different heights. Two repeated experiments are compared, and maximum discrepancies on the averages velocities are always below 3 cm/s locally, which is coherent with the expected accuracy of the measurements.

In order to achieve this kind of result, we had to take care of the following points: image quality, experimental set-up geometrical alignments, experimental conditions, quasi steadiness.

Image quality: We have already mentioned that pre process was made on the obtained pictures to remove background noise, and amount of seeding has to be thoroughly controlled. We repeat the following steps:

- We use a smoke generator for a few seconds in the garage.
- After smoke generation, we mix the garage atmosphere with a mechanical ventilation.

This process has probably a minor impact on reproducibility but is applied anyway.

Experimental set-up alignment: We already mentioned that using Bosh profile helped to ensure the correct angles and verticality of the system. This is of great importance, we have noticed that a slightly non vertical system (as slight as half a degree) has an impact on the expected plan-symmetries of the results. Also, it is very important to position the laser plan where it should be. We use micrometer screws and light sensitive paper to accurately position the laser plan. We expect an accuracy better than 1 mm in the positioning which is almost the thickness of the laser plan.

Experimental conditions: It mainly consists in controlling a steady temperature and the absence of perturbing air movement in the GARAGE. As we said the GARAGE is well insulated and sealed. Residual velocities should dissipate in a few minutes, especially with the absence of heat source and ventilation in the room (power supplies, PCs are located outside).

Steadiness: In order to reach and record data during a steady state:

- Acquisition starts 5 min after closing the access door of the garage.
- Steady state will be analysed in post treatment and final considered sequence might start sometimes between 5 up to 10 min after smoke injection.
- Helium is injected at the same time as the closing of the garage (the steady state is control ed both by helium injection start and the time unwanted air movement in the garage become negligible).

Scaling factor: at last, in order to convert dimensions in pixel into real lengths, we have to evaluate the scale factor which is the real equivalent size of 1 pixel. In order to do that we place a meter in the laser plan (it is very important that this meter is located in the plan where the lens focus is done, since focusing slightly modifies the focal length and therefore the image zooming). This operation must be redone for each experiment, Fig. 9. Geometrical dimension can be estimated to an accuracy better than 0.5 mm and therefore, the scaling factor error is lower than 1%. The scaling error leads to a multiplicative error on the calculated pixel/s velocities. It is a global error. It is impossible to guess on the PIV pictures where are the boundaries of the box due to multiple reflections, and therefore impossible to derive this scaling factor correctly. We made around 10% errors when we initially operated without a meter picture for each experiment.

2D slices for contour plots

Results of CFD and experiments are compared on 14 selected vertical two dimensional (2D) slices in the horizontal and span-wise directions, respectively x and y. The slices along the horizontal dimension are denoted by XZ, while YZ is used for slices along the span-wise direction. Locations of the slices are materialized on sub-figure (a) of Fig. 10 from a top view schematic representation, or on sub-figure (b) of Fig. 10 for a complete three dimensional (3D) observation. For completeness, a detailed description is reported in Table 2. CFD will provide the 3 components of the velocity in each of the selected plans, whereas PIV measurements only provide 2D...
components of the velocity in the plans. The orthogonal component hasn’t been measured due to the difficulty to use stereo PIV on such a small cavity.

Experiments have therefore been performed for each of the selected plans, whereas a single CFD calculation could be used to restrict the results on each of the selected plans.

Results produced both by experimental measurements and with a numerical simulation have to be post treated in a same manner. Since we are only interested in the quasi steady state, we have to ensure first that we are in such a state, and second to calculate time averaged quantities and rms values of the time fluctuations. At last, in order to evaluate the statistical

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**Table 1 – Physical properties of the working fluids.**

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Density [kg.m⁻³]</th>
<th>Dynamic viscosity [×10⁻³ kg.m⁻¹.s⁻¹]</th>
<th>Molar mass [×10⁻² kg.mol⁻¹]</th>
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<tr>
<td>Injected</td>
<td>μ_in = 0.16148</td>
<td>μ_in = 1.918</td>
<td>M_in = 0.4003</td>
</tr>
<tr>
<td>Ambient</td>
<td>μ_am = 1.36864</td>
<td>μ_am = 1.792</td>
<td>M_am = 2.897</td>
</tr>
</tbody>
</table>

**Table 2 – Position of the PIV studied vertical slices: Left: xz-plane, right: yz-plane.**

<table>
<thead>
<tr>
<th>xz-planes</th>
<th>Slice</th>
<th>y-position [cm]</th>
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<tbody>
<tr>
<td>XZ₁</td>
<td>y=0</td>
<td></td>
</tr>
<tr>
<td>XZ₂</td>
<td>y=0.5</td>
<td></td>
</tr>
<tr>
<td>XZ₃</td>
<td>y=1.5</td>
<td></td>
</tr>
<tr>
<td>XZ₄</td>
<td>y=2</td>
<td></td>
</tr>
<tr>
<td>XZ₂'</td>
<td>y=−0.5</td>
<td></td>
</tr>
<tr>
<td>XZ₃'</td>
<td>y=−1.5</td>
<td></td>
</tr>
<tr>
<td>XZ₄'</td>
<td>y=−2</td>
<td></td>
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<table>
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<tr>
<th>yz-planes</th>
<th>Slice</th>
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<tr>
<td>YZ₁</td>
<td>x=0</td>
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<tr>
<td>YZ₂</td>
<td>x=0.5</td>
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<tr>
<td>YZ₃</td>
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<tr>
<td>YZ₄</td>
<td>x=2</td>
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<tr>
<td>YZ₂'</td>
<td>x=−0.5</td>
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<td>YZ₃'</td>
<td>x=−1.5</td>
<td></td>
</tr>
<tr>
<td>YZ₄'</td>
<td>x=−2</td>
<td></td>
</tr>
</tbody>
</table>

**Fig. 9 – Meter image to calculate the scaling factor.**

**Fig. 10 – Schematic representation of the vertical slices used in the PIV measurements. Left: 2D top-cavity view, right: 3D representation for some selected slices.**
Fig. 11 – Examples of time evolutions of the norm $|u|_a$ at three locations (a) ($x = 0.5$ cm, $z = 14$ cm), $xz_1$ plan, (b) ($x = -1.8$ cm, $z = 1.8$ cm), $xz_1$ plan, (c) ($y = -2$ cm, $z = 8$ cm), $yz_3'$ plan.
accuracy of the data, we need to characterize the time correlation lengths which will determine the number of uncorrelated data.

**Quasi steady state**

In order to check that we obtain a quasi steady state, each experiment or CFD calculation has to be reviewed individually. Of course, once we have established a time after which steadiness is observed, it remains more or less the same for all the others (since only the laser map location changes for example). Nevertheless data have always to be reviewed to avoid the presence of unpredicted errors. Steadiness is checked by plotting the time evolution of the velocity norm at different locations in the enclosure, Fig. 11.

For example, 3 points are chosen on 2 different vertical plans. We notice that at the top of the cavity, where turbulence is developed, the velocity norm fluctuation seem random and to change rapidly in time and the values seem already at a steady state when data acquisition started, Fig. 11 (a). At the bottom of the enclosure, near the jet, fluctuation seem organized and almost periodic with a low frequency (period of a 100 s), Fig. 11 (b), this phenomenon is strange and the amplitude of the oscillation (around 5 cm/s) seem to indicate unsteady interaction with an unsteady ambient atmosphere in the garage entering the cavity. This might occur in the door is not properly closed, or acquisition starts soon after the smoke injection. At last we choose a point located at mid height near the jet, Fig. 11 (c), the time evolution seem to remain unsteady at 500s, with variations abnormal peaks of fluctuation around 220s and 450s. Such analysis of the time histogram indicates that this experiment is still unsteady after 500s. This conclusion is confirmed looking at the xz3’ plan velocity norm 2D plot. All plots in constant y plans should be symmetrical versus x = 0 plan. We see that a structure clearly dominates on the left side

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![Fig. 12 — Time correlations of the vertical velocity at x=y=0 and respectively z=3cm, z=6cm and z=10cm - experimental measurements.](image)

![Fig. 13 — Horizontal velocity time evolutions and time correlations at two different locations of the flow - CFD calculation.](image)
while the should be symmetrical structure is smaller and slightly shifted to the right side.

As a conclusion, both time histograms of the velocity norm should be checked for steadiness and 2D plot in vertical plans parallel to the vents wall should be checked for symmetry. When unsteadiness is detected, a larger time sample is used until steadiness is reached. In a rare case where no steadiness is achieved, experiment is checked to understand the problem (mostly verticality of the set-up or accidental smoke generation during the experiment). Experiment is redone.

**Statistical errors**

For a local quantity varying with time $\tau(t)$, we define the time averaging operator $<\cdot>$, between a starting time $t_{\text{start}}$ and ending time $t_{\text{end}}$:

$$<\tau> = \frac{1}{t_{\text{end}} - t_{\text{start}}} \int_{t_{\text{start}}}^{t_{\text{end}}} \tau(t)dt$$  (1)

The fluctuation $(\cdot)'$ is given by:

$$\tau'(t) = \tau(t) - <\tau>$$  (2)

The time autocorrelation $r(t')$ is:

$$r(t') = \frac{<\tau'(t),\tau'(t+t')>_{\tau}}{<\tau^2>_{\tau}},$$  (3)

where $<\cdot>_{\tau} = \frac{1}{t_{\text{end}} - t_{\text{start}}} \int_{t_{\text{start}}}^{t_{\text{end}}} (\cdot)(t)dt$.

The norm of the fluctuation is:

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**Fig. 14** — Computational domain.

**Fig. 15** — Time averaged velocity norm on left picture (PIV), the 2 first pictures on the right are instantaneous snapshot of the flow in the xoz plan at different times and the last picture on the right is a zoom to show the seeding quality.
And the statistical error for the time average is:

$$\text{Err}(\tau) = \frac{\text{rms}(\tau)}{\sqrt{N}}$$  \hspace{1cm} (5)$$

where $N$ is the number of uncorrelated data used to calculate the average.

We will see next that we manage to obtain more than 400 uncorrelated velocity fields per experiment (a thousand actually for 1 Hz acquisition). The statistical error for the averages is then lower than 5% of the measured standard deviation of the quantity. The standard deviation of the velocity norm being lower than 50% in a large majority of the flow region, the statistical error never exceeds 2.5% of the average quantity. In fact it is the PIV measurement accuracy which is the limiting factor in term of global accuracy.

**Time correlations**

On a steady experiment, we calculate cross-correlation functions for time evolutions of the vertical velocity at different heights of the vertical axis $x=y=0$. The same operation is also performed for the CFD calculations. For the experiments, we used the fast camera because PIV acquisitions at 1 Hz with the PIV camera show only random fluctuations the sample time being quite beyond the physical correlation time.

We plot vertical velocity time correlations, Fig. 12, at various heights of the vertical $oz$ axis. We observe a fast decay of the correlation ranging from approximately 0.01s up to 0.1s. This corresponds to the correlation time length of fast fluctuations (probably turbulence). Slow oscillations of periods around 0.5 up to 1s are also observed. Even faster oscillations can be seen in the second curve, with periods around 0.02 up to 0.1s. A spectrum calculation of those correlations doesn’t show peaks associated to an oscillatory behavior. Those fluctuations are mainly due to jet pseudo oscillatory behavior in the $z=4$cm region, where large eddies appear and the jet

**Fig. 16** – Time averaged velocity norm field in a horizontal plan at $z=3$cm. CFD calculation from Saikali [20]. This shows the interaction of the jet and the lateral flow entering the bottom vent.

**Fig. 17** – Time averaged velocity field in the plan $xoz$. CFD calculations on the left and PIV results on the right.
interacts with air entering the bottom vent. Larger times of acquisition would be necessary to see the correlations decrease to 0, but it is impossible due to memory limitations of fast cameras. It is nevertheless confirmed by the absence of correlation on 1 Hz acquisition sequences. Our main goal was to ensure no pure oscillatory behavior would exist at the acquisition frequency of 1 Hz.

We conclude that correlation lengths for rapid fluctuation are below 0.1s and intermediate correlation time exist around 0.5s corresponding to larger interactions between the cavity and the outer domain. We therefore validate the fact that 1 Hz acquisition allows acquisition of statistically independent samples. The same work has been performed for CFD calculation, Fig. 13. We draw similar conclusions with small scale correlation lengths being below 0.2s and larger ones around 0.5 up to 1s. Although of interest, we won’t analyse further the velocity correlations obtained with both approaches. It will be the subject of future works.

Comparisons of PIV results with L.E.S simulations

The objective of the section is to present comparisons with L.E.S simulations of this experiment provided by E. Saikali [20,21]. We first recall main characteristic of the CFD simulations as well as the quantities which are being compared. Then general characteristics of the flow are presented. At last quantitative comparisons between velocity profiles or 2D contour plots are presented.

![Fig. 18](image)

**Fig. 18** – Time averaged velocity norm profiles at different heights in the plan xoz: comparisons between CFD calculations and PIV results.
CFD calculations are well described in Refs. [20,21]. We therefore just recall a few elements about the simulations. The CEA code TrioCFD [23] was used with the software TRUST. The physical model is a low Mach approximation with Navier-Stokes equations for the flow and transport of the helium, perfect gas law, and both pressure and temperature are constant. Physical parameters dependence on the mixture composition is properly modeled. The L.E.S method relies on a Smagorinsky model for viscosity where the characteristic filter length is the cubic root of the cell volume.

The spatial discretization was a finite volume difference on a staggered grid with rectangular elements. A projection method is used for velocity and pressure decoupling. A two stages second order Rational Runge-Kutta scheme (RRK2) is employed for the temporal discretization. RRK2 scheme was first introduced by Wambecq in Ref.[24] to simulate steady flows and showed to be accurate, second order and A0 stable. Angrand et al.[25] show that RRK2 is more efficient than the first order Euler method, especially in cases where a central spacial scheme is considered. Convection terms are centered for the flow equations and uncentered (QUICK) for concentration equations, both are time explicit. Diffusive terms are implicit. Therefore time steps are imposed to respect the CFL criteria and range between $10^{-4}$s and $3 \times 10^{-5}$s. The convective scheme being explicit, the maximum CFL on the cells is kept to 1 and time step is deduced. The mesh being made of cubic cells, the reference length for the CFL is the unique cell size.

The mesh, although composed of rectangular elements, is unstructured and realized with CEA cast3m code and converted with Salome open source code. Cells are about 0.7 mm wide which is about 3 times the Kolmogorov scale estimated by Saikali and about the same size as the PIV sub-windows. A thorough convergence study has been completed both for the discretization and also for the boundary conditions, applied to a selected meshed external domain. The study for the selection of a correct external domain is the main subject of the paper [20]. A view of the mesh is given, Fig. 14.

CEA TRUST-TrioCFD has been executed on a local cluster of CEA—SACLAY (Intel Xeon, E5-2680 V2, 2.8 GHz, 128 Go memory per node and infiniband QDR 40 Gbit/s). MPI option has been specified for the parallel computation over 100 communicating processors, where the total mesh corresponds to $6.10^{848} \times 10^{6}$ cells. The simulation is carried on to 110s of physical time. A steady state is proven to be reached after 40s, but data are only used between 80s and 110s to calculate the statistical quantities which is enough to have a negligible
statistical error compared to the discretization error. L2 norm convergence study indicates that velocity should be converged at approximately 10% for L2 norm.

**Flow structure in the xoz plan**

*Jet structure* We are observing the flow structure in the xoz plan which is vertical, perpendicular to the vents and contains the oz axis. We represent, Fig. 15, instantaneous pictures of the seeded flow as well as the time averaged velocity norm.

Black regions of the flow are corresponding to a lack of fog droplets and therefore higher helium concentration (injected helium has no particles). We assert that 2 cm above the injection, seeding is enough to measure PIV velocity fields as shown on the velocity plot. We can see that except in the injection, the black regions without droplets are very narrow (around 0.2 mm wide) and allow correct velocity measurements as discussed earlier.

We note that the level of fluctuations along the plume varies at different times. Nevertheless fluctuations start to develop slightly above the upper part of the bottom vent. We consider that a laminar to turbulent flow occur in the jet for a z height ranging between 3 and 5 cm. This instability seems to be the result of the interaction of air entering the bottom vent and bending the plume with unsteady structures development. Black structures are also seen along the left wall facing the vents, behind the plume. Those structures have to be understood as a “turning movement of the jet” due to the interaction of lateral entrance of air and vertical movement of the jet flow, illustrated in a top view from Ref. [20], Fig. 16.

It is important to note that a low Mach model is required on the CFD calculation, the interaction between entering air and ascending helium is strongly diminished if density ratios are not properly taken into account. Indeed, we also observe that the jet is inclined toward the back wall (left) facing the vents.

*Comparison between PIV and CFD*: We represent, Fig. 17, a comparison between PIV and CFD velocity norm in the Xoz plan.

To start with differences, we notice a stronger interaction of the jet and the left wall for the PIV measurements. That interaction starts earlier, approximately at z=4 cm whereas this interaction develops at z=7 cm for CFD. In order to have better understanding of those differences, we plot velocity norm profiles in the same plan at varying heights, Fig. 18. Velocity norm intensity differences might be as large as 20 cm/s up to z=7 cm and even larger at the top of the cavity. It is clearly above numerical and experimental expected errors. Nevertheless, the profiles show strong similarities: the main jet (from helium
injection) sees its intensity decreasing while an ascending structure develops near the left wall. The main difference is that the main jet remains dominant in CFD while starting at $z = 5.5$ cm the wall structure becomes dominant in PIV. We will see later on that it is mainly due to a lack of fluctuation in the jet for CFD (or too much fluctuations for the experiment).

We also note strong similarities: the inclination of the jet is identical in both approaches. At the top wall, a similar thin jet layer is observed and exits the cavity through the top vent. A small eddy develops at the top left corner and another one develops near the bottom of the top vent, we illustrate this with a zoom on instantaneous vector fields Fig. 19.

We also plot the horizontal time averaged velocity profiles at the bottom and the top vent, Fig. 20. Here again, strong similarities exist. We note at the bottom vent the same parabolic inverted profile. Velocities are stronger at the edge of the vent while smaller at the center. The absolute difference of velocity is around 3–4 cm/s. The higher measured PIV velocity is again due to higher turbulent rms fluctuations for the experimental results. The resulting higher mixing inside the cavity requires higher inflow of air. At the top vent, both profiles show the presence of an exiting jet layer, but its thickness is more important for the experiments.

yz plans

We now interest ourselves in plans parallel to the vent with a fixed x position. We don’t intend to reproduce all the results. In Fig. 21 we see that the contour structure of the velocity norm is qualitatively very similar for PIV and CFD.

Differences are easily illustrated on velocity norm profiles, Fig. 22 where PIV and CFD profiles are quite similar at the bottom of the box but the main jet seems truncated (around $y = 0$ and $z = 13$ cm) for the PIV.

We place the observation plan closer to vent, Fig. 23. We plot the corresponding velocity norm profiles at different heights, Fig. 24. Similar conclusions can be made. Nevertheless the profiles are a lot closer, since the main different between PIV and CFD are located in the region between the jet and the back wall facing the vent. The slightly higher velocity observed for PIV experiment at the lowest positions is due to a higher air velocity entering the bottom vent as shown in the previous section.

RMS levels

The main discrepancies in the results for PIV and CFD is actually due to a difference of fluctuation level in the jet for lower heights $z < 7$ cm. This is illustrated by plotting the rms level of velocity fluctuations along the jet center, Fig. 25. Fluctuations are clearly at least 4 times higher in the experiments than in CFD calculations.

On the other hand the general shape of the curve is similar, as shown Fig. 26, where rms fluctuations for LES are multiplied by 4 on the right figure. This indicates that laminar to
turbulent transition occurs at the same height around $z = 4\text{ cm}$ where fluctuations are at a maximum. As said, this will be the object of further work.

**Linden bi-layer structure**

As underlined in the introduction, it is difficult to explain the existence of Linden bi-layer structure without looking at the velocities. On the other side, it is difficult to assert that we are in presence or not of a bi-layer without looking at the concentrations. We want to assess a numerical method to model such experiments because it is difficult to perform simultaneously velocity and concentration measurements, whereas this is a standard result of the CFD simulations.

In the YZ1 plan, we draw the velocity field at the top of the cavity, Fig. 27. We observe on both results two eddies of approximately 3 cm width. This structure is typical of a Linden layer formation. However, Saikali [20] indicates that vertical concentration profiles contradicts the existence of such a layer due to the strong interaction between the jet and the left wall in xoz plan and recirculations near the top vent. The observed symmetrical eddies in the YZ1 plan are not strong enough to establish the bi-layer structure.

**Fig. 24** – Time averaged velocity norm contour profiles at different heights in two yz vertical plans located at $x = 1.5\text{cm}$ and $x = 2\text{cm}$. PIV and CFD comparisons.

**Fig. 25** – Velocity fluctuations rms profile along the plume axis. PIV and CFD comparisons.

**Fig. 26** – Velocity fluctuations rms profile along the plume axis, scaled 4 times on the right for experiments. PIV and CFD comparisons.
We intentionally don’t show the concentration profiles in Ref. [20] to underline the need for such a data in Linden structure analysis.

**Conclusion**

Comparisons between the LES simulations and the PIV results are qualitatively in good agreement. Quantitative comparisons show more discrepancies, with similar contour shapes of the averaged quantities but significant differences in the spreading of the jet and its interaction with the back wall facing the vents. Overall, maximum velocities L2 errors are lower than 15% on average and L.E.S tend to over-predict the concentration due to reduced rms fluctuations and lower air flow entering through the bottom vent (15% lower).

Our conclusion is that L.E.S is therefore a suitable approach to model plume dispersion in hydrogen safety studies being a conservative approach and reasonably accurate compared to RANS models. On the other hand we wouldn’t advise this approach as a substitute for experiments until the observed discrepancies are explained. Although L.E.S can’t yet be considered as a perfect substitution to experiments, it is nevertheless qualitatively good enough to be used as an assistance to experiments design.

Therefore our next work will focus on finding explanations for the observed discrepancies. It seems that finer grid (although we are at three times the Kolmogorov length) should be investigated as well as DNS calculations, even though the turbulent viscosity of Smagorinsky model is a third for the observed discrepancies. It seems that finer grid assistance to experiments design.

**R E F E R E N C E S**


![Fig. 27 — Velocity vectors at the top of the cavity in YZ1 plan. PIV and CFD comparisons.](image-url)


