Design and construction of a standard gases portable measurement setup

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Abstract: We present the design and construction of a compact and portable standard gases measurement setup, mainly intended for colorimetric based sensors. The setup consists of a transparent methacrylate chamber and a methacrylate and 3D-printed plastic case, which has a Raspberry Pi, which single-board microprocessor, that manages a touch-screen and camera module. Prototype in nature, the setup has been intended to be used in research tasks. Hence it is designed to be fully detachable and thus easily modified or improved. The whole setup has been made with off the shelf components and designed and run by FOSS -Free and Open-Source Software-.

I. INTRODUCTION

Nowadays there is huge social concern about harmful and malodorous gases present in the air we breathe. Gas concentration readings are required for the security and wellbeing of people and environment in many situations, from chemical, food or almost any industry to cities or natural phenomena like volcanic activity. This wide spectrum of applications carries the need for cheap and readily available detection methods. The compact or even mobile nature of the sensors system needed requires those systems to be as small and energy-efficient as possible.

In this context, colorimetric sensors have virtually zero power consumption in the gas-to-colour transition. Also, most of the colour changing indicators used in this kind of sensors are cheap and can be printed and dried on inexpensive disposable substrates. They are small, low-cost and energy-efficient devices.

In comparison with other electronic devices, colorimetric sensors can determine the presence and concentration of specific chemical compounds in complex chemical environments, as they rely on a highly specific reaction that only proceeds in the presence of the gas we are targeting. Therefore, colorimetric sensors are a great choice for multiplex sensing arrays by combining different gas-specific indicators [1].

Maybe the weakest point of colorimetric sensors is their sensibility to external factors like ambient light or camera setup. Therefore the goal is to research and develop software that allows us to read gas concentrations accurately, even with bad ambient light, or to use RGB sensors with high accuracy for the colour measurements [2-3]. Those are some of the experimental uses for our setup.

In the same way, it is essential to have an environment where all those parameters are under control, in order to characterize the colorimetric sensors' response and to test the software developed. Housing the device in an enclosure to provide a stable optical environment could be an easy and effective way to improve the accuracy of the records.

As we have said, bad focusing of the camera, reflection from the chamber cover or bad lighting in general can make hours or even days of recorded data useless. This led us to incorporate a screen on this setup, so as to allow us to have a preview image before the experiment starts, which can save us considerable time.

II. ELECTRONICS AND MATERIALS

The electronic part consists of a *Raspberry Pi Camera V2*, an 8MP camera module, a *Raspberry Pi 7" Touchscreen Display*, a *Raspberry Pi 3 Model B+* run by *Linux* and a Hue Phillips strep lighting. Also, we choose a four-inlets chamber design so one of them could easily be used to put a temperature, pressure and humidity sensor (*BME280)* inside the chamber.

As we use *Raspberry Pi* components we can use their software [6] to manage both the camera and the screen. Additionally, we use some previously self-developed software for further management tools needed to run experiments.

The lighting consists of a LED strep stuck to the methacrylate case at half height, to prevent direct reflections from the chamber cover on the camera. Lighting intensity and colour can be managed from the *Raspberry Pi*, so we can get colour and intensity response dependence in a single exposure by changing the lighting parameters periodically and taking images for each lighting.

As we need to record with the camera the colour changes of the colorimetric sensor, we choose transparent methacrylate to make the chamber. Also, methacrylate can be cut in almost any shape, so we choose to use it both for the chamber and the case. We have used the department's 3D printer for the screen's own case.

III. CHAMBER DESIGN

In order to choose the chamber shape, we designed three models; a square one, a round one (as both with the squared one are the most common ones) and an ellipsoidal one in order to see how the gas flux turbulences improve removing all 90^{o} corners, Fig.(1). And we used *Simscale*, an online simulation software, to run some compressible fluid simulations on each chamber model.

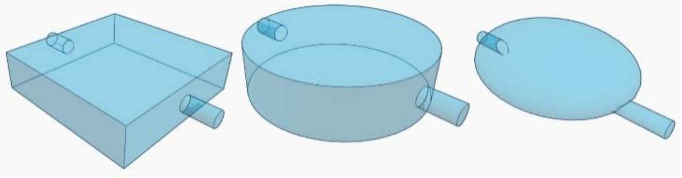

FIG. 1: Chamber model's 3D inner volumes.

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A. Simulations

To evaluate each chamber performance, we ran some air flow simulations of each one with *SimScale*, a computer-aided engineering software product based on cloud computing. *SimScale* offers a wide number of physics and engineering simulation options; fluid dynamics, solid mechanics, thermodynamics and thermomechanics. We were interested on its compressible CFD (Computational Fluid Dynamics) simulations.

Reynolds number (*Re*) determines the laminar or turbulence behaviour of a fluid flow. For flow in a circular tube of diameter D at an average velocity V it is defined as follows.

$$Re = \frac{DV\rho}{\mu} = \frac{DV}{\nu}$$

Where, μ is the dynamic viscosity of the fluid, and ρ is the density of the fluid. In our case Re takes values from 250 to 400 among the different chamber parts of the different chambers. Since for values of $Re<2300$ laminar behaviour dominates the flow [4], we ran laminar model simulations.

Whether or not the flow rate change during the simulation, the simulation time dependency would be transient or steady-state. In our case the flow rate is constant. For steady-state laminar compressible CFD simulations *SimScale* uses the *rhoSimpleFoam* solver, from *OpenFOAM®*, which is based on SIMPLE (Semi-Implicit Method for Pressure Linked Equations) [5].

We have set a dry air flow with a 21% oxygen-78% nitrogen composition and 28.97 *kg/mol* molar mass. We have also set other air parameters like specific heat (717 *J/kg·K*) and dynamic viscosity ($1.83 \cdot 10^{-5}$ *kg/s·m*).

As boundary conditions we set the inlet flow rate at the inlet pipe (2*L/min*), atmospheric pressure (101325 *Pa*) at the outlet pie, and fixed temperature (293 *K*) at the other walls.

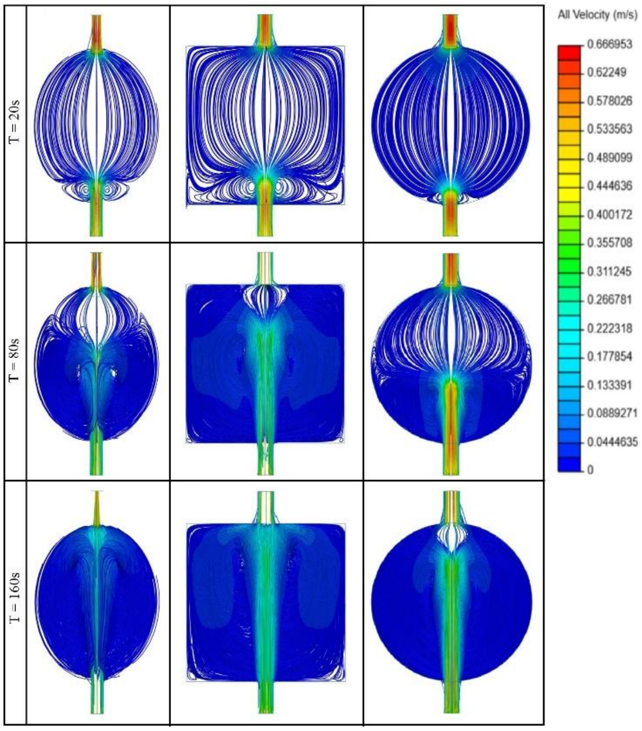

FIG. 2: Velocity field plot. From left to right ellipsoidal, squared and round shaped chamber models' simulations for T=20s, 80s, 160s.

Fig.(2) is a velocity field plot comparation between the three models we have simulated, for a 180s simulation, which allows as to evaluate for each chamber the time it takes to reach a steady state situation. The square one takes 80-100s, the ellipsoidal one takes 120-140s and the round one takes 160-180s. These times are quite small compared with the exposure time a gasometric sensor is exposed during an experiment, which goes from several minutes to some hours. Therefore, each of the 3 configurations is valid to calibrate gas sensors.

If we look at the steady state of each chamber, we can also get some conclusions. We can see in all three cases that a very clear cylindric laminar flow is formed between the inlet and the outlet pipes. Also, a symmetric turbulence is formed in each side of this central flow, with a vorticity point at the outlet half of the chambers in each side too. If we take lateral views of the velocity field, we realize those vorticity points are where the only vertical air transport takes place; the rest of the volume is ruled by laminar behaviour. Comparing the velocity of the turbulence area and the central flow, we have one magnitude order of difference. So, in the steady state the effective cross section of the flow is almost reduced to the central cylindric flow.

Chamber's air refreshing time is an important attribute that cannot be directly derived from the post-process results. Taking in account the previous considerations, reducing the turbulence area, as it is the slowest part, will improve the air refreshing time. Moreover, looking at the steady-state we realize that in the square chamber, near 90° vertical corners, occasionally some secondary turbulences and vorticity points are formed. While, neither on the square or the round one, any secondary turbulence is created on the lateral-to-covers walls' corners. That is consistent with the laminar behaviour and the very little vertical air transport. As an example, to clean the chamber we use a synthetic air (oxygen + nitrogen) pulse, and gases like NH_3 used to get stuck everywhere, so reducing extra turbulence areas or shapes must be considered.

B. Chosen chamber design

For the final chamber design chose, we made the following considerations:

- The simulations don't give us big differences between the three models, apart from a relative quickness reaching the steady state with the square one. However, it has a bigger turbulence area and secondary turbulences near the corners.
- The ellipsoidal one was rejected because its significantly higher production cost does not balance out with notably better simulations results.
- We know square shaped methacrylate chambers need top and bottom metal covers; otherwise they have leaks in the middle area of each side, because with just four bolts holding it, its sides folds. As round shaped structures have a better pressure distribution, we would like to evaluate if those metal covers are also needed or not.

Therefore, we choose the round shaped chamber model. Fig.(3) is a 3D view of the final chamber design. Its outer diameter has 140*mm* and the inner one has 100*mm*. It has two transparent methacrylate covers of 5*mm* thickness, one central part of 20*mm* transparent methacrylate with four inlets of 10*mm* diameter, and two rubber slabs between the methacrylate pieces. Also, each part has a 6*mm* diameter hole for each of the four folds we use to hermetically close the chamber.

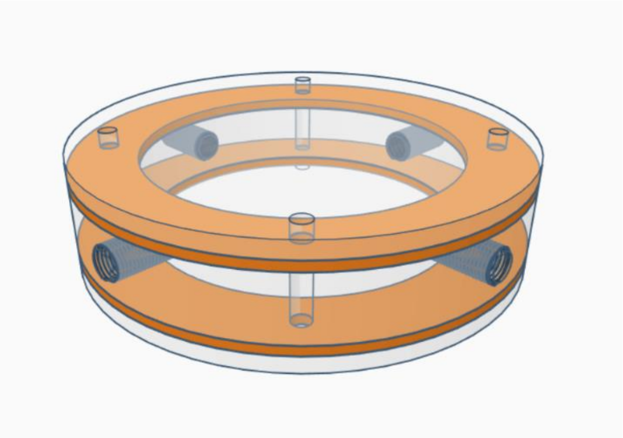

FIG. 3: Round shaped chamber 3D design.

IV. CASE DESIGN

The case consists of five laser cut methacrylate pieces and a screen case made of 3D printed PLA. Due to the prototype character of this project our aim was to make it as detachable as possible.

We use as screen a *Raspberry Pi 7" Touchscreen Display*, that is driven by a *Raspberry Pi 3 Model B+*, a single-board microprocessor, attached to its back side. As it's seen in Fig(4) the screen case, at the top, has a window in the middle to allocate the Raspberry Pi. This printed part its attached to the screen by screws but its not attached to the top methacrylate piece because it must be easy to take it out if we need to manipulate the camera position or anything on the *Raspberry Pi* board.

The methacrylate pieces got four holes on the bottom part for gas tubes, and an opening on the top part for the electronics power outlets.

FIG. 4: 3D case design.

Considering illumination is one of the main error sources of colorimetric sensor-based experiments, we cover the methacrylate part with an opaque material.

V. SET UP

Fig.(5) illustrates the final set up before the methacrylate case is cover with an opaque material. If we look at Fig.(5) we can see how the set up looks like completely assembled and ready to start the experimental data record.

Previously we have explained how the screen and the single-board microcontroller are assembled to the case. Since, as we said, the microcontroller and all the electronics attached to it must be easily detachable from the methacrylate case, and the camera is also linked to the *Raspberry Pi*, it must be detachable as well. We printed a Raspberry Pi camera case with the 3D printer, with a two-degrees-of-freedom mobile support. The support is attached to one of the methacrylate case sides with a strip of Velcro (Fig.(5)).

For experimental use the hole set up is divided into as many three parts. The electronic pack, which consist of the microcontroller, the screen and the camera, is easily removable from the case by removing the methacrylate cover. The remaining four methacrylate pieces are glued to improve the stability of the case. As we said the lighting is also attached to the methacrylate case. Both the electronic pack and the case can be solidary moved to manipulate the chamber and the gas tubes. The chamber and the gas tubes, which are connected to a gas flow-rate controller, are the third part of our set up. As the chamber is not attached to the case we can use any other chamber with this set up.

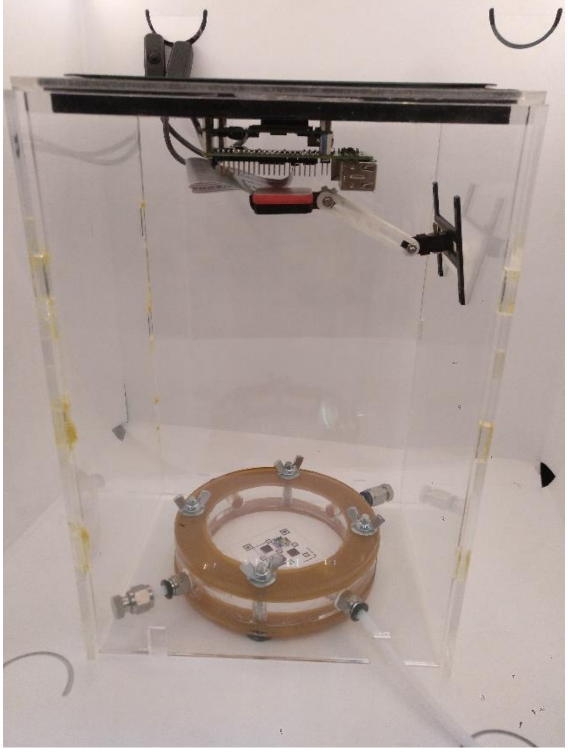

FIG. 5: Final set up.

VI. EXPERIMENTAL TEST

Finally, we made an experimental test of our setup with a CO_2 colorimetric sensor. We used a CO_2 colorimetric sensor printed on a QR code Fig.(6), even though in this case we didn't use the QR code. The test consisted of a 5*min* pulse of synthetic air to clean the chamber, followed by a 20*min* pulse of CO_2, with a 50% concentration at 50% humidity rate, and a 40*min* return pulse of synthetic air.

FIG. 6: CO_2 colorimetric sensor printed inside a QR code. Synthetic air pulse picture(left), CO_2 pulse picture(right).

Also, we tested the lighting management. We took a picture every 25*s* for three different lightings, corresponding to 4500*K*, 5000*K* and 5500*K* colour temperature.

As we used a camera module, we needed to process the images to quantify the response. We took some pixels from each detector, and we get it's 1D projections on the RGB space ($\sum$). At this point we had to choose which $\sum$ we want to plot, in this case the response in the Red space was significantly higher.

All the $\sum$ have a background response value, so we were interested on the response growth respect that value. Then we define $\sum_{norm}$ as follows:

$$\sum\nolimits_{norm} = \frac{\sum(t) - \sum_{min}}{\sum_{min}}$$

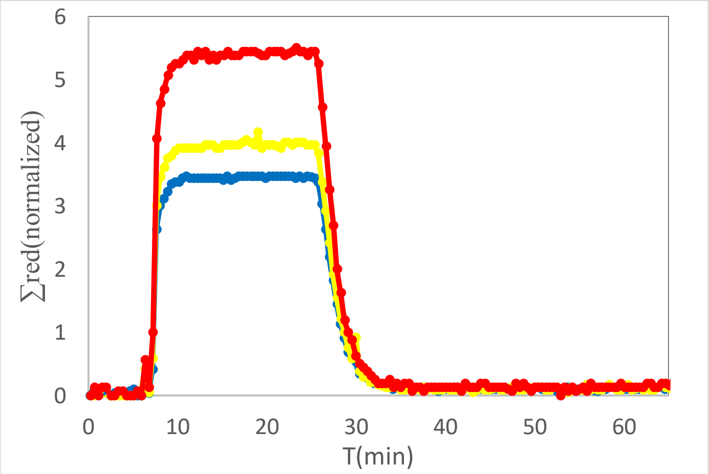

FIG. 7: Red response normalized for 4500*K* (blue), 5000*K* (yellow) and 5500*K* (red).

From a qualitative point of view we can see from Fig.(7) that for any lighting the response is clear and quite fast. There is no derive response during the return pulse. And since the response is over 500% higher than the background response for 5500*K* colour temperature lighting, indeed we can conclude that for this sensor the response increases significantly as we increase the lighting temperature.

VII. CONCLUSIONS

- The simulations implemented with *SimScale* shows that there are not significant differences between the chosen shape models, but we could not properly evaluate chamber parameters like air refreshing time due to computational restrictions.

- A compact experimental set up for colorimetric sensor-based experiments can be fully design and run with FOSS. The hardware and electronic components used are easy to find. Methacrylate and 3D printing are also accessible, and furthermore the full case could easily be replaced by cheaper and more accessible material. Hence, we have described how a compact set up for colorimetric sensor-based experiments can be design and build without big investment or complex technological needs.

- We succeeded in running an experimental test for colorimetric sensor-based experiments. We showed how, by managing the lighting, the optimal one can be easily found in a single pulse for each sensor.

- The setup can be easily upgraded with software; better and more complex camera and lighting management, and hardware; humidity, pressure, temperature electronic sensors can be placed inside the camera. Better lighting is also a possibility.

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