Design and Produce a Dynamic Animated Tool for Simulation of Doplet’s Propagation through Space in Modeled Areas

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***Abstract*— Predicting the spread of respiratory droplets can be an important factor in preventing the dissemination of airborne diseases in different environments. As can be seen through the Sars-Cov2 pandemic, where one of its main means of propagation is the air and has already caused more than 6 million deaths worldwide [1], the study in question is of utmost importance. As such, in this paper it is presented the initial creation of an animated tool that allows the simulation and analysis of respiratory droplets’ dissemination in different environments. This paper also intends to study the influence that the emission of respiratory droplets under certain conditions has on particles’ dissemination. This work is part of the 3-year PAFSE project funded by the European Union, which aims to boost young people's awareness of public health challenges, protective factors and patterns of risky behaviour, and the role they can play in their community preparedness. [2].**

A series of projects are being developed within the scope of the PAFSE project, by several Universities where the project in which this paper focuses is being developed by Instituto Superior de Engenharia de Lisboa (ISEL). Fundamentally the tool created was composed of 4 interconnected software. Essentially, to execute the simulation of droplets’ dissemination in this work it is necessary to perform 2 steps, first it’s necessary to simulate the airflow developed inside the room, and subsequently the respiratory droplets’ propagation. Firstly, to create the physical space to be simulated as well as to implement the CFD (Computational Fluid Dynamics) boundaries inherent to the simulation, CFD tool DesignBuilder 7.1.0.098 Beta-Student version was operated.

Then, to start off the airflow simulation it was necessary to manually execute required configurations to the CFD simulations that weren´t included in the default CFD folder generated by DesignBuilder in the act of creation of the CFD simulation. To perform this task as well as to run the particle flow simulation, OpenFOAM 8 was operated. To perform the post-processing of the results generated in the simulations, ParaView 5.6.2 64-bit, was employed allowing the better observation of the streamlines developed inside the physical space as well as the particles’ distribution. To obtain the output of the tool, it was compiled a series of scripts generated by Paraview that were disposed in a Microsoft Excel spreadsheet, followed by the elaboration of charts which demonstrated the particles’ behaviour inside the room, by referring (in terms of percentage of total particles emitted) how many of them attached in each surface, the number of particles that were removed from the room as well as the fraction that was still airborne in the room at the end of the simulation.

To evaluate the tool’s performance a series of simulations were created with different settings and a comparison between them was established. The results of the simulations showed that the tool performed well, thus allowing the withdraw of some conclusions regarding the particle flow process such as the particle percentage that was removed from the room due to a ventilation system (mechanical or natural), which surfaces inside the room were most contaminated, or in which scenario the occupants were most infected. Nevertheless, considering the level of information contained in the scripts generated on the post-processing stage, the data obtained in the charts are still rudimentary, addressing the fact that it’s still required to boost the tool with the emphasis being on versatility, dynamism, and greater ability to discretize post-processing results, being those, the main goals to achieve in the remaining time of the project developed by Instituto Superior de Engenharia de Lisboa within the scope of the PAFSE project.

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I. INTRODUCTION

Fundamentally, this work is motivated and encouraged by the recent pandemic crisis of the Sars-Cov2 virus (COVID-19), since it is still uncertain how the virus spreads, although in the scientific community, it is commonly held that the virus is transmitted mostly through air. [3] [4] [5]

In this sense, the guideline to combat the pandemic adopted by health organizations in each country has been the confinement of populations, to restrict contact between them, and in certain countries, like Portugal were Instituto Superior de Engenharia de Lisboa is located, in specific places such as an hospital or a nursing home it is mandatory to use of masks to limit the spread of such airborne disease. [6]

From this perspective, the physical space under study in this work is, fundamentally, a closed environment, with different configurations containing ventilation systems, whether they are mechanical (HVAC system) or natural (Windows/and or Doors open), where restrictive measures are felt more rigorously. With the technological advances achieved today, it makes perfect sense to use a tool such as CFD simulation, to predict and simulate the propagation of respiratory particles, thus identifying, for example, locations with greater propensity for airborne transmission between individuals, or proposing changes to the projects of HVAC systems and QAI, in order to mitigate the spread of airborne diseases such as Sars-Cov2.

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II. Literature Review

During the literature review conducted, it was found a vast panoply of works related to the creation of CFD methodologies, with an intention of simulating respiratory particles’ distribution in closed spaces. However, none of the papers mentioned all the aspects required to develop the tool, that is, they didn’t address the second step of the tool creation, the criteria necessary to simulate the particle flow, as they skipped to the presentation of the post-processing results.

In addition, only a few papers referred to have corroborated the numerical results obtained with experimental results. This aspect was crucial for the development of the tool since the first step of its creation was the validation of the airflow developed inside the physical space performed by recreating a CFD model withdrawn from one of the papers of the literature review followed by a comparison between the numerical results obtained and the experimental results contained in the paper.

Furthermore, many of the papers found only refer to the input of boundary conditions and the post-processing phase through the comparison of numerical and experimental results, not mentioning the steps taken to create the physical model, or how they performed the particle flow simulation.

Nevertheless, it is considered that the work developed by Z. Zhang and Q. Chen [7], as well as the work developed by F.Romano, L. Marocco, J. Gústen and C. M. Joppolo [8], are the state of the art regarding the simulation of the airflow inside the physical model with the main intention of simulating particles’ transport as they provide a good overview on how to perform resembling tasks.

To conduct the second step of the tool, the simulation of particle transport, with was necessary to resort to several papers containing pivotal information regarding some aspects related to the respiratory particle such as its dimension and the respective size range, the spreading angle, velocity of exhalation, the number of particles exhalated as well as the external forces that influenced the particles transport. More details regarding particle transport could have been addressed, but the initial aim of the project was not to explore the physics of particle transport, but to construct a tool that allowed the simulation of particle distribution in different environments.

Even though, the particle physics can be studied more deeply by continuing the work developed in this paper. The referred characteristics regarding respiratory droplets can be found in [9], [10], [11], [12], [13], [14], [15], [16] and [17].

III. Tool Development

To create the tool, it was necessary to employ 4 different software:

- *DesignBuilder 7.1.0.098 Beta-Student Version.*
- *OpenFOAM 8.*
- *ParaView 5.6.2 64-bit.*
- *Microsoft Excel 2016.*

A. DesignBuilder

This was the first software to be employed in the creation of the tool. DesignBuilder was used to create the physical model to be simulated as well as to input the CFD boundary conditions inherent to the simulation. In first instance, to perform the validation of the airflow developed inside the room, DesignBuilder was utilized to recreate the CFD model presented in [7].

Then, the default configurations of the software were employed to create more complex geometries as mentioned in the introduction. In the DesignBuilder desktop, on the left, it can be seen the current geometries that composed the created model. If one of the geometries is selected, on the right section of the desktop the respective CFD boundary implemented is exhibited. DesignBuilder desktop as well as an example of a model plausible to be created in the software are illustrated in figure 1.

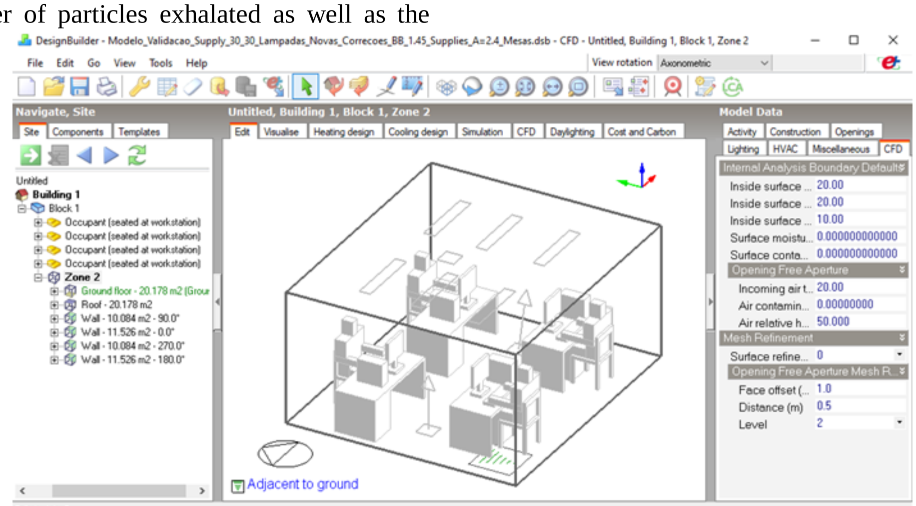

Fig. 1: *DesignBuilder* Desktop

B. OpenFOAM 8

OpenFOAM is a CFD software that was used to generate the mesh, and to manually run the airflow simulations as well as the particle flow simulations. It was also possible to run the airflow simulation in *DesignBuilder*, but there were some specific CFD boundary conditions referred in [7], such as the turbulence intensity of the supplies that weren´t possible to define in *DesignBuilder*.

Therefore, it was necessary to manually implement the aforementioned parameters. To perform the mesh generation as well as to run the simulation, it was necessary to run a series of scripts through *OpenFOAM*, such as *Clean.Mesh.sh* for cleaning the mesh generated, *Run.Mesh.sh* to generate the mesh, *Clean.Sim.sh* to clean the results obtained from the simulation, or *Run.Sim.sh* to run the simulation.

All the referred scripts were automatically generated when a CFD simulation was developed in *DesignBuilder*, and they were ensembled in a zipped folder named *project.bcfdk*, along with other folders inherent to the simulation. Some scripts encountered in the *workflow* folder contained in *project.bcfdk* allowed the manual implementation of the referred parameters for turbulence intensity mentioned in [7].

To run the particle flow simulation it was necessary to add some folders to the *worflow* folder, called *Sim.10.particleFoam*, *Sim.11.particleFoam* and *Sim.12.particleFoam*. In this step, was also necessary to run some scripts such as *Clean.Particle.sh* to clean the particle flow simulation results, and *Run.Particle.sh* to run the particle flow simulation. The content of the zipped folder *project.bcfdk* along with the content of the *workflow* folder are exhibited in figure 2.

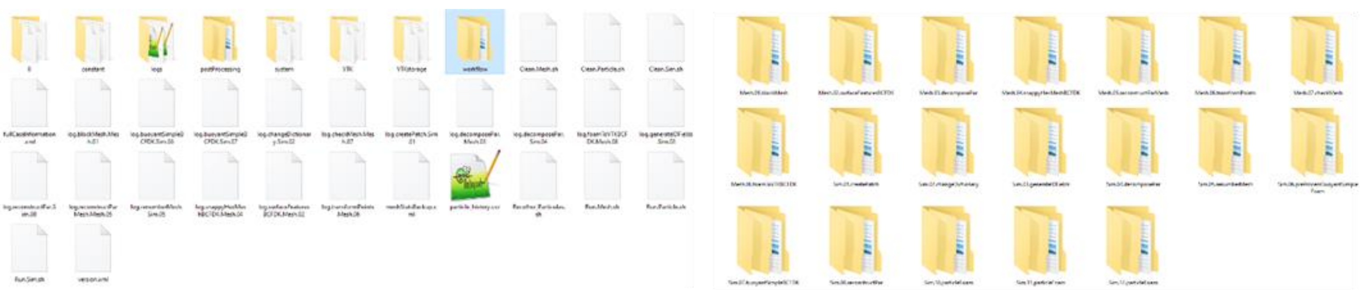

Fig. 2: Folder Content: *project.bcfdk (left)* and *workflow(right)*

It is also necessary to mention that all the *log.* scripts ilustrated on the left image of figure 2 were generated simultaneously with the airflow simulation and served to verify the simulation status and to convert the computational results into readable data.

C. ParaView

ParaView was utilized in the post-processing phase and allowed the observation of the mesh generated along with the airflow and particle flow simulations. In addition, the software also allows the analysis of several parameters that influence the airflow such as the temperature, pressure, air velocity, etc…

The particle flow simulation is widely overviewed as a one-way simulation. It was an issue addressed in papers [7] and [8] mentioned in the literature review, and it means that the airlflow strongly influences the particle flow, but the other way arround doesn´t occur due to the fact that the liquid particle concentration is significantly lower compared to the airflow inside the room. Therefore, one of the ways to study the airflow developed inside the room and also to have a gimplse on how the particle flow will unfold, is to analyse the streamlines generated by the airflow, something conceivable with *ParaView*.

In *ParaView* it is also possible to analyse every time-step of the particle transport, for a given simulation time. Additionally, through *ParaView*, the data produced by the simulation results, in first instance, will be compared with the experimental results of [7] to validate the airflow simulation, and on the other hand, it will be used to perform a comparison between the several scenarios developed to study the particle flow. In figure 3 is illustrated for one of the scenarios analysed, both the streamlines surrounding the particle emitter, the temperature developed inside the room as well as the particle flow at a certain time-step, as these are all aspects available to be studied in *ParaView*.

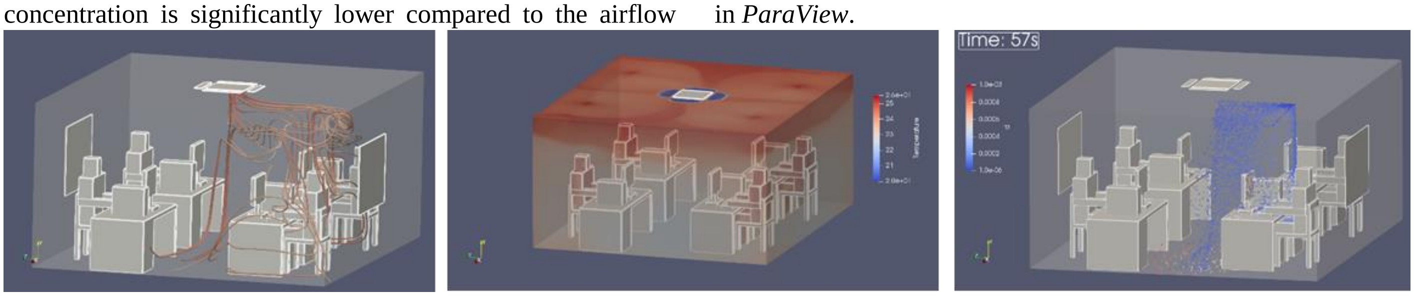

Fig. 3: Parameters Observed in *ParaView* (from left to right): Streamlines, Temperature inside the room, Particle flow at 57 seconds from the start of the simulation

D. Microsoft Excel 2016

Microsoft Excel was the last software to be implemented in the tool and was used as an output for the data produced in the simulation results. The data regarding the simulation results was exported from ParaView and then compiled in an Excel spreadsheet thus allowing the comparison between the numerical results and the experimental results obtained in [7] to validate the airflow simulated, and later, the comparison between the results achieved in the several particle flow simulations conducted.

IV. Tool Application

This section intends to demonstrate the tool implementation, considering the functionalities explored for each software in section 3, and by demonstrating the processes inherent to the two steps necessary to correctly execute the tool: the validation of the airflow developed inside the physical space and the subsequent particle flow simulations.

A. Airflow Validation

As it was mentioned in section 3.1, the CFD model recreated to validate the airflow simulation was the one addressed in paper [7], whose authors were Z. Zhang and Q. Chen. The first step to perform such task was to use DesignBuilder, and then input the CFD boundaries referred in [7].

The model was composed of 6 lamps and an air extractor on the celling, 4 human simulators, and an under-floor air distribution system (UFAD). The recreated model, and its geometries' dimensions are exhibited in figure 4 and table 1, respectively. The CFD boundaries implemented for each geometry can be consulted in [7]. The only details worth mentioning are that the total airflow rate referred in [7] was equally distributed between the two air supplies illustrated in figure 1 and that 2 CFD boundaries were attributed to the human simulators, but only the heat boundary was implemented in this work. The parameters regarding the mesh generation as well as the simulation costs performed by the tool for the validation scenario can be analysed in table 2.

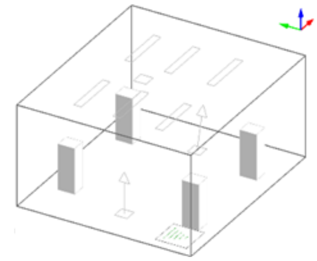

Fig. 4: CFD model of [6] Recreated

TABLE I: Mesh Features and Simulation Computational Costs of The Validation Case

Mesh Cell Size [m]	Mesh Cell Geometry	Mesh Total Number of Cells	Refinement Level	Number of Iterations until Convergence
0,05	Prismatic	419024	0 in all surfaces	10000

TABLE II: Room Geometries and Dimensions

Geometries	Dimensions [m]		
	Length	Width	Height
Room	4,8	4,2	2,4
Human Simulators	0,35	0,4	1,1
Lamps	1,2	0,2	-
Air Extractor	0,3	0,3	-
Air Supplies	0,3	0,3	-

It is necessary to refer that several simulations were conducted to obtain the best correlation between the numerical results and the experimental data of [7]. The modus operandi in [7] to validate the airflow simulation was to compare the velocity and temperature profiles measured in different locations of the room in the experimental activity, with the ones obtained in the numerical simulations.

Therefore, the comparison between the numerical results achieved with the tool and the experimental data in [7] is illustrated in figure 5. More details regarding the positions in the room where the measures were taken as well as the simulation results obtained in [7] can be consulted in the referred paper.

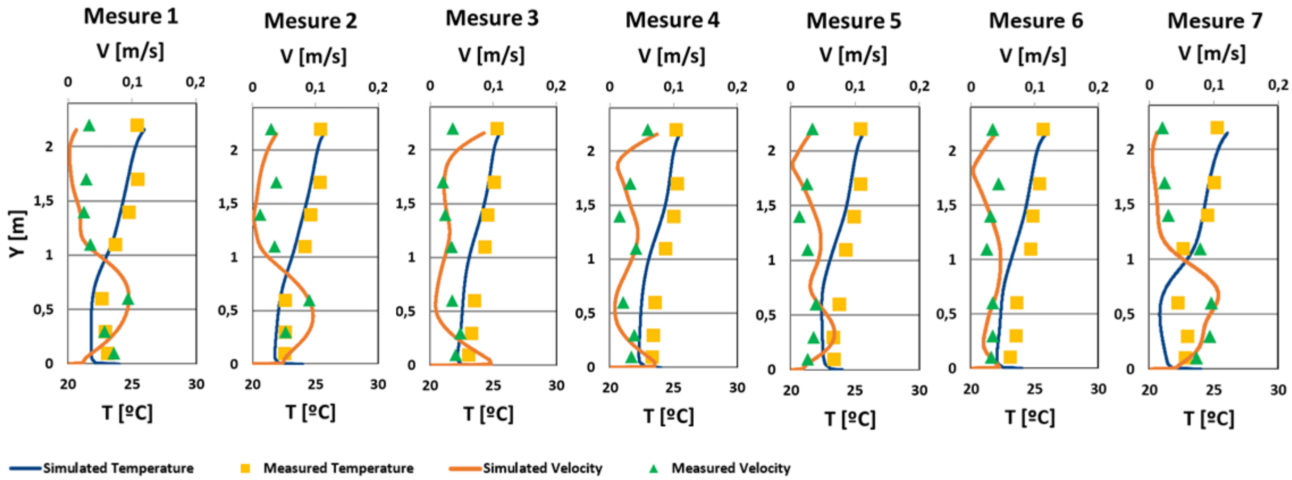

Fig. 5: Comparison of simulated and measured temperature and velocity profiles

As can been seen in figure 5, there were taken measures of velocity and temperature at 7 different locations in the experimental activity conducted in [7], and the simulated and experimental profiles are very similar.

B. Particle Flow Simulations

Having performed the airflow validation, now it was possible to simulate the case studies of particle flow. To be able to execute such simulations, like it was referred in 3.2 it was necessary to add to the workflow folder, the particleFoam folders where the parameters mentioned in the literature review regarding the respiratory particle were introduced.

As discussed in the aforementioned sections, there were several scenarios performed, where different configurations of the room along with distinct parameters regarding the respiratory particle were studied. For each configuration addressed in the scenarios, 3 different breathing regime situations were simulated: coughing, sneezing, and talking, where only one occupant emitted particles. In table 3, are exhibited all the parameters implemented for each breathing regime.

TABLE III: Parameters Implemented in the Tool Regarding Breathing Regimes

Breathing Regime	Spreading Angle [º]	Velocity [m/s]	Full Duration [s]	Total Emitted [particles/s]	Particle dimension [μm]	Simulation Time
Coughing	15,4	15	0,5	10846	[0,1;1000]	60 minutes
Sneezing	15,4	6,85	0,5	2445300	[0,1;1000]	60 minutes
Talking	42,9	6,05	300	195	[0,1;2000]	60 minutes

It is necessary to refer that the total number of particles emitted for each breathing regime represented in table 2 is a sum of the number of particles emitted for each particle size range, therefore the dimension intervals illustrated in table 2 also symbolize the total particle size range simulated in the case studies. [9] [13]

The different configurations analysed in each case study involved geometries with more complexity compared with the ones simulated in the validation model observed in figure 4, since they were more similar to the ones exhibited in figure 1. The room configurations evaluated for the particle flow simulations taking already into account the geometries noticed in figure 1, were as follows:

- Room with the settings illustrated in figure 1 (with UFAD)
- Room totally closed without a ventilation system (mechanical or natural)
- Room with 2 windows opened at 10% and a door opened at 10%
- Room with 2 windows opened at 50% and a door opened at 50%
- Room with 2 windows opened at 10% and a completely closed door
- Room with 2 windows opened at 50% and a completely closed door
- Room with HVAC located on the celling with two closed windows and no lamps
- Room with a vertical design radiator

Analysing all the referred cases as well as all the parameters that influenced the particle flow, thoroughly, were not the aim of this work as it was only intended to create a tool that could be implemented to simulate and describe particle flow inside different environments.

To verify the tool's ability to perform the referred simulations, a comparison between the results obtained for 3 of the aforementioned configurations for the most contagious breathing regime was performed. The situation where the occupant sneezed was the most contagious one as this was the case where particles were released in greater number as can be seen in table 3. The 3 configurations to be compared in this paper were:

- Room totally closed without a ventilation system
- Room with the settings illustrated in figure 1 (with UFAD)
- Room with 2 windows opened at 50% and a completely closed door

The reason why these two configurations were chosen to demonstrate the tool´s performance, in addition to the standard scenario in which the room had the settings observed in figure 1 is due to the fact that these were the cases where more distinct results were obtained in terms of particle removal capacity, that is, in the case where the room didn´t have a ventilation system, none of the particles initially emitted were removed. In the scenario where the room had 2 windows opened at 50% and a completely shut door, it was found that this was the case where the particle removal was more efficient.

To be able to point out these conclusions, inside the particleFoam folder there were several files that accounted, for the given simulation time, the number of particles that attached in each surface as well as those removed by the extractor and the fraction that was still airborne.

Then a log. file was generated and performed the conversion of the computational numerical results obtained into a readable file. Subsequently, the data contained in the log. file was transmitted to a script and then the information was compiled in an Excel spreadsheet. Bearing in mind the configurations analysed, in figure 6 are exhibited 4 graphs comparing for each room configuration, the particle percentage rate that attached on humans, was removed by the extractor, is still airborne, and attached on the room geometries.

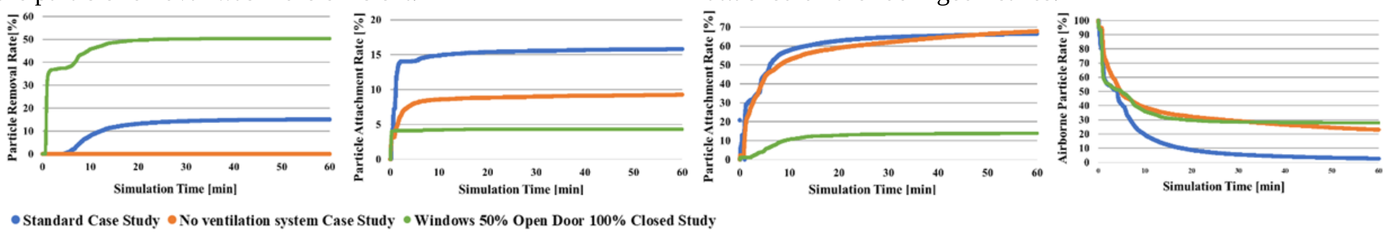

Fig. 6: Case Studies Conclusions (From Left to Right): Particle Removal efficiency, Particle Attachment in Humans, Particle Attachment in Room Geometries and Particles Still Airborne

As can been seen in the charts, and as it was already mentioned it was found that the scenario where the windows were opened at 50% and the door was completely closed was the one where the particle removal was more efficient (≈51%) at the end of the simulation. Consequently, this was the scenario in which the particles were less attached in the room geometries (≈14%) and the humans were less infected (≈5 %).

However, this was the case where a higher percentage of particles were still airborne (≈28 %) at the end of the simulation. In opposition, both the unventilated and standard case studies registered a high percentage of particles attached to the room geometries at end of the simulation (≈70%). Additionally, it was found that between the 3 analysed scenarios the standard case was the one where the humans were most infected.

In the scope of the PAFSE project, and to better visualize the numerical results obtained, several animated videos animated were produced where, for the duration of the simulation, it was possible to observe how the particles behave. To have a glimpse of the outcome of the videos, in figures 7 and 8 are described, for each case scenario, the streamlines developed as well as the particle flow at a certain time-step of the simulation, respectively.

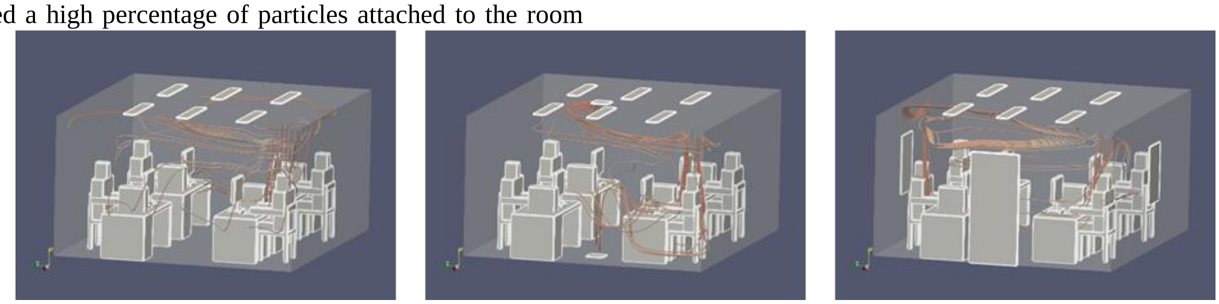

Fig. 7: Case Scenarios Streamlines (From Left to Right): Unventilated Room, Standard Case, Windows Opened at 50% Door 100% Closed

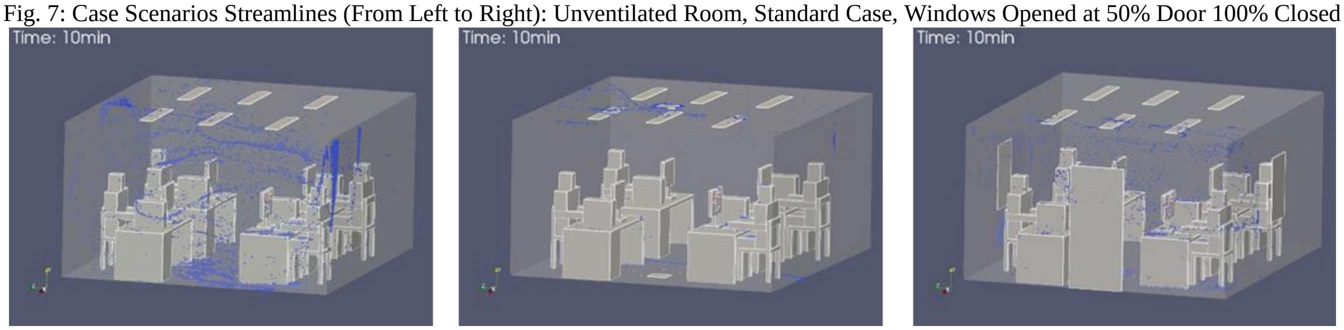

Fig. 8: Particle Flow At a certain time-step for each case scenario (From Left to Right): Unventilated Room, Standard Case, Windows Opened at 50% Door 100% Closed

Essentially, the tool performed well thus allowing the withdraw of some conclusions regarding particle flow process. Although, the tool’s inferences are still rudimentary, as more details can be addressed in a future work such as the production of a histogram regarding the particle dimensions that attached in relevant surfaces, as well as the residence time for those particle ranges in order to correlate each size interval to a certain danger level in function of time and particle size.

V. Conclusion

This paper focused on the development and implementation of an animated tool that allowed the simulation of particle flow in different environments. The animated tool established was composed of 4 different software interconnected: *DesignBuilder*, *OpenFOAM*, *ParaView* and *Microsoft Excel*.

In particle flow simulations two steps are required to be fulfilled: first, it is necessary to simulate the airflow developed in the physical space and only then, it is possible to perform the particle flow simulation. To test the tool development, different scenarios were analysed by variating the configurations of the room as well as the breathing regimes simulated. However, as mentioned, first it was required to simulate and validate the airflow, having used for this purpose the work conducted in [7].

It was found that the tool performed well, since it was possible to withdraw some conclusions regarding the particle flow, since in the comparison made between 3 of the several scenarios, for the given simulation time, it was possible to determine the particle removal efficiency by the ventilations systems implemented in the room, whether they were mechanical or natural, the scenario where the humans were most infected, as well as the particle percentage that was still airborne.

Nevertheless, the tool can still be improved, since several factors inherent to the particle flow process were not addressed such as the production of a histogram regarding the particle dimensions that attached in relevant surfaces, as well as the residence time for those particle ranges in order to correlate each size interval to a certain danger level in function of time and particle size. In addition, in a future work the tool can also be upgraded with the emphasis being on interconnectivity, and dynamism between the different software implemented, as these aspects are still rudimentary at the current stage.

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