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Safety In Research Institutions: How to Better Communicate the Risks using Numerical Simulations

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What are the risks for the personnel following a gas leak in a laboratory? How effective are the safety measures (gas detection) put in place? Are users aware of how fast they can be exposed?
These questions have been approached with the intent to better communicate to the users the risks involved in their daily activities by showing how a gas is dispersed in their laboratory. In order to do so, a software tool performing Computation Fluid Dynamics (CFD) simulations of a pollutant gas dispersion in a room has been developed by the Chemical and Physical Safety Group (GSCP) at EPFL in collaboration with Optimad Engineering srl.
The software and its physical model have been based on experimental data obtained by the GSCP used as a benchmark for the numerical simulation results. As side deliverables, these results are been used to place gas leak detectors in the most efficient location, thus optimizing the cost of safety measures.
Furthermore, the simulation results have then been used to create videos showing the pollutant gas dispersion in the laboratory. A real case is presented in order to reveal the power of the used dual methodology: modelling as a mean of communication for an effective training/teaching of the personnel. The visual representation of the risks has a greater impact than any other means of communication available.

1. Introduction

The use of several compressed gases as well as cryogenic liquids in modern laboratories is so common nowadays that the large majority of the laboratory users do not perceive anymore the hazards posed by the presence of a pressurized gas bottle (Leslie and Birk, 1991) or of a large amount on liquid nitrogen in the confined space of a laboratory (Gubinelli and Cozzani, 2009).
In this regard, the Ecole Polytechnique Fédérale de Lausanne (EPFL) is not different than any other modern university. The vast majority of research groups handle toxic (H_2S, BF_3, B_2H_6 and F_2 among others), flammable (H_2, CH_4, C_2H_6, C_3H_8) and inert gases (N_2, Ar, He) on a daily basis and the use of large quantities of liquid helium and liquid nitrogen is daily practice for the analysis platforms and research groups present at the school.
The aim of the Group of Chemical and Physical Safety (GSCP) is to study and develop tools and applications towards a proactive approach to the health and safety management. On a daily basis, GSCP supports the work of the Safety Competence Center (DSPS-SCC) in the management of the risk in laboratories by means of laboratory safety audits, risk analysis, hazard specific trainings, development of new research tools as well as regular updates and communication with the research community at EPFL.
Considering the large amount of pressurized gas cylinders as well as cryogenic liquids used at EPFL, it is of great interest to understand the behavior of a fluid in case of an accident (Rigas and Sklavounos, 2005), in order to ensure that the corrective preventive measures have been put in place and/or assess the effectiveness of the ventilation systems in a laboratory (Khan and Abbasi, 1998).

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Furthermore, it is even more important to properly inform and train the laboratory personnel regarding the hazards to which they might be exposed in case of an accident. Showing them how a gas is dispersed in their laboratory by visualization of the gas diffusion is an effective method to raise their awareness as it has a much stronger impact compared to any other tool currently available.
The goals of this project are therefore, several:

1. To better understand gas diffusion inside confined spaces, under different ventilation conditions,
2. To improve the effectiveness of the safety measures by choosing the best location for a gas detector,
3. To raise the awareness of the personnel exposed to a hazard by improving the communication methods and making the scientific results easily understandable by a large audience.

For all these reasons, the GSCP, in collaboration with Optimad Engineering srl., started the development of a software tool performing Computation Fluid Dynamics (CFD) simulations of a pollutant gas dispersion in a laboratory. The results of the simulations are then use to create videos showing the gas diffusion in a pre-render reconstruction of the simulated laboratory.

2. Experiments and simulations

2.1 Experimental setup

A series of experiments has been performed by the GSCP in a laboratory at EPFL in order to understand the diffusion processes involved during the leak of gases or the spill of liquid cryogenics in relatively large indoor ventilated spaces. The experimental results have then been used to implement the appropriate detection methods as well as to feed and validate the physical model implemented in the CFD simulations.
More specifically, three different types of experiments have been performed:

1. Evaporation of approximately 26 L of liquid nitrogen, corresponding to approximately 600 L of gaseous nitrogen volume, poured inside an aluminum tray,
2. Evaporation of approximately 26 L of liquid nitrogen spilled on the floor of the laboratory,
3. Leakage of approximately 1 m^3 of O_2 in the laboratory.

The first type of experiments, the evaporation of liquid nitrogen poured into an aluminum tray, has been designed to study the gas diffusion in a ventilated environment under slow evaporation rates (approximately 11 mL s^{-1}) and to test the limits of the CFD physical model under small variations of the pollutant concentrations.
The second set of experiments, the evaporation of a large quantity of liquid nitrogen spilled directly on the floor of the laboratory, aims to study an event that is not covered yet by our simulation model: the catastrophic complete leak of a large Dewar inside a relatively small environment and the fast drop of oxygen concentration that will result from it.
Finally, the leak of oxygen in the laboratory (at a rate of approximately 32 L s^{-1}) aims to reproduce the leakage of a pollutant gas from a point source.
The ventilation system in the laboratory allowed the use of three different ventilation set-ups during each type of experiments: high ventilation (HV, air renewal rate of 13.5 h^{-1}), low ventilation (LV, air renewal rate of 8.9 h^{-1}) and no ventilation (NV).
During each experiment, the concentration levels of oxygen have been measured at a sample rate of 1 Hz using 18 O_2 detectors (model GfG O2.ZO, type GMA 011) carefully placed around in the laboratory. Temperature, pressure and humidity where also monitored at a rate of 0.2 Hz using 10 temperature/humidity dataloggers (model Extech RHT10) as well as 2 pressure/temperature/humidity dataloggers (model Extech SD700). The experimental setup of the laboratory is shown in Figure 1.
The experimental results, namely the O_2 concentration measurements as well as the temperature and pressure profiles, are used as a benchmark for the CFD simulations results as a mean of validation of the physical model implemented.
Furthermore, the point of lowest concentration of O_2 measured in the laboratory is used as the best location for the placement of a detector under the different ventilation conditions.

2.2 CFD simulations

Optimad Engineering srl. has developed the semi-automated software tool that performs the CFD simulations. The tool is based on a set of classes of OpenFOAM, an open-source C++ platform for the development of meshing software and numerical solvers used in CFD (OpenFOAM, 2016).
The computation tool consists of two parts:

1. A CFD model based on the OpenFOAM platform,
2. A library of scripts devoted to control the CFD model, dispatch the simulation runs and post processing the results.

Figure 1: Experimental setup of the chosen laboratory.

The software tool has been developed for end-users without in-depth expertise in CFD simulations: the library of scripts allows the users to run the required CFD simulations by performing the following steps:

a. Pre-processing: import of a 3D CAD model of the indoor environment to simulate; generation of the surface and volume mesh,
b. Setup of the CFD model: setup of the physical model; enforcement of the initial and boundary conditions (ventilations system of the room, pollutant sources); placement of the point and surface probes that monitor the evolution of the pollutant dispersion,
c. Run the simulation: setup of the parallel computing and launch of parallel simulation runs,
d. Post-processing: extraction of the flow fields, generation of the reports and visualization of the solutions.

In the following subsections a short description of the steps to run a simulation is reported. The leak of O_2 in an indoor laboratory from a point source is also reported as an example.

Pre-processing

The aim of the pre-processing procedure is to generate the computational volume mesh from the provided 3D CAD model of the simulated indoor environment which is an input of the computational tool. The mesh is then automatically generated via a refinement process that increases the number of elements around particularly important elements of the environment (inlets, outlets, boundaries).

The refinement is chosen by the end-user depending on the size of the computational domain, the simulation time as well as the characteristic velocities of the flow and the complexity of the environment geometry. Figure 2 shows the imported 3D CAD model of the chosen laboratory as well as a view of the generated mesh in the proximity of the aluminum tray where the liquid nitrogen has been poured in.

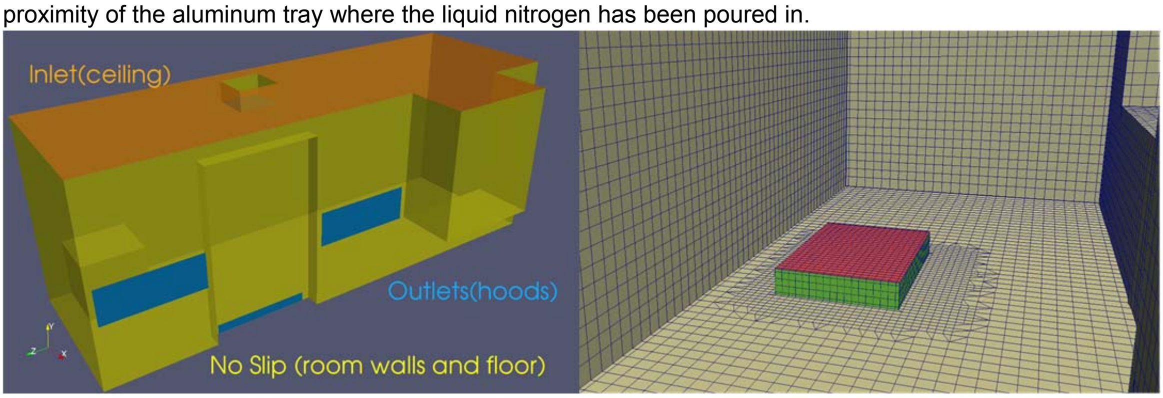

Figure 2: Simplified 3D CAD model geometry of the simulated laboratory (left) and view of the generated mesh in proximity of the aluminium tray.

CFD model

The CFD model is based on the solution of the laminar compressible unsteady Navier-Stokes equations for a mixture of non-reacting gases. Buoyancy and heat-exchange effects are taken into consideration.

The user has to, via the scripting interface, set the sources and the chemical characteristics of the pollutants, the initial environmental conditions (pressure and temperature) as well as the parameters of the ventilation. Furthermore, he also has to choose the time step and duration of the simulation. Figure 3 shows an example of the mesh generation around a point gas source defined by the user. In this particular case, the point source is used to simulate the leak of O_2 inside the ventilated environment.

Finally, the user can also place point as well as surface probes in the environment, to select the desired physical quantities (i.e. concentration of a specific species, thermodynamic properties, flow velocities, etc.) to be observed during post-processing.

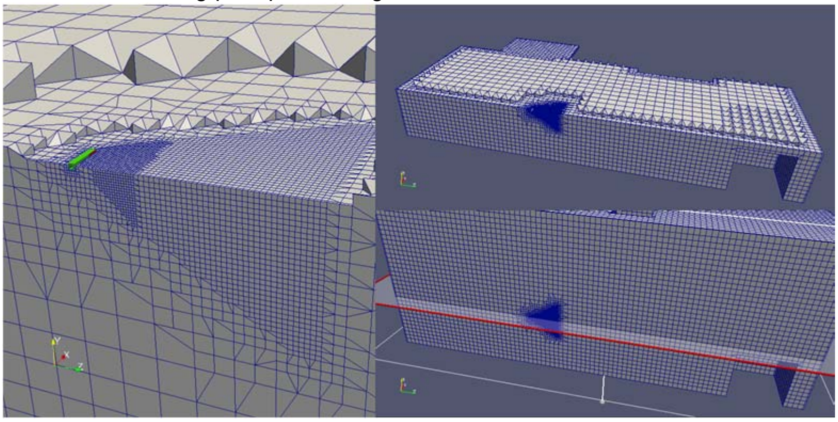

Figure 3: Gas point source and its mesh generation.

Post-processing

In post-processing, the user can extract the desired flow quantities and properties from the computed flow fields. Since the dispersion of air pollutants is a typically unsteady process, it is important to monitor the evolution in the of the desired quantities for which probes have been placed during the model definition.

The CFD solver OpenFOAM provides the computed flow field into a standard VTK format which is then processed by means of a visualization software, the open source and multi-platform application ParaView (ParaView, 2018). The visualization process is also semiautomated: via the scripting interface the user can select the probes and quantities of interest and generate screenshots and reports without directly access the visualization software. Figure 4 shows an example of generated screenshots for the leak of O_2 inside the ventilated laboratory at chosen times. The physical quantities shown are the O_2 concentration in the laboratory with its temperature.

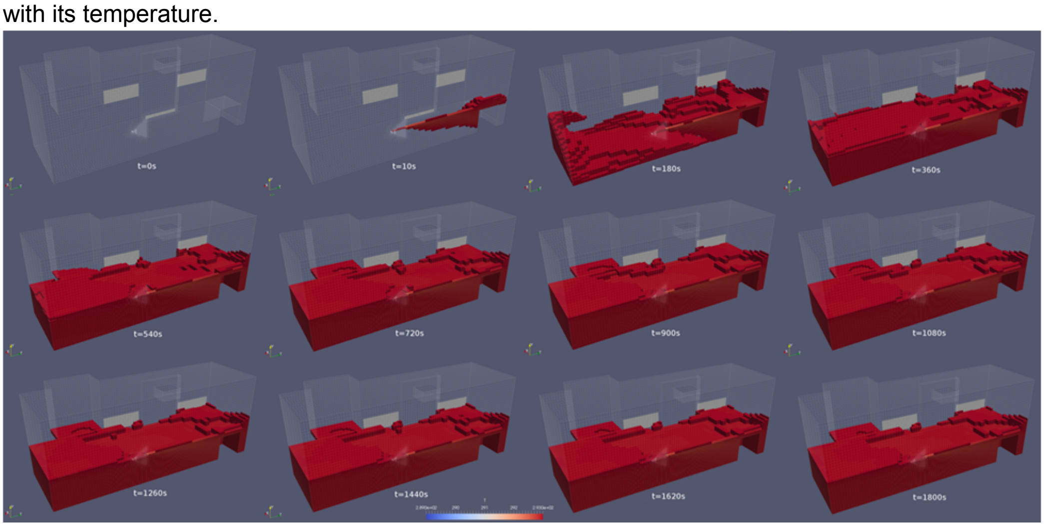

Figure 4: Oxygen concentration simulation results at preselected times.

3. Scientific data visualization

In order to be effective, scientific visualization needs to convert complex numerical simulation data into a form than can be displayed and understood easily. As mentioned by Alexander and Wang (2006), this conversion ultimate goal is to communicate scientific results in a way that is easy to digest for humans.
Even though the application used, ParaView, is a popular choice for scientific visualization due to its support to many data types (Sherman, 2014) and the post-processed results shown in Figure 4 are rather comprehensible to personnel with a scientific background in flow dynamics and general physics, these results might still be difficult to understand for a broader scientific and non-scientific audience.
The current technology, techniques as well as computing power allow for advanced methods to be implemented for an immersive, effective and easily understandable visualization of scientific data. The limits to modern advanced visualization lie in the user's imagination. Since the best way to show scientific data depends heavily on the type of data itself, the methods chosen have to reflect these differences.
For human sized simulations as the gas diffusion inside a room, immersive technologies such as virtual reality (VR) are extremely beneficial to get a first-person view of the results and a better scale of the environment. The user's immersion can be further enhanced using sensory feedbacks from computer generated stimuli: 3D visual imagery, spatialized sound and/or tactile feedbacks (Bowman and McMahan, 2007).
Starting from the results of the CFD simulations, the data points have been imported into Blender, a free and open source software for 3D creation. Blender is a popular tool for modeling, rendering and animating 3D, often used for video editing and game creation (Blender, 2018).
The laboratory environment has been recreated in Blender by reconstructing image texture from realistic photographs of the surfaces of the room. Furthermore, character models have been inserted into the scene to provide additional scale reference. Figure 5 shows a snapshot of the virtual simulation environment recreated in Blender.

Figure 5: Virtual rendering of the simulation environment.

In order to have a realistic rendering of the simulation results, the volume flow of evaporating nitrogen has been represented as a condensation cloud. A compromise had to be done between a realistic representation of clouds vs computational rendering times. Therefore, the clouds resulting from the rendering process have more liquid appearance than cloudy. Regardless, the overall results, of which an example is shown in Figure 6, are quite satisfactory for this early stage of the development.
In order to make the understanding of the simulation results as easy as possible, a 360° animation of the simulation environment has been created to visualize the gas diffusion. Virtual reality (VR) lets the user experience a computer-generated world as if it is real, in this case the reconstructed environment is a "real" laboratory that can be freely explored by the user during the animation.
The rendering time is the bottleneck of the process: to render a high resolution, 45 seconds video animation (600 frames) approximately 10 days were necessary on a workstation powered by 4 NVIDIA GeForce GTX TITAN graphics cards.
The final video can be watched on any computer using an appropriate 360° viewing software, such as GoPro VR Player. Of much higher impact for training purposes, the video can be used with one of the many VR applications for smartphones combined with a head mounted display for a more realistic immersion experience.
Overall, the awareness of hazards that cannot normally be seen or touched is increased using easy-to-understand 3D immersive animations thus providing a sensible gain towards the safety of the personnel.

Figure 6: Rendering of the simulated results.

4. Conclusions

A better understanding of gas diffusion inside complex confined spaces, the determination of the best place to install a gas detector based of experimental results, the validation of a simulation models as well as a full immersion VR video of the evaporation of liquid nitrogen. These are the results that have been accomplished during this project and they prove the effectiveness and power of a dualistic approach to modelling: as a tool for understanding a complex problem as well as a mean to improve the communication and training of personnel exposed to different hazards via advanced modern visualization techniques.
The 3D animation has been already used during gas hazard trainings for the laboratory personnel. The use of head mounted displays also appeals to the younger students that are receptive and participative during classes and trainings. Using these new means of communications, we are able to provide clear, visible examples of otherwise invisible and complex hazard risks. Those are easily understandable not only by the trained personnel but also by yet untrained students as well as a broader general public.
Further improvements are under study: new experiments will be performed in order to validate the simulation physical model under particular conditions; following the feedbacks of users, same scientific content will be added to the 360° animation to show the time scale of the diffusion as well as an indication of the O_2 concentration levels during the animation.

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