CFD SIMULATION OF HEAVY GAS DISPERSION IN VENTILATED ROOMS AND VALIDATION BY TRACING EXPERIMENTS

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Abstract
In order to improve the risk assessment related to accidental release of UF₆ (high density product used in some nuclear facilities), IRSN has conducted an experimental and numerical study on heavy gas dispersion in ventilated rooms. This study relies on upward injections of large amounts of SF₆ (heavy tracer gas) inside two different ventilated rooms. About twenty experimental configurations have been performed by varying the injection and ventilation conditions. Gas stratification is highlighted in all cases, even for small concentrations, and comparison between simulation and experiment shows a good agreement, especially during the gas injection and for low flow velocities inside the rooms. Nevertheless, complementary studies remain to be carried out in order to explain some phenomena, such as sudden concentrations decrease.

INTRODUCTION

Within the framework of internal emergency plans analysis of nuclear facilities, IRSN has to assess accidental scenarios, as well as their consequences in environment. Some of these facilities involve the risk of an accidental release of uranium hexafluoride (UF₆), heavy gas whose dispersion in a ventilated room, and thus its hydrolysis with ambient humidity, are mainly governed by its high density (equal to 12). In order to study heavy gas dispersion in a ventilated room and to assess the ability of a CFD tool to simulate accidental scenarios of UF₆ release, an experimental and numerical study has been carried out at IRSN. This study relies on upward injection experiments of SF₆ (heavy tracer gas whose density is equal to 5) inside two ventilated rooms of 36 m³ and 1 500 m³ volume.

METHODOLOGY

Time evolutions of SF₆ concentration were measured in various locations inside each room, using infrared spectrometry: in bottom (Bi), median (Mi) and high (Hi) points. The two geometries and the location of measurement points are shown on Figure 1.

![Figure 1: Room geometries and measurement points](image)

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Concerning the largest room, two air exhaust configurations have been studied, as shown in Figure 2: a lower exhaust (B) and an upper one (H).

![Figure 2: Two air exhaust locations](image1)

About twenty experimental configurations have been performed by varying the injection conditions (diameter $\phi_{\text{inj}}$, velocity $V_{\text{inj}}$ and duration $t_{\text{inj}}$) and the room ventilation conditions (air change rate $R$, continuous/discontinuous mode). Experimental conditions, derived from accidental scenarios analysis, are shown on Figure 3 for both geometries. It can be noticed that, for the largest room, conditions of SF$_6$ emission are quite similar: the main difference between all tests is the air change rate.

![Figure 3: test grids used for the 36 m$^3$ (a) and the 1500 m$^3$ (b) room](image2)

Subsequently, these experiments have been simulated using the Computational Fluid Dynamics (CFD) code CFX-5 [1], in order to contribute to the interpretation of the experimental results, and to validate this code for subsequent simulations of UF$_6$ dispersion. The gaseous mixing, constituted by air and SF$_6$, was assumed perfect and the flow was assumed turbulent, isothermal and dilatable. A classical RANS (Reynolds Averaged Navier-Stokes) multi-species formulation in weakly compressible and buoyant flow has been used, with standard $k$-$\varepsilon$ turbulence model. This approach was also used in other studies dealing with heavy gas dispersion in environment [2, 3].

![Figure 4 shows the computational domain and the mesh grid used for both rooms.](image3)

For discontinuous mode, air change rate is expressed as follows: $[2 \times 3^3 ; 0.4 \times 4^3 ; 0.8]$ means that $R = 2$ h$^{-1}$ during 3 min, then $R = 0.4$ h$^{-1}$ during 4 min and finally $R = 0.8$ h$^{-1}$.
**MAIN RESULTS**

Global validation
Figure 5 shows the SF$_6$ mass fraction field in the median vertical plane of each room obtained with CFX-5 (only the first 9 tests for the 36 m$^3$ room). Gas stratification is highlighted in most cases, due to the accumulation of SF$_6$ in the lower part of the room. Moreover, it can be observed that the influence of the gas injection characteristics is very important for the smallest room, whereas the results are quite similar for the largest one, due to very close values of injection parameters.

A first validation of these results was performed by comparing the maximum jet height obtained by the code to the one derived from the model of Baines et al. [4]. Figure 6 shows that the agreement is very satisfactory.
A second validation was performed by comparing, for each test, the maximum concentration at lower plane obtained by CFX-5 with the experimental one. Figure 7 shows that the results are coherent on the whole.

Figure 7: Comparison of the maximum concentration between CFX-5 and experiment

Highlighting the most influential parameters

- Tests at high flow velocities
  One of the parameters identified as very influential on heavy gas dispersion is the level of flow velocities inside the room, linked to the air mixing intensity. Because of the scale effect, this parameter is controlled primarily by the gas injection for the smallest room and by the room ventilation for the largest one. Thus, Figure 8 shows a comparison between the computation results and the experimental ones in the case of the test 3 carried out in the first room. In this test, the range of the SF₆ jet is very high, leading to an important flow mixing inside the room. The comparison of the concentrations evolution at the bottom (in red), median (in green) and high (in blue) points during the injection phase (120 s) is very satisfactory. Only the comparison of the concentration decrease, after the injection break, shows some discrepancies (this conclusion applies to all the tests carried out in this room). Indeed, in calculation, this decrease is primarily due to the air change rate, whereas in experiment, an effect due to the fall of SF₆ in the room is added. Nevertheless, on the whole, the concentration levels are well predicted by the code.

Figure 8: Test at high flow velocity in the 36 m³ room

The comparison between calculation and experiment is also satisfactory in the case of the tests 18B and 18H, carried out in the largest room and characterized by the highest...
air change rate (see Figure 9). The gas stratification, the concentration levels, and the influence of the air exhaust location are well predicted (concentration levels increase with upper exhaust at median and high points).

**Tests at low flow velocities**

The most important discrepancies with the experimental results were obtained for the tests at low flow velocities in the room: tests at low injection velocity in the first room (tests 2, 6 and 13) and tests at low air change rate in the second one (tests 16 and 19). Indeed, as shown in Figure 10 related to tests 2, 6 and 19B, a very strong disparity is highlighted in experiments between the bottom points. This disparity is not observed in calculation. Moreover, the concentration levels reached at these points are generally overestimated. Nevertheless, all these tests were characterized by great instabilities and reproducibility problems, which confirm the strong influence of the flow velocities on heavy gas dispersion.

Figure 9: Test at high flow velocity in the 1500 m³ room

Figure 10: Tests at low flow velocity
• Tests at high concentration

Another influential parameter seems to be the maximum concentration level reached in the room. Indeed, during the tests 8 and 9 carried out in the smallest room and characterized by concentration levels up to 30 000 ppm at the low points (cf. Figure 11), a very fast concentrations fall at the median points was observed in experiments, either just after the injection break (test 8) or during the injection (test 9), showing the great instability of the gas stratification. However, this behaviour was not predicted by the simulation: no concentrations fall is observed during the injection, and the concentrations decrease after the injection break is relatively slow, due mainly to the air change rate.

![Figure 11: Tests at high concentration in the 36 m³ room](image)

CONCLUSION

The SF₆ concentrations levels predicted by the simulation are overall in good agreement with experiment results, especially during the injection phase. Moreover, the heights reached by heavy jets are very close to the ones derived from literature model. The comparison between simulation and experiment is all the more satisfactory as flow velocities are high in each ventilated room. However, complementary studies remain to be carried out in order to explain some phenomena, such as sudden concentrations decrease either during or at the end of tracer injection.

REFERENCE