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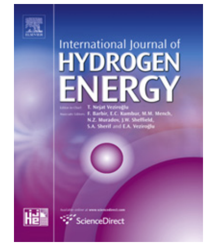

LES modelling of hydrogen release and accumulation within a non-ventilated ambient pressure garage using the ADREA-HF CFD code

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ABSTRACT

Computational Fluid Dynamics (CFD) has already proven to be a powerful tool to study the hydrogen dispersion and help in the hydrogen safety assessment. In this work, the Large Eddy Simulation (LES) recently incorporated into the ADREA-HF CFD code is evaluated against the INERIS-6C experiment of hydrogen leakage in a supposed garage, which provides detailed experimental measurements, visualization of the flow and availability of previous CFD results from various institutions (HySafe SBEP-V3). The short-term evolution of the hydrogen concentrations in this confined space is examined and comparison with experimental data is provided, along with comments about the ability of LES to capture the transient phenomena occurring during hydrogen dispersion. The influence of the value of the Smagorinsky constant on the resolved and on the unresolved turbulence is also presented. Furthermore, the renormalization group (RNG) LES methodology is also tested and its behaviour in both highly-turbulent and less-turbulent parts of the flow is highlighted.

1. Introduction

Given the shortage of fossil fuel and the environmental concerns from their use, hydrogen's special characteristics as an energy carrier have attracted the interest of the scientific community in recent years [1]. Indeed, in Europe for example, hydrogen and fuel cells are the first research topic of the 2.35 billion euro non-nuclear energy budget of the 50.5 billion euro total Seventh Framework Programme funds [2]. This trend reflects both the high potential of hydrogen energy and the safety concerns from its possible generalized use.

Hydrogen used in transportation has 2.5 times the energy efficiency of improved gasoline vehicles [3], being at the same time renewable and environmentally friendly, especially if clean energy is used for its production [4].

On the other hand, hydrogen is colourless, odourless, very buoyant under atmospheric conditions, with a wide flammable range between 4 and 75% by volume, a low ignition energy and a relatively high burning velocity, making its storage and handling hazardous and challenging [5].

On those grounds, the understanding of potential accidental release in a garage, as well as the ability to model it, is of particular importance and has attracted both experimental and numerical CFD studies [6–20]. The numerical studies [8–20] resulted in the conclusion that CFD is a convenient means for examining hydrogen dispersion and can provide reasonable agreement with the experimental data.

CFD is indeed a very strong and relatively low-cost tool that can help in exploring various hydrogen dispersion scenarios and support not only design procedures, but also decision

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making and emergency response; it can be thus considered a strategic means for the hydrogen safety assessment. The most common approach of this numerical method is the Reynolds Averaged Navier Stokes (RANS) technique that has historically accompanied CFD from its very early stages. Most of the above-mentioned numerical studies use the RANS technique. On the other hand, RANS is not very suitable for transient calculations, since it is based on averaging and it models the whole turbulence spectra. A more recent approach is the LES, which is natively transient and solves explicitly the bigger, energy containing eddies. Low-cost computational power increase has made LES an attractive alternative CFD approach, despite the fact that LES needs substantially more calculation time than RANS. LES has been successfully used in hydrogen dispersion studies in confined spaces in the recent past [17–20].

Given the fact that the LES methodology has a high potential, it has been recently incorporated into ADREA-HF, which is a well-established CFD code in atmospheric and hydrogen release dispersion applications [21,22]. The LES ability of ADREA-HF has already been evaluated against both flow field [23] and pollutant dispersion [24] calculations. In this work, the ADREA-HF LES code is used in modelling of hydrogen release and accumulation in a confined space and the results are compared with experimental data.

2. Description of the experiment

The experiment simulated was INERIS-test-6C, performed by INERIS (Institut national de l' environnement industriel et des risques; http://www.ineris.fr) within the activity InsHyde (http://www.hysafe.net/InsHyde), internal project of the HySafe network of excellence (http://www.hysafe.org). The experiment was used to evaluate various CFD codes in predicting the short and long term mixing and distribution of hydrogen releases in confined spaces.

The INERIS experiment was conducted in a rock cave of an approximately rectangular shape of dimensions 3.78 × 7.2 × 2.88 m in width, length and height respectively [7,15,25] (Fig. 1). At a more or less central point of this supposed garage, at 3.8 m from the front side and 0.265 m from the floor, a 1 g s^{-1} vertical hydrogen release for 240 s from an orifice of 0.02 m diameter was realized. The front side of the room consisted of a sealed plastic wall, with two small openings at the bottom to assure constant (ambient) pressure. During the test,

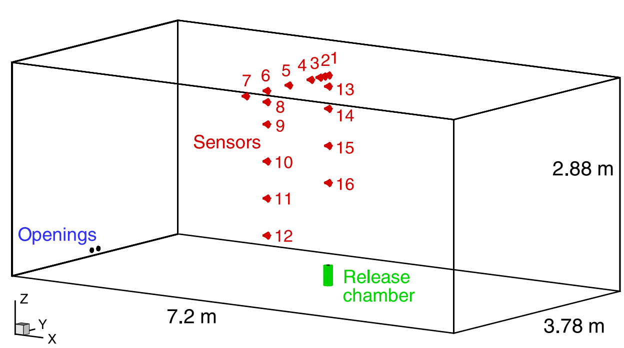

Fig. 1 – Geometry of the garage and locations of the sensors.

hydrogen concentration was measured regularly at 12 positions in the garage (Fig. 1; at sensors 2, 3, 5 and 15 no measurements are available), for a period up to 5160 s after the end of release, covering both the release and the subsequent diffusion phases. Fig. 2 presents photos from both the inside and outside of the room. More details about the experiment and its results can be found in Lacome et al. [7].

Before and after the experiment, the inter-comparison exercise SBEP (Standard Benchmarking Exercise Problem) - V3 was performed within the activity InsHyde [15], which helped in obtaining consensus regarding issues associated with prediction of hydrogen releases in confined spaces. CFD results were in general quite good, while the turbulence model, the resolution and the discretization scheme were found to be the most important simulation parameters.

3. Numerical methodology

3.1. Governing equations

In LES, the large turbulent scales containing most of the energy are resolved explicitly, while only the Sub-Grid Scales (SGS) containing a small fraction of the energy are modelled. A spatial filtering is applied to every variable of the flow field, decomposing it into a resolved (or filtered) component and an SGS component. The filtered governing equations neglecting the terms not used in this study are:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial\left(\bar{\rho}\tilde{u}_i\right)}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial\left(\bar{\rho}\tilde{u}_i\right)}{\partial t} + \frac{\partial\left(\bar{\rho}\tilde{u}_i\tilde{u}_j\right)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial\left(\tilde{\tau}_{ij}^{l} + \tau_{ij}^{R}\right)}{\partial x_j}, \tag{2}$$

$$\tilde{\tau}_{ij}^{l} + \frac{2}{3}\mu\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij} = 2\mu\tilde{S}_{ij}, \tag{3}$$

$$\tilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right), \tag{4}$$

$$\bar{p} = \bar{\rho} r \bar{T}, \tag{5}$$

where ρ is the density, t is the time, u_i is the velocity components, x_i is the distance, p is the pressure, τ_{ij} is the stress tensor components, μ is the kinematic viscosity, δ_{ij} is the Kronecker delta, S_{ij} is the rate-of-strain tensor, r is the gas constant, T is the absolute temperature.

The instantaneous variables here are space-averaged and not time-averaged as in RANS, while the tilde denotes density weighted Favre-averaging. $\tilde{\tau}_{ij}^{l}$ is the instantaneous shear stress tensor due to molecular forcing and $\tau_{ij}^{R} = -\bar{\rho}\widetilde{u_i u_j} + \bar{\rho}\tilde{u}_i\tilde{u}_j$ is the residual stress tensor due to the subgrid turbulence, modelled using the classical Smagorinsky subgrid scale model, as:

$$\tau_{ij}^{R} + \frac{1}{3}\tau_{kk}\delta_{ij} = 2\mu_t\tilde{S}_{ij}, \tag{6}$$

$$\mu_t = \bar{\rho}(C_s\Delta)^2\sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}, \tag{7}$$