Comparison of Standards Requirements with CFD Simulations for Determining Sizes of Hazardous Locations in Hydrogen Energy Station

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Abstract

This paper presents the comparison of IEC60079-10, CSA B108:99, NFPA 52 and API Standards requirements for determining sizes of hazardous locations with simulation results obtained by computational fluid dynamics (CFD) modeling. International standard IEC60079-10 determines the size of a hazardous location by a calculation of the hypothetical combustible volume caused by a fluid leak under specific temperatures, and ventilation rates. Canadian standard CSA B108:99 and American standard NFPA 52 use a prescriptive method to assign the size of a hazardous location depending on fuel quantities contained in the equipment. Considering hydrogen high buoyancy and diffusivity, requirements of both standards are likely too conservative. The PHOENICS CFD software package was used to solve the continuity, momentum and concentration equations with the appropriate boundary conditions, buoyancy model and turbulence models. Numerical results on hydrogen concentration predictions were obtained in the real industrial environment, which is the Hydrogen Energy Station (HES) produced by Stuart Energy Systems Corporation.

Keywords: Standard, hazardous location, CFD modeling, PHOENICS, hydrogen, numerical simulation.

Introduction

In the absence of specific regulations, codes and standards that would address installation of hydrogen systems, IEC60079-10, and CSA B108:99, as well as NFPA 52 have been extensively used for design and installation of Stuart Energy's Hydrogen Energy Stations (HES) in various jurisdictions. API 505 is also being used as a reference document.

It has been long suspected by hydrogen experts that, due to hydrogen high buoyancy and diffusivity, requirements of both standards are likely too conservative and result in inaccurate combustible volumes for hydrogen and higher than necessary hazardous zones. This, in turn, results in higher than necessary use of "classified" components that eventually increase the overall cost of the Hydrogen Energy Station.

To address this issue, Computational Fluid Dynamics (CFD) software was used to model potential releases of hydrogen under various conditions of the Hydrogen Energy Station. The obtained CFD numerical simulation results were compared with the requirements of the above standards.

Modeling Scenario Description

This paper discusses one of the potential failure scenarios – hydrogen release into the Generator Room of the Hydrogen Energy Station from the electrolytic hydrogen generator CF450 during self-purging start-up procedure.

At start-up, to ensure only high purity gas is directed for compression, hydrogen is being vented for 10 min. After 10 min a regulator driven by PLC logic re-directs hydrogen flow from vent to process. The point of potential release – the vent pipe at the roof of the hydrogen generator. The outlet pipe size is 2" and the constant flow rate is 0.0035 Nm3/s. This is a low- pressure release (P = 1 psig). This worst case scenario assumes, conservatively, that at the start-up the generator vent pipe comes off and all hydrogen that is generated during these 10 min is vented inside the Generator Room, and hydrogen sensors fail to detect the leak until after 10 minutes. Thus, this potential hydrogen release has maximum duration of 10 min.

Modeling Approach

The solid objects inside the Generator Room and on the roof were accurately represented in modeling domains as per provided engineering drawings of the Hydrogen Energy Station.

Hydrogen convection, diffusion, buoyancy and transience were modeled based on the general 3-D conservation equations and the details of various scenarios were introduced via the proper initial and boundary conditions. PHOENICS software was chosen for the purpose of modeling of these scenarios. PHOENICS is a well-recognized general-purpose CFD software package that has been validated and successfully used around the world for more than 20 years [1]. One of the advantages of PHOENICS is that it contains the LVEL model, a proper turbulence model allowing for both laminar and turbulent flow conditions to be considered. The local Reynolds numbers in every cell of the computational mesh can be computed so that they accurately reflect the local effective viscosities, which include both laminar and turbulent components. This allows for accurate modeling of fluid flow conditions within the whole domain.

Another important feature of the modeling approach was the use of transient conditions for computing the releases and dispersion of hydrogen clouds according to the requirements of different scenario conditions. First, the modeling was performed under steady-state conditions without any hydrogen leak. The velocity profiles obtained from the steady state were then used as the initial conditions for the during-the-release simulations, which were performed with a hydrogen leak at the specified rate and time increments. After- release simulations predicted the hydrogen dispersion in the room below 10% of the LFL. Note that both during- release and after- release simulations were transient, allowing for: (i) inclusion of the transient behavior of all calculated variables (pressure, gas density, velocity and hydrogen concentration); (ii) simulation of the movement of hydrogen clouds with time; as well as, (iii) evaluation of the hydrogen generator room safety by analyzing the iso-surfaces of the hydrogen concentration. To account for the effect of hydrogen buoyancy, the gas mixture density was calculated as an inverse-linear function of the mass concentration of hydrogen, C1, with coefficients based on the physical densities of air and hydrogen under the specified conditions. The buoyancy force, acting on the fluid particles, was proportional to the difference between the transient local gas mixture density and the constant reference density of air under the specified conditions. As a result, the significance of the buoyancy force in various room locations depended on the transient 3-D hydrogen mass fraction distribution. The latter was calculated from the standard mass conservation equation of hydrogen (see [1] for more details).

This modeling approach was validated by comparing Stuart Energy System Corporation's (SESC) PHOENICS CFD modeling results to the experimental and computational data of Swain et al. [2] for a case of slow hydrogen release and dispersion in a hallway. PHOENICS predictions of the transient behavior of hydrogen compared well with the experimental results [3].

Results

"Before Leak" Simulation

The existence of a louver and a exhaust fan in the Generator Room creates a steady-state airflow with 3-D fluid flow pattern. This airflow was simulated first, before trying to simulate the transient 3-D behaviour of hydrogen cloud introduced by a particular hydrogen release, since it provides initial fields of gas velocity and pressure for the release scenario considered below. Figure 1 shows ventilation velocities created by the louver and the exhaust fan.

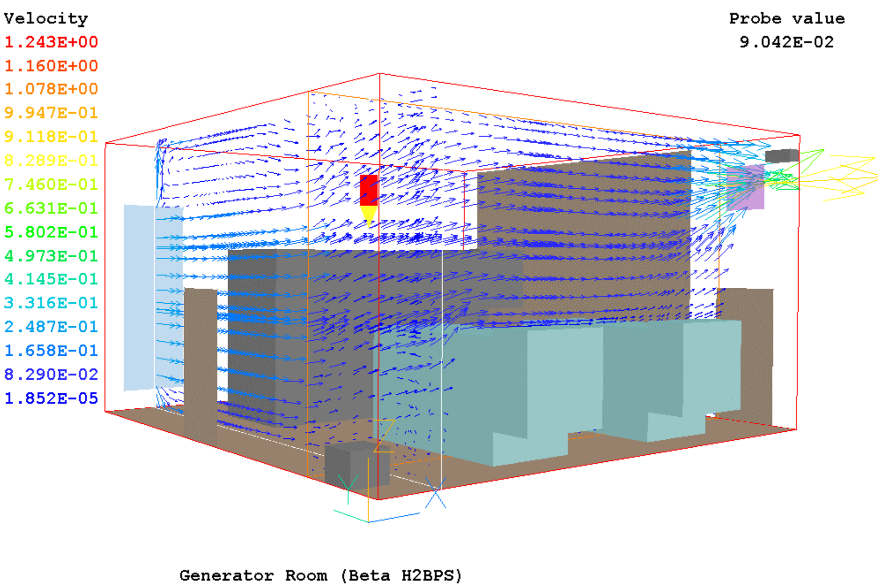

Figure 1. Ventilation velocities (X- and Y-planes) before leak.

“Leak” Simulation: Release from hydrogen generator vent line

The leak scenario considers the case when, for whatever reason, during the CF hydrogen generator start-up self-purging procedure the hydrogen vent line on the roof of CF comes off, thus causing all hydrogen being produced during the self-purging procedure (10 min) to leak into the Generator Room. It is also assumed that all hydrogen sensors intended to shut down the CF during the self-purging procedure are disabled. Room ventilation is provided by the louver and the exhaust fan (1 m^3/s). CFD predictions of 3-D hydrogen concentration distribution are shown in Figures 2 and 3. Figure 2 illustrates the H_2 (4% vol.) iso-surface at the end of the release (10 min) and Figure 3 shows the H_2 (2% vol.) iso-surface at the end of the release. It is seen that the sizes of these two clouds are very different.

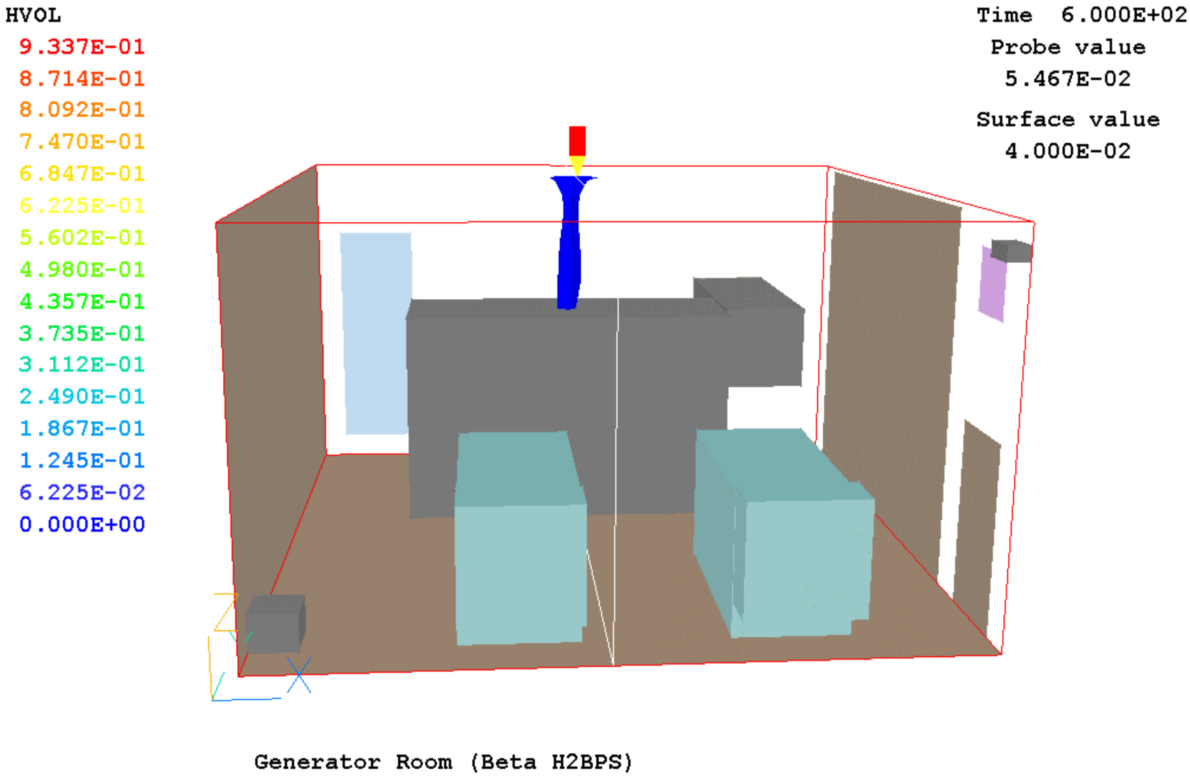

Figure 2. End of 10-min release from the CF vent line (4% hydrogen cloud).

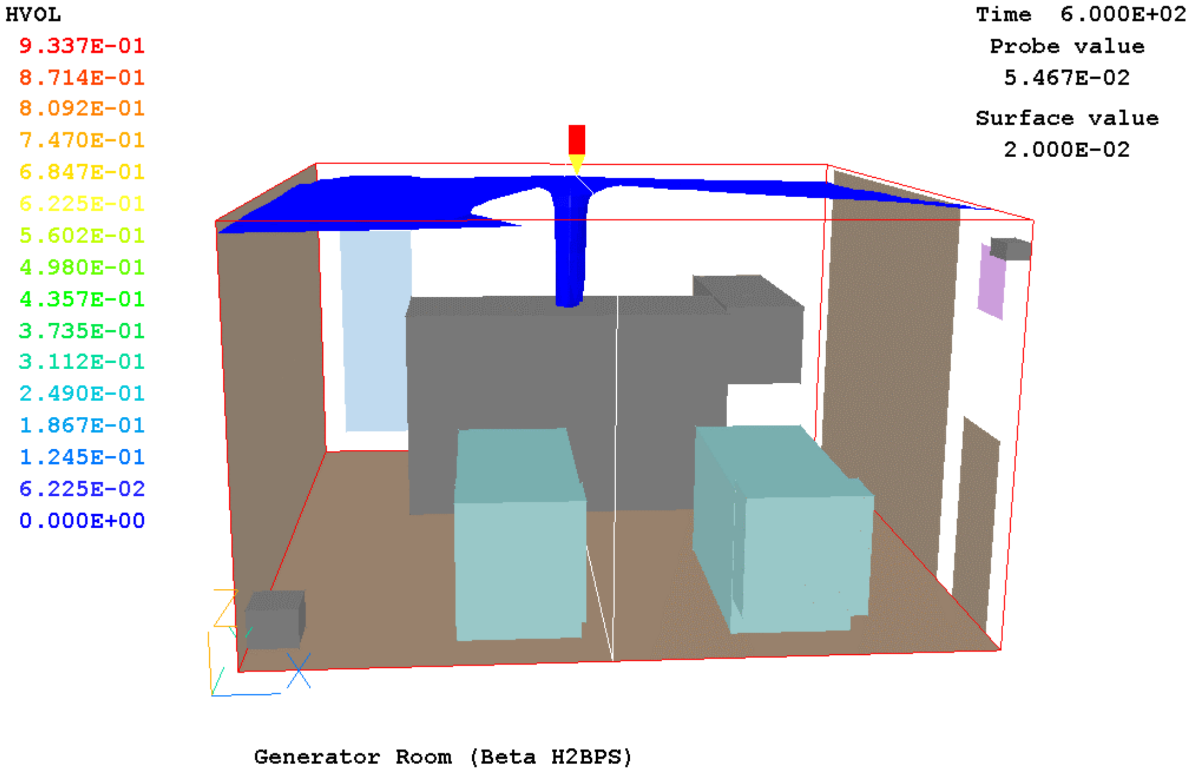

Figure 3. End of 10-min release from the CF vent line (2% hydrogen cloud).

Size of flammable mixture cloud (CFD approach)

The size of the flammable cloud was calculated, using the programmability of the PHOENICS CFD software. Three global quantities, DOMV, P4H and P2H were defined as the volume (in m^3) of the whole domain (DOMV), the volume of the hydrogen cloud with more than 4% volume concentration (P4H) and the volume of the hydrogen cloud with more than 2% volume concentration (P2H) respectively.

The printout from the global calculations file is shown below

Global calculations:

DOMV	=	229.9500
P4H	=	8.0717586E-02
P2H	=	6.225283

It is seen that the 4% cloud volume (P4H), which is about 0.081 m^3, is much smaller than the volume of cloud with 2% volume concentration (P2H), which is about 6.225 m^3. Both clouds are much smaller in volume than the whole domain volume (DOMV), which is about 230 m^3.

Requirements of IEC 60079-10

IEC 60079-10 sets out the essential criteria against which the risk of ignition can be assessed, and gives the guidance on the design and control parameters that can be used in order to reduce such a risk. The important criteria are:

- the LFL of the gas, leak rate, concentration and grade of release
- the degree and availability of ventilation and if there are any obstacles

Calculation to ascertain the degree of ventilation within Container Gas Compartment

The following method of ventilation calculation was taken from IEC 60079-10 2002.

Characteristics of release

Flammable material	Hydrogen gas
Source of release	vent pipe
Lower Explosive limit (LFL)	3.3 x 10^{-3} kg/m^3 (4% vol)
Grade of release	Secondary
Safety factor, k (applied to LFL)	0.5 (secondary release)

Release rate (dG/dt) = 12.6 Nm^3/hr = (H_2 density = 0.084 kg/m^3 at 20C, = density = 0.090 at 273C)
12.6 Nm^3/hr = 0.00305 m^3/sec x 0.090kg/m^3 = 0.000275 kg/sec
Gas concentration in release X_o = 100%

Ventilation Characteristics

Generator room Volume = 7.3m x 7.5m x 4.2 m = 230 m^3 – equipment volume = 185 m^3
Fan airflow = 1 Nm3/sec = 3600 Nm^3/hour
Number of air changes, C = 3600 m^3/hr/185m^3 = 19.5/hr = 0.0054/sec
Quality factor, f = 2 (There are few obstacles to impede airflow)
Ambient temperature, T = 35C (308K)
Temperature coefficient, (T/293 K) = 1.05

Minimum volumetric flow rate of fresh air:

$$(dV/dt)_{\min} = \frac{(dG/dt)_{\max}}{k \times LEL} \times \frac{T}{293} = \frac{2.75 \times 10^{-4}}{0.5 \times 3.3 \times 10^{-3}} \times \frac{308}{293} = 0.175 m^3/\text{sec}$$

Evaluation of hypothetical volume V_z

$$V_z = \frac{f \times (dV/dt)_{\min}}{C} = \frac{2 \times 0.175}{0.0054} = 64.8 m^3$$

Conclusion

The hypothetical volume V_z of 65 m^3 is significant relative to the room volume of 230 m^3 and would likely result in a Zone 2 room classification for at least the upper third of the room.

Requirements of CSA B108:99

Section 7.14 of CSA B108 states "a vent shall be provided to direct any natural gas being purged or released from the piping system of a fuelling station to a safe outdoor location".

Table 7.1 Electrical Classification of Space Surrounding Vents (Relief valve vents)

	Class I Zone I	**Class I Zone II**
Distance from vents	The distance shall be 100 vent orifice diameters, within 15 deg. of the line of discharge	1.8 m (6 ft. in all directions from the opening, excluding the Zone 1 space.

For a 2 inch vent the area classification is = 200 inches = 16.7 ft. = 5 m plus an additional 1.8 m around this volume for a total of volume of 33 m^3. (This requirement is for a pressure relief device which assumes a high pressure/volume leak).

NFPA 52 Requirements - Table 6.4.3.8 Electrical Installations

Location	**Division or Zone**	**Extent of Area Classification**
Discharge from relief va lves or vents Outdoors Outdoors	 1 2	 5 ft (1.5 m) in all directions from the point source Beyond 5 ft (1.5 m) but within 15 ft
Discharge from relief valves within 15 degrees of the line of discharge	1	15 ft (4.6 m) in all directions from point of discharge
Dispensing equipment - indoors	2	Entire room with adequate ventilation

API 505 Requirements

Section 6.6.2 defines: adequate ventilation (natural or artificial) that is sufficient to prevent the accumulation of significant quantities of vapor-air or gas-air mixtures in concentration above 25 percent of LFL). Section 6.6.2.4.2 states adequate ventilation for enclosed areas is at least 1 ft^3/min per square foot of floor but at least 6 air changes per hour. The air changes required for the 55 m^2 (589 ft^2) generator room would be 35340 ft^3/hr for 8122 ft^3 room which = 4.35 per hour. As 6 air changes minimum are required, the fan capacity must be 8122 x 6/60 = 812 cfm = 23 m^3/min = 0.38 m^3/sec, about one third the actual fan capacity. With this fan installed, the calculated hypothetical volume from IEC 60079-10 would be 167 m^3.

Comparison of results

Model	Hazardous location volume m^3
CFD modeling of 100% LFL H_2 cloud (4% vol. H2 in air)	0.081 m^3
CFD modeling of 50% LFL H_2 cloud (2% vol. H2 in air)	6.2 m^3
IEC 60079-10	65 m^3
CSA B108 NFPA 52	15 deg. 5m high cone 6.8 m dia. at base = 33 m^3 4.57 m sphere = 50 m^3
API 505	Requires a minimum fan capacity of 0.38 m^3/sec resulting in 167 m^3 hypothetical volume

NFPA 52 and CSA B108 consider the discharge from high pressure CNG.

Summary

The analysis performed in this paper suggests that requirements of IEC60079-10, CSA B108:99 and NFPA 52 for the size of hazardous locations could be considered too conservative. CFD numerical simulations indicate that the size of potentially flammable cloud, even in the case of all hydrogen generator production leaking into the Generator Room of the Hydrogen Energy Station, is one tenth of that prescribed by the above standards. For this situation API 505 may not require sufficient ventilation but also refers to IEC 60079-10.

The prime reason for the discrepancies is that CSA, NFPA and API do not consider the actual leak rate. IEC 60079-10 gives a very conservative result.

References

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